SIMCA®

SIMCA® 15 User Guide

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Trademark	Descriptor
Umetrics®	Suite of Data Analytics Solutions
MODDE®	Design of Experiments Solution
SIMCA®	Multivariate Data Analysis Solution
OPLS®	Method for improved regression analysis
O2PLS®	Method for data integration
OPLS-DA®	Method for group separation
PLS-TREE®	Top down clustering
S-PLOT®	Highlighting discriminatory variables
EZinfo®	Embedded Waters solution
VALUE FROM DATA®	We are value providers

ID #0000

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1 How to get started

1.1 Introduction

This chapter holds information about the installation, including system requirements and such, as well as a short introduction to using SIMCA.

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1.2 License information

Before installing the SIMCA product, carefully read the license agreement included with your SIMCA software package. This license agreement is also accessible by clicking the General license conditions link on the **File | Help** page in SIMCA.

In case you do not fully accept the terms of the license agreement, you should immediately return all parts of the package to your local supplier.

1.3 What is in the package

The SIMCA package contains the following:

- Installation files.
- SIMCA User Guide (.pdf).
- Installation instructions document.

1.4 System requirements

The minimum recommended system requirements:

- Pentium based computer (PC) with a 1.5 GHz or faster processor.
- 1 GB RAM or more.
- 1 GB available hard disk space.
- 1024x768 screen resolution color display.
- Microsoft Windows 7, 8 or 10.
- Graphics card that has hardware 3D acceleration and supports Open GL.

1.5 Installation

To install, follow the installation instructions delivered with the installation program.

Note: You must have administrative privileges to be able to install the software.

1.5.1 Registration and activation

To register and activate, follow the instructions delivered with the installation program. See also the Activate subsection in the Help section in Chapter 5, File.

1.6 Starting SIMCA

Start SIMCA by double-clicking the icon or by starting it from the **Start**-menu or start screen.

Continue by:

- Reading about the SIMCA software in the Help or User Guide. Both contain the same information.
- Starting a new project: click **File** | **New**.
- Running tutorial examples: Find the tutorials and tutorial datasets at the Sartorius Stedim Data Analytics website www.umetrics.com, or contact your Sartorius Stedim Data Analytics sales office. Select a suitable tutorial example, import the listed dataset used in the tutorial and follow the described steps.

1.7 SIMCA projects

What is a project?

SIMCA is organized into projects. A project is a .usp file containing the results of the analysis of one or more datasets.

Creating a new project

Start a new project by importing one or more datasets. The default unfitted model is created when exiting the SIMCA import and is displayed in the **Project Window**.

Project window

The project window displays, for every model, one line summarizing the model results. The active model, the one you are working with, is marked in the project window.

Default workset and model

The default **Workset** consists of the first dataset and all its variables and observations, imported with the roles defined in the import. All variables are default centered and scaled to unit variance. How the variables were defined at import also defines which type the default model is. For batch projects the default workset includes all imported batch evolution datasets.

Creating a new model

Unfitted models are implicitly created by SIMCA when:

- Specifying a workset or
- When changing the model type of a fitted model (fitted model is the active model).

Activating and opening the model window

To activate a model click it in the project window.

All plots and lists created from the **Home**, **Analyze** and **Predict** tabs are created for the active model.

To open the model window:

- Double-click it in the project window or
- Mark the model in the project window and then select the **Model window** check box on the **View** tab.

The model window opens with the details of the model results, displaying one line per component.

Step	Objective	How to do it
1.	Creating a new project.	Click **File | New | Regular project,** and then select the dataset file or files to import. In the import spreadsheet define identifiers, X, Y, and qualitative variables etc.
2.	Viewing and preprocessing the data.	When warranted, preprocess your dataset using the available **Spectral filters** or **Time series filters on the Data tab.**
3.	Specifying the workset and model type.	On the **Home** tab, open the **Workset** dialog by clicking **New/Edit** in the **Workset** group. Select the variables and observations to include or exclude, define classes, transform, scale, or lag variables, and Trim-Winsorize the variables. Optionally select **Model type** before clicking **OK** to exit the dialog.
4.	Fitting the model.	In the **Fit model** group click **Autofit.**
5.	Reviewing the results and performing diagnostics.	Create plots found in the **Diagnostics & interpretation** group to detect trends, groupings, deviations, etc.
6.	Using the model for predictions.	On the **Predict** tab, use the predictionset to see how new data fit with the active model. Import another dataset with the new observations or use observations not included in the model as predictionset.

Opening the workset dialog

To open the workset dialog of an existing model use one of the following methods:

1. Right-click the model in the **Project Window** and then select **Edit Model x**.
2. Click the **Workset** button in the **Model Window**.
3. On the **Home** tab click **Edit | Model x**.

1.8 Work process for regular projects

The work process in SIMCA consists of the following steps:

1.8.1 Creating a new project by importing a dataset

Create a new project by importing a dataset and specifying data properties in the SIMCA import spreadsheet.

1.8.1.1 Selecting the dataset

Click **File | New | Regular project** and then browse to find the file or files to import.

To import from a database, **Cancel** the **Open** dialog and then click **Add data | From database** on the **Home** tab in SIMCA Import.

You can import more than one dataset at the same time in SIMCA Import by clicking **Add data**. Selecting another file adds a new spreadsheet to the SIMCA import. These spreadsheets are imported individually at **Finish** and you can create the workset from all or a selection of the datasets.

1.8.1.2 Indicating file contents

Specify **Primary ID** and as many **Secondary IDs** as desired for both variables and observations.

Specify qualitative and date/time variables when present.

Click **Finish** to import all currently open spreadsheets.

1.8.2 Viewing and preprocessing the data

Click **Dataset**, on the **Home** or **Data** tabs, to open any available dataset. Use the **Data** tab features to manipulate and preprocess datasets.

1.8.2.1 Viewing the dataset

Before preprocessing your data you may want to display the variables or observations in a plot. You can do this directly from the dataset spreadsheet by marking the variables or observations and on the **Marked items** tab clicking one of the plots in the **Create from marked items** group, or **Drill down** group or by opening the **Quick Info** pane on the **View** tab.

To plot all the X observations as line plot, click **Data | Spectra |** *dataset*.

1.8.2.2 Preprocessing the dataset

Quick Info

The **Quick Info** pane holds interactive plots tied to the dataset displaying variables or observations in the time or frequency domain. When displaying variables, **Trimming / Winsorizing** for a single or all variables is available.

Generate new variables

Generate new variables as functions of existing ones or from model results by clicking **Data | Generate variables**.

Filter the dataset

Filter your dataset (**Data | Spectral filters**), for example using:

- Multiplicative Signal Correction (MSC).
- Standard Normal Variate (SNV).
- Wavelet transform and compression.
- Wavelet transform time series data using compression, decimation/denoising.

1.8.3 Specifying the workset

The default **Workset**, at the project start, is the first dataset with variables defined as X and Y as specified at import, centered and scaled to unit variance. The associated model (unfitted) is listed in the project window.

To fit the default model click **Autofit** in the **Fit model** group (**Home** tab).

An unfitted model is generated by SIMCA when clicking **OK** in the **Workset** dialog and when switching model type for a fitted model by clicking the **Change model type**-button.

1.8.3.1 New

In the **Workset** group click **New** to create a workset of the entire firstly imported dataset with X and Y as defined at import and scaling as defined in **File** | **Options** | **Project options**.

1.8.3.2 New as model

In the **Workset** group click **New as | Mx** to use the workset of the selected model as starting point.

1.8.3.3 Edit

In the **Workset** group click **Edit** to open an already created workset.

1.8.3.4 Modifying the workset

To fit a model different from the default model, with maybe other or more datasets included, excluded variables and observations, or transformations, or different scaling, it is necessary to modify the default **Workset.**

The following pages are available as tabs in the **Workset** dialog:

Page	Functionality available
Select data	Selecting which datasets to include. Only available when there are more than one dataset to choose from.
Overview	Excluding variables and observations, redefining variables as X or Y, setting class belonging for observations, changing missing value tolerance and checking variables and observations for missing values.
Variables	Excluding and including variables. Defining variables as X or Y.
Observations	Including and excluding observations. Grouping observations into classes for classification.
Transform	Applying transformations for variables. Trim-Winsorizing variables. Note that trimming / Winsorizing the workset does not affect the dataset but just that particular workset.
Lag	Defining lag structure.
Expand	Expanding terms with cross, square, and cubic terms.
Scale	Scaling variables.

Page	Functionality available
Spreadsheet	Trim-Winsorizing variables. Note that trimming / Winsorizing the workset does not affect the dataset but just that particular workset.

1.8.3.5 Simple mode

You can select to have the workset wizard guide you through the specification and automatically fit the model by clicking the **Use simple mode** button in the **Workset** dialog. To turn it off, click the **Use advanced mode** button.

1.8.4 Specifying and fitting the model

1.8.4.1 Selecting the model type

You can change the model type, when the workset specification allows it, by selecting another fit method than the default in the **Model type** box in the **Workset** dialog. Or by clicking **Change model type** in the **Workset** group and clicking a model type.

1.8.4.2 Selecting a new model type after fit

You can, after fitting the model, select a new model type. SIMCA then creates a new unfitted model with the selected model type.

For example, if you have defined your Workset variables as X and Y, you can first fit a PCY (PC of the responses), then change the model type to PLS and fit a PLS model (another model) to the same data.

1.8.4.3 Fitting the model

Fit the model using one of the fitting types listed.

1.8.4.3.1 Autofit

Rule based fitting of the marked model or group of models.

1.8.4.3.2 Two first

Calculates two components whether they are significant or not. Often used to get a quick overview of the data.

1.8.4.3.3 Add

Calculate one component at a time. Here it is possible to force components to be calculated regardless of significance rules.

1.8.4.3.4 Remove

Remove the last component.

1.8.5 Reviewing the fit and performing diagnostics

After fitting, the whole spectrum of plots and lists are available for model interpretation and diagnostics.

Important plots

- Summary plots
- Scores: t1 vs. t2, t1 vs. u1, etc.
- Loadings: p1 vs. p2, w*c1 vs. w*c2, etc.
- Hotelling's T2Range
- Coefficients
- Variable Importance (VIP)

Important plots for diagnostics

- Distance to Model
- Residuals N-Plot (**Analyze** tab)
- Contribution plots

- Permutations (**Analyze** tab)

Note: By default, all cumulative plots and lists are displayed for the last component. To select a different component for display in the plots, and/or a different variable, introduce the change in the **Properties** group, on the **Tools** tab.

1.8.6 Using the model for predictions

When you are content with your model you can use it for prediction.

1.8.6.1 Importing datasets for prediction

Later you may import additional data for use in predictions. Click **Data | Import dataset**.

1.8.6.1.1 Building the predictionset

Click **Specify** on the **Predict** tab to build your predictionset from ***any or all datasets***. You can display the predictionset as a spreadsheet or just plot or list results.

If you do ***not*** specify a predictionset, the predictionset is by default the first dataset.

1.8.6.1.2 Displaying the predictions

Use any fitted model to:

- Classify the observations from the predictionset with respect to a PC or PLS model.
- Predict responses (values of Y variables) for the observations in the predictionset with respect to a PLS and OPLS model.

All the prediction results (scores, y-values, etc.), computed with the active model, can be displayed as plots or lists.

1.8.6.2 Plots and lists

On the **Plot/List** tab you can find general plot and list commands. Here it is possible to plot and list any data, results and predictions.

There are scatter, line, column, 3D scatter, list, time series, control charts, histogram, dot plot, normal probability plots, response contour, response surface, wavelets plots, and step response plots available.

Note: With *an active plot or list, use* ***Change type*** *group, on the* ***Tools*** *tab, to generate lists from plots and plots from lists.*

1.9 Work process for batch modeling

A SIMCA batch project consists of one or more batch evolution datasets and models and optionally one or more batch level datasets and models:

1. The batch evolution datasets have several observations per batch with the variables measured during the evolution of the batch.
2. The batch level datasets consisting of the completed batches, with one batch being one observation (matrix row). The variables of the batch level datasets are the scores, original variables (raw), or statistical summary variables (raw data statistics) of the batch evolution model, BEM, at every aligned time point folded out side-wise. The BLM may also contain batch condition variables.

Batches may be divided into phases.

The work process in SIMCA consists of the following steps:

Step	Objective	How to do it
1.	Creating a new project.	Click **File | New | Batch project**. Select the dataset file or files to import. In the SIMCA import spreadsheet, define **Batch ID**, **Phase ID**, X, qualitative, time or maturity as Y, and if present **Batch conditions**. With phases, in the **Batch & Phase** pane optionally **Rename**, **Merge**, **Delete**, switch the order or time/maturity for the phases, or apply **Conditional delete**. Batch, phase and phase iteration conditions can be imported with the batch evolution dataset, or as a separate dataset. SIMCA import assumes that a dataset with only one row per batch contains batch conditions.

Step	Objective	How to do it
2.	Viewing and preprocessing the data.	When warranted, preprocess your dataset using the available **Spectral filters** or **Time series filters** on the **Data** tab.
3.	Specifying the workset.	On the **Home** tab, open the **Workset** dialog by clicking **New/Edit** in the **Workset** group. Select the variables and observations to include or exclude, crop, transform, scale, expand or lag variables, and Trim-Winsorize the variables. Use the **Variables** page to configure the x and y-variables to the relevant phases, and y-variables smoothing/shifting/normalizing.
4.	Fitting the model.	Click **OK** in the Specify Autofit dialog automatically opened when exiting the Workset. Alternatively, mark the wrapper BEM and click **Autofit**.
5.	Reviewing the batch evolution results and performing diagnostics.	Create BCC-plots found in the **Analysis control charts** group on the **Batch** tab to detect trends, groupings, deviations, etc.
6.	Using the model for predictions.	Create the BCC-plots found in the **Prediction control charts** group to see how new data fit with the active model.
7.	Creating the batch level dataset.	On the **Batch** tab, click **Create batch level** and go through the wizard.
8.	Importing batch, phase and phase iteration conditions.	To import batch, phase and/or phase iteration conditions, click **Data | Import dataset**, select the file or files to import and specify ID.
9.	Specifying the workset.	The **Workset** dialog opens at **Finish**. Note that the **Create a batch level model** check box at the top of the **Select data** page is selected. Select the batch level and batch conditions datasets to use and then continue to the variables and observations pages to include or exclude etc.
10.	Fitting the model.	In the **Fit model** group click **Autofit**.
11.	Reviewing the batch level results and performing diagnostics.	Create plots found on the **Home** tab to detect trends, groupings, deviations, etc.
12.	Using the model for predictions.	On the **Predict** tab, use the predictionset to see how new data fit with the active model. The batch evolution predictionset is automatically rearranged to a batch level predictionset.

1.9.1 Batch project overview

1.9.1.1 Batch evolution

With batch data, you start by importing the batch evolution data and create the batch evolution model, BEM.

Batch and phase identifiers and maturity variable

In the data, you must have a *Batch ID* (identifier), indicating the start and end of the batch, and if phases are present, also a *Phase ID*. If a batch is run more than once in one or more phases a Phase iteration ID is also required. You may also have a variable indicating the evolution of the batch or phase and its end point. This variable can be *Time* or *Maturity.* You can have different Maturity variables for different phases.

Default unfitted models

Unfitted batch evolution models are implicitly created by SIMCA. When batches have phases, each phase is fitted as one PLS-class model with Time or Maturity as Y for each phase. By default all variables in a phase are centered and scaled to unit variance.

Fitting the model

Click **Autofit** with the BEM marked to fit all models at once.

Reviewing the results

Display the results of the analysis of the workset batches in the **Analysis control charts** group on the **Batch** tab, either as scores, DModX, Hotelling’s T2Range, predicted time or maturity, or as individual variables.

Predictions

More datasets can be imported with new batches. The predictions can also be displayed in batch control charts in the same way by selecting the plot from the **Prediction control charts** group on the **Batch** tab.

1.9.1.2 Batch level

The batch level dataset is based on scores, original variables, or statistics of the original variables for completed batches, obtained from the BEM. The model created from these batch level datasets is named batch level model, BLM.

Creating batch level dataset

Create the batch level datasets by clicking **Create batch level**, in the **Dataset** group, on the **Batch** tab. Specify the properties of the batch level datasets to create.

Creating batch level model

Clicking **Finish** in the **Create Batch Level Dataset** wizard opens the **Workset** dialog with the **Create a batch level model** check box selected. Here you can select any batch, phase, or phase iteration conditions in combination with batch level dataset created from the same BEM. To import conditions, click **Data | Import dataset**.

You can change the default model type to any desired model type allowed by the workset specification. Alternatively specify hierarchical (**Create hierarchical batch models** on the **Batch** tab) or partial (select the **Create partial models for each phase** check box in the **Workset** dialog) models.

Reviewing the results

Display the results of the analysis of the workset batches in the **Diagnostics & interpretation** group, on the **Home** tab.

Predictions

The batch evolution predictionset is automatically rearranged to a batch level predictionset. This means that to make predictions for a BLM you select data from batch evolution datasets and SIMCA takes care of the rest.

Project window for batch projects

The project window displays, for every model, one line summarizing the model results.

When batches have phases the PLS phase models (class models) are grouped in a wrapper, BEM. Both the BEM and BLM are grouped under an umbrella called BMxx, where xx is a sequential number.

Use the tutorials to get a guided tour for building PC and PLS models.

Find the tutorials at www.umetrics.com, under Downloads | SIMCA.

2 Introduction to multivariate data analysis

2.1 Introduction

This chapter gives an introduction to multivariate data analysis of regular and batch processes.

Content

- Process data analysis
- Batch data analysis
- Traditional data analysis: One or two variables at a time
- Multivariate approach
- Conclusion

2.2 Process data analysis

Any investigation of a real process or system is based on measurements (data). Fifty years ago, measurement devices were expensive and few, and consequently the amount of data, measured on processes, was limited; a temperature and a pressure here, a flow rate there. The monitoring, display, and analysis of these few data was relatively simple, and a few running charts of the data provided all available information about the state of the process.

Today, batteries of sensors and on-line instruments are providing data from all parts of the process in various forms, often at very short intervals. The masses of data are fed into computers, re-computed into moving averages (per minute, hourly, daily, weekly, etc.) and displayed and stored.

This change from a situation with few, fairly infrequent measurements, to many, almost continuously measured variables has still not affected the manner in which process data are treated, potentially leading to large losses of information. With appropriate multivariate analytical methods, such as Principal Components (PC) and Projection to Latent Structures (PLS), and the recent extensions OPLS and O2PLS, in the SIMCA package, the masses of process data can provide easy to grasp graphical information about the state of the process, and relations between important sets of process variables. These multivariate methods make efficient use of all pertinent data, with little loss of information.

2.2.1 Process data properties

Before going into the analysis of process data, it may be useful to discuss their nature. The data are usually measured at regular intervals over time; say every day, every hour, or every minute. These intervals are often different for different variables. We can recognize five categories, types, of process data: controlled process variables, result variables, characteristics of raw material, intermediate result variables, and uncontrolled variables. The variable types are described in the text that follows.

2.2.1.1 Controlled process variables

Related to the controlled setting of the conditions of the process, these are variables that, in principle, can be changed, thereby affecting the results, the output, of the process. We shall denote the values of these variables by x_{ik} (observation i, variable k).

Examples of such variables are:

- T1, T2: the measured temperatures in reactors 1 and 2.
- P1, P2: the pressures in reactors 1 and 2.
- f12: the flow rate from reactor 1 to reactor 2.

2.2.1.2 Result variables

The availability of multivariate result variables (output, responses) measuring important properties of the products coming out of the process dramatically increases the possibilities to better understand and optimize a process. The result variables, are denoted y_{im} (data point i, y-variable m).

Examples of such variables are:

- y_{i1} = yield of main product (%).
- y_{i2} = impurity level (%).
- y_{i3} = amount of side product no. 1 (%).
- y_{i4} = tensile strength of product.

2.2.1.3 Characteristics of raw material

The characteristics of the raw material (inputs) are also denoted by x_{ik}. These variables are often of great importance for the process and the product properties, but usually difficult or impossible to control.

Examples of such variables are:

- Concentrations of iron, coal, nickel and vanadium in feed.
- Fiber length distribution in input pulp.
- Gas chromatographic and spectroscopic (NMR, IR, etc.) analysis of feed stock.

2.2.1.4 Intermediate result variables

Intermediate result variables are denoted by x_{ik}, y_{im}, or z_{it}.

Examples of such variables are:

- Viscosity of output from reactor 1 (=input to reactor 2).
- Concentration of oxygen in output from reactor 1.

2.2.1.5 Uncontrolled variables

Uncontrolled variables are denoted by x_{ik}, or z_{it}.

Examples of such variables are:

- Air humidity, temperature of cooling water.
- Amount of oxygen in sparging nitrogen.

The purposes of measuring the data on the process and its input and environment are to:

- Provide information allowing a better understanding of the process, relationships between different parts of the process, which chemical or other reactions occur inside reactors, etc.
- Yield information about the "state" of the process, recognizing trends, peculiarities, etc., all to keep the process under proper control.
- Discover how the output is affected by the process and input variables in order to improve product quality and minimize manufacturing costs, pollution, etc.

2.3 Batch data analysis

With batch processes, K variables are measured on N batches at regular time intervals. This gives a J x K matrix for each batch (J time points (X) times K variables). Consequently, a set of N normal batches gives a three-way matrix of dimension (N x J x K).

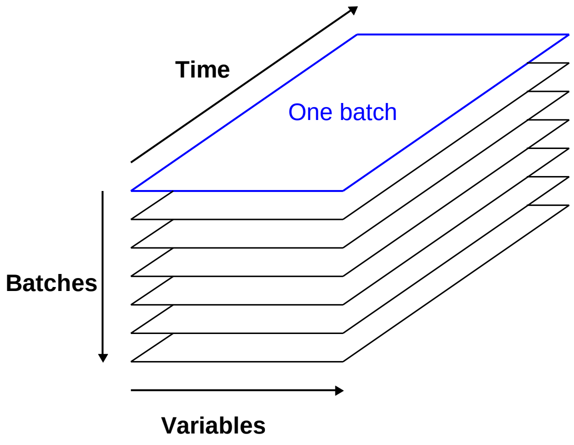


Figure 1: Three-way table of historical data of, for example, N batches with J time points, and K variables. Often the batches have different length (not shown in the picture) and may also be divided in phases.

2.3.1 Batch data properties

One of the differences between batch data and process data is that the batch process has a finite duration. Each batch can also go through several phases, optionally several times, before completion.

Since the batch data are collected batch wise they need reorganization before importing.

2.3.2 Reorganization of 3D table before import

To be able to import the dataset, the 3-way data table has to be unfolded to preserve the direction of the K variables (see figure 2). The resulting matrix has **n_{obs} = N x J** observations (rows) and **K** columns. Hence this matrix, **X**, has the individual observation as a unit, and not the whole batches.

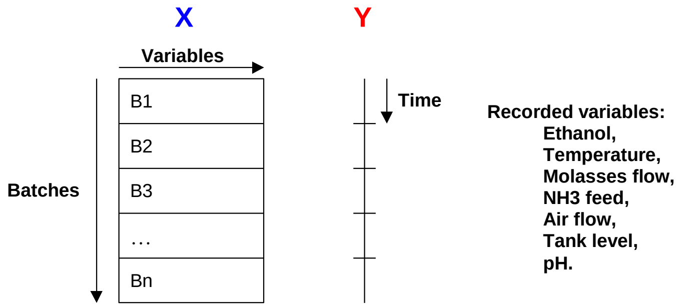


Figure 2. The three-way matrix of figure 1 unfolded along the batch direction to give a two-way matrix with N x J rows and K columns. Each row has the data (x_{ijk}) from a single batch observation (batch i, time j, variable k).

2.4 Traditional data analysis: One or two variables at a time

To gain insight into the state of a process it is common to display important variables and their change over time (figure 3). This works fairly well with up to 5 to 10 variables, but thereafter becomes increasingly difficult to comprehend. Furthermore, these "time traces" reveal little about the relationships between different variables.

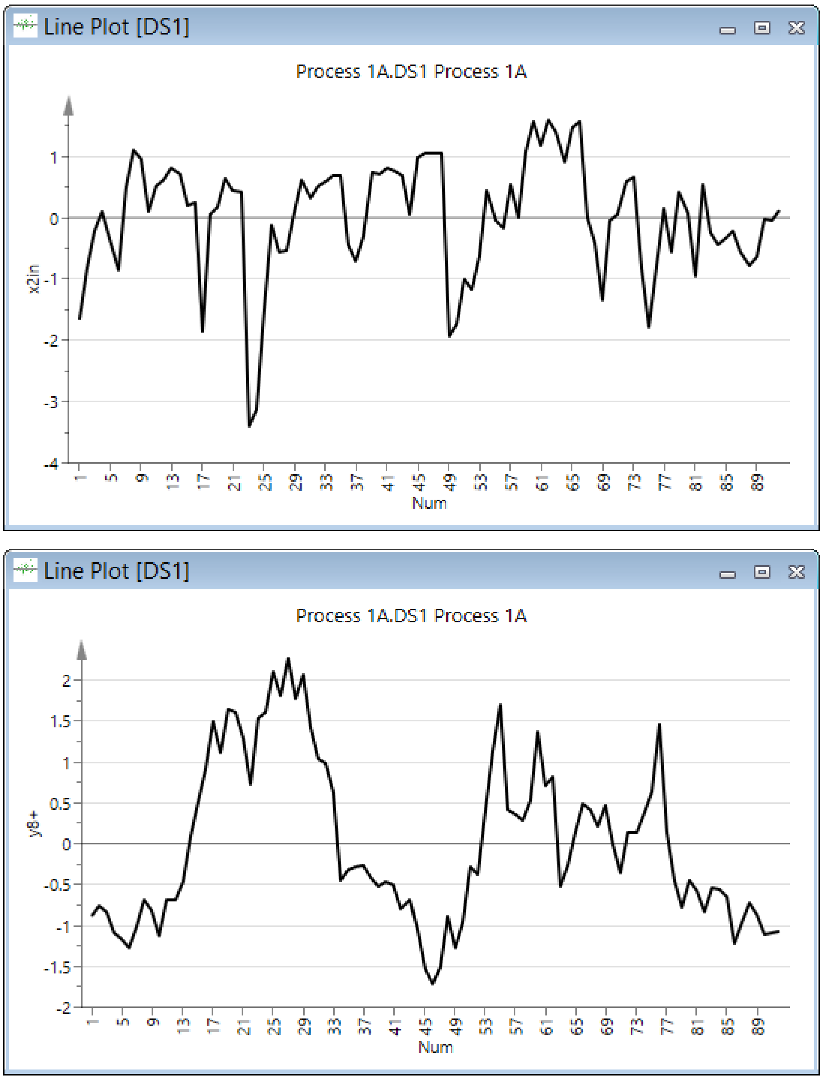


Figure 3. Two of the variables plotted against time on horizontal axis.

Scatter plots of pairs of variables are common complements to time traces (figure 4). One hopes to identify correlations, thereby identifying important process variables causing changes in the output variables.

The basic problem with pair-wise scatter plots is that they provide little information about the real relationships between, on the one hand, input and process variables, and, on the other hand, output variables. This is because the output (y) is influenced by combinations of the input and process variables (x).

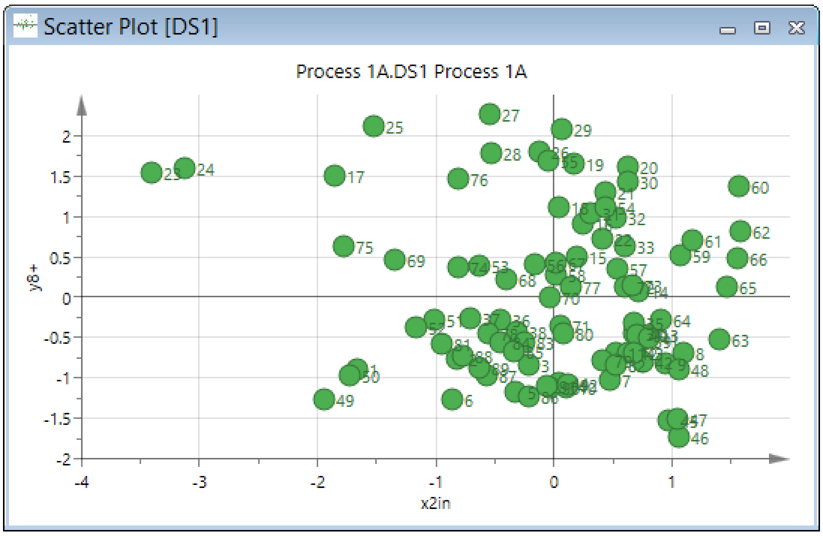


Figure 4. Scatter plot of y8* (impurity) against x2in (one of the inputs).

2.5 Multivariate approach

With multivariate methods, one can investigate the relations between all variables in a single context. These relationships can be displayed in plots as easy to understand as time traces and pair-wise scatter plots.

The methods for multivariate process data analysis included in SIMCA are PC analysis and modeling, PLS modeling, OPLS modeling, O2PLS modeling and more. The principles and mathematics of the fit methods are briefly described later in the introduction, and more thoroughly in the Statistical appendix. References are also given to additional pertinent literature.

Here we will indicate how to use these methods to solve typical problems in process data analysis.

2.5.1 Summarizing a set of process variables

Data measured on a process are usually stored in some kind of database. A process database containing the values of K variables for N data points can be regarded as a table, a matrix. We denote the whole table by X. Each column in the table corresponds to one variable (x_k), and one row (x_i) corresponds to the values observed at one point in time.

Inputs or outputs or both can be displayed in multivariate control charts.

2.5.2 Summarizing batch data

Data measured batch wise are also often stored in some kind of database. One of the differences between batch data and process data is that the batch process has a finite duration. Each batch can also go through several phases before completion.

Inputs or outputs can be displayed in batch control charts.

2.5.3 PCA - Principal Component Analysis

Principal component analysis of a data table gives vectors of scores, with values t_{ia}, which summarize all the variables entering the analysis. It is customary to calculate two or three **score** vectors, and then plot them against each other (tt-plots). This gives a picture that is the best summary of the process behavior over time! In this plot we can see trends, unusual behavior and other things of interest. With experience, one will be able to recognize an area in this PC score plot in which the process remains under "normal" operation, thus providing a multivariate control chart.

The score plot in combination with the *loading* plot, indicate the responsible variables for deviations from normal operation.

The PCA also gives residuals, deviations between the data and the PC model, named *DModX*. When these residuals are large, this indicates an abnormal behavior in the process. To see this, we make a plot of the residual standard deviation, DModX (residual distance, root mean square).

Observations with a DModX larger than the DCrit are outliers. When DModX is twice DCrit they are strong outliers. This indicates that these observations are different from the normal observations with respect to the correlation structure of the variables.

2.5.4 PLS - Partial Least Squares Projections to Latent Structures

2.5.4.1 Relating the result variables to input and process variables

A common problem is “process diagnostics”. That means identifying those input and process variables, X, that are “responsible” for the change in output variables, result variables, Y. For this purpose, one often attempts to use multiple regression, which, however, leads to great difficulties because process data usually do not possess the correct “properties” for regression modeling. In particular, regression deals with each result variable (y_m) separately, and one therefore ends up with a set of models, one for each output of interest. This makes interpretation and optimization difficult or impossible.

To allow strict interpretation of "cause and effect", the data should be collected in a careful experimentation using statistical design (with software such as MODDE). To search for relationships between input and output in process logs is risky and often less successful. This is because a process does not provide data with good information content when the important factors are well controlled within small "control intervals".

2.5.4.2 PLS - Scores

PLS modeling has been developed explicitly for this type of situation with numerous, often-correlated input and process variables and several to many result variables. One just specifies which variables in the database that are predictors (X), and which variables are dependent (Y), and PLS finds the relation between the two groups of variables.

The PLS model is expressed as a set of X-score vectors, Y-score vectors, X-weight and Y-weight vectors, for a set of PLS model dimensions. Each dimension (index a) expresses a linear relation between an X-score vector (t_a) and Y-score vector (u_a). The weight vectors of each model dimension express how the X-variables are combined to form t_a, and the Y-variables are combined to form u_a. In this way the data are modeled as a set of "factors" in X and Y and their relationships. Plots of the scores and weights facilitate the model interpretation.

2.5.4.3 PLS - Loadings

The PLS analysis results in model coefficients for the variables, called PLS-weights or loadings. The loadings for the X-variables, denoted w, indicate the importance of these variables, how much they “in a relative sense” participate in the modeling of Y. The loadings for the Y-variables, denoted by c, indicate which Y-variables are modeled in the respective PLS model dimensions.

When these coefficients are plotted in a w*c plot, we obtain a picture showing the relationships between X and Y, those X-variables that are important, which Y-variables are related to which X, etc.

2.5.4.4 PLS - Residuals

Analogous to PC, PLS gives residuals, both on the Y-side and on the X-side. The standard deviations of these (residual distances) can be plotted just as for PCA to give a third "SPC" plot (Statistical Process Control) showing if the process is behaving normally or not in DModX and DModY plots.

2.5.5 OPLS and O2PLS - Orthogonal Partial Least Squares

OPLS is an extension of PLS and addresses the regression problem. OPLS separates the systematic variation in X into two parts, one part that is correlated (predictive) to Y and one part that is uncorrelated (orthogonal) to Y. This gives improved model interpretability. In the single-Y case, there is only one predictive component, and all components beyond the first one reflect orthogonal variation. However, with multiple Y-variables there can be more than one predictive OPLS component.

O2PLS is yet another extension of PLS and addresses the data integration problem. Thus, in the two-block (X/Y) context, O2PLS examines which information overlaps between the two data tables and which information is unique to a specific data table (X or Y). O2PLS accomplishes this task by a flexible model structure incorporating three types of components, that is,

(i) components expressing the joint X/Y information overlap,

(ii) components expressing what is unique to X, and

(iii) components expressing what is unique to Y.

For both OPLS and O2PLS the different components are interpretable the usual way, since the scores, loadings, and residual-based parameters with a familiar meaning are preserved.

2.5.6 Batch modeling in SIMCA

A SIMCA batch project consists of one or more batch evolution models, BEM, and optionally one or more batch level models, BLM:

1. The BEM has several observations per batch with the variables measured during the evolution of the batch. Batch evolution models are commonly applied for real time process monitoring.
2. The BLM consists of the completed batches, with one batch being one observation (matrix row). The variables of the BLM are the scores, original variables, or summary variables (statistics of the original variables) of the BEM at every time point folded out side-wise. Batch level models are commonly applied to investigate variations between batches, sites, campaigns or to study impact of process variations on product quality.

A BM, sequentially numbered, holds the BEM and the BLM-models built on datasets created from that BEM.

Batches may be divided into phases, i.e. process steps. If a batch is iterated in a phase, phase iteration ID needs to be specified for SIMCA to correctly handle the batch.

2.5.6.1 Batch evolution modeling

When importing the dataset in SIMCA, an index y-variable starting at 0 is constructed if no maturity is specified. This is the "relative local batch time".

The default model, after completed import in SIMCA, is a PLS or OPLS model for the centered and scaled X and y, or "relative local batch time" as y if no other y was specified. If a maturity variable, recorded relative to the start of each batch, was defined as y, it is the variable used as y.

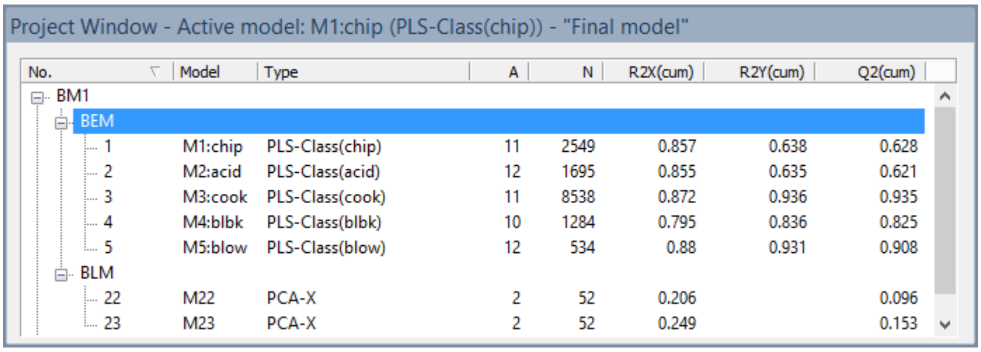
When fitting the batch evolution PLS model, “Autofit” will stop when 85% of X has been explained, but will also give at least 3 components, as long as the number of components does not exceed number of variables/2. This is necessary in order to ensure that much of the X-matrix is "explained". This results in an ($\mathbf{n_{obs}}$ **x A**) score matrix, **T**, plus PLS weight and loading matrices **W** and **P** (of dimensions K x A).

When fitting the batch evolution OPLS model the regular OPLS cross validation rules for autofit are used.

2.5.6.1.1 Modeling the evolution of batches in the workset

At the start of a batch project, when phases are present, the BEM workset is created with an unfitted model for every phase. The BEM is the wrapper grouping all the OPLS or PLS class models (one for every phase). Maturity or time, as specified for each phase, is used as Y, the other variables as X, and all are centered and scaled to Unit Variance.

When batches have no phases, there is only one model in the BEM, with time or maturity as Y and all other variables as X, centered and scaled to Unit Variance.

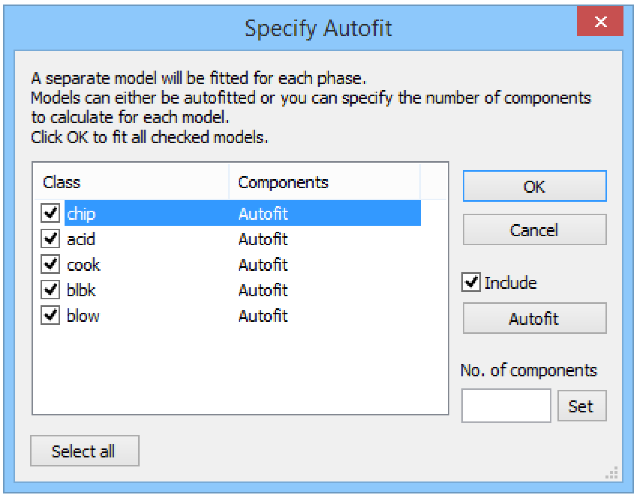


Project Window - Active model: M1:chip (PLS-Class(chip)) - "Final model"

No.	Model	Type	A	N	R2X(cum)	R2Y(cum)	Q2(cum)
BM1							
BEM							
1	M1:chip	PLS-Class(chip)	11	2549	0.857	0.638	0.628
2	M2:acid	PLS-Class(acid)	12	1695	0.855	0.635	0.621
3	M3:cook	PLS-Class(cook)	11	8538	0.872	0.936	0.935
4	M4:blbk	PLS-Class(blbk)	10	1284	0.795	0.836	0.825
5	M5:blow	PLS-Class(blow)	12	534	0.88	0.931	0.908
BLM							
22	M22	PCA-X	2	52	0.206		0.096
23	M23	PCA-X	2	52	0.249		0.153

Note: A model is positioned in a BEM only when the data was imported as batch and it is an OPLS or PLS model with one variable specified as y (Time or Maturity).

To fit the model(s), mark the BEM and click **Autofit**.



A separate model will be fitted for each phase.
Models can either be autofitted or you can specify the number of components to calculate for each model.
Click OK to fit all checked models.

Class	Components
☑ chip	Autofit
☑ acid	Autofit
☑ cook	Autofit
☑ blbk	Autofit
☑ blow	Autofit

☑ Include

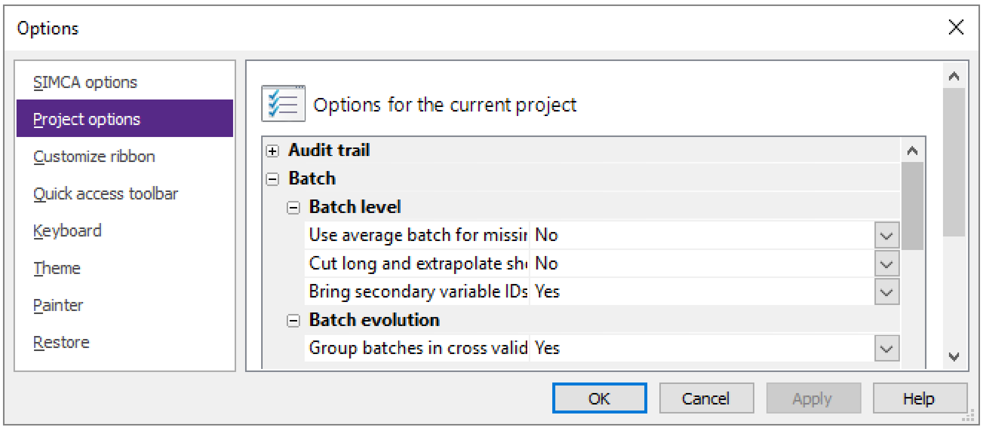
The BEM is built on the good batches when the goal is to define a process monitoring model with the ideal evolutionary trace. Around this trace, 3 SD limits are used to define the acceptable variation.

Examine the batch evolution models using the Batch control charts (BCC), starting with the Variable BCC to ensure that the process data is good and reliable for all batches. Look for outlier batches in batch control chart scores and/or the DModX plots. Interpret deviating batches with contribution plots.

2.5.6.1.2 Batches with different length

Alignment of data is done differently depending on Y-setting configuration of the time/maturity variables at Batch evolution level. How shorter or longer than median batches are treated at Batch level depends on Batch level settings in Project options. For batches of similar length the impact is small. This is not relevant when the Y-setting is *Normalized*.

There was a change in default behavior in management of batches with different length between SIMCA 14 and 14.1. Below are the default settings in Project options for SIMCA 14.1 onwards. To apply defaults as SIMCA 14 and earlier, change the Cut long and extrapolate short batches option from No to Yes.



Options for the current project

⊞ Audit trail
⊟ Batch
⊟ Batch level

Use average batch for missi	No
Cut long and extrapolate sh	No
Bring secondary variable IDs	Yes

⊟ Batch evolution

Group batches in cross valid	Yes

The used length in average batch is the shorter of the median batch length and the average batch length rounded down.

If Cut long and extrapolate short batches option is Yes, then all batches will be aligned to median (or average) batch length. Shorter than median (or average) batches will be filled up with last good value from their actual endpoint to median batch length. Longer than median (or average) batches will be cut.

If Cut long and extrapolate short batches option is No, then the alignment will continue after median (or average) batch length and batches will be filled up with last good value from their actual endpoint to the next maturity value. Note that the steps between maturities will increase after median (or average) batch length has been reached. Shorter batches will have missing data up until the last maturity at Batch level.

2.5.6.1.3 Batches with several phases

When batches have several phases, observations are organized in classes, one class for every phase. Separate PLS or OPLS-class models are fitted for every phase.

2.5.6.1.4 Smoothing the maturity variable

If a maturity variable is used as the response variable Y, indicating the degree of completion of a phase, the maturity variable has to be strictly monotonic in a given phase, but can be ascending or descending.

Different phases can have different maturity variables. Different phases can have ascending or descending maturity.

When maturity variables are not strictly monotonic, they are smoothed within each phase. The smoothing is done by fitting a constrained quadratic polynomial, using a piece wise least squares algorithm. This is to ensure that the maturity is strictly monotonic within a phase. The smoothed maturity is used by default, both as the response variable Y, and for alignment.

A difference between SIMCA 14 and SIMCA 13 is that in SIMCA 14 and later the smoothing increment was decreased so that when a maturity isn't increasing/decreasing it appears flat visually (in plots). That was sometimes not the case in SIMCA 13 and earlier.

2.5.6.1.5 Result variables

The score matrix T is a good summary of X, and PLS focuses this summary on y (local time). Hence the first column of t (t_1) will contain strong contributions of those X-variables that vary monotonously with y, i.e., either increase or decrease with time. The second component (t_2) is an aggregate mainly of those variables that change “quadratically” with time, i.e., first go up to a maximum, and then decrease, or first go down, and then up. The third component catches the variables having a cubic behavior, etc.

The value of "local time" predicted by the PLS model (with the number of components determined by cross validation), y_{pred}, is very suitable as a "maturity index" that can be used to indicate how far the batch has evolved, if it is ready for termination, etc.

For the OPLS model all variation relating to Y is captured in the first component.

2.5.6.1.6 Calculating limits to build control charts

To monitor the evolution of new batches, one calculates the typical evolution trace of a normal batch in terms of the scores, DModX, etc. This is in short done as follows:

1. **Reorganization**: First the scores of the BEM are chopped up and reorganized so that the scores of one batch form one row vector (t_1 followed by t_2 for PLS and t_{o1} for OPLS, followed by t_3 for PLS and t_{o2} for OPLS, etc.) in a matrix S_T. This matrix has N rows (one per batch) and A x J (AJ) columns from the A score vectors and the J "time points" per batch. When batches have phases, the scores of each batch are collected from the different PLS phase models and the calculations are done separately for the different phases.

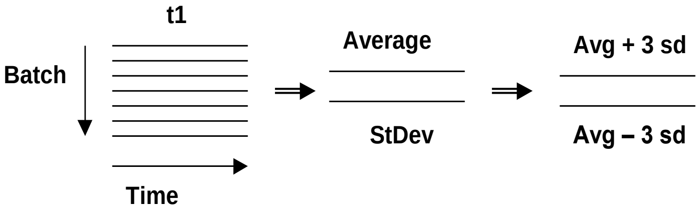


Figure 4. The score values for each batch are arranged as row vectors under each other, giving an N x (J x A) matrix, S_T. Above we see only the first part of S_T corresponding to the 1st component (t_1). From this matrix one calculates the averages and standard deviations (SDs) of the matrix columns, and then control intervals as the averages ± 3 SD.

2. **Calculating tolerance limits for score batch control charts**: Now the matrix S_T is used to derive minimum and maximum tolerated values at each time point (j) of t_{j1}, t_{j2}, t_{j3}…, t_{jA} from the column averages and standard deviations of S_T, as indicated in figure 4. In MSPC one would typically use tolerance intervals of the average ± 3 SD at each time point. Hence, we now have for each score vector an average trace with upper and lower tolerance limits (figure 4). This specifies the normal evolution traces, one for each score component, of new batches.
3. **Calculating tolerance limits for y predicted batch control chart**: An additional trace is constructed from the values of predicted y (local time or maturity), for each time point of each batch. The predicted y-values should be fairly close to the "real" y-value for a batch evolving at the "normal" rate. SIMCA forms a matrix R_Y with the traces of predicted y of each batch as rows, and then analyzing it in the same way as S_T above, and gives tolerance intervals of y_{pred} for each time point.

4. **Calculating tolerance limits for DModX batch control chart**: An additional trace is constructed from the values of the residual standard deviation (distance to the model, DModX), for each time point of each batch. The residual standard deviation (DModX) is calculated from the residuals, i.e., after subtracting t_i x P' from the scaled and centered observation x-vector. For an observation to be judged OK (non-deviating), DModX should be smaller than a critical limit, D_{crit} calculated from the F-distribution.

Note: When batches have phases, the limit calculations are done by phase.

2.5.6.1.7 Monitoring the evolution of new batches

The batch evolution data of new batches are inserted into the PLS or OPLS model, giving predicted values of the score values t_1 to t_A. These results can now be plotted in the appropriate batch control charts, with limits derived as described in the Calculating limits to build control charts subsection. These charts indicate whether the batches are starting normally or not. If the values are outside the normal ranges, contribution plots based on the x-values or the residuals indicate which variables together are related to the deviations.

In addition, the PLS model gives predicted values of y (local time or maturity index). Plotting y_{pred} vs. y_{obs} gives a very interesting indication of whether the batches are developing too quickly (over-mature, $y_{pred} > y_{obs}$) or too slowly (under-mature, $y_{pred} < y_{obs}$).

When batches have phases, the appropriate PLS phase model is used to predict the t scores of every phase. The scores are collected for every batch and results are plotted in the control charts.

2.5.6.2 Batch level modeling

This section describes modeling of entire batches as observations (rows) using batch level modeling.

2.5.6.2.1 Why batch level modeling?

At the batch level multivariate models are developed addressing two typical use cases, i.e., (i) batch qualification analysis and (ii) product quality variation assessments. Different modeling strategies and multivariate techniques are used in these two situations.

In *batch qualification analysis* PCA is used to create a reference model based on data of good and ‘qualified’ batches. This model defines normal operation and is used to verify if a new batch is similar or not to the good and ‘qualified’ batches. If a new batch conforms with normal operation it may be released if system is real time release. If a new batch deviates from normal operation drill-down analysis will show what is causing the deviation from normal operation conditions. With this model also slow drifts in the processing conditions may be revealed and examining batch-to-batch trends will guide preventive maintenance. A batch qualification model is validated using known qualified AND disqualified batches. Provided that the model correctly can distinguish between qualified and disqualified batches, alarm and warning limits may be stored in the usp and thereafter distributed to SIMCA-online.

In *product quality variation* assessments OPLS is employed to develop quality prediction model(s). The overriding goal is to understand how variations in critical process parameters (CPPs) affect final product quality attributes (CQAs). Usually, the OPLS model is based on all available batches that are not outliers and where CQA data are available. Using all available batches ensures better prediction of Y-data as there will be larger numerical variations in the response(s). This kind of predictive modeling is applied both in early development and for continuous processing improvements.

Regardless of multivariate model type, the batch level model (BLM) allows the full interpretation of the batch data of completed batches. Groups of batches may be discovered, outliers will be found, and so on. Critical time periods will be indicated by "periods" of large weights, loadings, and VIP values. Analogously, important factors in the batch conditions will stand out.

2.5.6.2.2 Creating the batch level model

The batch level model can be created based on scores, original variables, summary variables (raw data statistics), duration and endpoint, plus batch conditions (Z).

2.5.6.2.3 Modeling batch level

The objective of batch level modeling is to make a model of the whole batch in order to understand how Y is influenced by the combination of batch conditions and the batch evolution. This model will be based on (when available) the batch conditions (Z), the evolution trace matrix S_T, and when applicable the properties and quality of the completed batch (Y), as shown in figure 5. The resulting model is used to predict Y for new batches from their batch conditions and their evolution traces.

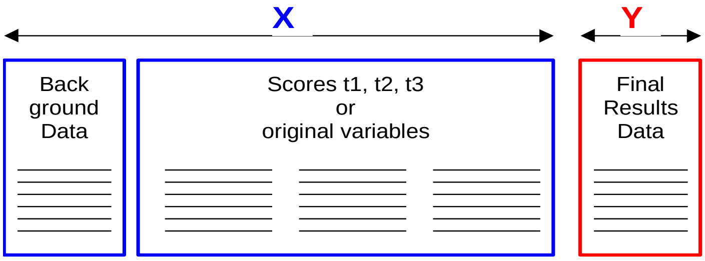


Figure 5: The data for batch level modeling. Each row has the data from one batch. The left matrix contains data describing initial batch conditions. The middle matrix contains the unfolded scores/raw variables, which describe the evolution of each batch. The optional right matrix (Y) contains the responses, the properties of the complete batch such as yield, purity, activity, etc.

In the case that Y-values do not exist, the X-matrix can still be used to develop a PC model. We see that this is the same type of model as the X-part of PLS in the batch evolution model. The difference is that in PCA the scores (T) are calculated to give an optimal summary of X, while in PLS this optimality is somewhat relaxed to make T scores better predictors of Y.

This PC model can then be used to classify new batches as normal (similar = well fitting to the PC model) or non-normal (far from the model).

2.5.6.2.4 Predicting results or classifying whole new batches

The batch level model is used to predict quality of the final batch (Y), or classify the batch as normal good batch or bad batch or predict their final quality.

If you have fitted hierarchical models of the batch level data at different percentage of completion, you can classify or predict the final quality of new batches as they are evolving when they reach the percent of completion of the models.

If the values are outside the limits, contribution plots indicate which variables together are related to the deviations.

2.5.6.2.5 Create a batch level model

When creating a batch level dataset, clicking **Finish** opens the **Workset** dialog with the **Create a batch level model** check box selected.

Select the datasets to use and then use the other pages in the dialog for editing the workset as desired. Clicking **OK** in the **Workset** dialog creates the unfitted **BLM**.

Note: Changing the order of the selected datasets resets the workset. Additionally selecting/clearing dataset check boxes in the **Select data** page may result in resetting the workset. When resetting the workset, all variable and observation/batch settings are cleared along with any changes in transformations, lags, expansions, scaling and trimming and the result is the default workset.

2.5.6.2.6 Hierarchical batch models

For batch level datasets you can fit hierarchical models of the whole batch, for different levels of completion:

- One model for each phase and component in BEM.
- One model for each phase.
- Sequential models covering parts of the batch completion, for example for 25%, 50%, 75% and 100% completion for models without phases.

These models can predict the final batch quality or classify the batch, before the batch is finished.

2.6 Conclusion

Projection methods such as PCA, PLS, OPLS and O2PLS find the information in masses of process data by projecting these data down on a few "scores". These scores provide a very good summary of process data tables (X and Y), and score plots display this in an easy to grasp form. The coefficients of the projections, i.e., how the variables are combined to form the scores, are called loadings or weights. Their plots show the importance of the variables, their similarity, their connection, and other things of interest.

The parts of the data not seen in the score plots, i.e., the residuals, are displayed (in summarized form) in the DModX and DModY plots (row residual standard deviations).

For further reading, see the **Multi- and Megavariate Data Analysis** book and the reference list.

3 Overview of SIMCA

3.1 Introduction

This chapter describes the following:

- Application icon and symbol.
- SIMCA projects.
- SIMCA window interface.
- Ribbon content.
- Shortcut menu.
- Conventions including limitations and missing values representation.
- Presentation of SIMCA results

3.2 Application icon and symbol

The application icon is a purple circle with a white S inside (below).

3.3 Projects

Multivariate data analysis in SIMCA is organized into ***projects***. You can think of a project as a file folder containing all the information related to the analysis of a number of datasets. Projects are by default named after the first selected dataset in SIMCA import.

This information is organized in the following components:

- Datasets used for the analysis.
- Other datasets used for predictions and model validation.
- Workset and multivariate models.

3.3.1 Datasets

For continuous processes, the data are observations made sequentially in time, usually at a constant sampling interval. Such data are called time series. In the analysis of time series, the observed outcome at time t is often modeled as a function of the previous observations at time t_1, $t_{2,}$ etc.

With PLS, the time series analysis is performed by creating lagged variables, i.e., variables shifted in time, and fitting the model. For PLS time series analysis to give correct results the observations must be contiguous in time (the sampling interval is constant), and with no missing observations.

A batch process has a finite duration. Each batch can go through several phases before completion. Since the batch data are collected batch wise they need reorganization before importing.

3.3.2 Workset

A workset is a subset or all of the data in the selected datasets with a particular treatment of the variables, i.e., role (predictor variables X, or responses Y), scaling, transformation, lagging, etc.

The workset is by default the first dataset with all imported variables and observations included and the variables centered and scaled to unit variance, for regular projects. For batch projects the default workset is all batch evolution datasets imported when creating the project.

When you define a workset, SIMCA creates an unfitted model, and both the model and the workset are identified by the same name.

3.3.3 Models

Models are mathematical representations of your process and are developed using the data specified in the workset and with a specified model type, for example, PCA-X, PCA-Y, PCA-X&Y, PLS, etc.

With a specified workset, you may be able to fit several models by selecting different model types. For example, if you have specified a workset by defining the X-variables (predictors) and the Y-variables (responses), you may first fit a PC of the responses (Y-block) and then fit a PLS model, by just selecting another model type.

Models are created by SIMCA when:

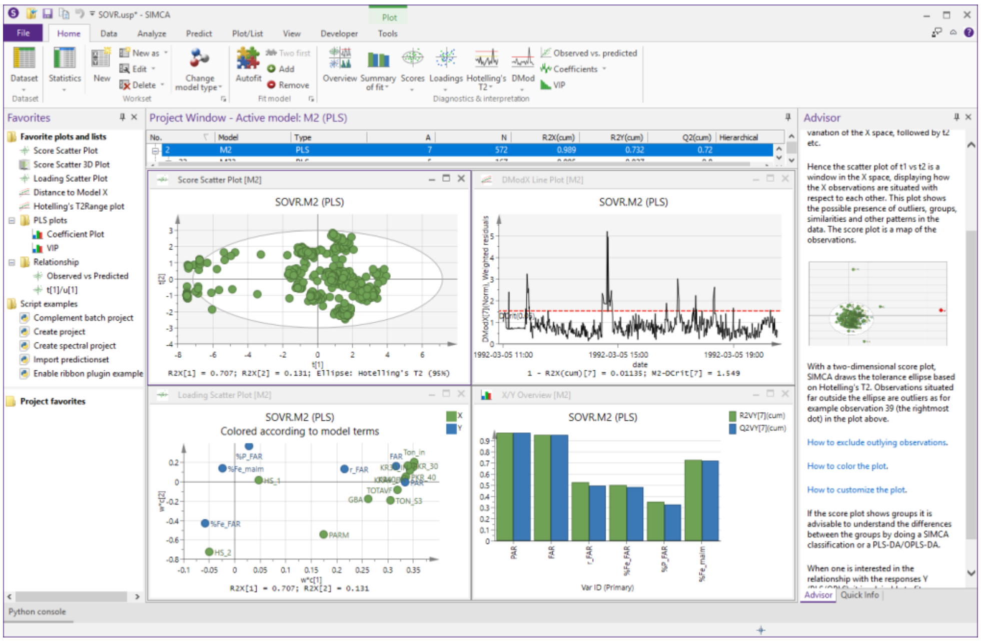
1. You specify a workset, **New/New as model**.
2. You make a selection under **Change model type** with a fitted model.

You work with one model at a time, the active model. This model is marked in the **Project Window** and its name and title are displayed in the caption of the project window.

There is always an active model. You may have several models open, but only one of them is active.

3.4 SIMCA window

The SIMCA window consists of the ribbon with regular and context tabs, the quick access toolbar, and panes.



No.	Model	Type	A	N	R2X(cum)	R2Y(cum)	Q2(cum)	Hierarchical
2	M2	PLS	7	572	0.989	0.732	0.72	

variation of the X space, followed by t2 etc.

Hence the scatter plot of t1 vs t2 is a window in the X space, displaying how the X observations are situated with respect to each other. This plot shows the possible presence of outliers, groups, similarities and other patterns in the data. The score plot is a map of the observations.

With a two-dimensional score plot, SIMCA draws the tolerance ellipse based on Hotelling's T2. Observations situated far outside the ellipse are outliers as for example observation 39 (the rightmost dot) in the plot above.

How to exclude outlying observations.

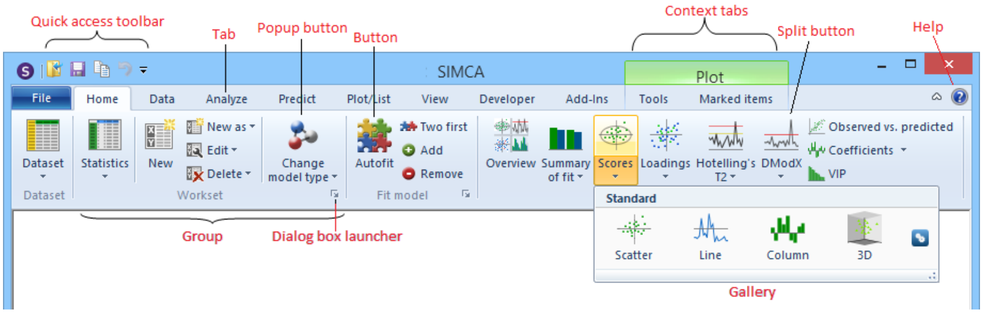
How to color the plot.

How to customize the plot.

If the score plot shows groups it is advisable to understand the differences between the groups by doing a SIMCA classification or a PLS-DA/OPLS-DA.

When one is interested in the relationship with the responses Y

3.5 SIMCA ribbon description



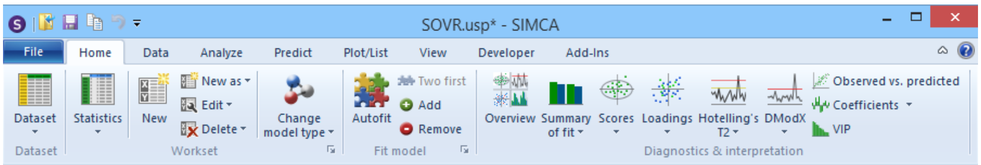
Description of the ribbon using terminology according to Microsoft:

- The ***File*** tab holds commands that involve doing something to or with a document, such as file-related commands.

- *Quick Access Toolbar* is a customizable toolbar that displays frequently used commands.
- *Core tabs* are the tabs that are always displayed.
- *Contextual tabs* are displayed only when a plot or list is open, **Tools**, or when items are marked in a plot or list, **Marked items**.
- *Galleries* are lists of commands or options presented graphically. A results-based gallery illustrates the effect of the commands or options instead of the commands themselves.
- *Dialog box launchers* are buttons at the bottom of some groups that open dialog boxes containing features related to the group.

3.6 Ribbon

Available functionality can be accessed through the SIMCA interface.



The SIMCA interface includes:

- the **Quick Access Toolbar**
- the regular tabs **File**, **Home**, **Data**, **Batch**, **Analyze**, **Predict**, **Plot/List**, and **View**
- the context tabs **Tools** and **Marked items**
- and the help-button

On the tabs the commands are parted in groups. Some of the groups have a dialog box launcher which opens a dialog closely connected to the features in the group.

For a short introduction see the sections that follow here. For more, see the respective chapters.

3.6.1 Quick Access Toolbar

The Quick Access Toolbar allows you to have your favorite commands easily accessible.

3.6.2 File

The following is available on the File tab:

- **Info** – **Manage** allows encrypting and compacting the project. **Report** creates a report. **Configure limits and alarms for SIMCA-online** to specify limits and alarms that can be imported in SIMCA-online.
- **New | Regular project/Batch project –** Creates new SIMCA projects after selecting a dataset in SIMCA import. If you have skins installed and enabled, application specific project types can be selected here automatically switching to the application skin.
- **Open** – Opens old project. Contains Recent projects and Recent folders lists.
- **Save** – Saves the current project.
- **Save as** – Saves the current project to the specified path and name.
- **Print –** Automatically displays a preview of the active window. Print setup and other print feature are available.
- **Share** – Uploads the project to SIMCA-online, provided a compatible version is available.
- **Close** – Closes the current project.
- **Help –** Contains license info, the possibility to **Activate**, and support features such as the help file.

- **Options –** Contains **SIMCA options** with the current default options for SIMCA, **Project options** with the current default options for the current project, and **Customize** which enables customization of the ribbon.

3.6.3 Home

On the Home tab you can change the model type, fit the model and review the fit. Plots and lists to analyze the model are available from this tab.

On the **Home** tab the following is available:

3.6.3.1.1 Dataset group

- **Dataset** – Lists and opens all available datasets.

3.6.3.1.2 Workset group

The workset is a working copy of the selected datasets with certain properties defined.

Note: *The datasets are NOT affected when you exclude variables/observations or by any other operation in the workset.*

In the **Workset** group the following is available:

- **Statistics | Workset statistics** – Displays statistics of selected variables of the active model.
- **Statistics | Correlation matrix** – Displays the correlations between the variables for the active model.
- **New** – Creates the default workset consisting of the first listed dataset with the variables set as X or Y as specified at import, and scaled according to the specified scaling in **Project Options**. For batch all batch evolution datasets imported when creating the project are included in the default workset.
- **New as –** Creates a new workset as a copy of the selected model.
- **Edit** – Opens the selected specified model for editing. If the model has already been fitted that model will be replaced by a new unfitted model at OK.
- **Delete** – Deletes the selected workset, and consequently also the model.
- **Change model type -** Displays the available model types:
    - **Overview - PCA-X, PCA-Y, PCA-X&Y, O2PLS**
    - **Regression** - **PLS**, **OPLS**
    - **Discriminant analysis** - **PLS-DA**, **OPLS-DA**, **O2PLS-DA**
    - **Class - PCA**, **PLS**, **OPLS**, **O2PLS**
    - **Clustering - PLS-Tree**
- **Model options** – Available from the dialog box launcher (arrow beneath the **Change model type** arrow) and displays the options of the active model.

3.6.3.1.3 Fit model group

For the model or model group (CM/BEM):

- **Autofit** – Autofits according to the autofitting rules.
- **Two first** – Calculates the two first components.
- **Add** – Calculates the next component.
- **Remove** – Removes the last component.

3.6.3.1.4 **Diagnostics & interpretation group**

Overview:

Displays the 4 default plots X/Y Overview, Scores, Loadings, DModX.

Summary of fit:

- **Summary of fit plot and list** – Displays the cumulative fit over all variables for each component.
- **X/Y overview plot and list –** Displays the cumulative fit of all variables for each x-variable for PCA and each y-variable for PLS, OPLS and O2PLS.
- **X/Y component –** Displays the fit of a variable for each component.
- **OPLS/O2PLS overview -** Displays OPLS and O2PLS specific R2.
- **Component contribution –** Displays the contribution of a model component to the fit.

Review the fit and investigate diagnostics:

- **Scores** t1 vs. t2, Num vs. t1, etc. – Displays trends, groupings, outliers.
- **Loadings** p1 vs. p2, w*c1vs. w*c2, etc. – Displays important variables, variable correlations.
- **Hotelling's T2** – Displays a measure of how far each observation is from the model center.
- **DModX** for X or Y – Displays the distance from the observation to the model, by default after the last component.
- **Observed vs. predicted** – Displays the actual value versus that observation predicted by the model for the selected response (y) variable.
- **Coefficients** – Displays the coefficient of the model for each response (y) variable cumulatively over all components.
- **VIP** – Displays the overall importance of each variable (x) on all responses (Y) cumulatively over all components.

3.6.4 Data

On the **Data** tab the following is available:

- **Import dataset** – Imports selected datasets.
- **Dataset** – Lists and opens all available datasets.

3.6.4.1.1 Modify dataset group

- **Merge** – Merges the selected datasets and deletes the second dataset (source).
- **Split -** Splits the selected dataset as specified in the dialog. Only available for independent datasets.
- **Transpose** – Transposes the selected dataset and deletes dependent models and datasets. **Not available for batch projects or dependent datasets**.
- **Delete dataset -** Deletes the selected dataset and any dependent models and datasets.
- **Generate variables –** Creates new variables as functions of the existing ones or from model results.
- **Local centering** - **Import** local centering or **View** already imported local centering data.

3.6.4.1.2 **Filters group**

- **Spectral filters -** Filters the selected dataset using the selected filter creating a dataset in the current project. The available filters are: Derivative (1st, 2nd, and 3rd derivative), Multiplicative Signal Correction (MSC), Standard Normal Variate (SNV), Row Center, Savitzky-Golay, EWMA, Wavelet Compression, Wavelet Denoising, Orthogonal Signal Correction (OSC) and chained filters.
- **Time series filters -** Time series filters the selected dataset using Wavelet Compress Time Series and Wavelet Denoising/Decimation creating a new dataset in the current project.

3.6.4.1.3 **Summary group**

- **Dataset summary –** Displays a summary of the performed filtering. Available for filtered datasets.
- **Missing value map -** Displays an overview of a dataset with respect to missing values.

- **Trimming overview –** Opens an overview window of the trimming. Only available after trimming.
- **Spectra** - Displays ObsDS, for the variables specified as X, of the selected dataset.

3.6.4.1.4 **Base model group**

- **Hierarchical** - Specifies the current model as hierarchical base model creating a hierarchical dataset.
- **Non hierarchical** - Removes the hierarchical base dataset.

3.6.5 Batch

On the Batch tab batch related commands are available.

3.6.5.1.1 Analysis control charts and Prediction control charts groups

- Batch control charts that display scores, distance to model, variable, Hotelling's T2, or predicted y with limits in plots and lists for models and predictions (BEM only).

3.6.5.1.2 Time/Maturity group

- **Observed vs. smoothed Y** - Displays the maturity for selected batch in original and treated form (BEM only).
- **Unaligned vs. aligned** - Displays the selected vector for the selected batch aligned and unaligned (BEM only).

3.6.5.1.3 **Dataset group**

- **Create batch level** – Creates the batch level dataset according to the selections made by the user. **Available with a BEM marked only**.
- **Create hierarchical batch models –** Creates hierarchical batch models according the selections in the dialog. **Only available for batch level datasets**.

3.6.5.1.4 **Variable summary group**

- **Variable importance plot** – Displays the overall importance of the variable over the whole evolution on the final quality of the batch. Available for BLM only.

3.6.6 Analyze

On the Analyze tab the analysis related features not available on the **Home** tab are available.

3.6.6.1.1 **Analysis group**

- **Biplot** – Displays scores and loadings superimposed.
- **Inner relation -** Displays t1 vs u1, t2 vs u2 etc.
- **S-plots - S-plot**, **S-line**, and **SUS-plot** display p in forms informative for OPLS with one Y.
- **Contribution** – Displays variables likely to be causes for upsets in the score, DModX, Hotelling's T2Range, or predicted response plots.
- **RMSECV** - Indicates predictive power.
- **Y-related profiles -** Coefficients rotated displaying the pure profiles of the underlying constituents in X using the assumption of additive Y-variables for OPLS and O2PLS.
- **Residuals N-plot** – Displays the residuals on the normal probability chart for the selected Y.

3.6.6.1.2 Validate group

- **Permutations** – Displays the validity and the degree of overfit for the model (only PLS).
- **CV-ANOVA** – For assessing the reliability of the model.
- **CV scores** - Displays the cross-validated complement to the regular scores plot

3.6.6.1.3 Clustering group

- **HCA –** Displays the clusters from the cluster analysis in a tree diagram.

- **PLS-Tree** - Displays the cluster analysis result using PLS-Trees.

3.6.7 Predict

On the **Predict** tab you can select a predictionset, display the predictionset as a spreadsheet, and display the prediction results using the active model.

The following is available:

3.6.7.1.1 Specify predictionset group

- **Specify** – Defines the predictionset in the **Specify Predictionset** dialog.
- **As dataset** - Predictionset is the selected dataset.
- **As workset** - Predictionset is the current workset.
- **Complement workset/Complement WS batches** - Predictionset is the observations/batches not included in the current model.
- **Class** - Predictionset is the selected class.
- **Delete predictionset** - Deletes the selected predictionset.

3.6.7.1.2 List group

- **Prediction list** – Displays the predictionset, some predicted vectors such as membership probability, scores, and the predicted response for PLS models.

3.6.7.1.3 Plots group

- **Y PS** – Displays the predictions for the selected response (y).
- **Scores PS** – Displays the predicted scores.
- **Hotelling's T2 PS** – Displays a measure of how far the predicted value for the observation is from the center
- **DModX PS+** for X or Y – Displays the distance from the predicted value for the observation to the model.
- **Control charts PS** – Displays the selected vector in the selected control chart: **Shewhart**, **CUSUM**, **EWMA**, or **EWMA/Shewhart**.
- **Contribution PS** – Show variables likely to be causes for upsets in the predicted score, distance to model X, Hotelling's T2Range, or predicted response plots.
- **Time Series PS** - Displays the selected vector in a line plot.
- **ROC -** Displays FPR (False Positive Rate) and TPR (True Positive Rate) for the marked DA or class models.
- **Coomans' plot** – Shows class separation for two selected models.
- **Classification list** - Displays the classification of a predictionset with respect to all the class models.
- **Misclassification table** – Summarizes the number of observations, with known class belonging, correctly classified in class or DA models.

3.6.8 Plot/List

The **Plot/List** tab holds general facilities for plotting and listing model and prediction results.

The following types of plots are provided:

3.6.8.1.1 Standard plots group

- **Scatter**
- **Scatter 3D**
- **Line**
- **Column**

- **List**

3.6.8.1.2 Control charts group

- **Time series**
- **Control charts**

3.6.8.1.3 Custom plots group

- **Histogram**
- **Dot plot**
- **Normal probability**
- **Response contour**
- **Response surface**
- **Wavelet structure**
- **Wavelet power spectrum**
- **Step response plot**

3.6.9 View

On the **View** tab the following is available:

Show group – Shows or hides the following panes:

- **Advisor** - Describes plots on the **Home** tab.
- **Audit trail** – Displays all actions taken that result in changes or additions to the project.
- **Favorites** – Holds a shortcut to selected plots, lists, and commands.
- **Item information** – Displays information about the marked items (points).
- **Marked items** – Displays the items, observations or variables, marked in a plot.
- **Model window** – Displays the model window of the active model.
- **Notes** - Pane where you can take notes about the project; automatically saved with the project.
- **Observations** – Displays the observations in the active model.
- **Project window -** Displays the models of the current project in the **Project Window**.
- **Quick info** – Displays information about the marked observation or variable.
- **Variables** – Displays the variables in the active model.
- **Status bar** – The Status bar displays an explanation when positioning the cursor over a button.
- **Full screen -** Displays the ribbon when clicking a tab but not otherwise.

3.6.9.1.1 Window group

Use the **Window** group to access the standard window commands.

3.6.10 Developer

The **Developer** tab is available when Python scripts are enabled in the license file, and provides access to scripting features.

3.6.11 Tools contextual tab

The **Tools** tab becomes available when opening a plot or list. The content is context sensitive. Changes introduced on the **Tools** tab apply to the active plot or list.

3.6.11.1 Layout group

Add plot element contains;

- **Maximize plot area** - Quick access to showing/hiding the header, legend, footer etc.
- **Header**
- **Footer**
- **Legend**
- **Axis titles**
- **Axes**
- **Regression line** - Displays the regression line and equation in the current plot.
- **Timestamp**

Templates contains;

- **Save templates** section with **Save as default** (saves the current plot formatting to the default plot formatting) and **Save as** (saves the current plot formatting to a plot formatting file).
- **Load template** - Switches to the selected template for all open and future plots.
- **Manage templates** section with **Open templates folder** (opens the folder where the custom templates are stored) and **Restore default settings** (restores the default template and switches to it).

3.6.11.2 Plot tools group

- **Select** – Selection modes.
- **Zoom –** Zooms according to the selected zooming type.
- **Zoom out** - Zooms out one step.
- **Highlight series** - Grays all but the series hovered in the legend.
- **Screen reader** - Displays the coordinates for the current position in a plot.
- **Sort** - Sorts lists, spreadsheets and column plots as specified.
- **Find** - Opens the **Find** dialog.

3.6.11.3 Properties group

The **Properties** group contains features also available in the **Properties** dialog for the current plot or list. The **Properties** group displays the properties of the plot or list.

- **Model -** Displays the active model.
- **Comp** - Displays the current component.
- X-axis comp - Displays the vector component.
- X-axis, Y-axis - Displays the vector displayed on the axis.
- **Batch** - Displays the selected batches.
- **Variable** - Displays the selected variable in for instance a BCC variable plot.
- **Observation** - Displays the selected observations in for instance a spectral plot.
- **Color by -** Displays and applies the selected coloring.
- **Labels -** Displays the selected labels.
- **Size by -** Displays and applies the selected sizing.

- Dialog box launcher - Opens the **Properties** dialog.
- **Resolve coefficients** - Available for hierarchical top models and results in coefficients for base models.

3.6.11.4 Create group

- **List -** Creates a list of the content of the current plot. For dendrograms (HCA, PLS-Tree) the created list displays the background to the plot.

For batches:

- **Sources of variation -** Converts the column plot to a sources of variation plot. Only available with BLM including one or more raw or score-variables.
- **Out of control summary -** Displays the percentage outside the displayed limits.
- **Batch control chart** - Available when the Out of Control Summary plot (OOC plot) is displayed and displays the batches in the OOC plot.

For dendrograms (HCA)

- **Merge list** - Displays the calculations behind the HCA dendrogram.

Change type of plot to;

- **Scatter**
- **Line**
- **Column**
- **Other plot types** - Opens the Create Plot dialog allowing you to select among all plot types.

3.6.11.4.1 Add group

- **Add to favorites** – Adds the current plot or list to the **Favorites** pane.
- **Add to report –** Adds the current plot or list to the HTML report in SIMCA.

Format plot - Opens the **Format Plot** dialog.

3.6.12 Marked items contextual tab

On the **Marked items** tab features available after marking items are available.

3.6.12.1 Create from marked items group

- **Scatter -** Creates a scatter plot holding only the marked items.
- **Line -** Creates a line plot holding only the marked items.
- **Column -** Creates a column plot holding only the marked items.
- **List** - Creates a list holding only the marked items.

3.6.12.2 Drill down group

3.6.12.2.1 Contribution plots

- **Point to average comparison**
- **Group to average comparison**
- **Point to point comparison**
- **Point to group comparison**
- **Group to group comparison**
- **Combined contribution -** Available only for BLM with scores marked.

3.6.12.2.2 Line plots

- **Plot XObs -** Plots the marked observations X-part in a line plot using a numerical ID as x-axis if available.
- **Plot YObs -** Plots the marked observations Y-part in a line plot using a numerical ID as x-axis if available.
- **Variable trend plot -** Plots the marked variables in a line plot.

3.6.12.2.3 Modify model group

- **Exclude -** Excludes the marked observations or variables.
- **Create new BEM and BLM without marked batches -** Available under **Exclude** after marking in a BLM score plot. Excludes the batches in the BEM, fits the BEM and automatically creates the new BLM holding the new batch level datasets and the batch condition datasets from the original BLM.
- **Include** - Adds the observations or variables to the unfitted model. Creates a new model holding only the included observations or variables if there is no unfitted model.
- **Class** - When marking observations *No Class*, *Class*, *Create class models*, *Create OPLS-DA*, and *Create PLS-DA* may be available enabling quick creation of class/DA models.

3.6.12.2.4 Layout group

- **Labels -** Displays the selected label on the marked points.
- **Hide -** Hides the marked points.
- **Show All -** Shows all items.
- **Format symbol -** Opens the **Format Plot** dialog with the new *Custom* node enabling customizing the marked items style.
- **Format label** - Opens the **Format Plot** dialog with the new *Custom* node enabling customizing the marked items labels.

3.6.13 Minimize/Expand the ribbon

Select whether to show the contents of the tabs or automatically slide away the tab content after clicking a command.

3.6.14 View help

Opens the SIMCA help.

3.7 Workspace

When the option to save a workspace in SIMCA is turned on, all plots, lists and spreadsheets are saved in their current state and position when the project is saved. This means that when opening this particular project again, the plots, lists and spreadsheets are reopened and positioned as before.

Customizations of the plots, such as axis scale or title wording, are also saved in the workspace.

3.7.1 Clearing the Workspace

If your workspace has become so large that it is time consuming to open the project and you want to get rid of the workspace;

1. Open SIMCA without opening the project.
2. Turn off the save workspace option on the **General** page in the **SIMCA options** dialog.
3. Open the .usp with the workspace and save it. This results in that the .usp is saved with an empty workspace.

3.8 Shortcut menu

Right-clicking any plot or list in SIMCA opens the context sensitive shortcut menu that includes general commands, such as **Copy**, **Print**, **Format plot**, and **Properties**.

3.9 Conventions

3.9.1 Limitations in project names

The project name length (including path) cannot be larger than 255 characters.

3.9.2 Limitations in observation and variable identifiers

Observation and variable identifiers (names) can be up to 256 characters long.

The primary observation and variable identifiers must be unique. When importing more datasets you are forced to have unique primary identifiers.

To be able to use a dataset as predictionset, the primary variable identifiers have to be identical to those of the model.

3.9.3 Case sensitivity

SIMCA is case insensitive. Lower or upper case in names will be displayed as entered, but for all comparisons lower or upper case are considered the same.

3.9.4 Menu and tab reference syntax

In this user guide we use the following syntax when referring to the **File** tab commands:

- Click **Tab** | **Command**. An example: Click **File** | **Save**.
- On the **Tab** tab, click **Command**. An example: On the **File** tab, click **Save**.
- Click **Command** on the **Tab** tab. An example: Click **Save** on the **File** tab.

In this user guide we use the following syntax when referring to tab commands/buttons:

- On the **Tab** tab, in the **Group** group, click **Command**. An example: On the **Home** tab, in the **Workset** group, click **New**.
- Click **Command**, in the **Group** group, on the **Tab** tab. An example: Click **New** in the **Workset** group on the **Home** tab.
- Click **Tab** | **Command** | **Menu item**. An example: Click **Home** | **Statistics** | **Workset statistics**.

In this user guide we use the following syntax when referring to a tab/menu item or gallery item accessed by clicking a button:

- On the **Tab** tab, in the **Group** group, click **Button | Menu item**. An example: On the **Home** tab, in the **Diagnostics & interpretation** group, click **Summary of fit | X/Y overview**.
- On the **Tab** tab, in the **Group** group, click **Button**, and then click **Menu item/Gallery item**. An example for menu: On the **Home** tab, in the **Diagnostics & interpretation** group, click **Summary of fit**, and then click **X/Y overview**. An example for gallery: On the **Home** tab, in the **Diagnostics & interpretation** group, click **Scores**, and then click **Line**.
- Click **Tab | Button | Menu item**. An example for menu: Click **Home | Summary of fit | X/Y overview**. An example for gallery: Click **Home | Scores | Line**.

3.9.5 Select and mark

Select or **Mark** an item in plots, lists, or menus signifies clicking the item leaving it highlighted.

3.9.6 Vector and matrix representation

Capital letters signify matrices, for ex. X, Y, P, T.

Letters typed in lower case signify vectors, for ex. x, y, p, t.

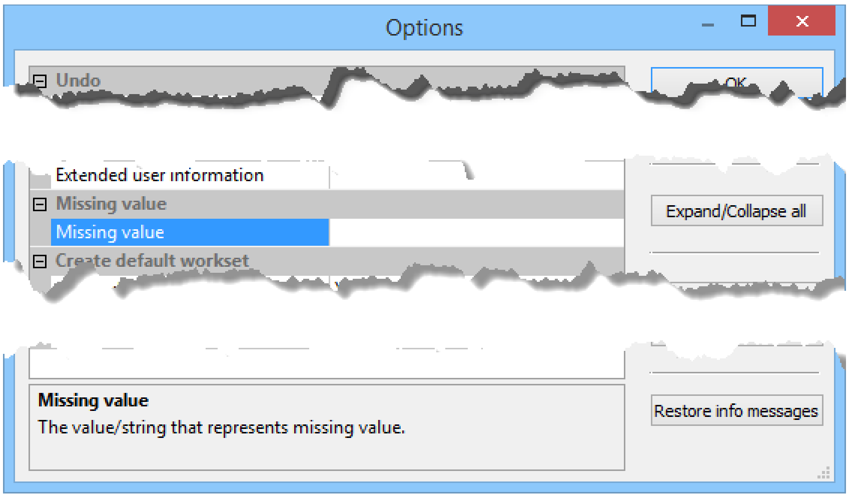
Prime <’> represents that the vector is a row vector. For example, t signifies a column vector with the values found under each other while p’ signifies a row vector where the values are found after each other.

3.9.7 Missing values representation

Missing values are represented by blank or space < >.

You can select another value to also represent missing in **Options** dialog, opened from the **File** tab in the SIMCA Import, by entering it in the **Missing value** field.

Note: -99 is assumed to be a valid value and is therefore automatically changed to -99.0001. If -99 represents missing value, enter -99.0001 in the **Missing value** field in Options dialog in the SIMCA import.



Missing value
The value/string that represents missing value.

3.9.7.1 Consequences of missing values

The present NIPALS algorithm works with missing data as long as they are relatively randomly distributed, i.e., do not occur with a systematic pattern. Otherwise the results of a model fitting can be very misleading. The default is to warn when the missing value content in an observation or variable exceeds 50%.

3.10 Presentation of SIMCA results

3.10.1 Plots for publications

For publications, use the **Print quality** field in the **Copy to Clipboard**/**Save As**-dialog. For more, see the Copy plot subsection in Chapter 4, Quick Access Toolbar.

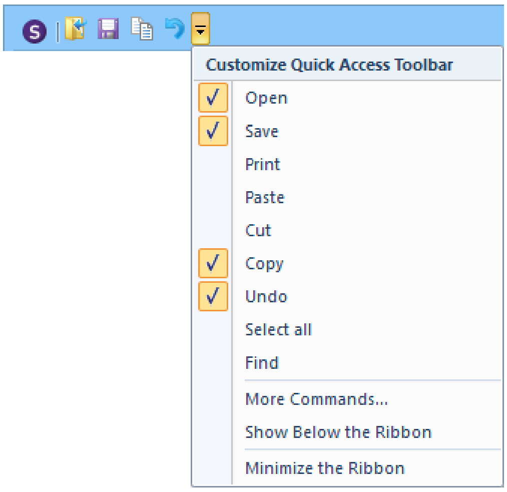
3.10.2 Plots for reports

For suitable formats to copy or save, use one of the Umetrics predefined, see the Save as subsection in Chapter 5, File.

4 Quick Access Toolbar

4.1 Quick Access Toolbar

The Quick Access Toolbar is by default positioned at the top above the tabs and allows you to have your favorite commands easily accessible. The Quick Access Toolbar is standard in Windows software with ribbons.



The Quick Access Toolbar in SIMCA default displays the following features:

- **Open** - CTRL+O
- **Save** - CTRL+S
- **Copy** - CTRL+C
- **Undo** - CTRL+Z

Note: **Undo** is unavailable after adding or deleting rows/columns or changing any content of a dataset spreadsheet.

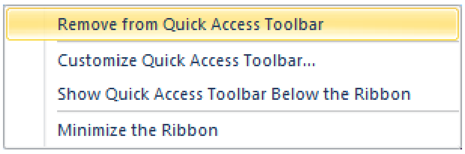
4.2 Customizing Quick Access Toolbar

You can add buttons to and remove buttons from the Quick Access Toolbar both using the methods described below and by opening the **File | Options** dialog and making the changes on the Quick access toolbar page.

4.2.1 Removing buttons from Quick Access Toolbar

To remove a button from the Quick Access Toolbar:

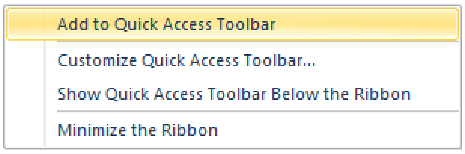
- Right-click the button and click **Remove from Quick Access Toolbar**.
- Click the arrow to the right of the available Quick Access Toolbar buttons and clear the relevant check box.


Remove from Quick Access Toolbar
Customize Quick Access Toolbar...
Show Quick Access Toolbar Below the Ribbon
Minimize the Ribbon

4.2.2 Adding buttons to Quick Access Toolbar

To add a button to the Quick Access Toolbar:

- Right-click the button on the ribbon and click **Add to Quick Access Toolbar**.
- Click **More commands** on the Quick Access Toolbar menu and make your changes in the **Customize** dialog.



Add to Quick Access Toolbar

Customize Quick Access Toolbar...

Show Quick Access Toolbar Below the Ribbon

Minimize the Ribbon

4.2.3 Moving the Quick Access Toolbar

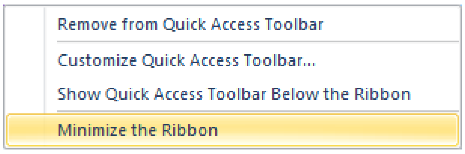
To position the Quick Access Toolbar closer to the work area you can select to position it below the ribbon by clicking the **Show below the ribbon** in the Quick Access Toolbar menu. Click **Show above the ribbon** to move it back to its original position.

4.3 Minimizing the ribbon

To maximize the work area you can minimize the ribbon so that it folds away like a menu.

The **Minimize the ribbon** command is available:

- When you right-click a button in the Quick Access Toolbar.
- In the Quick Access Toolbar menu.
- When you right-click a button in the ribbon.
- To the far right of the tabs just left of the help-button.



Remove from Quick Access Toolbar

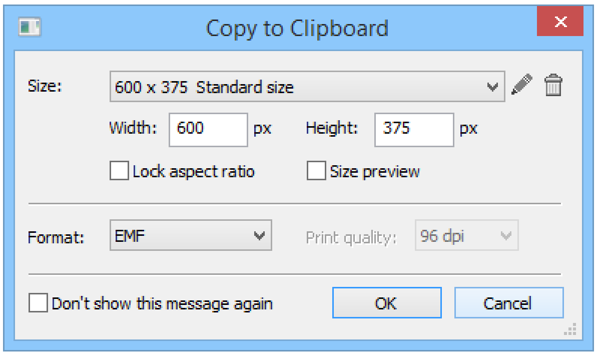
Customize Quick Access Toolbar...

Show Quick Access Toolbar Below the Ribbon

Minimize the Ribbon

4.4 Copy and save plot

The **Save Plot** and **Copy to Clipboard** dialog boxes are very similar, merely the presence/absence of the Format drop down differentiates them. When copying, the plot format can be selected in this dialog box while, for save, it is selected in the **Save As** dialog which opens after **OK**.



Copy to Clipboard

Size: 600 x 375 Standard size

Width: 600 px Height: 375 px

□ Lock aspect ratio □ Size preview

Format: EMF Print quality: 96 dpi

□ Don't show this message again

4.4.1.1 Size

The size of the plot is defined by the values in the Width and Height fields. These fields are automatically updated when switching between the predefined sizes in the Size box. Likewise, the content of the Size box is updated when changing the width and height.

Note: To keep the aspect ratio of the plot while customizing the size, select the **Lock aspect ratio** check box before changing.

The available options in the Size drop down box are,

- Original size - the current plot size

Suitable for documentation

- 600x375 - standard size
- 300x300 - square, fits two side by side

- 600x600 - square

Suitable for presentations

- 755x465 - fits one plot per slide
- 755x270 - fits two above and below
- 375x465 - fits two side by side

Custom sizes

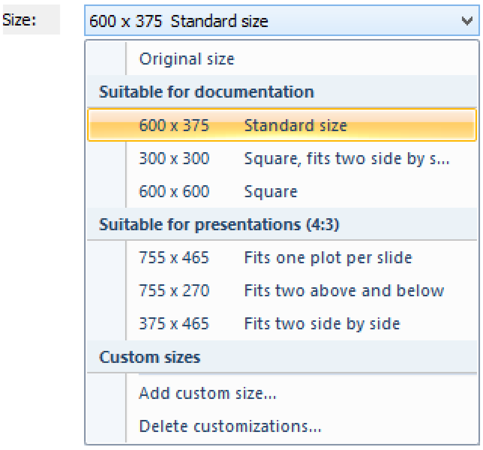
- Add custom size - opens the **Add Custom Size** dialog box with the current plot size predefined. Clicking **OK** adds the specified size under the Custom sizes header.

4.4.1.2 Edit, delete and restore

To edit the current size, click the **Edit current size** pencil to the right of the Size drop down.

To delete the current size, click the **Delete current size** garbage bin.

To delete all customized sizes at once and restore the built-in formats, click **Delete customizations** under **Custom sizes** in the **Size** drop down box.


Size:
600 x 375 Standard size
Original size
Suitable for documentation
600 x 375 Standard size
300 x 300 Square, fits two side by s...
600 x 600 Square
Suitable for presentations (4:3)
755 x 465 Fits one plot per slide
755 x 270 Fits two above and below
375 x 465 Fits two side by side
Custom sizes
Add custom size...
Delete customizations...

4.4.1.3 Size preview

Selecting the Size preview check box displays the plot exactly as it will be saved or copied. This feature allows you to verify that the layout and text formats harmonize with the selected save/copy size before inserting/pasting it.

4.4.1.4 Print quality and plot format

The default print quality is 96 dpi. This is sufficient for the web and presentations, but not for high quality print where 300 dpi is recommended.

The plot formats available are Bitmap (BMP), EMF (only 2D), PNG, JPG, Encapsulated PostScript (EPS), and SVG (only 3D and only when saving).

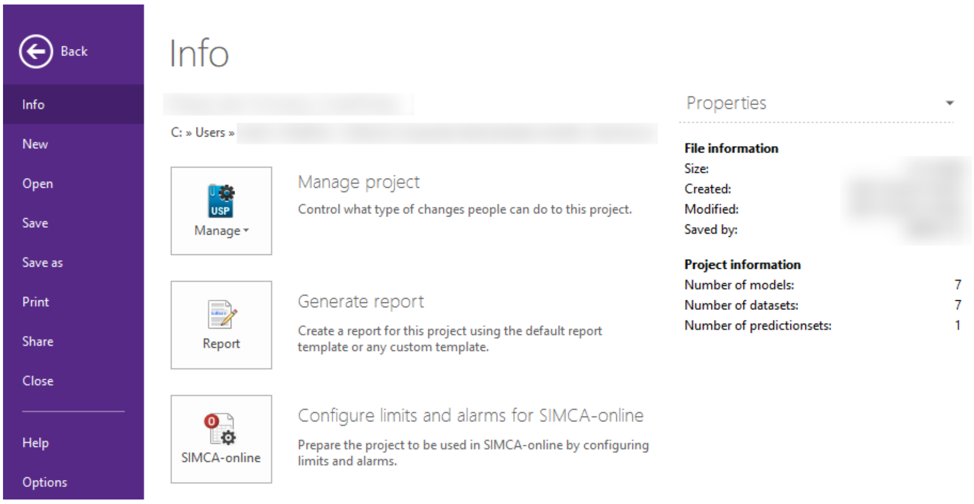
Note: Using EPS with high dpi creates a very large plot file.

5 File

5.1 Introduction

This chapter describes all features available on the **File** tab.

The following commands are available: **Back** (closes the backstage view and returns focus to the previously active tab), **Info**, **New**, **Open**, **Save**, **Save as**, **Print**, **Share**, **Close**, **Help** and **Options**.



Manage project

Control what type of changes people can do to this project.

Generate report

Create a report for this project using the default report template or any custom template.

Configure limits and alarms for SIMCA-online

Prepare the project to be used in SIMCA-online by configuring limits and alarms.

File information

Size:
Created:
Modified:
Saved by:

Project information

Number of models:	7
Number of datasets:	7
Number of predictionsets:	1

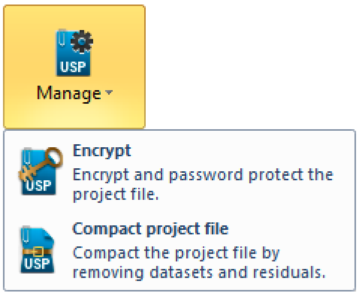
5.2 Info

The Info section on the File tab provides access to **Compact project file** and **Encrypt** under **Manage**, delete project and creation of the **Report**, **Configure limits and alarms for SIMCA-online**, as well as giving a quick summary of the project properties.

5.2.1 Project properties

Project properties shows information about,

- Size
- Creation date
- Modified date
- Number of models
- Number of datasets
- Number of predictionsets
- SIMCA-online metadata such as server origin, source project ID, etc.



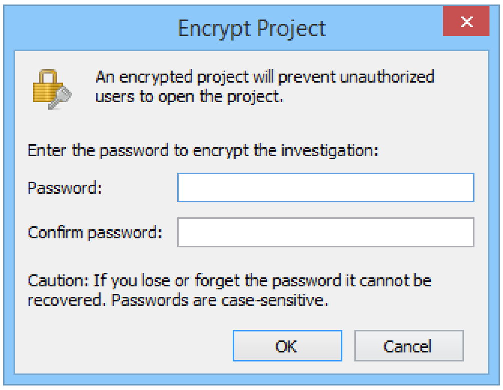
Encrypt
Encrypt and password protect the project file.

Compact project file
Compact the project file by removing datasets and residuals.

5.2.2 Encrypt

To encrypt and lock a project, click **File** | **Info** | **Manage** | **Encrypt**. The Encrypt Project dialog opens and you are prompted by SIMCA to enter a password.

After entering the password twice and clicking **OK**, the project is locked and can only be opened by providing the password.



An encrypted project will prevent unauthorized users to open the project.

Enter the password to encrypt the investigation:

Password:

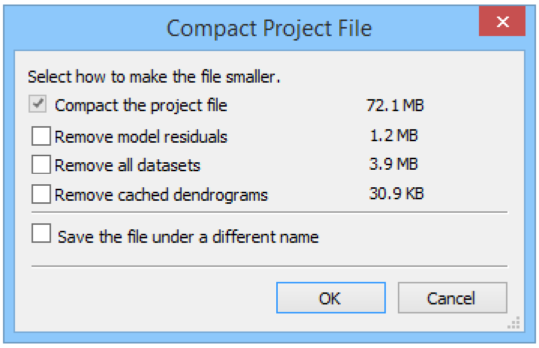
Confirm password:

Caution: If you lose or forget the password it cannot be recovered. Passwords are case-sensitive.

5.2.3 Compact project file

When compacting a project file, this is done by removing unnecessary data and optionally data considered unnecessary by the user. Compacting a project file is particularly useful when models or datasets have been deleted in the project.

Click **File** | **Info** | **Manage** | **Compact project file** to open the Compact Project File dialog.



Select how to make the file smaller.

☑ Compact the project file 72.1 MB

□ Remove model residuals 1.2 MB

□ Remove all datasets 3.9 MB

□ Remove cached dendrograms 30.9 KB

□ Save the file under a different name

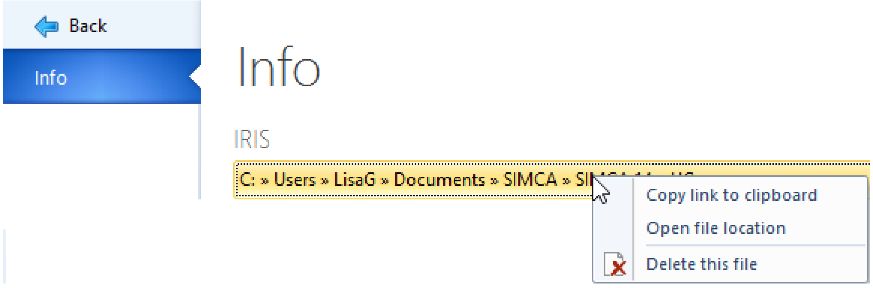
In the **Compact Project File** dialog, select which data to remove. The available choices are listed in the table.

Check box	Select the check box and click OK
Compact the project file	Removes all deleted models and datasets. **Compact the project file** is the default selection and is always selected.
Remove model residuals	Deletes and removes model residuals. **NOTE**: If you remove the model residuals from a project, SIMCA will not be able to open it again. Project files without model residuals can only be used by a few Umetrics Suite products, e.g. SIMCA-Q. Therefore the project will be saved to a new file with the extension .rusp. (r for reduced).
Remove all datasets	Deletes and removes all datasets. **NOTE**: If you remove all datasets from a project, SIMCA will not be able to open it again. Project files without the datasets can only be used with a few Umetrics Suite products, e.g. SIMCA-Q. Because of this, the project will be saved to a new file with the extension .rusp.
Remove cached dendrograms	Deletes cached dendrograms.
Save the file under a different name	Saves the compacted project under a different name and leaves the original project untouched.

Note: Compact cannot be undone. The compacted project file is saved when clicking **OK**.

5.2.4 Delete project

To delete the current project, click **File** | **Info** and left-click the path of the project.



5.2.5 Report

5.2.5.1 Introduction

SIMCA has an automatic report generator available by clicking **File** | **Info** | **Report**.

In the report generator, basic formatting functionality for writing text is available.

Plots, lists, and model results of SIMCA can be added to the report at any time. These items are added to the report as *placeholders*.

A placeholder stands in the place of contents which SIMCA will provide; let it be a plot, list, text or number.

The placeholders enable using the same report, as a template, in different projects. Edit the text, and just click **Update report** to update all SIMCA results using the active model.

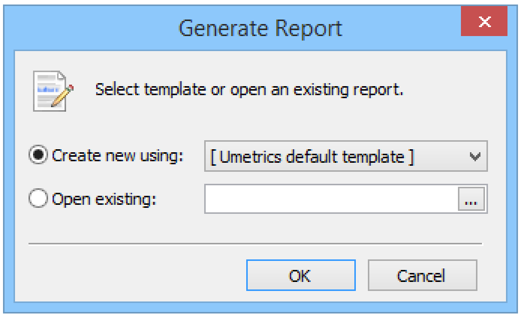
Note: To avoid updating a plot, you must remove the placeholder. For more, see the Tools menu in report subsection later in this section.

For details about how to send a report by e-mail, see the knowledgebase at the Sartorius Stedim Data Analytics website www.umetrics.com.

5.2.5.2 Starting to generate a report

To create a report:

1. Click **File** | **Info** | **Report**.
2. In the **Generate Report** dialog select to:
   a. Create a new report selecting **Create new using** and selecting [Blank] or [Umetrics default template] or
   b. Open a report by clicking **Open existing** and selecting an existing report.
3. Click **OK**.

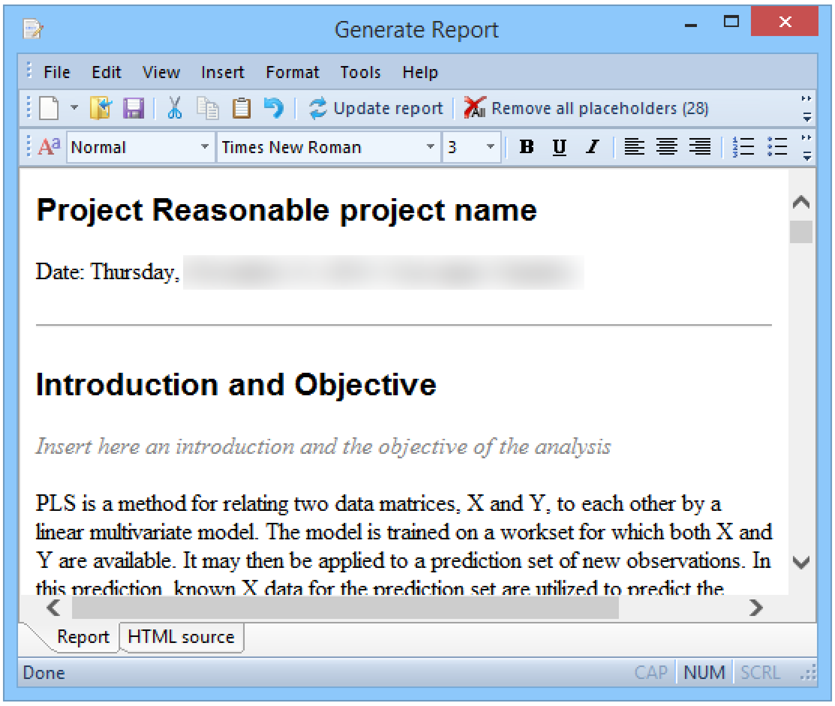

Select template or open an existing report.

● Create new using: [Umetrics default template]

○ Open existing:

5.2.5.3 Generate Report window

The report for the active model opens in a new window, the **Generate Report** window. This window is separate from SIMCA but is closed when SIMCA is closed.



Project Reasonable project name

Date: Thursday, [redacted]

Introduction and Objective

Insert here an introduction and the objective of the analysis

PLS is a method for relating two data matrices, X and Y, to each other by a linear multivariate model. The model is trained on a workset for which both X and Y are available. It may then be applied to a prediction set of new observations. In this prediction, known X data for the prediction set are utilized to predict the

The **Generate Report** window contains the following:

- Menu bar holding the menus **File**, **Edit**, **View**, **Insert**, **Format**, **Tools**, and **Help**.
- Generate report toolbar with commonly used commands.
- Formatting toolbar with commonly used formatting commands.
- Main window showing the report template.
- **Placeholders** window with a list of built-in placeholders.
- **Report Generator FAQ** window with a short introduction to how to use the report generator.
- **Properties** window where plot size and placeholder properties can be edited.

5.2.5.4 Default templates

SIMCA has a default template for the following models:

- PCA
- PLS, OPLS, O2PLS
- PLS-DA, OPLS-DA, O2PLS-DA
- Batch

5.2.5.4.1 Default template content

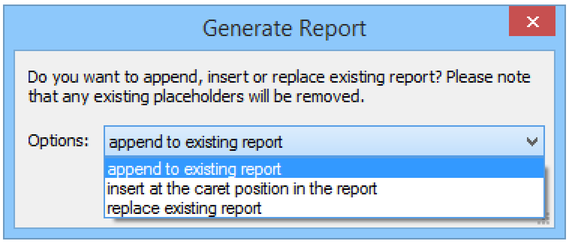
The SIMCA default template consists of:

1. Introduction and Objective (text to be filled by user).
2. Description of the included datasets.
3. Pre-processing such as spectral filters etc., if any.
4. Model summary.
5. Transformation and scaling.
6. Goodness of fit.

7. Model results.
8. Predictions (plots and lists to be added by the user).
9. Conclusion (text to be filled by user).

5.2.5.5 Appending to, inserting in, or replacing existing report

With an open report, right-clicking a model in the **Project Window** and clicking **Generate report** opens the following dialog:



Generate Report

Do you want to append, insert or replace existing report? Please note that any existing placeholders will be removed.

Options: append to existing report

append to existing report
insert at the caret position in the report
replace existing report

This enables:

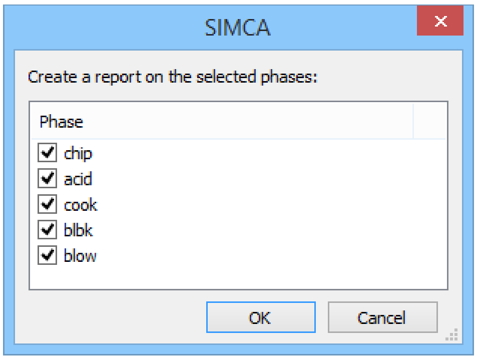
1. Appending the report updated for the active model to the current report by clicking **append to existing report**.
2. Inserting the report updated for the active model to the current report at the caret position in the report by clicking **insert at the caret position in the report**.
3. Replacing the existing report with an updated report using the active model by clicking **replace existing report**.

Note: After selecting 1 or 2 above and clicking **OK**, the placeholders for the previous report are removed.

5.2.5.6 Creating a report including several phases

To generate a report for all the phases of the batch evolution model:

1. Right-click the BEM in the **Project Window**.
2. Click **Generate report** and select the Umetrics template (or one you have prepared).
3. Select the phases to include in the report.
4. Click **OK** to open the report.



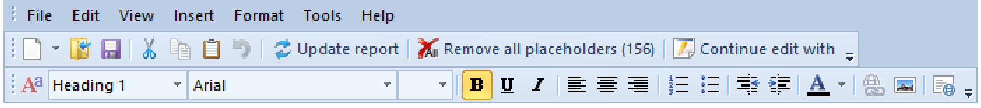
SIMCA

Create a report on the selected phases:

Phase
☑ chip
☑ acid
☑ cook
☑ blbk
☑ blow

5.2.5.7 Menu bar in report

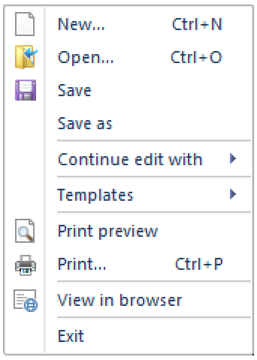
The menu bar consists of the **File**, **Edit**, **View**, **Insert**, **Format**, **Tools**, and **Help** menus.



5.2.5.7.1 File menu in report

Under the **File** menu the general Windows commands **New**, **Open**, **Save As**, **Print Preview**, **Print** and **Exit** are available.

Additionally the report generator commands **Continue edit with**, **Templates** and **View in browser** are available.



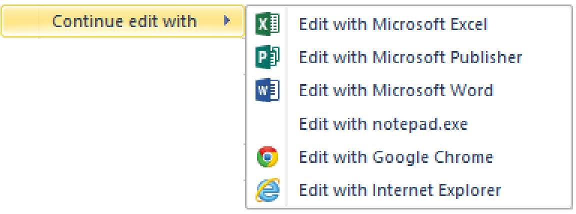
General windows commands

The functions of the general windows commands are described in the table.

Command	Use to
New	Create a new report from the selected template or report.
Open	Open a report saved in HTML format.
Save as	Save the report in HTML format. The report is saved with placeholders and can be used as template.
Print, Print preview	Print the report. Preview the report.
Exit	Close the report.

Continue editing report with

Continue to work with the report in the editor of your choice by under the **File** menu clicking **Continue edit with**, and then selecting the editor. The applications listed here are the applications that have registered with Windows that they can edit HTML text.

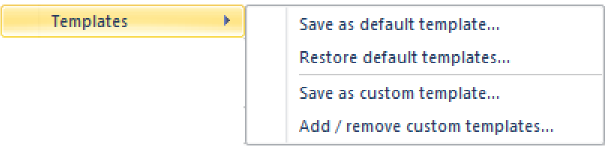


Continue edit with is also available as a button on the **Generate report** bar.

Templates

Save templates, restore templates and add or remove custom templates by clicking **Templates** under the **File** menu.

- Select **Save as default template** when you have changed/created a template according to your wishes and want to use it as the default template next time you generate a report for the same model type.
- Select **Restore default templates** if you have made changes to the default templates and want to remove those changes.
- Select **Save as custom template** when you have changed/created a template according to your wishes and want to save it to be able to use it again. Custom templates will be listed in the **Select template or open existing** dialog (after clicking **File | Info | Report** in SIMCA) and when clicking **Insert | Template**.
- Select **Add / Remove custom templates** when you want to add an already created template or remove one of your custom templates.


Templates
Save as default template...
Restore default templates...
Save as custom template...
Add / remove custom templates...

View in browser

To view the current report in your default internet browser, on the **File** menu click **View in browser**.

5.2.5.7.2 Edit menu in report

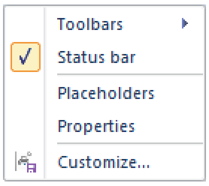
Under the **Edit** menu the commands **Undo** (CTRL+Z), **Redo (CTRL+Y)**, **Copy** (CTRL+C), **Paste** (CTRL+V), **Paste unformatted** (CTRL+SHIFT+V), **Clear** (DELETE), **Select all** (CTRL+A), and **Find** (CTRL+F) are available.

Paste unformatted is useful when the text copied is formatted.

5.2.5.7.3 View menu in report

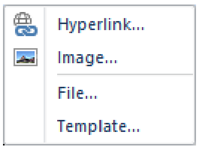
Under the **View** menu, select to hide or show the **Toolbars**, **Status bar**, **Placeholders** window, and **Properties** window. You can also customize the toolbars, command menus and toolbar and menu options in **Customize**.

- To show or hide the toolbars click **Toolbars** and then click **Generate report** or **Format**. Both toolbars are displayed by default. For more about the toolbars, see the Generate report bar and Format bar subsections later in this chapter.
- To show or hide the **Status bar**, click it. The **Status bar** displays an explanation when positioning the cursor over a button.
- Click **Placeholders** to display the window. For more see the Placeholders window subsection later in this chapter.
- Click **Properties** to display the window. The properties of plots and images can be customized in the **Properties** window. For more see the Properties window subsection later in this chapter.



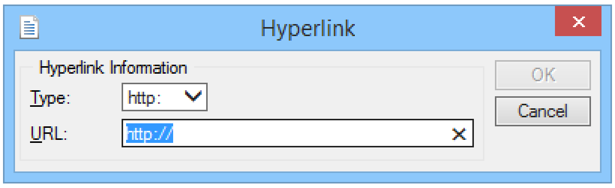
5.2.5.7.4 Insert menu in report

Use the **Insert** menu to insert a **Hyperlink**, **Image**, **File**, or **Template** in the current report.



Hyperlink

To insert a hyperlink, mark the text or plot in the report and then click **Insert** | **Hyperlink**. The following dialog opens:



Hyperlink Information

Type: http:

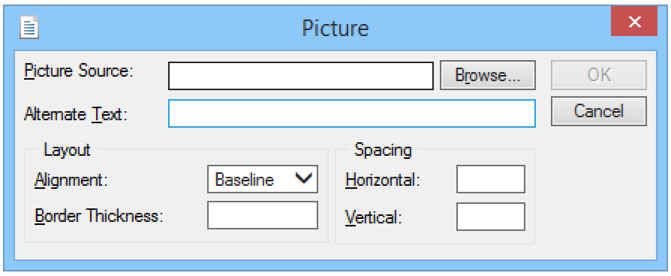
URL: http://

In the URL field, enter the hyperlink address.

Insert hyperlink is also available in the Format bar.

Image

To insert a picture in the report, click **Insert** | **Image**, and then click **Browse** to find the file.



Alignment: Baseline

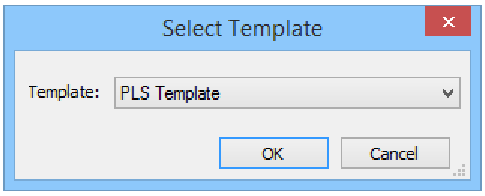
Insert image is also available in the Format bar.

File

To insert a Web page file (*.htm, *.html), a Text file (*.txt), or a picture file (*.jpg, *.png, *.gif, *.bmp.), click **Insert** | **File**. In the **Open** dialog, select the file.

Template

To select a template to insert in the report, click **Insert** | **Template**. In the **Select Template** dialog, select the template to insert in the report.

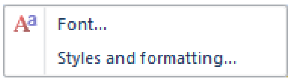


Template: PLS Template

For a template to be available in this dialog, it must either come with the program or first have been saved using **File** | **Templates** | **Save as custom template**.

5.2.5.7.5 Format menu in report

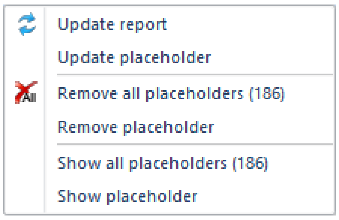
Use the **Format** menu to customize **Font** and **Styles and formatting** when specifying your style sheet.



5.2.5.7.6 Tools menu in report

Under the **Tools** menu find the commands **Update report**, **Update placeholder**, **Show all placeholders**, **Show placeholder**, **Remove all placeholders**, and **Remove placeholder**.

Command	Result after selected
Update report	Updates all placeholders with the plots and lists of the active model. **Update report** is also available as a button on the Generate report bar.
Update placeholder	Updates the marked placeholder.
Remove all placeholders	Removes all placeholders. Use this option when you do not want any items, plots, or lists to be updated. **Remove all placeholders** is also available as a button on the Generate report bar.
Remove placeholder	**Removes the marked placeholder. Use this option** when you do not want a certain item, plot, or list to be updated.
Show all placeholders	Shows all underlying placeholders.
Show placeholder	Shows the underlying placeholder of the marked plot, list, or item.



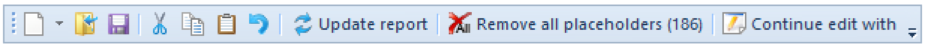
5.2.5.7.7 Help menu in report

To access the FAQ of the report generator, click **Welcome page and FAQ** on the **Help** menu. The **Report Generator FAQ** window opens to the right.

5.2.5.8 Generate report bar

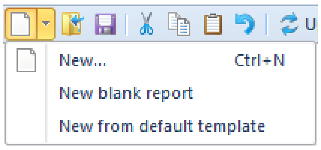
The **Generate report** bar includes the general commands **New**, **Open**, **Save**, **Cut**, **Copy**, **Paste**, and **Undo**. All these commands work according to Windows standard except for the **New** command described here.

The generate report bar additionally includes the commands **Update placeholders**, **Remove all placeholders**, and **Continue edit with**.



5.2.5.8.1 New

Click the arrow next to **New** and the following commands are displayed.



- Click **New** from the menu displays the generate report dialog from which you can select which report/template to use or to open an existing report/template.
- Click **New blank report** to start a new report with no text.
- Click **New from default template** to create a report from the default template. Save a report as a default template by clicking **File** | **Templates** | **Save as default template**. Umetrics’ default template is used if no other template has been specified.

5.2.5.8.2 Generate report bar additional buttons

For info about the **Placeholder** functions **Update report** and **Remove all placeholders**, see the Tools menu section.

For info about **Continue edit with**, see the File menu section.

For info about **View in browser**, see the File menu section.

5.2.5.9 Format bar

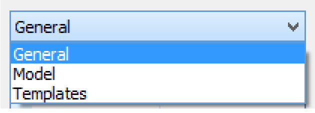
The **Format** bar is the standard toolbar for formatting text with three additional buttons: **Insert hyperlink** , **Insert image** , and **View in browser** .

For more, see the Insert menu and File menu sections in this chapter.

5.2.5.10 Placeholders window

The placeholders are organized into the following categories:

- General
- Model
- Templates



5.2.5.10.1 Open the Placeholder window

Open the Placeholder window by clicking **View** | **Placeholders**.

5.2.5.10.2 Inserting a placeholder

To insert a placeholder in the report:

1. Place the cursor in the desired position in the report.
2. Mark the placeholder by clicking it in the **Placeholders** window.
3. Click **Insert**.

5.2.5.10.3 Placeholders window - General

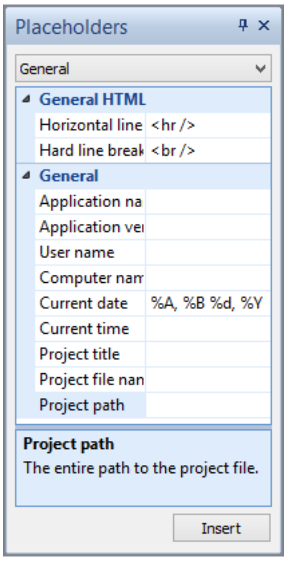
The general placeholders available are listed here with the expected result after clicking **Insert** and updating the placeholder.

General HTML

- **Horizontal line** - horizontal line.
- **Hard line break** - line break as when pressing **SHIFT** + **ENTER**.

General

- **Application name** - 'SIMCA'.
- **Application version** - 15'.
- **User name** - the user name used to log in to Windows.
- **Computer name** - the internal computer name.
- **Current date** - today's date.
- **Current time** - the time when updating the placeholder.
- **Project title** - the name of the SIMCA project.
- **Project file name** - the SIMCA project name including extension, e.g. FOODS.usp.
- **Project path** - the path to the SIMCA project file.



Horizontal line	<hr />
Hard line breal	<br />
Application na	
Application vei	
User name	
Computer narr	
Current date	%A, %B %d, %Y
Current time	
Project title	
Project file nan	
Project path	

Project path
The entire path to the project file.

5.2.5.10.4 Placeholders window - Model

The model placeholders available are listed here with the result after clicking **Insert** and updating the placeholder. The placeholders refer to all datasets included in the model.

Numbers

- **Num. variables** - number of variables included in the model when counting both X and Y.
- **Num. X variables** - number of x-variables in the model.
- **Num. Y variables** - number of y-variables in the model.
- **Num. excluded variables** - number of excluded variables.
- **Num. observations** - number of observations in the model.
- **Num. excluded observations** - number of excluded observations.
- **Num. batches** - number of batches in the model. Batch projects only.
- **Num. classes** - number of classes.

Text

- **Variable primary ID** - lists all primary variable identifiers in the model.
- **X variable primary ID** - lists the primary variable identifiers for x-variables in the model.
- **Y variable primary ID** - lists the primary variable identifiers for all y-variables in the model.
- **Excluded variable primary ID** - lists the primary variable identifiers for excluded variables.
- **Included batch ID** - lists the batch identifiers of the batches included in the model. Batch projects only.
- **Excluded batch ID** - lists the batch identifiers of excluded batches. Batch projects only.
- **Observation primary ID** - lists the primary observation identifiers in the model.
- **Model name** - lists the model name, e.g. M1. For batches, with the phase name, e.g. M1:chip.
- **Model title** - lists the user entered model title. 'Untitled' if no title was entered.
- **Model type** - lists the model type, e.g. PCA. For batches with the phase name, e.g. PLS-Class(chip).
- **Phase ID** - lists the phase identifier of the active model.
- **Dataset names -** lists the names of all datasets included in the model.

Summaries

- **Dataset import log** - the text from the import log. Can be viewed in SIMCA by opening the **Dataset properties**, tab **General**.
- **Preprocessing summary** - the text in **Data | Dataset summary**. Available for filtered datasets.
- **Expanded terms** - lists all expansions.
- **Lagged variables** - lists all lags.
- **Transformed variables summary** - lists the transformed variables and their transformation.
- **Scaled variables summary** - lists the variables not centered and scaled to Unit Variance with their scaling.
- **Trimmed variables summary** - lists the trimming performed in the workset.

Results

- **Num. components** - lists the number of components extracted for the active model.

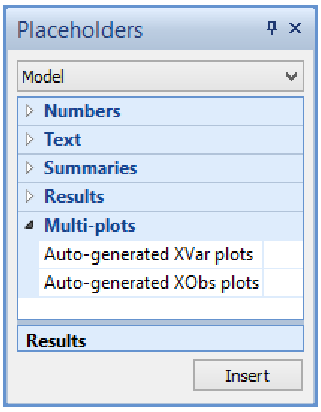
- **R2X, R2X(Cum), R2Y, R2Y(Cum), Q2, Q2(Cum)** - lists the values for all components or cumulatively for the last component for the vectors. For details about the vectors, see the Function of component vectors section in the Statistical appendix.

Note: The vectors are by default displayed for the last component. For how to display all components, see the Properties window subsection later in this chapter.

Multi-plots

- **Auto-generated XVar plots** - displays each x-variable in a separate line plot.
- **Auto-generated XObs plots** - displays each observation in a separate line plot. Only the values for the x-variables are displayed.

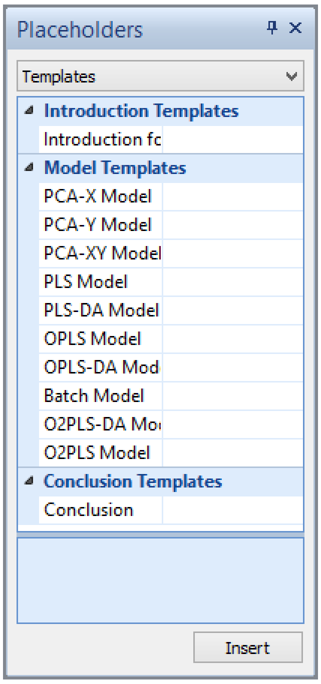
Using these placeholders it may take a long time to update the report. Press the **ESC**-button to abort the multi plot update.



5.2.5.10.5 Placeholders window - Templates

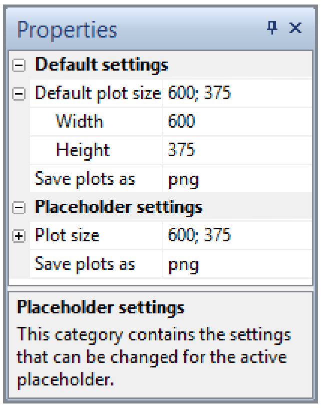
The **Templates** placeholders consist of model templates.

Use the templates placeholders to insert a template into a report.



5.2.5.11 Properties window

The properties window is opened by clicking **View** | **Properties**. The properties for a placeholder are displayed when clicking the placeholder with the **Properties** window open.



Properties

⊟ **Default settings**	
⊟ Default plot size	600; 375
Width	600
Height	375
Save plots as	png
⊟ **Placeholder settings**	
⊞ Plot size	600; 375
Save plots as	png

Placeholder settings
This category contains the settings that can be changed for the active placeholder.

In the **Properties** window the following can be customized:

- The **Default plot size** and format under **Default settings**.
- The **Plot size** and format for the current plot (placeholder) under **Placeholder settings**.

The format for plots is by default .png. The available formats are .png, .bmp, and .jpg.

Placeholders for vectors can be modified to display a part of the vector or the entire vector. For instance, R2X is by default displayed for the last component. To display all components, type: 'R2X[{0}] = {1}{separator: }<BR>' in the **Data** field.

Note: The properties of the placeholder for the date can be changed by selecting it and using the Properties window.

5.2.5.12 Adding plots and lists to the report

To add a plot or list to the report, click the desired position in the report and then use one of the following methods:

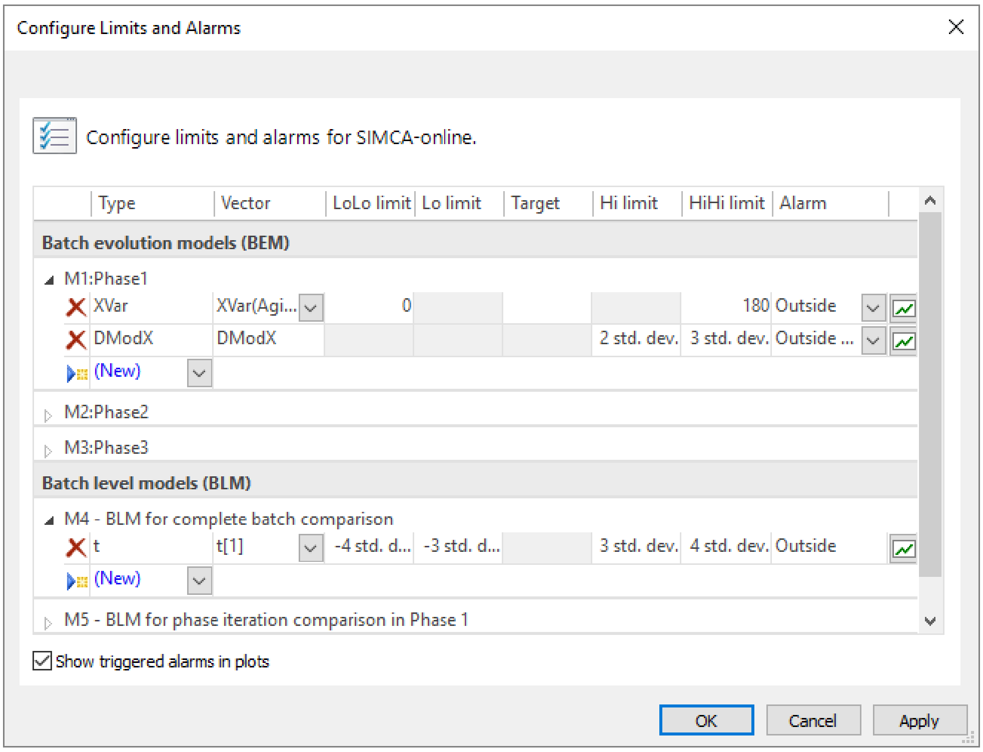
- Right-click the plot or list window in SIMCA and click **Add to report**.
- On the **Tools** tab, in the **Add** group, click **Add to report**.

The plot or list is inserted into your report.

5.2.6 Configure limits and alarms for SIMCA-online

Alarm rules and limits to be used in SIMCA-online can be defined already in SIMCA. The settings are stored in the SIMCA project and transferred to the SIMCA-online configuration when using **File | Share**.

Click the plot icon at the end of the alarm specification row to open the relevant prediction plot. Triggered alarms are displayed in the SIMCA project as long as the **Show triggered alarms in plots** check box is selected in this dialog.



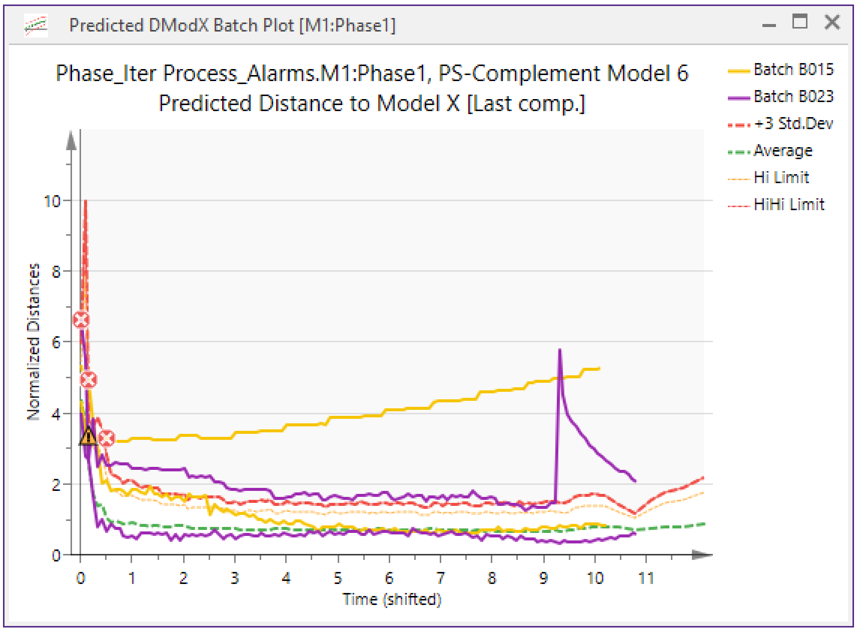
Configure Limits and Alarms

Configure limits and alarms for SIMCA-online.

Type	Vector	LoLo limit	Lo limit	Target	Hi limit	HiHi limit	Alarm
Batch evolution models (BEM)							
M1:Phase1							
XVar	XVar(Agi...	0				180	Outside
DModX	DModX				2 std. dev.	3 std. dev.	Outside ...
(New)							
M2:Phase2							
M3:Phase3							
Batch level models (BLM)							
M4 - BLM for complete batch comparison							
t	t[1]	-4 std. d...	-3 std. d...		3 std. dev.	4 std. dev.	Outside
(New)							
M5 - BLM for phase iteration comparison in Phase 1							

☑ Show triggered alarms in plots

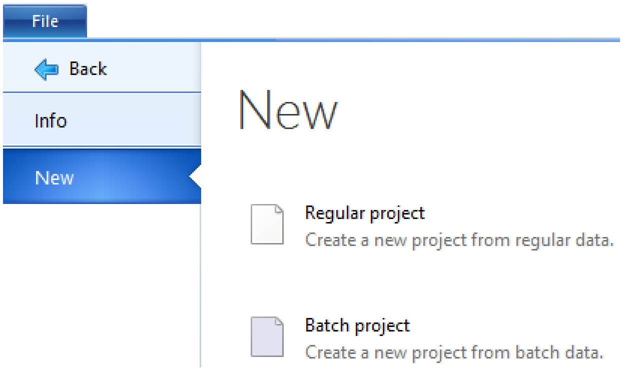
Clicking the plot icon on the DModX alarm opens the plot below there a number of alarms have been triggered.



Note: When here is a time variable, that variable will be placed on the x-axis while the Num axis is used to define which observation is the first to be triggered in an alarm. This means that if the time-variable is not consecutive, the alarms may be triggered out of sync with the x-axis.

5.3 New - Creating a new project

When creating a new project you have to select which type: **Regular project** or **Batch project**. Optionally, with skins installed, such projects can be created by clicking the respective command here.



New

Regular project
Create a new project from regular data.

Batch project
Create a new project from batch data.

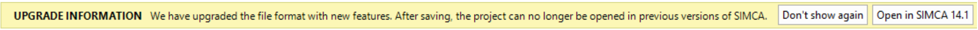
Click **File** | **New** | **Regular project** or **Batch project** to open SIMCA import, select your data and create a new project. See Chapter 6, SIMCA import for more.

5.4 Open - Opening an existing project

Click **File | Open** to open an existing SIMCA project by selecting the corresponding SIMCA project *.usp-file.

Each instance of SIMCA can only open one project while several instances of SIMCA can be open in parallel.

When opening an project created in a previous version, that information is displayed to alert you of this fact. If that version is installed, you can select to open the project there instead if you want to avoid updating the file format.



UPGRADE INFORMATION We have upgraded the file format with new features. After saving, the project can no longer be opened in previous versions of SIMCA.

5.4.1 Opening pre-13 projects

Projects from SIMCA-P 9 to SIMCA-P+ 12 are automatically converted when opened. All models are refitted except for hierarchical top models. The hierarchical base specification is also lost in the conversion and must be re-specified.

Note: Datasets from projects created in SIMCA-P 9 and later can be imported.

Projects and datasets from SIMCA-P version 8.0 and earlier cannot be opened or imported by this version of SIMCA.

5.4.2 Opening pre-13 filtered projects limitations

When converting a filtered project the following functionality is unavailable in SIMCA:

- Reconstruct.
- **Spectral filters** and **Time series filters**.
- **Data** | **Import dataset**.

5.4.3 Opening pre-13 batch projects

When opening a batch observation level project, all connected batch level projects are listed and you can choose which one to convert resulting in a project with both the observation level models and batch level models. For more, see Chapter 9, Batch.

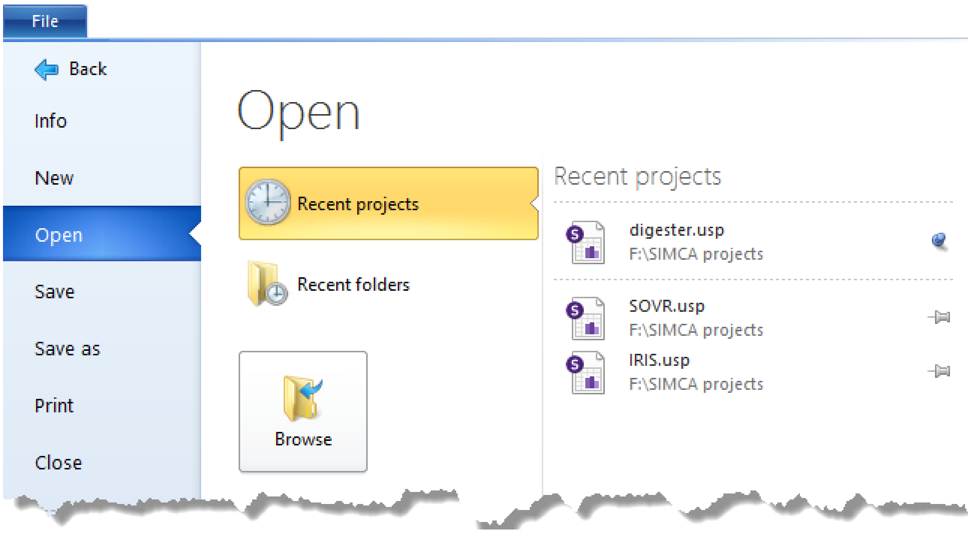
Batch projects have been reorganized to include both levels in the same project. The observation level model and dataset have been renamed batch evolution model and dataset, abbreviated BEM and BE DS, while the batch level model and dataset names remain batch level model and dataset, abbreviated BLM and BL DS. Both the BEM and the BLM are positioned in a BMx, where x is a sequential number.

5.4.4 Recent projects and folders

Recent projects lists the most recently opened projects.

Recent folders lists the most recently opened folders.

Clicking the pin to the right of the recently opened project or folder turns the pin and keeps that item in the recent list even after it should have fallen off.

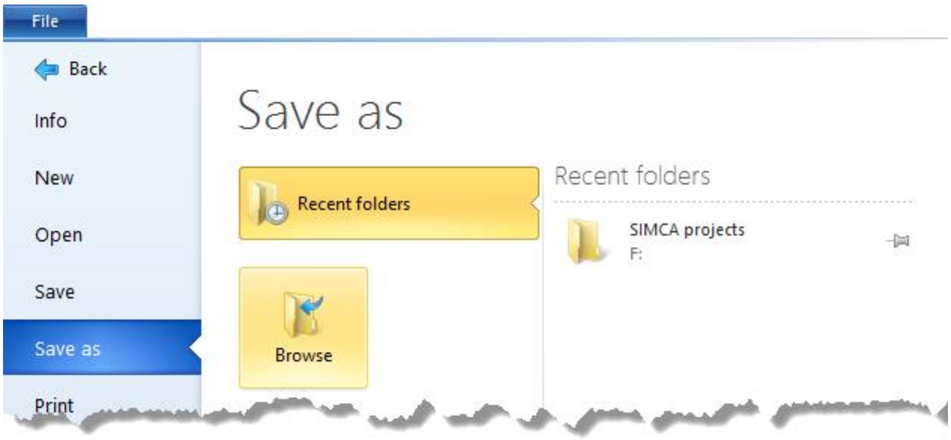


5.5 Save project

To save the open project to the current name and location, click **File** | **Save**.

5.6 Save project as

Under **Save as** you can select to save the active project to a specific file name and path.



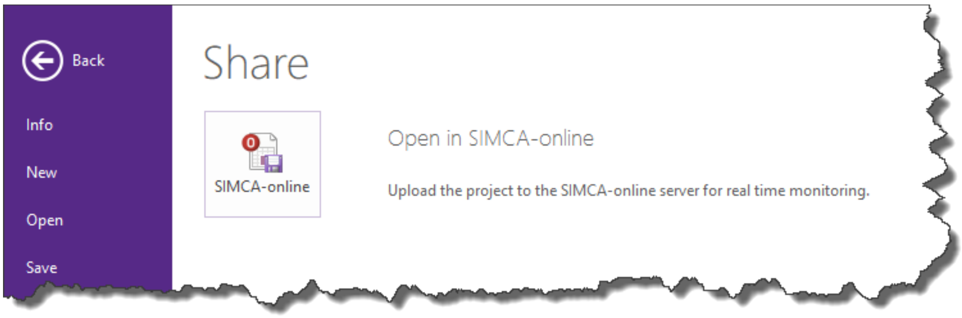
5.7 Print

To print, preview or change the print setup click **File** | **Print**.

Note: Plots are printed as viewed on the screen except when printing to a pdf writer.

5.8 Share with SIMCA-online

The currently open project can be exported to SIMCA-online, provided a compatible version is available. For more, see the SIMCA-online help.



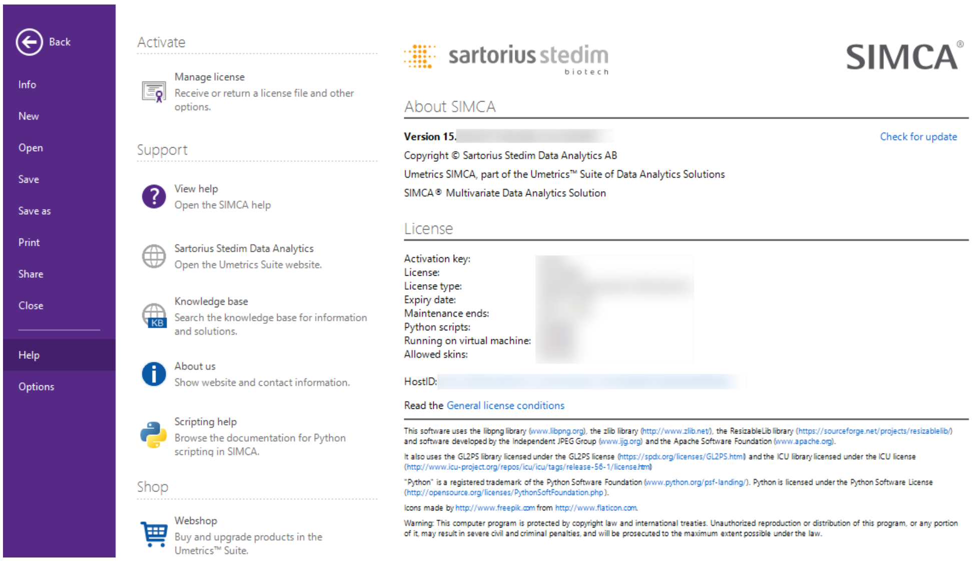
Upload the project to the SIMCA-online server for real time monitoring.

5.9 Help

5.9.1 Introduction

This section describes all commands available when clicking **File** | **Help**.

Use the **Help** section to: activate SIMCA, access the help, access the Sartorius Stedim Data Analytics website, or view version, license details, HostID, general license conditions, etc.


Back
Info
New
Open
Save
Save as
Print
Share
Close
Help
Options
Activate
Manage license
Receive or return a license file and other options.
Support
View help
Open the SIMCA help
Sartorius Stedim Data Analytics
Open the Umetrics Suite website.
Knowledge base
Search the knowledge base for information and solutions.
About us
Show website and contact information.
Scripting help
Browse the documentation for Python scripting in SIMCA.
Shop
Webshop
Buy and upgrade products in the Umetrics™ Suite.
sartorius stedim biotech
SIMCA®
Check for update

About SIMCA

Version 15.[redacted]

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Umetrics SIMCA, part of the Umetrics™ Suite of Data Analytics Solutions

SIMCA® Multivariate Data Analytics Solution

License

Activation key:
License:
License type:
Expiry date:
Maintenance ends:
Python scripts:
Running on virtual machine:
Allowed skins: [redacted]

HostID: [redacted]

Read the General license conditions

This software uses the libpng library (www.libpng.org), the zlib library (http://www.zlib.net/), the ResizableLib library (https://sourceforge.net/projects/resizablelib/) and software developed by the Independent JPEG Group (www.ijg.org) and the Apache Software Foundation (www.apache.org).

It also uses the GL2PS library licensed under the GL2PS license (https://spdx.org/licenses/GL2PS.html) and the ICU library licensed under the ICU license (http://www.icu-project.org/repos/icu/icu/tags/release-56-1/license.html)

"Python" is a registered trademark of the Python Software Foundation (www.python.org/psf-landing/). Python is licensed under the Python Software License (http://opensource.org/licenses/PythonSoftFoundation.php).

Icons made by http://www.freepik.com from http://www.flaticon.com.

Warning: This computer program is protected by copyright law and international treaties. Unauthorized reproduction or distribution of this program, or any portion of it, may result in severe civil and criminal penalties, and will be prosecuted to the maximum extent possible under the law.

The help and the user guide are based on the same files. To read the Help file, Internet Explorer must be installed but does not need to be the default browser.

5.9.2 Activate SIMCA

After installing SIMCA it has to be activated. If you choose to activate later, click **File** | **Help** | **Activate** and follow the directions.

5.9.3 HTML help

The HTML help file is installed to include interactive and stand-alone help.

Open the help by:

- Clicking the **View help** button.
- Clicking the **Help**-button Help in one of the dialogs or wizards.
- Pressing F1.

Use the Contents, Index, or Search tabs to find what you are looking for.

Note: Using citation marks <"> allows searching of phrases.

Additionally, the Advisor is available to guide you through the analysis. Open it by selecting the **Advisor** check box in the **Show** group on the **View** tab. For more, see the Advisor subsection in Chapter 13, View.

5.9.4 Sartorius Stedim Data Analytics on the Web

Visit the Sartorius Stedim Data Analytics website (www.umetrics.com) to get the latest news and other information by clicking **File** | **Help** and then **Sartorius Stedim Data Analytics**.

To find the latest information and solutions to problems, search the Knowledge base. Click **File** | **Help** | **Knowledge base** to open it.

5.9.5 About SIMCA

To find the version number of SIMCA and current license information, click **File** | **Help**.

5.10 Options

Options in SIMCA can be set at 3 levels:

- **SIMCA options** - apply to the software. Changes in these options apply to all projects opened after the change. For more about these general options, see the SIMCA options section later in this chapter.
- **Project options** – set at the project level and are in effect for that project and all models created after applying changes. New projects inherit the factory settings options. To make new projects inherit the current project options settings, click **Save as default** on the **Project options** page. For more about the project options, see the Project options section later in this chapter.
- **Model options** – set at the model level and are local to that particular model. Some options can only be set in model options. New models inherit the options from the project level. For more about the model options, see the Model options section in the Workset section in Chapter 7, Home.

File | Options opens the **Options** dialog with the pages **SIMCA options**, **Project options**, **Customize ribbon**, **Quick access toolbar**, **Keyboard**, **Theme**, **Painter**, and **Restore**.

5.10.1 Theme

On the **Theme** page, a few relevant themes are selectable. SIMCA is the default theme.

5.10.2 Keyboard shortcuts

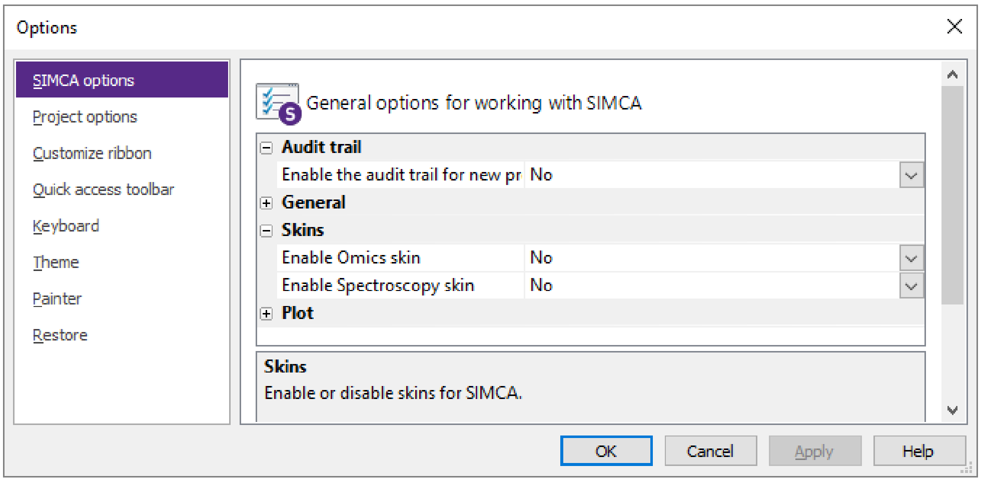
You can also customize the shortcut commands used by SIMCA by clicking **Keyboard** and make changes.

5.10.3 SIMCA options

The options available from SIMCA options apply to SIMCA and not just the current project.

The sections on the SIMCA options page are **Audit trail**, **General**, **Skins**, and **Plot**. The **General** and **Plot** sections are described here.

Clicking the **Reset** button returns all settings to the factory settings for the SIMCA options page.

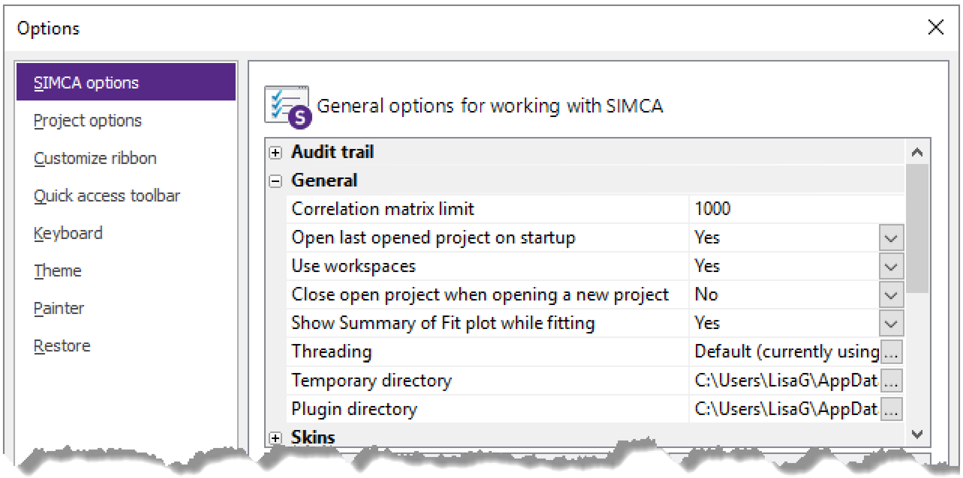


Audit trail
Enable the audit trail for new pr No
General
Skins
Enable Omics skin No
Enable Spectroscopy skin No
Plot

Skins
Enable or disable skins for SIMCA.

5.10.3.1 General

The **General** page includes default behavior when starting SIMCA, creating a new project, and fitting the model.



⊞ Audit trail

⊟ General

Correlation matrix limit	1000
Open last opened project on startup	Yes
Use workspaces	Yes
Close open project when opening a new project	No
Show Summary of Fit plot while fitting	Yes
Threading	Default (currently using
Temporary directory	C:\Users\LisaG\AppDat
Plugin directory	C:\Users\LisaG\AppDat

⊞ Skins

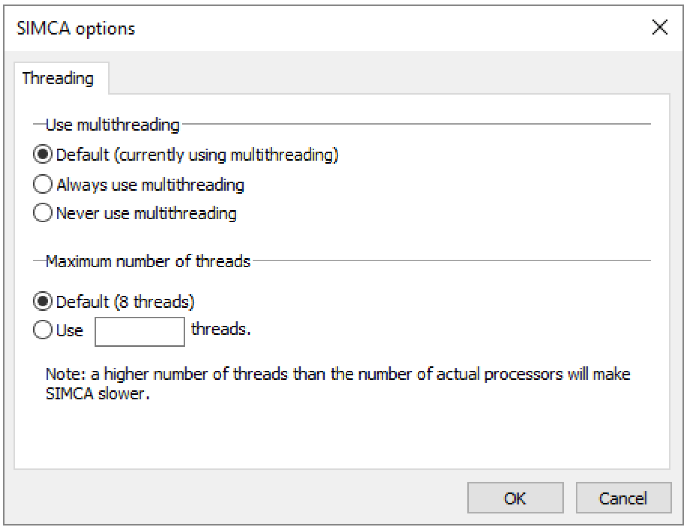
All check boxes, starting from the top, are described in the table below:

Option	Description	When	Default
Correlation matrix limit	Limit in the correlation matrix to avoid slowing the software down.	Increasing from the default allows displaying the correlations of more variables.	1000
Open last opened project on start-up	Opens the last opened project when opening SIMCA.	The project you worked with last is often the one you start off with. Clear this check box when working with very large projects, to avoid opening a project when planning to work with another.	Yes
Use workspaces	Opens the workspace when opening a project.	You want all plots and lists to reappear when you reopen a project. Clear this check box when working with very large projects as opening the workspace can be very time consuming.	Yes
Close open project when opening a new project	The open project will be closed and the new created one will be the only open.	When you want only one project open. Clear this check box if you want the current project to remain open. The new project is then opened in another instance of SIMCA.	Yes
Show Summary of Fit plot while fitting	When fitting a model, the summary plot is displayed.	Clear the check box if you don't want to see the summary plot.	Yes
Threading	In SIMCA certain calculations can use multithreading to speed up the calculations.	When the computers has several processors or several process cores. Threading can speed up calculations for large projects but will have little effect on small to medium sized projects.	Default
Temporary directory	The path to the **Temporary directory**, used by SIMCA to save temporary files, is displayed.	When opening SIMCA projects.	%temp%/umetrics/SIMCA/15.0
Plugin directory	The path to the **Plugin directory**, used by SIMCA to load plugins, is displayed. Plugins supported by SIMCA are spectral filters, import, and item information.	When loading plugins.	A plugin folder in the *application data* folder of the current user.

5.10.3.2 Selecting multithreading

In SIMCA certain calculations can use multithreading to speed up the calculations, if it detects that the computer has several processors or several processor cores. Threading can speed up calculations for large projects but will have little effect on small to medium sized projects.

In the **Threading** page opened by clicking the button at the end of the Threading row in the **General** section on the **SIMCA options** page., Threading can be turned on and off and the number of processors to use can be specified.



Use multithreading

● Default (currently using multithreading)

○ Always use multithreading

○ Never use multithreading

Maximum number of threads

● Default (8 threads)

○ Use [   ] threads.

Note: a higher number of threads than the number of actual processors will make SIMCA slower.

5.10.3.2.1 Using multithreading

In the **Use multithreading** section, select one of the following options:

- **Default** – SIMCA checks if the computer has more than one processor and turns multithreading on if it does. In parenthesis the status is displayed as ‘**currently using multithreading**’ or ‘**currently not using multithreading**’.
- **Always use multithreading** – SIMCA uses multithreading without first checking for number of processors.
- **Never use multithreading** – SIMCA does not use multithreading.

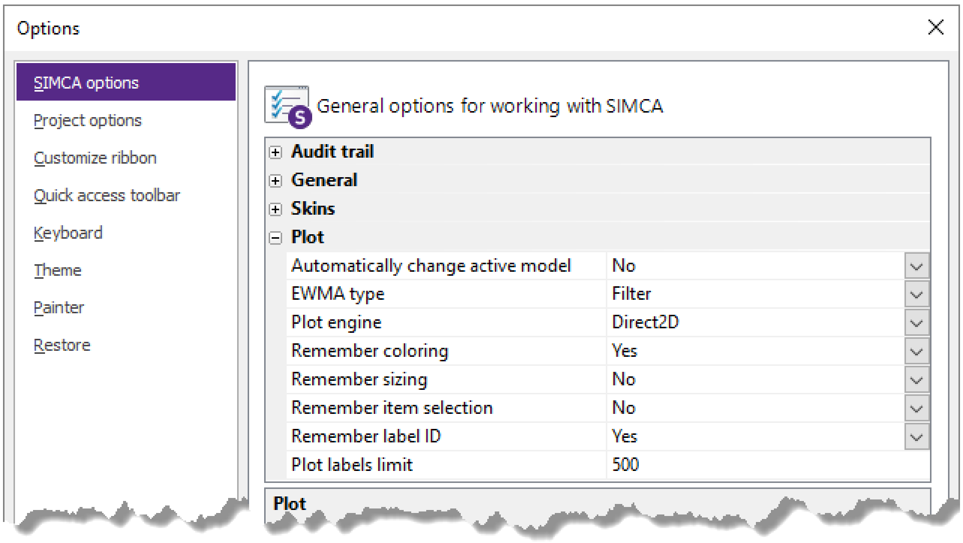
5.10.3.2.2 Selecting number of threads

In the **Maximum number of threads** section, select one of the following options:

- **Default** - SIMCA threads using the number of processors found. That number is displayed in parenthesis.
- **Use x threads**; enter the number of threads to use - This option is only viable when you want fewer threads than available processors to be used.

5.10.3.3 Plot options

The **Plot** section on the **SIMCA options** page displays and holds settings relevant for plots. The settings here define the defaults and default behavior for the plots.



Options

SIMCA options
Project options
Customize ribbon
Quick access toolbar
Keyboard
Theme
Painter
Restore

General options for working with SIMCA

⊞ Audit trail
⊞ General
⊞ Skins
⊟ Plot

Automatically change active model	No
EWMA type	Filter
Plot engine	Direct2D
Remember coloring	Yes
Remember sizing	No
Remember item selection	No
Remember label ID	Yes
Plot labels limit	500

Plot

In the table the options available under **Plot** in the **SIMCA options** page are described. Each option can be changed by clicking the current entry and changing it.

Option name	Description	Default
Automatically change active model	The active model is automatically changed when clicking a plot created from that plot.	Yes
EWMA type	The EWMA type that will be used in Control Charts, spectral filters and when transforming with EWMA on the Transformation page in the Plot/List dialog.	Filter
Plot engine	Switch between GDI+ and Direct 2D.	Direct2D when possible.
Remember coloring	Remembers the coloring specified in **Tools | Color by** or in the **Color** tab of the **Properties** dialog, between plots. That is, after selecting a certain coloring in one plot, the next plot opened will use the same coloring scheme.	Yes
Remember sizing	Remembers the sizing specified in **Tools | Size by** or in the **Size** tab of the **Properties** dialog, between plots. That is, after selecting a certain sizing in one plot, the next plot opened will use the same sizing.	No
Remember item selection	Remembers the item selection specified by marking and clicking **Hide** on the **Marked items** tab, or the **Item selection** tab of the **Properties** dialog, between plots. That is, after making the item selection for one plot, the next plot opened will use the same item selection.	No
Remember label ID	Remembers the label specified in **Tools | Labels** or on the **Plot labels** tab in the **Properties** dialog.	Yes
Plot labels limit	When the number of plot labels in a plot exceeds this number, no labels are displayed.	500

5.10.4 Project options

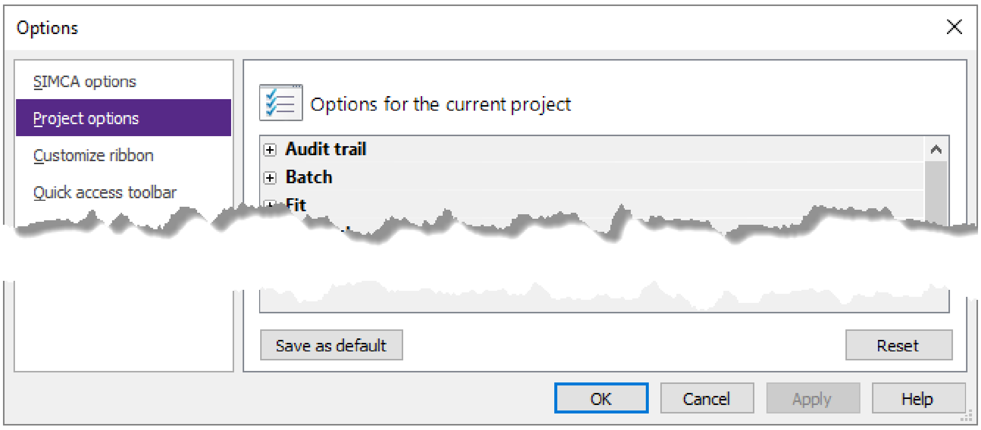
The Project options apply to the current project. For options also available in Model Options, changes in Project options apply to future models only.

The **Project options** page includes the sections: Audit trail, Batch (for batch projects only), Fit, General, Statistical options, and Predictions.

Clicking **Reset** returns all settings to the factory settings for the Project options page.

Clicking **Save as default** saves the current Project options as global options.

Project options and **SIMCA options** are accessed by clicking **File** | **Options**.



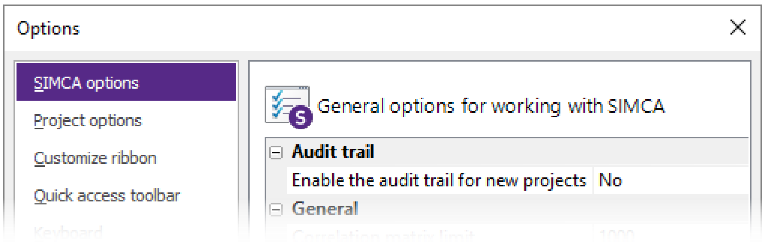
5.10.4.1 Administration of the audit trail

The audit trail can be turned on/off in SIMCA but for the audit trail to be automatically on or off for new projects it has to be turned on/off in SIMCA options before creating the project (**Enable the audit trail for new projects** *Yes* on the **SIMCA options** page*)*. To turn the audit trail on the for the current project, use Project options.

An administrator can enable or disable the entire Audit trail page and control the behavior of the Audit Trail, i.e., always on or off.

As the administrator of the system, contact your sales office for instructions on how to disable user administration of the audit trail, or search the knowledge base at www.umetrics.com.

For details about the audit trail, see the Audit Trail section in Chapter 13, View.



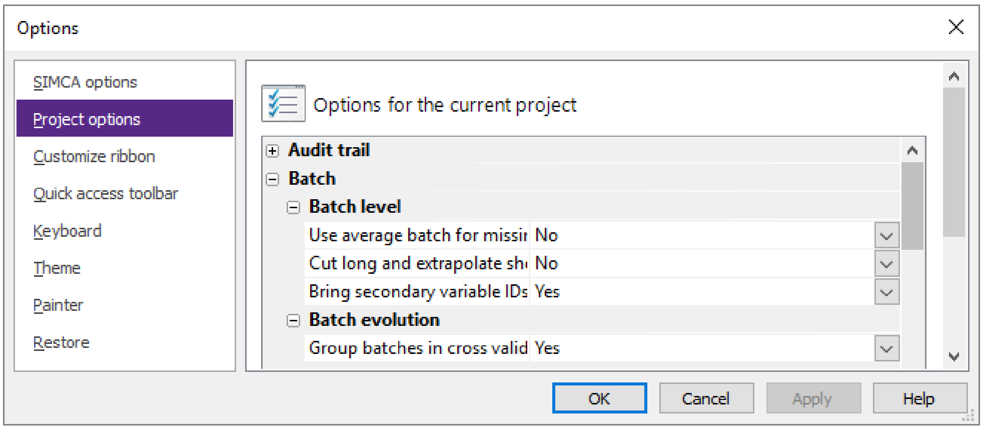
Enable the audit trail for new projects No

Clearing or saving the audit trail for a certain project is available by right-clicking the Audit trail pane.

5.10.4.2 Batch section

In the Batch section, on the Project options page, there are four options; three pertaining to the creation of batch level datasets and one that specifies the default cross validation groups for the batch evolution model, BEM.

- **Use average batch for missing phases -** Create batch level datasets displaying missing value for missing phases with the default option 'No'. Select 'Yes' to display average batch values for missing phases.
- **Cut long and extrapolate short batches** - Use all of the longer batches and display missing after short batches have finished with the default option 'No'. Select 'Yes' to cut the longest batches and extrapolate short batches using the last value. For projects create in SIMCA 14 and earlier, this option is locked 'Yes'.
- **Bring secondary variable IDs to batch level** - Bring all secondary variable IDs to the batch level datasets with the default option 'Yes'.
- **Group batches in cross validation** - Assigns all observations belonging to the same batch in the same cross validation group. See also the Cross validation group examples topic. This option was unavailable in SIMCA 14 and earlier.

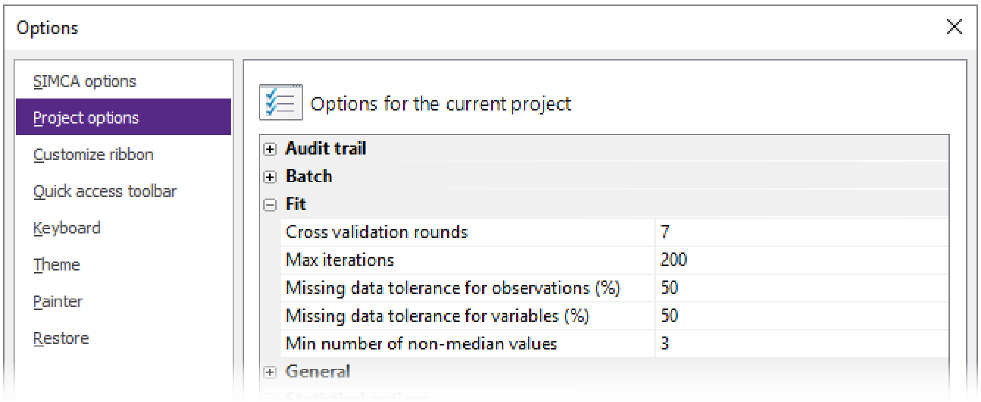


Options for the current project

- Audit trail
- Batch
  - Batch level
    - Use average batch for missir No
    - Cut long and extrapolate sh No
    - Bring secondary variable IDs Yes
  - Batch evolution
    - Group batches in cross valid Yes

5.10.4.3 Fitting options

The options available from the **Fit** page pertain to the fit of the model.



Options for the current project

- Audit trail
- Batch
- Fit
  - Cross validation rounds 7
  - Max iterations 200
  - Missing data tolerance for observations (%) 50
  - Missing data tolerance for variables (%) 50
  - Min number of non-median values 3
- General

All options are described in the table below:

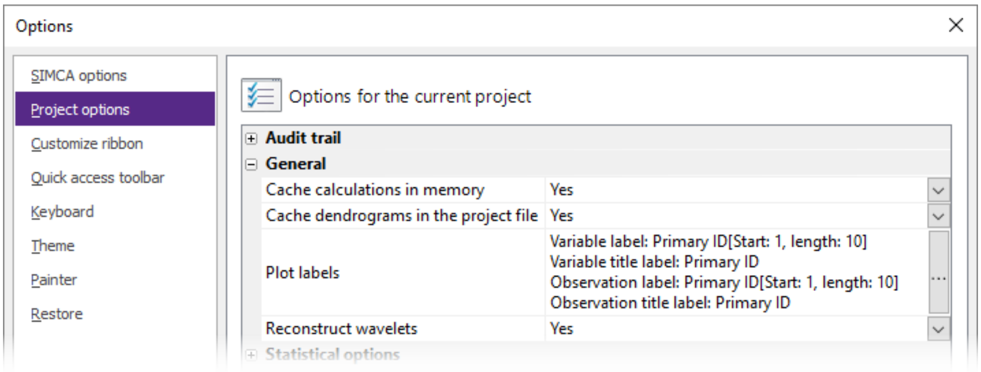
Option	Description	Default
Cross validation rounds	Each observation is left out once during the cross validation. The number in **Cross validation rounds** is the number of groups, that one by one is left out of the modeling and repredicted during the cross validation.	7
Max iterations	Maximum number of iterations until convergence when fitting the model.	200
Missing data tolerance (Obs)	Threshold of missing values for observations in percent. The threshold applies to both the workset and the predictionset. The threshold is displayed in the **Workset** dialog and can be changed there for the specific model.	50%
Missing data tolerance (Var)	Threshold of missing values for variables in percent. The threshold applies to both the workset and the predictionset. The threshold is displayed in the **Workset** dialog and can be changed there for the specific model.	50%
Min number of non-median values	Minimum number of values that have to differ from the median. When a variable has fewer values differing from the median than entered in **Min number of non-median values**, SIMCA will suggest excluding the variable since it is considered to lack variance.	3

5.10.4.4 General section, Project options

Under General the following options can be specified;

- **Cache calculations in memory** - by default turned on and caches calculations to speed up the computations. Turn off if the project takes too much RAM. The software will then be slower but the memory consumption smaller.

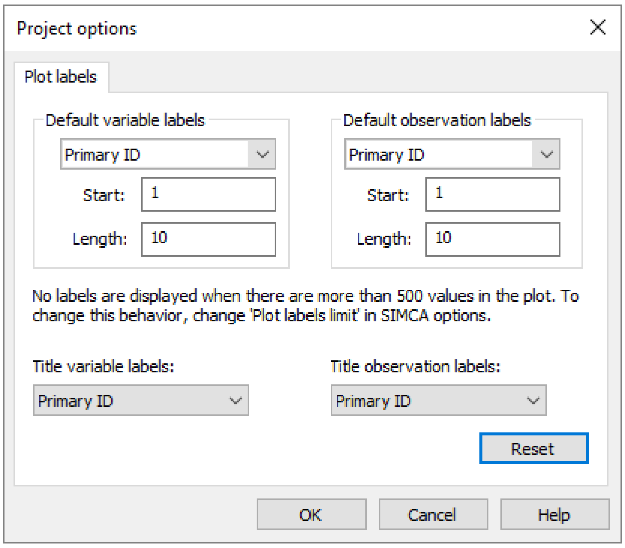
- **Cache dendrograms in the project file** - by default turned on and caches dendrograms to speed up regeneration of the dendrogram.
- **Plot labels** - default settings for plot properties, see more in the Selecting plot labels subsection.
- **Reconstruct wavelets** - When using the wavelet transform to compress the dataset variable wise (suitable for spectra such as NIR, or Raman etc.), SIMCA creates a new dataset and you can fit models to the compressed data. When variables have been compressed, the new variables are linear combinations of the original ones. Loading, coefficients, VIP or any plots displaying variables are difficult to interpret in the wavelet domain. Therefore it is possible to reconstruct not only the original variables, but also individual vectors such as loadings, coefficients, VIP, etc. This option is by default turned on.



Cache calculations in memory	Yes
Cache dendrograms in the project file	Yes
Plot labels	Variable label: Primary ID[Start: 1, length: 10] Variable title label: Primary ID Observation label: Primary ID[Start: 1, length: 10] Observation title label: Primary ID
Reconstruct wavelets	Yes

5.10.4.5 Selecting plot labels

The options available from the **Plot labels** page pertain to the presentation of labels in the plots.



Default variable labels: Primary ID, Start: 1, Length: 10

Default observation labels: Primary ID, Start: 1, Length: 10

No labels are displayed when there are more than 500 values in the plot. To change this behavior, change 'Plot labels limit' in SIMCA options.

Title variable labels: Primary ID

Title observation labels: Primary ID

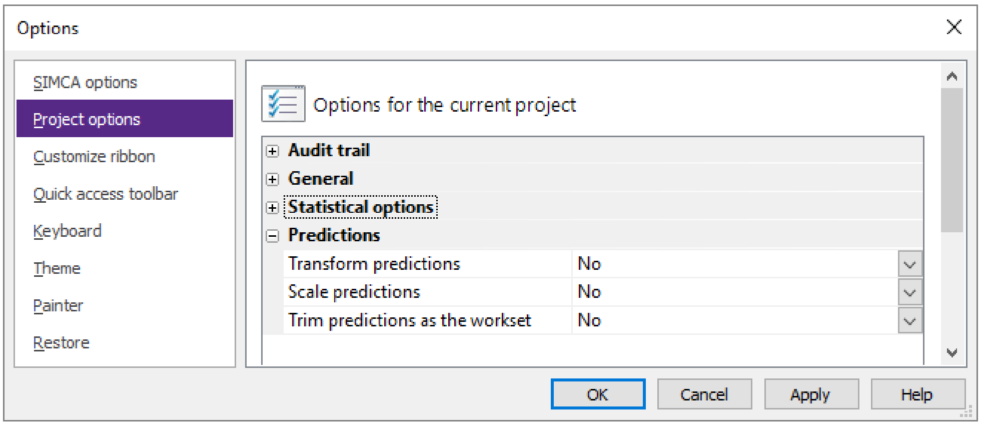
Select the identifier to be used as variable or observation label on all plots in the current project in the **Select default variable/observation labels** sections. Change the starting position and length as needed.

To display a specific label type in the title of plots, select the identifier in the **Title variable/observation labels** box.

These options are also available from the **Properties** dialog for the individual plots.

5.10.4.6 Predictions presentation

The options available in the **Predictions** section pertain to the presentation of the predictions.



Transform predictions: No
Scale predictions: No
Trim predictions as the workset: No

5.10.4.6.1 Transforming predictions

When the y-variables have been transformed, by default the predictions are back transformed to the original units.

Select **Transform predictions** *Yes* when you want to display the predicted Y in the transformed units.

5.10.4.6.2 Scaling predictions

To display the predicted Y in the same unit as the workset, select **Scale predictions** *Yes*.

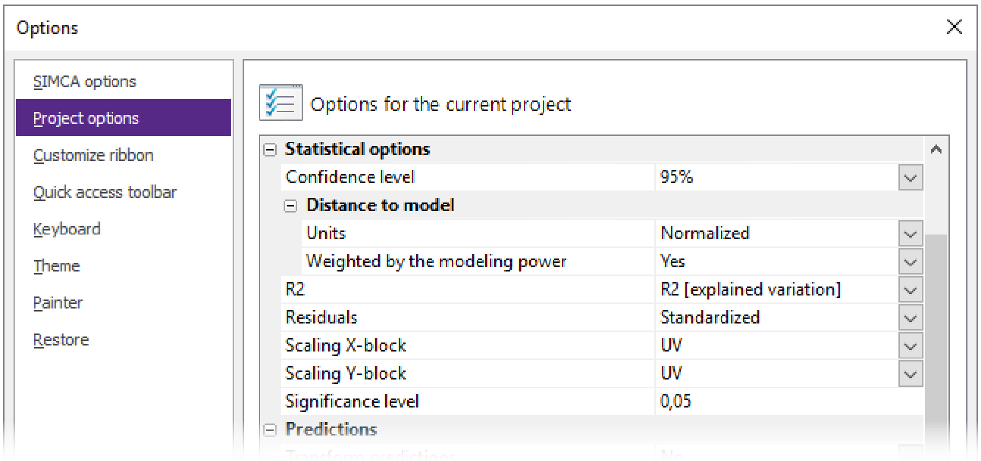
5.10.4.6.3 Trimming predictions as the workset

When the workset has been trimmed or Winsorized, the predictionset can be trimmed or Winsorized in the same manner by selecting **Trim predictions as the workset** *Yes*.

By default the predictionset is not trimmed nor Winsorized.

5.10.4.7 Fitting options

The options available from the **Fit** page pertain to the fit of the model.



Confidence level: 95%
Units: Normalized
Weighted by the modeling power: Yes
R2: R2 [explained variation]
Residuals: Standardized
Scaling X-block: UV
Scaling Y-block: UV
Significance level: 0,05
Transform predictions: No

All options are described in the table below:

Option	Description	Default
Confidence level on parameters	Confidence level used when computing confidence intervals on the parameters. **None**, **99%**, **95%** and **90%** are available.	95%
Distance to model - Units	The distance to the model of X or Y, DModX or DModY, can be expressed as an absolute value or a normalized value i.e., in units of standard deviation of the pooled RSD of the model. The default is **Normalized** in units of standard deviation.	Normalized

Option	Description	Default
Distance to model - Weighted by the modeling power	When computing the distance to the model, SIMCA by default weight the residuals by the modeling power of the variables. Change this default by changing to **Weighted by the modeling power** *No*. The distance to the model will then be computed without weighted residuals.	Yes
R2	R2 is displayed in all summary plots but the OPLS/O2PLS Overview plot. Select: • R² - **explained variation** to display the fraction of the Sum of Squares (SS) explained by the model (default). • R² **Adjusted - variance** to display the fraction of variance explained by the model, SS adjusted for the degrees of freedom.	R2
Residuals	The normal probability plot of residuals is available on the **Analyze** tab by clicking **Residuals N-Plot**. This plot can be displayed both in original units and in standardized units. The standardized residuals are the unscaled residuals divided by their standard deviation. Select: • **Raw – original units** to display the unscaled residuals. • **Standardized** to display the standardized residuals (default).	Standardized
Scaling X-block	Default scaling for X-block in the default workset. Changes here apply to the x-variables defined as such in the default workset.	UV
Scaling Y-block	Default scaling for Y-block in the default workset. Changes here apply to the Y-variables defined as such in the default workset.	UV
Significance level	Significance level used to compute the Hotelling's T^2 ellipse and the critical distance to the model.	0.05 (95%)

Note: To not display the Hotelling's T2 ellipse or the DCrit line, see the Limits and Line style subsections in Chapter 14, Plot and list contextual tabs.

5.10.5 Customize ribbon

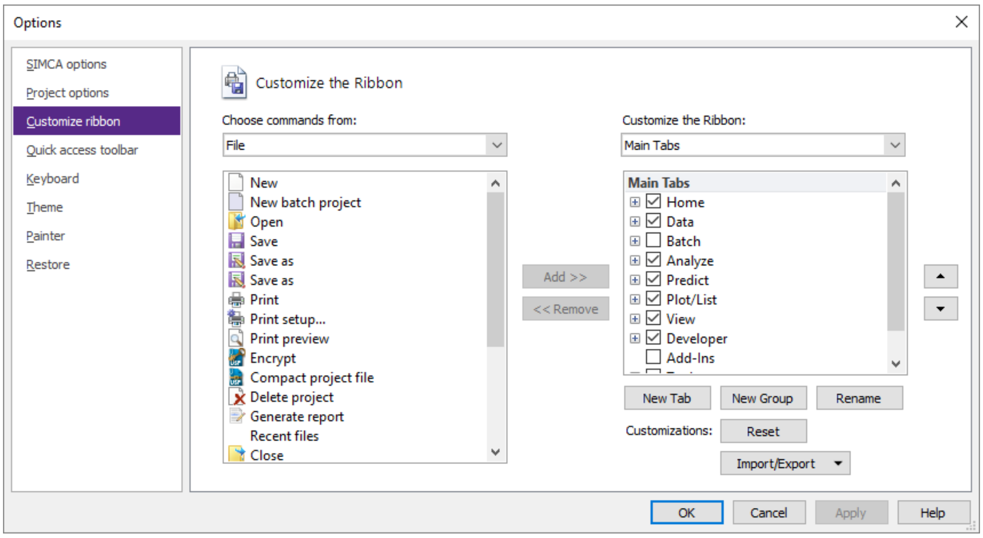
To access the Customize ribbon page, on the **File** tab, click **Options**, then click **Customize ribbon**.

With the Customize dialog box open you can interactively customize all available toolbars, tabs and menus

1. Select the command in the left box that you want to place.
2. Click the location in the right box where you would like the command to be shown.
3. Click **Add**.
4. Click **Close** to return to SIMCA.

Note: With this dialog open, all buttons and tabs currently displayed can be dragged to new positions. Buttons can be removed by pulling them down.

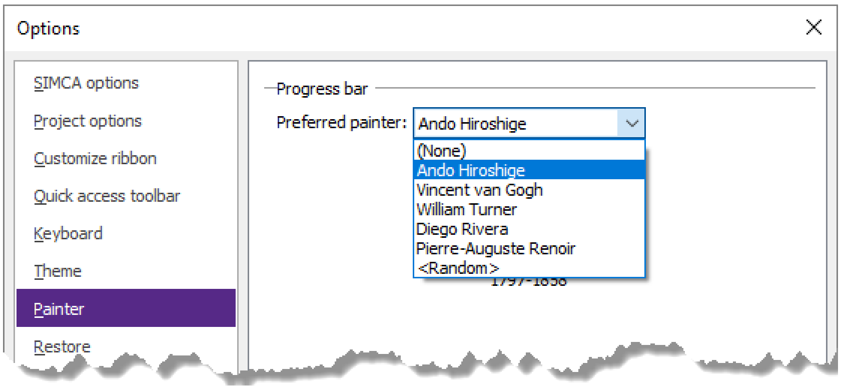
To customize the content of the Quick Access Toolbar, click **Quick Access Toolbar** to the left and choose commands to add.



5.10.6 Selecting progress bar pictures

The **Painter** page in the Options dialog provides the option to display nothing or the work of a painter during fit of models. Under Progress bar select your **Preferred painter**.

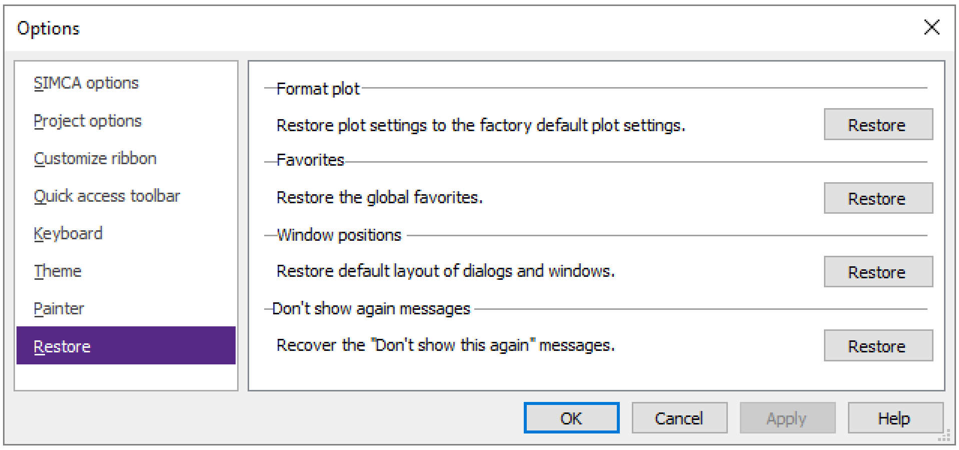
Painters possible to select are Ando Hiroshige, Vincent van Gogh, William Turner, Diego Rivera and Pierre-Auguste Renoir. Selecting *Random* displays the work of all artists in random order. Selecting *None* turns this feature off.



Preferred painter: Ando Hiroshige

5.10.7 Restoring to default

The Restore page in the **Options** dialog can be used to restore SIMCA defaults regarding Format plot, Favorites, Windows positions, and Don't show this again-messages, by clicking the relevant **Restore**.



Restore plot settings to the factory default plot settings.

Restore the global favorites.

Restore default layout of dialogs and windows.

Recover the "Don't show this again" messages.

The table describes the available restoring options.

Restore	Description	Restoring is useful when
Format plot	A file defining how all plots look, including fonts, colors, plot marks etc. See also the Switching plot formatting templates subsection in the Layout section in Chapter 14, Plot and list contextual tabs.	The changes saved in the default plot template are no longer desired.
Favorites	A pane displaying shortcuts to plots and lists.	The original Favorites items are desired.
Windows positions	The positions of dialogs and windows are saved.	A dialog ends up outside the screen, for instance when working with two screens and one screen is no longer available.
Don't show again messages	A **Don't show again**-message is an information dialog with a **Don't show again** check box that if selected hides the message the next time it could be displayed.	You want to know what a **Don't show again message** said.

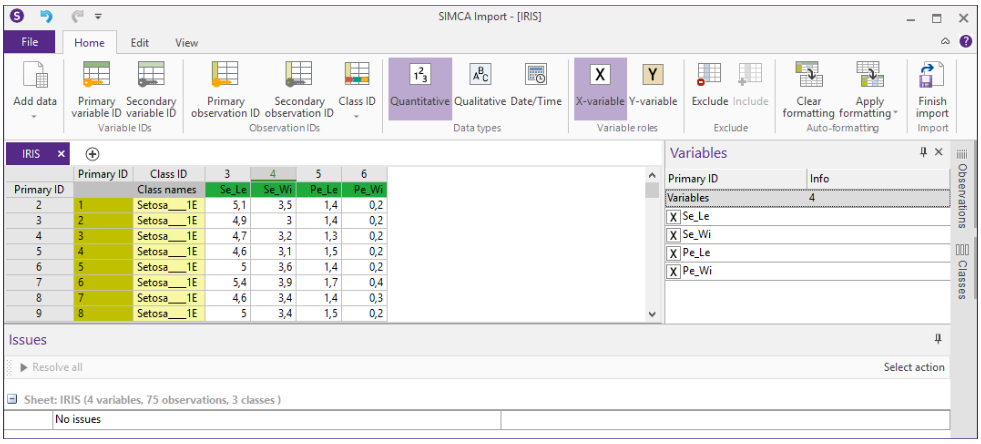
6 SIMCA import

6.1 Introduction

When creating a new project or selecting to import another dataset, the **SIMCA import** opens allowing you to import from file, database or just paste the data in an empty spreadsheet.

The first time you open the SIMCA import, the **Open** dialog for selecting a file is automatically opened.

The SIMCA import window consists of the ribbon, the Quick Access Toolbar at the top, panes and the **Find** toolbar.



	Primary ID	Class ID	3	4	5	6
Primary ID		Class names	Se_Le	Se_Wi	Pe_Le	Pe_Wi
2	1	Setosa___1E	5,1	3,5	1,4	0,2
3	2	Setosa___1E	4,9	3	1,4	0,2
4	3	Setosa___1E	4,7	3,2	1,3	0,2
5	4	Setosa___1E	4,6	3,1	1,5	0,2
6	5	Setosa___1E	5	3,6	1,4	0,2
7	6	Setosa___1E	5,4	3,9	1,7	0,4
8	7	Setosa___1E	4,6	3,4	1,4	0,3
9	8	Setosa___1E	5	3,4	1,5	0,2

Primary ID	Info
Variables	4
X Se_Le	
X Se_Wi	
X Pe_Le	
X Pe_Wi	

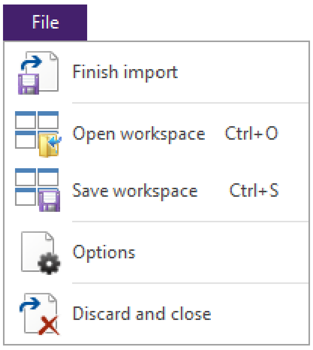
Sheet: IRIS (4 variables, 75 observations, 3 classes)

No issues

6.2 File

This section describes all features available on the File tab in SIMCA import.

The following commands are available: **Finish import**, Open workspace, Save workspace, Options, and Discard and close.



6.2.1 Workspace

In SIMCA import you can open and save workspaces. A workspace consists of one or more data spreadsheets formatted as specified at save.

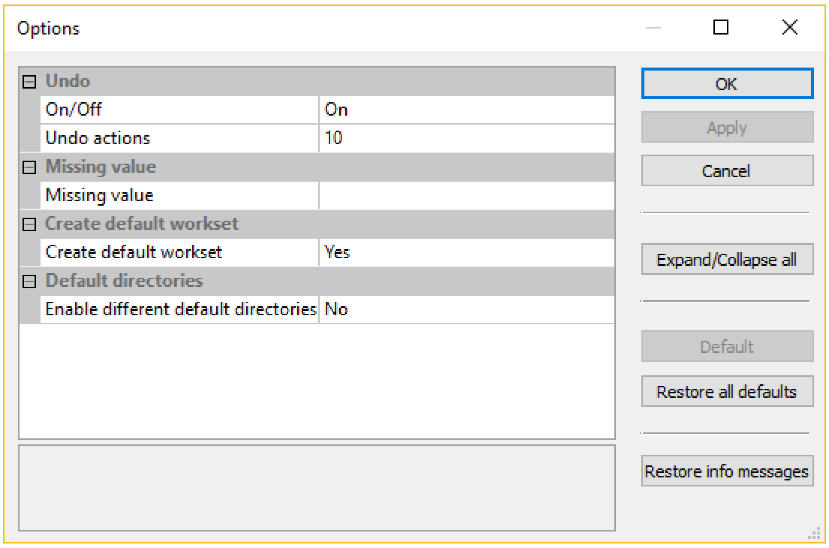
A workspace is saved as a .wusp and can be opened by the SIMCA import.

To save a workspace, click **File** | **Save workspace**.

To open a workspace, click **File** | **Open workspace**.

6.2.2 Options

Clicking **File | Options** opens the SIMCA Import **Options** dialog.



⊟ Undo	
On/Off	On
Undo actions	10
⊟ Missing value	
Missing value	
⊟ Create default workset	
Create default workset	Yes
⊟ Default directories	
Enable different default directories	No

Header	What and why	Default setting
Undo	You can select to turn the **Undo** memory off to speed up spreadsheet actions involving a lot of data.	**On/Off** is *On*. Undo actions is *10*.
Missing value	See the Missing value representation subsection for details.	Missing value is empty.
Create default workset	When creating the SIMCA project a default workset can be created. When the default workset is not of interest, the creation of the default workset can be turned off.	Create default workset is *Yes*.
Default directories	By default the directory where you select a data file to import is used for storing the project. If you store your SIMCA project files in a location different from where you fetch data for import, select *Yes*.	Enable different default directories is *No*

6.2.2.1 Missing value representation

Missing values are represented by blank or space < >.

You can select another value to also represent missing in **Options** dialog, opened from the **File** tab in the SIMCA Import, by entering it in the **Missing value** field.

Note: -99 is assumed to be a valid value and is therefore automatically changed to -99.0001. If -99 represents missing value, enter -99.0001 in the **Missing value** field in Options dialog in the SIMCA import.

For more, see the Conventions section in Chapter 3, Overview of SIMCA.

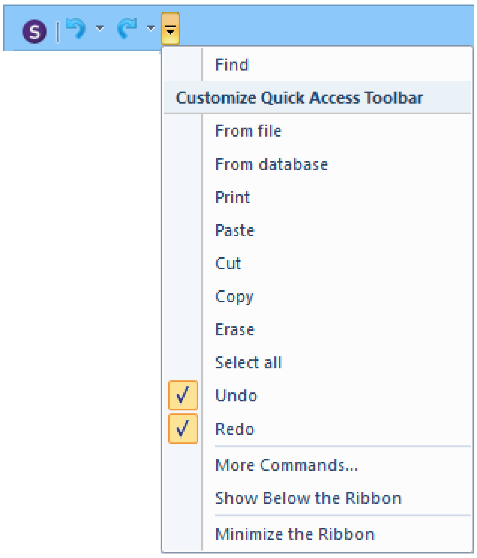
6.2.3 Discard and close

To close the current spreadsheet in SIMCA import, click the tab cross of that spreadsheet tab or click **File** | **Discard and close**.

6.3 Quick Access Toolbar

The standard editing commands **Undo** and **Redo** are by default available from the Quick Access Toolbar in the SIMCA Import. Any button in the SIMCA Import can be added to this toolbar.

For details about how to customize the Quick Access Toolbar etc., see Chapter 4, Quick Access Toolbar.

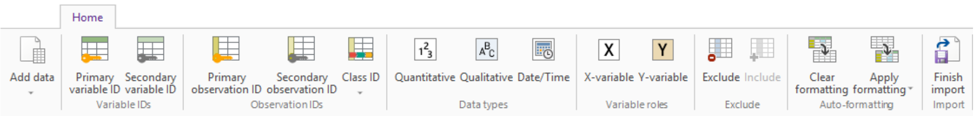


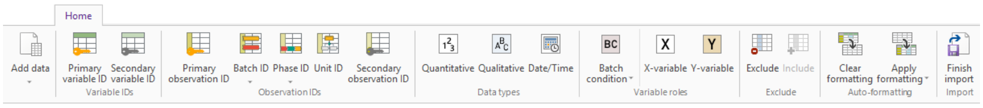
6.4 Home

When the SIMCA Import opens, the data to import needs to be specified. Then all identifiers, qualitative variables, time or maturity (y-variable for batch projects), and condition variables must be identified and specified. Optionally, regular projects can specify y-variables and classes defining the default workset.

The available commands differ depending on whether you are importing a regular or batch dataset.

Note: *A row, with slash </> as the leftmost character of the leftmost column of that row, is automatically formatted as excluded by SIMCA.*
A column with slash </> as the leftmost character in the top cell, is automatically formatted as excluded by SIMCA.





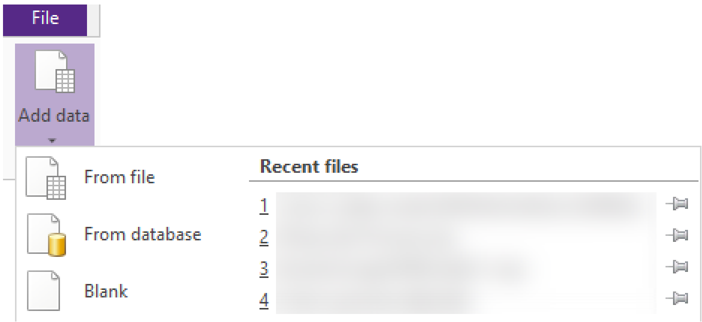
6.4.1 New spreadsheet

The SIMCA Import supports three types of import:

- From file - Opens a dialog where you can select the files to import.
- From database. For more see the Importing data from a database subsection later in this chapter.
- Blank - enables pasting in an empty spreadsheet. For details, see the Pasting dataset in import wizard subsection later in this chapter.

Select any type of import by clicking **Add data | From file/From database/Blank**. Repeat until all data you want to import are available in SIMCA Import.

Note: To rename the data sheet, double click the tab and enter a new name.



The right-side of the menu lists Recent files, see more in the Recent projects and folders subsection in Chapter 5, File.

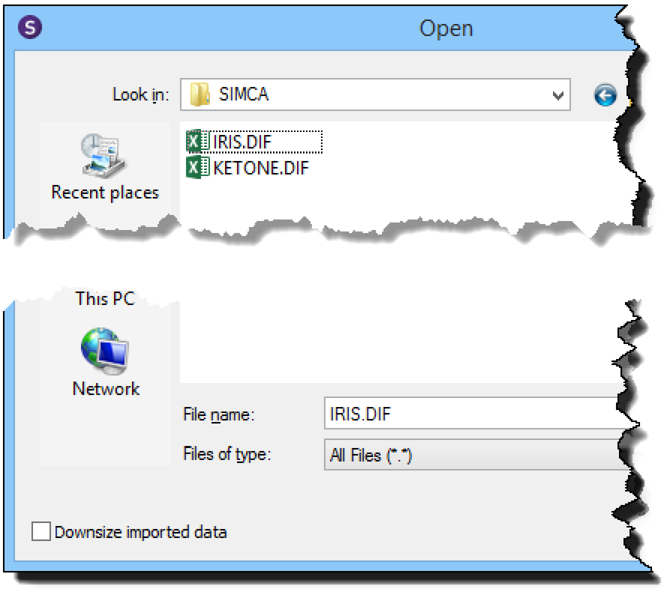
Note: The import type used is the default the next time you import.

6.4.1.1 Import from file

When selecting to import from file, the Open dialog opens. This dialog is a standard dialog box for selecting file type, name and source address of the data file to import. The selected file type in the **Files of type** box is the default file type next time a file is imported.

Note: Multiple sheets can be imported in separate sheets. The datasets in .usp files can be imported.

In this dialog you can also select to downsize the dataset *before* reading by selecting the **Downsize imported data** check box. For details, see the Downsizing dataset before reading it subsection later in this chapter.



Look in: SIMCA

IRIS.DIF
KETONE.DIF

File name: IRIS.DIF

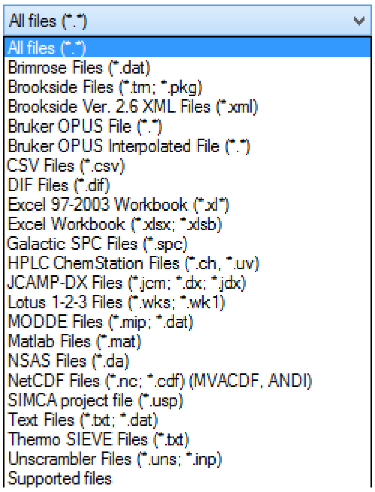
Files of type: All Files (*.*)

□ Downsize imported data

6.4.1.1.1 File types supported

In the **Files of type** list box, select your file type. SIMCA imports a number of file types. See the table.

Supported files is the default selected file type and results in that all files of the supported file types are listed.


All files (*.*)
All files (*.*)
Brimrose Files (*.dat)
Brookside Files (*.trn; *.pkg)
Brookside Ver. 2.6 XML Files (*.xml)
Bruker OPUS File (*.*)
Bruker OPUS Interpolated File (*.*)
CSV Files (*.csv)
DIF Files (*.dif)
Excel 97-2003 Workbook (*.xl*)
Excel Workbook (*.xlsx; *.xlsb)
Galactic SPC Files (*.spc)
HPLC ChemStation Files (*.ch, *.uv)
JCAMP-DX Files (*.jcm; *.dx; *.jdx)
Lotus 1-2-3 Files (*.wks; *.wk1)
MODDE Files (*.mip; *.dat)
Matlab Files (*.mat)
NSAS Files (*.da)
NetCDF Files (*.nc; *.cdf) (MVACDF, ANDI)
SIMCA project file (*.usp)
Text Files (*.txt; *.dat)
Thermo SIEVE Files (*.txt)
Unscrambler Files (*.uns; *.inp)
Supported files

Note: For JCAMP-DX, NetCDF, Galactic SPC, and Brookside XML files, importing several files from the same folder, and merging without (exact) matching, is available by marking them and clicking **Open**.

File type	**Description**
Brimrose files (.dat)	Brimrose files (*.dat) are created by Brimrose NIR instruments.
Brookside files (*.trn, *.pkg)	Process data files type used in the semiconductor industry.
Brookside Ver 2.6 XML files (.xml)	Process data files type used in the semiconductor industry.
Bruker OPUS file (*.*)	OPUS spectral files up to version 5.5, but not 3D data.
Bruker OPUS intrapolated file (*.*)	OPUS spectral files up to version 5.5, but not 3D data. All spectra are interpolated to the reference spectra (first).
CSV files (*csv)	Standard delimited text files with extension *.csv. The separators between observation IDs, variable IDs, and values must be tabs, blanks, semicolons, or commas. Each new observation must start on a new line, with only one line per observation. This file format is useful when the file contains "" around the values. With csv-files without the "" the regular Text file import is preferable.
DIF files (*.dif)	The DIF format is a common data interchange format used by software as a way to exchange data.
Excel 97-2003 Workbook (*.xl*)	Excel files (*.xl*) are files written by Microsoft Excel 97 to 2003.
Excel Workbook (*.xlsx, *.xlsb)	Excel files (*.xlsx, *.xlsb) are files written by Microsoft Excel. All versions, available before the release of this version of SIMCA, are supported. Generally import of .xlsb is faster.
Galactic SPC files (*.spc)	Galactic SPC files (*.spc) are files saved to a standard format in Galactic software.
HPLC ChemStation files (*ch, *.uv)	The *.ch files are Chromatographic/electropherographic signal data files. The file name comprises the module or detector type, module number and signal or channel identification. For example, ADC1A.CH, where ADC is the module type, 1 is the module number and A is the signal identifier and .ch is the chromatographic extension. The *.uv files are UV spectral data files. The file name comprises the detector type and device number (only with diode array and fluorescence detector).
JCAMP-DX files (*.jcm, *.dc, *.jdx)	JCAMP-DX is a Chromatography/Spectroscopy general file format saved with the extensions *.jcm, *.dx, and *.jdx. The following files are supported: • XYDATA, uniformly spaced XY pairs. • XYPOINTS • PEAKTABLE SIMCA supports JCAMP-DX V5.0 with multiple pages and multiple data blocks.

File type	Description
Lotus 1-2-3 files (*.wks, *wk1)	Lotus 1-2-3 version 2.2 and earlier, saved to *.wk1 or *.wks, are supported.
Matlab files (*.mat)	MATLAB (*.mat) formatted binary files version 5.0 and earlier are supported.
MODDE files (*.mip, *.dat)	MODDE files are created by Umetrics MODDE software in the formats *.dat (MODDE 4.0 and earlier) and *.mip (MODDE 5.0 and later).
NetCDF files (*.nc, *.cd)(MVACDF, ANDI)	The NetCDF files are saved with extensions *.nc and *.cdf. MVACDF and ANDI are extensions of NetCDF for raw-data files containing multivariate data and chromatography data.
NSAS files (*.da)	FOSS spectral file format saved to *.da files with supporting files with extension .cn. NSAS versions earlier than 2.2 are not supported.
SIMCA project file (*.usp)	SIMCA project files are created by SIMCA-P 9.0 and later.
Text files (*.txt, *.dat)	Standard delimited text files with extensions *.txt, *.dat. The separators between observation IDs, variable IDs, and values must be tabs, blanks, semicolons, or commas. Each new observation must start on a new line, with only one line per observation.
Thermo SIEVE files (*.txt)	SIEVE processed files from Thermo Scientific ion traps and triple quadrupoles.
Unscrambler files (*.uns, *.inp)	Unscrambler files are written by the Unscrambler software (*.uns, *.inp).
User defined format	SIMCA also supports user written import routines as plugins. For more information about writing plugins, contact your Umetrics sales office.

6.4.1.1.2 Downsizing dataset before reading it

Reading large datasets may be time consuming. In the case where you plan to downsize the dataset, selecting to downsize before reading the dataset can reduce the time.

To downsize the dataset before reading it:

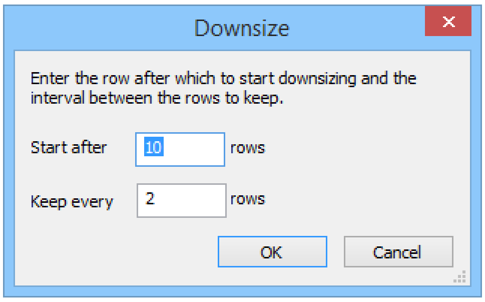
1. In the Open dialog, select the **Downsize imported data** check box, select the file, and then click **Open**.

☑ Downsize imported data

2. In the Downsize dialog:

   - In the **Start after xx rows** field, enter the last row to read before downsizing.
   - Enter the downsizing interval in the **Keep every xx rows**.

3. Click **OK** when done.



Downsize

Enter the row after which to start downsizing and the interval between the rows to keep.

Start after 10 rows

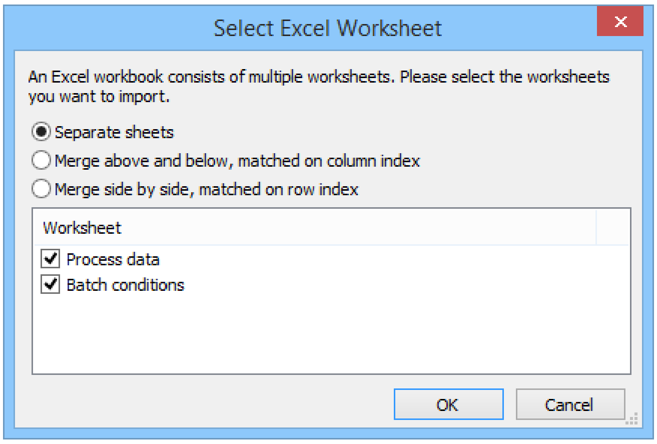
Keep every 2 rows

Downsizing is also available after opening the file in SIMCA Import. For more, see the Downsizing the dataset subsection later in this chapter.

6.4.1.1.3 Import of several datasets

When importing an Excel-file with several sheets you can select how to import them;

- As separate sheets, as they were in Excel.
- Merged above and below matching only on column index.
- Merged side by side matching only on row index.



Select Excel Worksheet

An Excel workbook consists of multiple worksheets. Please select the worksheets you want to import.

● Separate sheets
○ Merge above and below, matched on column index
○ Merge side by side, matched on row index

Worksheet
☑ Process data
☑ Batch conditions

When importing SIMCA project files, all files can be imported as separate sheets.

Note: To rename the data sheet, double click the tab and enter a new name.

6.4.1.2 Importing data from a database

To be able to use the database import utility in SIMCA, a data source and an interface to the data source already needs to be in place.

There are three main interface types supported:

- ODBC (Microsoft)
- OPC (OPC Foundation)
- SimApi's.

The SimApi is the API (Application Program Interface) connection that SIMCA-online needs to be able to connect to data sources. For instance OSIsoft PI and Siemens SIPAT have support for the SimApi interfaces.

The database import supports several extraction methods:

- *Continuous* - from a start time to an end time.
- *Batch* - batches that exists in the system during a time interval.
- *Relational* - a complete table in an ODBC data source.
- *SQL* - an SQL query through the ODBC driver from the database vendor.

In table 1, the different possible import combinations are shown.

Table1: Different combinations of data connections and retrieval types supported.

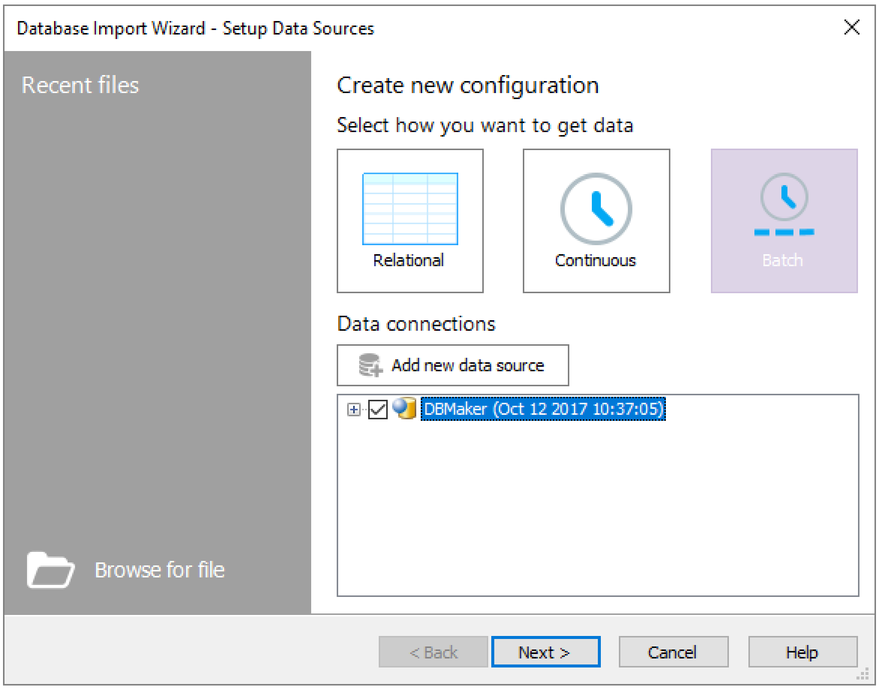
	Continuous	Batch	Relational	SQL
ODBC	X	X	X	X
OPC	X			
SimApi	X	X		

Since the configuration of some of these different combinations can be rather cumbersome, a SIMCA DataBase Settings file (*.sdbs) can store most parts of the configuration.

For more information about the database settings file, see the SIMCA Database Settings file subsection later in this section.

6.4.1.2.1 Setup data sources

On the **Setup Data Sources** page, the type of import (**Relational**, **Continuous**, or **Batch**) needs to be specified before clicking **Add new data source** to add a new data source connection.



Data sources connection information is stored in the registry. There are three types of connections possible:

- ODBC
- OPC
- SimApi

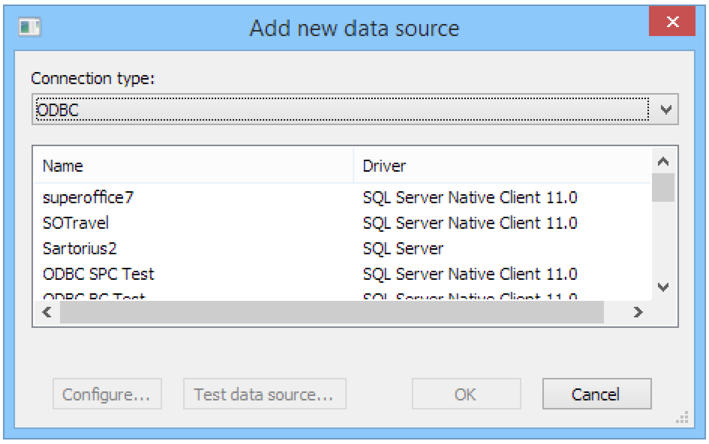
Unavailable connections appear in gray.

6.4.1.2.2 ODBC - Add New Data Source

To create an ODBC connection:

1. Click **Add new** in the **Setup Data Sources** page.
2. In the **Add new data source** dialog, select ODBC in **Connection type** box.
3. Select the data source name (DSN) that you have set up in the Windows ODBC Data Source Administrator application.

Note: Configuration of ODBC sources are driver specific, but can for instance contain log in information and server information.



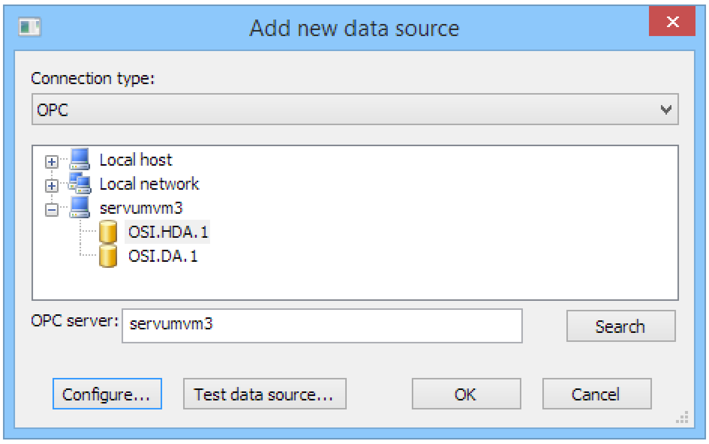
Connection type: ODBC

Name	Driver
superoffice7	SQL Server Native Client 11.0
SOTravel	SQL Server Native Client 11.0
Sartorius2	SQL Server
ODBC SPC Test	SQL Server Native Client 11.0
ODBC BC Test	SQL Server Native Client 11.0

6.4.1.2.3 OPC - Add New Data Source

To create an OPC connection:

1. Click **Add new** in the **Setup Data Sources** page.
2. In the **Add new data source** dialog, select OPC in the **Connection type** box.
3. Browse to the network computer to connect to.
4. Expand the network node to view all available servers on that computer. OPC servers with the historical data interface (HDA) are selectable.



Add new data source

Connection type: OPC

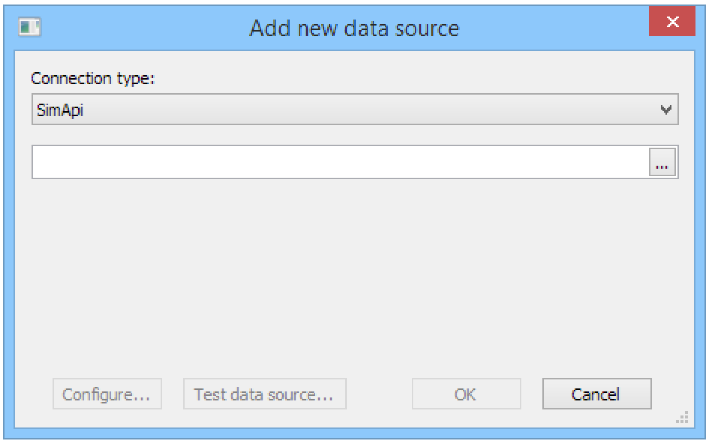
OPC server: servumvm3

6.4.1.2.4 SimApi - Add New Data Source

To create a SimApi connection:

1. Click **Add new datasource** in the **Create new configuration** page.
2. In the **Add new datasource** dialog, select SimApi in the **Connection type** box.
3. Browse for the SimApi DLL file.

Note: The configuration is specific to each SimApi.



Add new data source

Connection type: SimApi

6.4.1.2.5 Configure Data Source

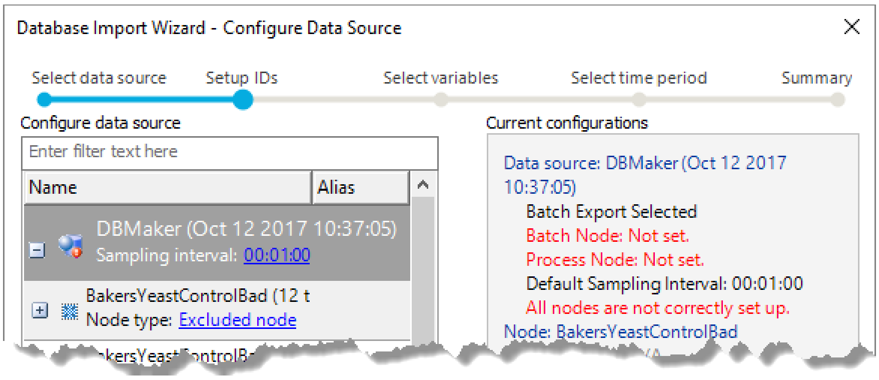
In the **Configure Data Source** page, of the **Database Import Wizard**, all data source connections are set up and necessary tag (variable) definitions are specified. The **Current configurations** window to the right (see figure) will help and guide you through the configuration of the data source.

The following tags can be specified:

- Sampling interval
- Timestamp
- Process node

- Batch node
- Batch ID
- Batch Start
- Batch Stop

The exclamation mark on the **Data Source** icon indicates that the configuration is incomplete. In the red text to the right we can see that the Sampling interval to import data with been default set to 1 minute, and that Batch and Process nodes are not set yet.


Database Import Wizard - Configure Data Source

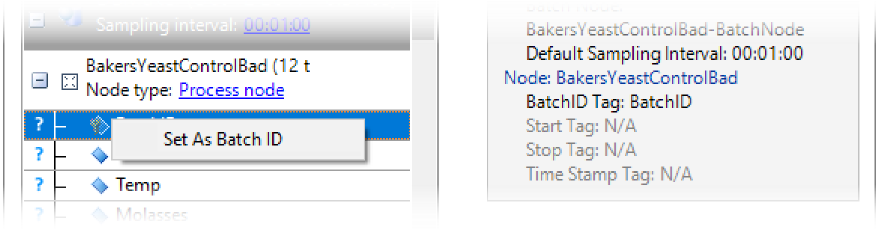
DBMaker (Oct 12 2017 10:37:05)
Sampling interval: 00:01:00

BakersYeastControlBad (12 t
Node type: Excluded node

Current configurations

Data source: DBMaker (Oct 12 2017 10:37:05)
Batch Export Selected
Batch Node: Not set.
Process Node: Not set.
Default Sampling Interval: 00:01:00
All nodes are not correctly set up.
Node: BakersYeastControlBad

- To change the sampling interval from the default, click the **Sampling interval** link. In the **Set sampling interval** dialog, enter the sampling interval to read data for the marked datasource.
- The batch and process nodes are specified by clicking the **Excluded node** link for the respective node and clicking the relevant node type.
- For the node specified as process node, the Batch ID has to be specified. This is done by right-clicking the Batch ID and clicking **Set As Batch ID**.

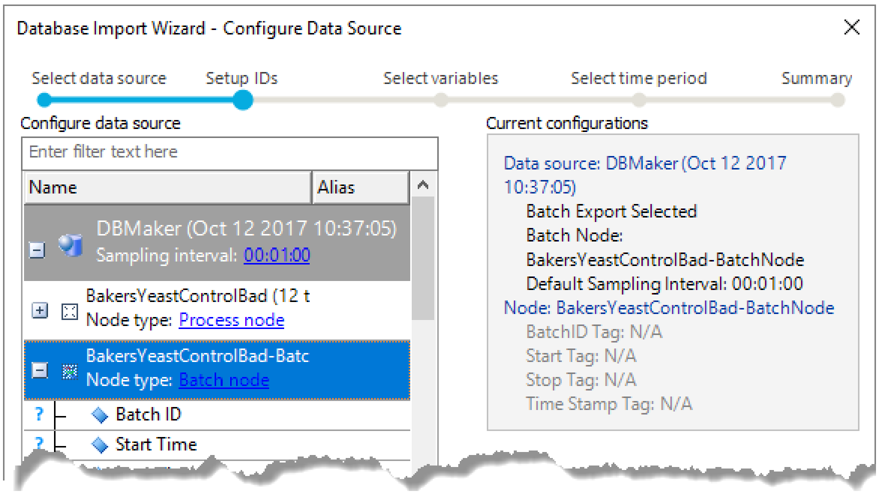

Sampling interval: 00:01:00

BakersYeastControlBad (12 t
Node type: Process node

BakersYeastControlBad-BatchNode
Default Sampling Interval: 00:01:00
Node: BakersYeastControlBad
BatchID Tag: BatchID
Start Tag: N/A
Stop Tag: N/A
Time Stamp Tag: N/A

Figure A displays a SimApi that is set up for Batch import with one process node (□) and one batch node (□)

Figure A. The **Configure Data Source** dialog for a batch import.


Database Import Wizard - Configure Data Source

DBMaker (Oct 12 2017 10:37:05)
Sampling interval: 00:01:00

BakersYeastControlBad (12 t
Node type: Process node

BakersYeastControlBad-Batc
Node type: Batch node

Current configurations

Data source: DBMaker (Oct 12 2017 10:37:05)
Batch Export Selected
Batch Node:
BakersYeastControlBad-BatchNode
Default Sampling Interval: 00:01:00
Node: BakersYeastControlBad-BatchNode
BatchID Tag: N/A
Start Tag: N/A
Stop Tag: N/A
Time Stamp Tag: N/A

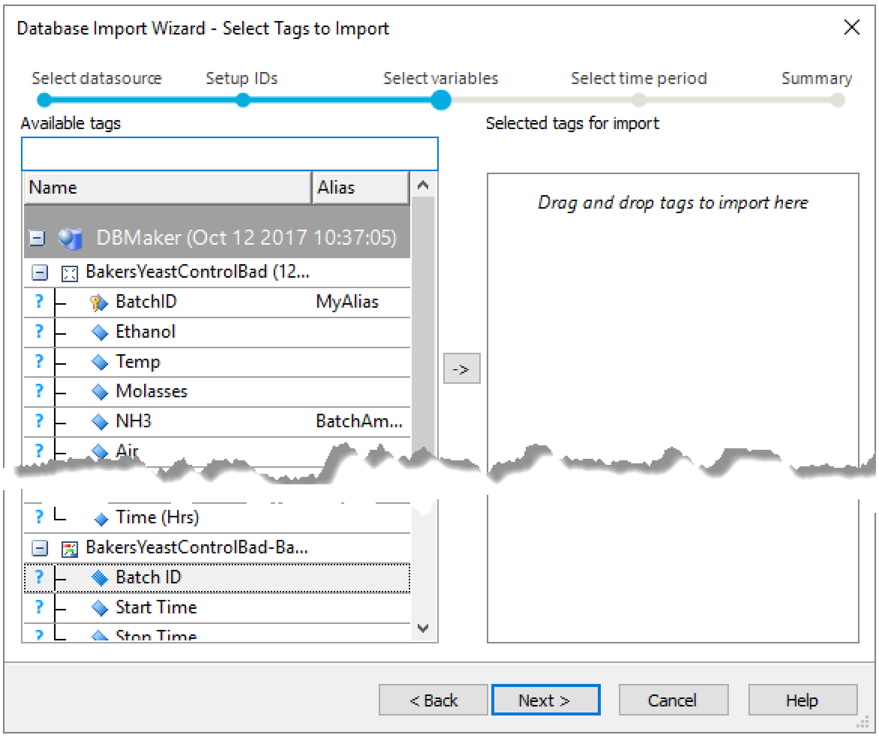
6.4.1.2.6 Select tags to import

The tags, or variables, that will be imported are selected on the **Select Tags to Import** page. Also, the user has the possibility to set aliases on the tag names, or add a data filter with a condition/logical expression on the tags that will be imported.

In this page, SQL queries can be entered by adding a SQL query folder. SQL (Structured Query Language) is a programming language to manage data in a database, however in SIMCA import we open the database as read only, which means that no alterations of the database will be introduced in the original database.

In figure C, the tag for the batch identifier can be recognized by its icon. The upper node “BakersYeast...” contains a number of tags and is a process node and the lower node with a similar name, also contains a number of tags and is a batch node.

Figure C. The **Select Tags to Import** page.



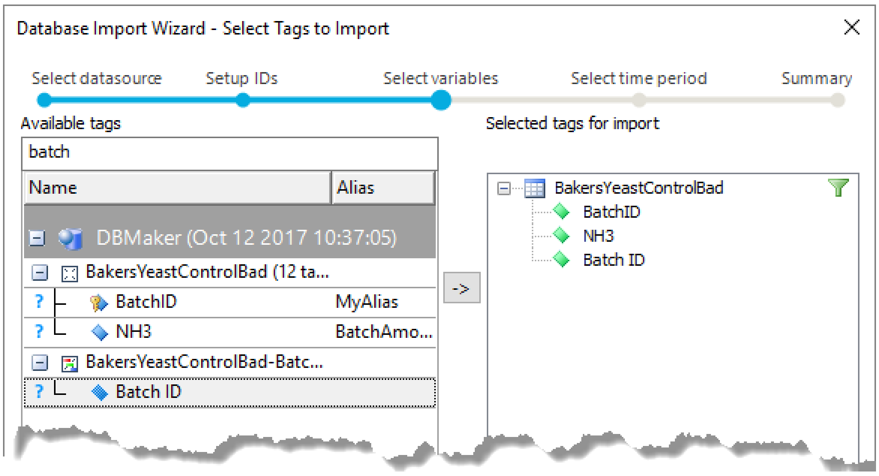
Name	Alias
DBMaker (Oct 12 2017 10:37:05)	
BakersYeastControlBad (12...	
? BatchID	MyAlias
? Ethanol	
? Temp	
? Molasses	
? NH3	BatchAm...
? Air	
? Time (Hrs)	
BakersYeastControlBad-Ba...	
? Batch ID	
? Start Time	
? Stop Time	

Drag and drop tags to import here

The text filter, at the top of the dialog on the Available tags side, searches in node names, in tag names and in aliases.

In figure D, we see the result after the word "Batch" was used to filter the available tags. The tooltip for the tags contains node information.

Figure D. The **Select Tags to Import** page after adding tags to import and with the text filter for "Batch".



batch

Name	Alias
DBMaker (Oct 12 2017 10:37:05)	
BakersYeastControlBad (12 ta...	
? BatchID	MyAlias
? NH3	BatchAmo...
BakersYeastControlBad-Batc...	
? Batch ID	

6.4.1.2.7 Data filters

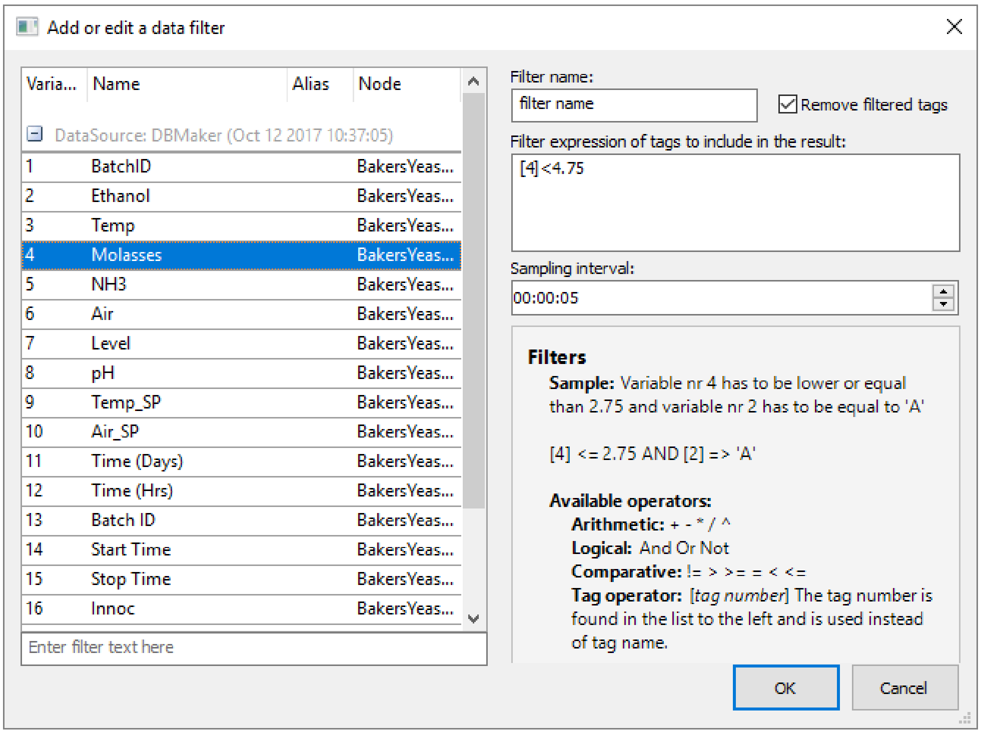
When adding a data filter, you have to specify a filter name, the logical expression for filtering and optionally a sampling interval. The data imported according to the filter are added to the SIMCA import in a new sheet named as the filter.

If the **Remove filtered tags** check box is cleared, all data will be imported from the database and a new variable specifying which data, among these data, that satisfy the filter.

When specifying the filter, each tag is referred to using the number in the dialog, not the name. When double-clicked, the tag number ends up in the **Filter expression** field.

In the example in figure e, the filter selects data where the level of MOLASSES is below 4.75. Note also that time interval for this variable is different from the default.

Figure E: The **Add or edit a data filter** dialog.



Add or edit a data filter

DataSource: DBMaker (Oct 12 2017 10:37:05)

Varia...	Name	Alias	Node
1	BatchID		BakersYeas...
2	Ethanol		BakersYeas...
3	Temp		BakersYeas...
4	Molasses		BakersYeas...
5	NH3		BakersYeas...
6	Air		BakersYeas...
7	Level		BakersYeas...
8	pH		BakersYeas...
9	Temp_SP		BakersYeas...
10	Air_SP		BakersYeas...
11	Time (Days)		BakersYeas...
12	Time (Hrs)		BakersYeas...
13	Batch ID		BakersYeas...
14	Start Time		BakersYeas...
15	Stop Time		BakersYeas...
16	Innoc		BakersYeas...

Enter filter text here

Filter name: filter name

☑ Remove filtered tags

Filter expression of tags to include in the result:

[4]<4.75

Sampling interval: 00:00:05

Filters

Sample: Variable nr 4 has to be lower or equal than 2.75 and variable nr 2 has to be equal to 'A'

[4] <= 2.75 AND [2] => 'A'

Available operators:

Arithmetic: + - * / ^

Logical: And Or Not

Comparative: != > >= = < <=

Tag operator: [*tag number*] The tag number is found in the list to the left and is used instead of tag name.

After the filter has been added, it is applied to all tags in the Selected tags for import list. The added tags specify which data to extract using the filter.

6.4.1.2.8 Select observation interval

When the data import type is *Continuous* or *Batch*, the time interval for which to import observations and batches can be selected in the **Select Observation Interval** page.

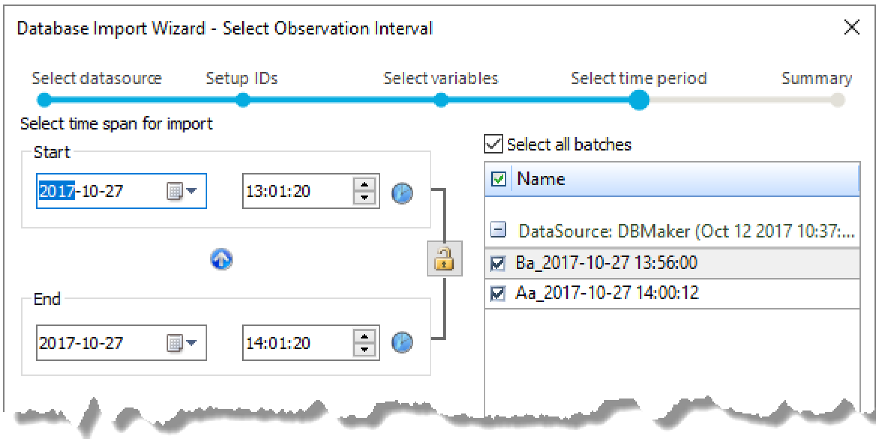
The selected **Start** and **End** times specify the time interval:

- The observations are imported for in the *Continuous* case.
- The batches are displayed for in the *Batch* case. Among the displayed batches, you can select to include all (default) or some by clearing the relevant check boxes.

Clicking the padlock locks the time interval so that changing either of the **Start** or **End** times automatically changes the other keeping the time interval constant. Clicking the arrow moves the date and time in **End** to **Start**. This means that by clicking the padlock you can specify a new time interval, spanning the same time and starting where the last interval ended, by just clicking the arrow.

In the example below there are several batches between the start and the end time and all are currently selected for import.

If too many batches are listed, clear the **Select all batches** check box and then select the batches to import.



Database Import Wizard - Select Observation Interval

Select time span for import

Start

2017-10-27 13:01:20

End

2017-10-27 14:01:20

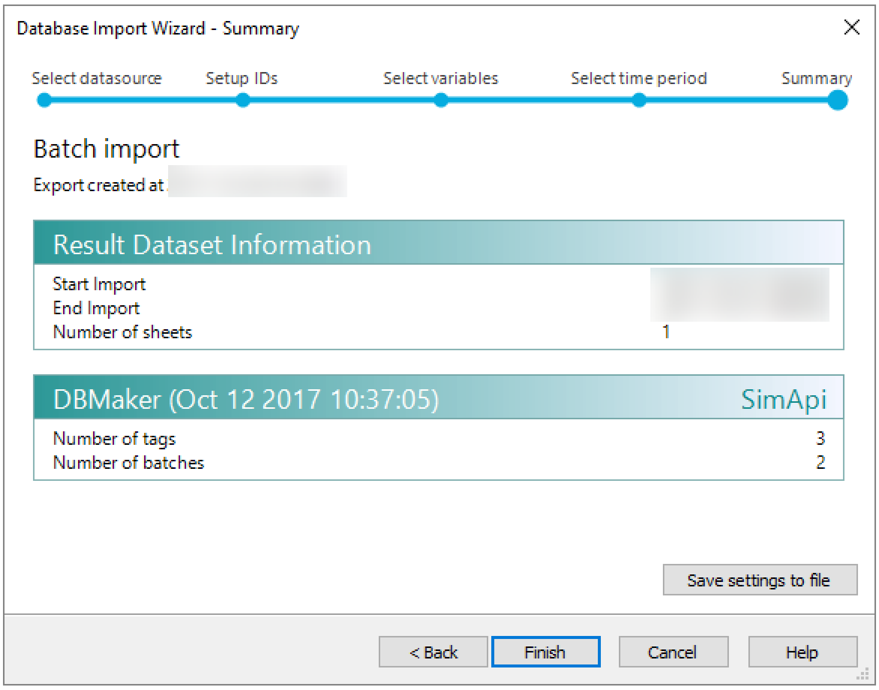
☑ Select all batches

☑ Name
⊟ DataSource: DBMaker (Oct 12 2017 10:37:...
☑ Ba_2017-10-27 13:56:00
☑ Aa_2017-10-27 14:00:12

6.4.1.2.9 Summary page

The last page in the database import wizard, the **Summary** page, provides information about the import. On the **Summary** page you can save all configurations made into a new or existing settings file by clicking **Save settings to file** and entering the file name for the settings file.

The example below shows the **Summary** page for a *batch* import. No settings file was selected.



Database Import Wizard - Summary

Batch import

Export created at

Result Dataset Information

Start Import	
End Import	
Number of sheets	1

DBMaker (Oct 12 2017 10:37:05) SimApi

Number of tags	3
Number of batches	2

6.4.1.2.10 SIMCA Data Base Settings file

The *.sdbs file will store the following settings:

- Data Source Configurations
- Aliases
- Filter information
- Tags
- Folders
- SQL queries

Settings not stored in the settings file, but in the registry of the local machine are:

- Data sources.

- Start and stop time in the **Select observation interval** page (if applicable).
- Recent SIMCA database settings files.

Note: Batches found and/or selected in the **Select observation interval** page are not stored anywhere.

6.4.1.2.11 Compatibility tested

The database import has been tested at Umetrics using the data source connectors listed in this subsection.

6.4.1.2.11.1 ODBC Drivers Compatibility

The following ODBC drivers have been tested:

- SQL Server 6.01
- PostgreSQL ANSI 9.0
- MySQL ODBC Driver 5.1
- Microsoft Excel/Access Driver 12.0
- Aegis ODBC Driver

6.4.1.2.11.2 OPC Compatibility

The SIMCA import can only read data through the HDA 1.1 interface of the OPC Foundation specifications. To see the compatibility of each server, please visit the OPC Foundation web page (www.opcfoundation.org).

6.4.1.2.11.3 SimApi Compatibility

The following SimApi's have been tested:

- OPC SimApi2
- OPC/ODBC SimApi2
- PISimApi2
- ODBC SimApi2

6.4.1.3 Pasting dataset in SIMCA Import

To paste data in the SIMCA import:

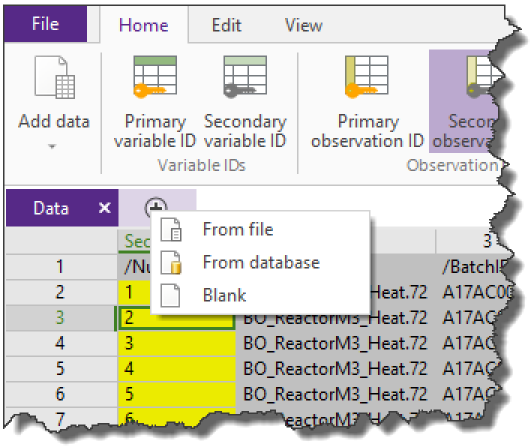
1. Click **Add data** | **Blank**. If a dialog is opened when the SIMCA import is opened, click **Cancel** to exit the dialog but not the import.
2. In the spreadsheet that opens, paste the data to import.

Note: In the empty spreadsheet you can type new values using the keyboard.

Hint: Remember to give your dataset a name. The default dataset name is Untitled.

6.4.1.4 Importing another dataset

To import another dataset in SIMCA Import, click **Add data** and the warranted type, or click the +tab.



For details about how to continue, see the New spreadsheet subsection earlier in this chapter or the Home section later in this chapter.

To merge with a dataset already open in SIMCA import, see the Merging spreadsheets subsection later in this chapter.

6.4.2 Specifying identifiers

Primary variable and observation identifiers (IDs) are used by SIMCA for the following tasks:

1. To keep track of variables and observations.
2. Variable and observation IDs are displayed in plots and lists.
3. The **Find** function in the **Workset** dialog can search in the identifiers.
4. In the **Observations** page of the **Workset** dialog the identifiers can be used to set classes.
5. For batch projects to define batch and optionally phase IDs and phase iteration IDs. See also the How to specify identifiers subsection next.
6. For batch projects Unit IDs can be specified facilitating the SIMCA-online configuration.
7. Class IDs can also be specified resulting in classes in the default workset. For more, see the Class ID specification subsection later in this chapter.

Note: IDs in plots are by default displayed using the first 10 characters.

Note: SIMCA is case insensitive.

6.4.2.1 How to specify identifiers

In the import spreadsheet the primary and secondary identifiers, and the batch and phase identifiers, can all be specified after marking the relevant rows or columns. Batch ID, Phase IDs, and Phase iteration IDs can only be specified in batch datasets.

1. Mark rows and click the relevant Identifier in the Variable IDs group.
2. Batch: Mark variables (columns) and click the relevant batch specific Identifier in the Observation IDs group; **Batch ID**, **Phase ID**, **Unit ID**. Note that with Phase iterations present in the data, these are specified by clicking the **Phase ID | Phase iteration ID**.
3. Regular: Mark row(s) and click the relevant identifier in the Observation IDs group.

For details, see Variable and observation ID description, Class ID specification and Batch and Phase ID specification.

Note: Leading zeros are included in identifiers. That is, while the number '001' is imported as '1' when specified as quantitative variable, it is imported as '001' when specified as identifier or qualitative variable.

Note: If no row is specified as primary variable ID, SIMCA automatically creates a primary variable ID as Var_1, Var_2, etc., when clicking **Finish**.

Note: If no column is specified as primary observation ID, SIMCA automatically creates a primary observation ID as 1, 2, 3, etc., when clicking **Finish**.

6.4.2.2 Variable and observation ID description

The identifiers, available in SIMCA, are described in the table. Variable IDs are found in rows and observation IDs in columns. ID is short for identifier.

ID	Description	Default
Primary variable ID	The primary variable ID is required and needs to be unique. The primary variable ID row is colored dark green.	The first row with unique entries is automatically specified as the primary variable ID.
Secondary variable ID	Secondary variable identifiers are optional and colored in light green.	No secondary variable IDs are automatically specified.
Primary observation ID	The primary observation ID is required and needs to be unique. The primary observation ID column is colored dark yellow.	The first column with unique entries is automatically specified as the p**rimary observation ID.**
Secondary observation ID	Secondary observation identifiers are optional and colored yellow.	The second column is automatically specified as secondary observation IDs when the first column is numerical and the second text.
Class ID	Specifying the Class ID at import defines classes in the default workset. Only one column can be defined as Class ID. Class ID is only available for regular projects.	No class identifiers are automatically specified.
Batch ID	When the dataset is a batch evolution dataset, batch identifier has to be specified. These specify the start and end of batches. Batch IDs are colored orange. Batch IDs are found in columns and there can only be one column per dataset defined as Batch ID. Batch IDs need to be contiguous within each phase and phase iteration.	When there is a column named 'Batch ID' it is automatically specified as batch ID.
Phase ID	For batch processes with several process steps or phases a Phase ID has to be specified for SIMCA to know which observations in one batch that belong to which phase. Phase IDs specify which phase and observation belongs to. Phase IDs are colored light yellow. Phase IDs are found in columns and there can only be one column per dataset defined as Phase ID. Phase IDs need to be contiguous within a batch. The phase is considered to start at the first occurrence of a specific Phase ID and end at the last contiguous occurrence of that specific Phase ID within a batch.	When there is a column named 'Phase ID' it is automatically specified as batch and phase ID.
Phase iteration ID	The Phase Iteration ID allows for modelling of processes where one phase appears several times in the same batch. This happens for instance if a batch is split into smaller units for one or more process steps, or if a phase has to be restarted. Phase Iteration IDs specify the start and end of each iteration of one phase.	When there is a column named 'PhaseIterationID' it is automatically specified as Phase iteration ID.

ID	Description	Default
	Phase Iteration IDs are colored light yellow. Phase Iteration IDs are found in columns and there can only be one column per dataset defined as Phase iteration ID. Phase iteration IDs need to be contiguous within each combination of batch and phase. The phase iteration is considered to start at the first occurrence of a specific Phase iteration ID and end at the last contiguous occurrence of that specific Phase iteration ID within each combination of batch and phase.	
Split	Splitting the contents of a column, or splitting out a number of characters, is available in the Batch ID and Phase ID menus as: **Batch ID | Split column into Batch and Phase ID**, **Batch ID | Split column into Batch ID** and **Phase ID | Split column into Phase ID**.	For more, see the Split column topic.
Unit ID	For batch processes it is optional to define a column as Unit ID. There can only be one Unit ID per dataset. The Unit ID is a Secondary ID type column which can be used for coloring plots and define groups of batches to investigate. Defining a Unit ID will assist the SIMCA-online configuration of the SIMCA project since the SIMCA-online project configuration reads the Unit ID and which models that originate from which units.	When there is a column named 'UnitID' it is automatically specified as Unit ID.

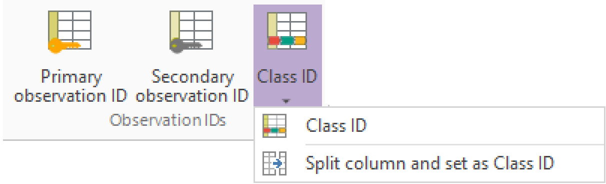
6.4.2.3 Class ID specification

Specifying the Class ID at import defines classes in the default workset. Specifying classes for the default workset can also be done in Dataset Properties after import. Only one column can be defined as Class ID and Class ID is only available for regular projects.

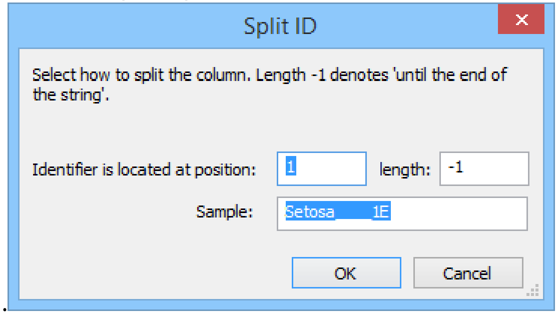
Specify class ID by marking a column and clicking **Class ID** in the Observation IDs group.

If you want to specify only a part as class ID;

1. mark the column and click **Class ID | Split column and set as Class ID**.



2. In the **Split ID** dialog, enter the start and length of the characters specifying the classes, or click **OK** to use the entire string. Length '-1' denotes 'until the end of the string'



Split ID

Select how to split the column. Length -1 denotes 'until the end of the string'.

Identifier is located at position: 1 length: -1

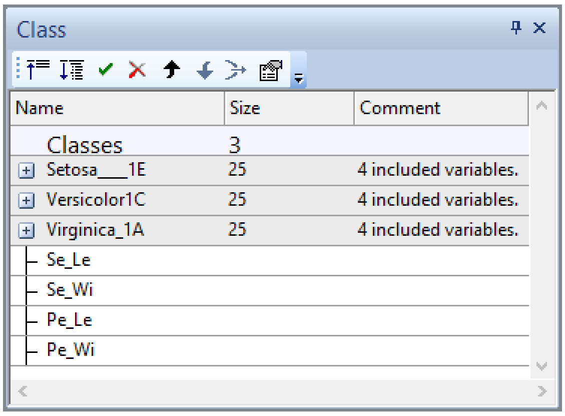
Sample: Setosa 1E

6.4.2.3.1 Class pane

After specifying a Class ID, the **Class** pane is updated accordingly.

Use the Class pane to **Rename**, **Merge**, **Delete**, and switch the order of the classes or excluding variables in certain classes. For more about these actions, see the **Batch & Phase pane phase part** subsection later in this chapter.

Note: Deleting classes here will omit them in the import while excluding variables only exclude them in the default workset.

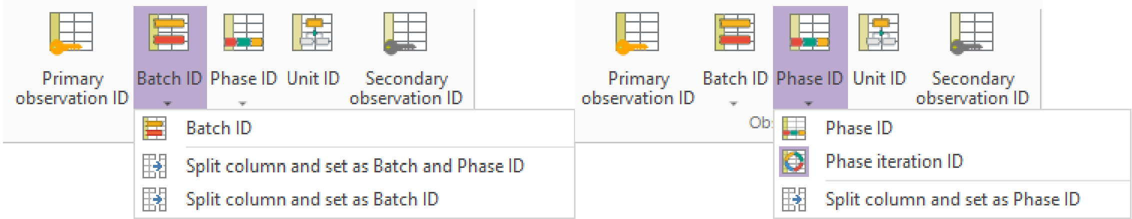


Name	Size	Comment
Classes	3	
Setosa___1E	25	4 included variables.
Versicolor1C	25	4 included variables.
Virginica_1A	25	4 included variables.
Se_Le		
Se_Wi		
Pe_Le		
Pe_Wi		

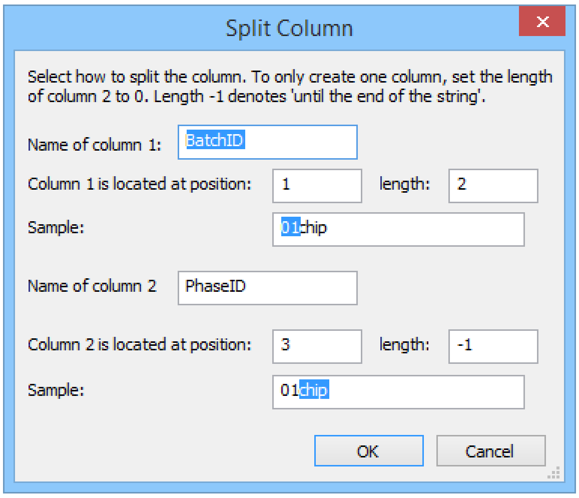
Note: When marking *classes, the marking may be somewhat difficult to see but is there.*

6.4.2.4 Batch and Phase ID specification

To specify the batch and phase IDs, mark the column and click **Batch ID** or **Phase ID**.



For the more advanced splitting of columns, or specification of Phase iteration ID, click the arrow and select from the Batch ID or Phase ID columns. The dialog opened when clicking Split column and set as Batch and Phase ID is show here and allows you to specify the position of the IDs by entering start character position and length.


Split Column

Select how to split the column. To only create one column, set the length of column 2 to 0. Length -1 denotes 'until the end of the string'.

Name of column 1: BatchID

Column 1 is located at position: 1 length: 2

Sample: 01chip

Name of column 2 PhaseID

Column 2 is located at position: 3 length: -1

Sample: 01chip

If the Batch or Phase IDs span several columns, click **Merge column** on the **Edit** tab to concatenate them.

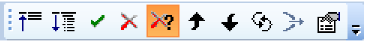
Specifying a Batch ID updates the content of the **Batch & Phase** pane. This pane is parted in two when Phase IDs have been specified; a phase part and a batch part.

Note: Leading zeros are included in identifiers. That is, while the number '001' is imported as '1' when specified as quantitative variable, it is imported as '001' when specified as identifier or qualitative variable.

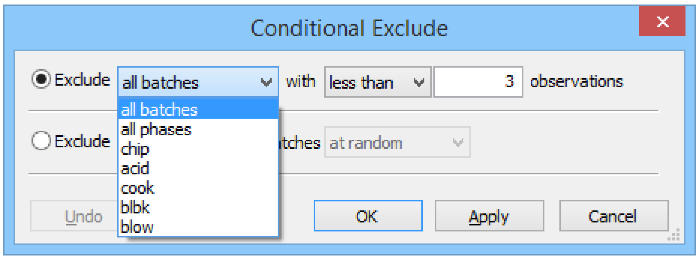
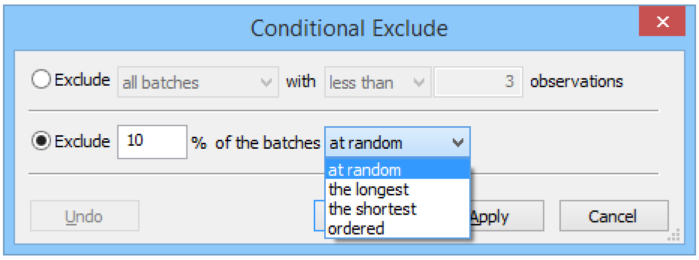
6.4.2.4.1 Downsizing using conditional exclude

When the file is large and contains many batches, conditional exclude can be used to downsize the number of batches.

Conditional exclude is available from the Batch & Phase pane by clicking **Conditional exclude** on the toolbar.



There are 2 types of conditional exclude available:

Conditional exclude type	Action by the user in the dialog
Excluding **all batches**, **all phases**, or the selected phase in each batch with **less than** / **more than** the user entered number of observations.	 Conditional Exclude ● Exclude all batches with less than 3 observations ○ Exclude ...tches at random all batches all phases chip acid cook blbk blow Undo OK Apply Cancel 1. Select the first **Exclude** option. 2. Select **all batches**, **all phases**, or one of the phases. 3. Select with less than or more than. 4. Enter the number of observations that defines the limit.
Excluding a user entered percentage of all batches **at random** / **the longest** / **the shortest** / **ordered**.	 Conditional Exclude ○ Exclude all batches with less than 3 observations ● Exclude 10 % of the batches at random at random the longest the shortest ordered Undo Apply Cancel 1. Select the second **Exclude** option. 2. Enter the percentage to use in the field. 3. Select how to delete the entered percentage of batches by clicking **at random/the longest/the shortest** or **ordered**.

6.4.3 Specifying data properties

For a regular project (non-batch), with no qualitative variables, it is necessary to include all variables (set them as x) but not necessary to specify y-variables. Specifying y-variables defines the default workset.

With batch data, the x variable, y variables (time or maturity), and variables pertaining to the whole batch, phase or phase iteration, such conditions, X or Y (quality of the batch) all need to be specified in the SIMCA Import.

6.4.3.1 All about specifying data

The table lists the **Variable types** available in the SIMCA Import, their description, the objective with specifying the type of variable, and the spreadsheet coloring after specification.

Specifying variable types is done as follows:

1. Mark the columns.
2. Click the relevant button in the **Variable types** group:
    - **Quantitative**
    - **Qualitative**
    - **Date/Time**
    - **Conditions** - requires that the column is also Quantitative or Qualitative and is available when importing batch data only.
    - **X variables**

- **Y variables**

Note: All data columns have to be specified as **X variables** or **Y variables** in addition to **Quantitative/Qualitative** or **Date/Time**.

Button	Description and objective	Coloring
Quantitative	Continuous variables. Imports a quantitative variable.	The variable is colored white.
Qualitative	Discrete variables that are split into dummy variables during the calculations. Imports a qualitative variable.	The variable is colored turquoise.
Date/Time variable	Specifies the selected variables according to the specified time format. For more, see the Specifying the Date/Time variable section later in this chapter. Date/time variables can be displayed on the x-axis showing time in the specified format.	The variable is colored orange.
Batch conditions	Batch condition variables can be imported with the batch evolution dataset or as a separate dataset arranged as a batch level dataset. Makes batch conditions available for modeling in batch level models.	The variable is colored light grey.
Phase conditions	Phase condition variables can be imported with the batch evolution dataset or as a separate dataset arranged as a batch level dataset. Makes phase conditions available for modeling in batch level models.	The variable is colored light grey.
Phase iteration conditions	Phase iteration condition variables can be imported with the batch evolution dataset or as a separate dataset arranged as batch level datasets, one per phase. Makes phase iteration conditions available for modeling in batch level models.	The variable is colored light grey.
X variable	All numerical variables, except the first column, are by default assumed to be x-variables. The x-variables are the explanatory variables. Includes the variable in the import.	The variable is colored white.
Y variable	Defines the default workset. The y-variables are the predictor variables.	The variable is colored light brown.

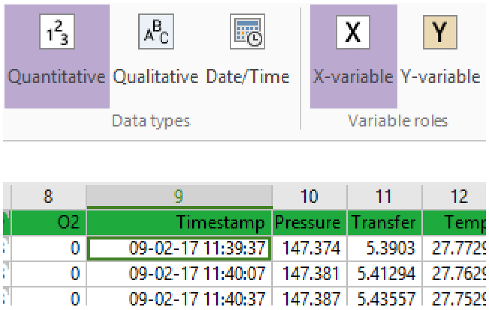
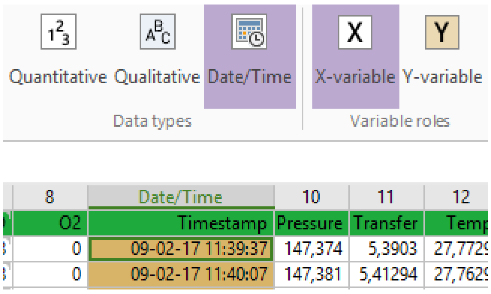
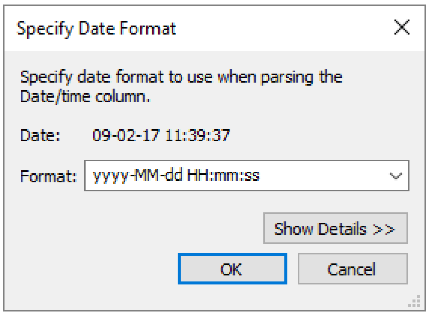
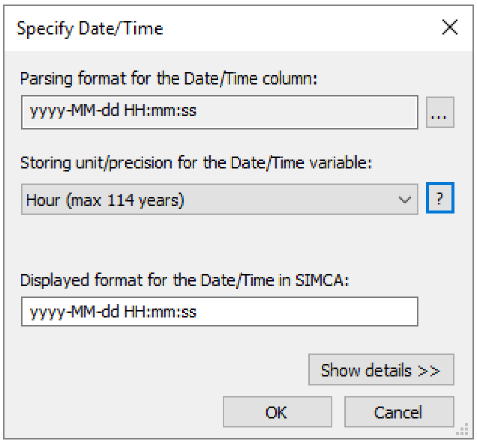
6.4.3.2 Formatting variable as Date/Time

A variable specified as **Date/Time** at import can be used:

- As a variable in the model. The date and time variable is then transformed into a regular value (float).
- As x-axis in plots. The **Date/Time** variable is by default displayed in line plots, for instance the score line plot and DModX.
- To dynamically lag variables in the workset.

6.4.3.2.1 Specifying the **Date/Time** variable

The auto formatting tries to recognize date/time variables and specify them as such. If the variable is not by default specified as date/time, follow the steps in the table:

Step	Description	Illustration
1.	Select the variable in the spreadsheet by clicking its column number. With more than one variable in the same format, mark them all.	 Quantitative Qualitative Date/Time X-variable Y-variable Data types Variable roles 8 | 9 | 10 | 11 | 12 O2 | Timestamp | Pressure | Transfer | Temp 0 | 09-02-17 11:39:37 | 147.374 | 5.3903 | 27.7729 0 | 09-02-17 11:40:07 | 147.381 | 5.41294 | 27.7629 0 | 09-02-17 11:40:37 | 147.387 | 5.43557 | 27.7529
2.	Specify the variable type by clicking **Date/Time**. If the variable is specified as X it is by default excluded from the default workset, if specified as Y, it is default included.	 Quantitative Qualitative Date/Time X-variable Y-variable Data types Variable roles 8 | Date/Time | 10 | 11 | 12 O2 | Timestamp | Pressure | Transfer | Temp 0 | 09-02-17 11:39:37 | 147,374 | 5,3903 | 27,7729 0 | 09-02-17 11:40:07 | 147,381 | 5,41294 | 27,7629
3.	If SIMCA cannot find an appropriate date/time format, the **Specify Date Format** dialog opens allowing you to specify it is displayed. Enter the format for the date/time variable and click **OK**. Click **Show details** to view the terminology, also displayed in the Date/Time formatting terminology subsection later in this section.	Specify Date Format Specify date format to use when parsing the Date/time column. Date: 09-02-17 11:39:37 Format: yyyy-MM-dd HH:mm:ss
4	If SIMCA can guess the date/time format, or after specifying it in step 3 and clicking **OK**, the **Specify Date/Time** dialog opens. In this dialog the parsing format for reading the data, the format for storage and the display format are selected. Worth noticing here is that: • The parsing format defines how the data is parsed. • The storing unit defines the unit used in plots with this time variable on the x-axis and the unit when defining subgroups based on this variable in control charts. Selecting to store the variable in seconds results in a warning when the time range is larger than 11 days. This does not affect how the data is imported, it's just a warning that is displayed depending on the storing unit selected. • Display format is the only setting here that can be edited after import, in Dataset Properties.	Specify Date/Time Parsing format for the Date/Time column: yyyy-MM-dd HH:mm:ss Storing unit/precision for the Date/Time variable: Hour (max 114 years) Displayed format for the Date/Time in SIMCA: yyyy-MM-dd HH:mm:ss
5	Clicking **OK** saves the format to use for parsing the variable.	

For reformatting after importing the dataset, see the Date/Time configuration in dataset properties subsection in Chapter 8, Data.

6.4.3.2.2 Date/Time formatting terminology

The following format details are available when clicking **Show details**:

Format	Description	Example
yyyy	Year using four digits.	2005
yy	Year using two digits.	05, 10
MMM	Month using three letters.	Aug
MM	Month using two digits.	08, 10
M	Month without leading 0.	8, 10
ddd	Day of week using three letters.	Mon
dd	Day in month using two digits.	05, 10
d	Day in month without leading 0.	5, 10
HH	Hour representing 24 hour day.	08, 10
H	Hour representing 24 hour day, no leading 0.	8, 10
hh	Hour representing 12 hour day.	01, 10
h	Hour representing 12 hour day, no leading 0.	1, 10
mm	Minutes using 2 digits.	01, 45
ss	Seconds using 2 digits.	01, 45
fff	Fractional seconds using 3 digits (milliseconds).	111
tt	AM/PM	AM or PM

6.4.3.3 Specifying time or maturity

Batch evolution models, BEM, require a y-variable, time or maturity. Neglecting to specifying a y-variable results in that $Time, automatically created by SIMCA, is used as y. $Time = relative local batch or phase time (i.e. the time restarts at the beginning of each batch and phase) with a sampling interval of 1.

6.4.3.4 Importing batch and phase conditions

When importing a dataset in a batch project and each batch only has one row, the data are assumed to be batch conditions. If some of the conditions variables are phase conditions, they need to be specified as such, see Batch and Phase ID specification. When there is one row per batch, phase and phase iteration, the variables in that dataset should be specified as phase iteration conditions. When importing phase iteration condition variables, the primary observation IDs are created to include batch ID, phase ID, and phase iteration ID and the phase iteration condition datasets are split to only hold data for one phase each.

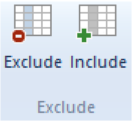
To import initial and final conditions, in SIMCA named *batch conditions*, *phase conditions,* and *phase iteration conditions*, after the batch project has been created, click **Data | Import dataset**. After import the new dataset can be selected in the **Workset** dialog when the **Create a batch level model** check box is selected.

Note: Beware of how you name your batch condition variables to not confuse them with the score names generated from the BEM. That is, do not use names such as t(1)_2_20.

6.4.4 Excluding/including rows or columns

To exclude or include a column or row in the import wizard spreadsheet: mark it and click **Exclude** or **Include**.

Excluded rows and columns are colored gray.



6.4.5 Apply formatting

Formatting specified for a file previously imported can be applied to the current spreadsheet by clicking **Apply formatting** and selecting the spreadsheet name. The files listed are those with matching variable and observation IDs.

To auto format (auto color) the dataset, click **Apply formatting | Auto format**.

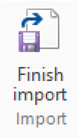
Clear formatting by clicking the **Clear formatting** button in the same group.

The formatting features are available in the **Formatting** group on the **Edit** tab.

Note: *A row, with slash </> as the leftmost character of the leftmost column of that row, is automatically marked as excluded by SIMCA. A column with slash </> as the leftmost character in the top cell is automatically marked as excluded by SIMCA.*

6.4.6 Finish and create project

After opening all datasets in the SIMCA import, click **Finish import** to create the SIMCA project.



In the dialog, select destination and enter project name.

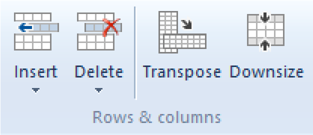
6.5 Edit

On the **Edit** tab editing commands are gathered in the groups: **Clipboard**, **Rows & columns**, **Merge**, and **Editing**. This section describes the features available in these groups with the exception of the Clipboard group which holds the standard commands **Paste**, **Cut**, and **Copy**.

6.5.1 Rows and columns

The standard editing commands **Insert** (with **Insert rows**, **Insert index**, **Shift** etc.) and **Delete** (with **Clear**, **Entire rows**, **Entire columns** etc.) are available in the **Rows & columns** group on the **Edit** tab.

Additionally Transpose and Downsize, described next in this section, are available.



6.5.1.1 Transpose

To transpose the dataset, on the **Edit** tab, in the **Rows & columns** group, click **Transpose**.

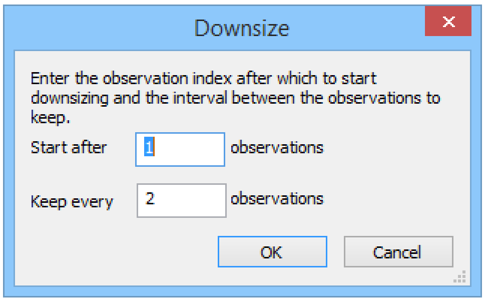
Transposing the dataset removes all formatting.

6.5.1.2 Downsizing the dataset

After importing a dataset you can select to downsize it before completing the import into SIMCA.

To use a subset of the imported dataset:

1. On the **Edit** tab, in the **Rows & columns** group, click **Downsize**.
2. In the **Start after** xx **observations** field, enter the starting observation. All observations, before and including this observation, remain included.
3. In the **Keep every** 'xx' **observations** field, enter the interval to use when downsizing.



Downsize

Enter the observation index after which to start downsizing and the interval between the observations to keep.

Start after 1 observations

Keep every 2 observations

Downsizing is not available here for batch projects. For batch projects, downsizing is available as **Conditional exclude** in the **Batches** page in the SIMCA import. For more, see the Batch & Phase pane batch part subsection later in this chapter.

6.5.2 Merge

6.5.2.1 Split column

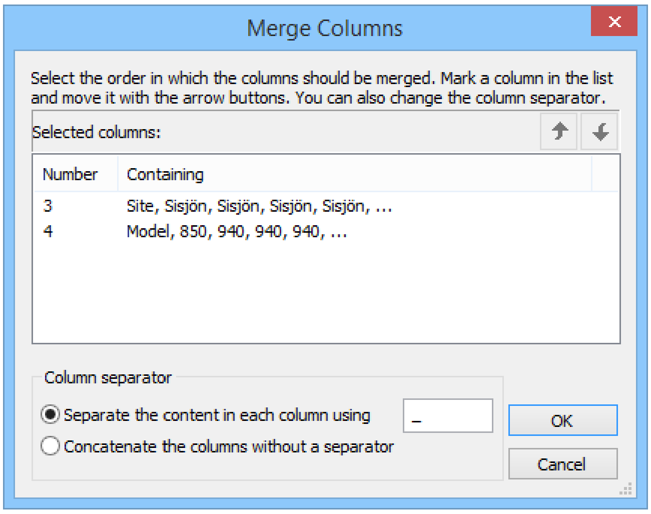
To split a column in two, mark the column and click **Split column** in the **Merge** group.

Splitting a column is useful when you have different information in the same column and would prefer them in separate columns.

6.5.2.2 Merging columns

To merge columns:

1. Mark the columns.
2. On the **Edit** tab, click **Merge columns**.
3. In the Merge Columns dialog, select the order in which the columns should be merged by marking and clicking the up and down arrows in the dialog.
4. If the columns should be merged with a separator, click **Separate the content in each column using** and enter a separator. If the columns should be merged without separator, select **Concatenate the columns without a separator**.
5. Click **OK** and the columns are merged and the original ones excluded.



Merge Columns

Select the order in which the columns should be merged. Mark a column in the list and move it with the arrow buttons. You can also change the column separator.

Selected columns:

Number	Containing
3	Site, Sisjön, Sisjön, Sisjön, Sisjön, ...
4	Model, 850, 940, 940, 940, ...

Column separator

● Separate the content in each column using _

○ Concatenate the columns without a separator

6.5.2.3 Merging spreadsheets

You can import one or more files using the SIMCA Import. When in SIMCA, datasets selected in the **Workset** dialog are merged by primary ID behind the scenes and merging is not necessary.

If you want to merge data before creating the project, on the **Edit** tab, in the **Merge** group, click **Merge spreadsheets**.

The table lists a description of the steps.

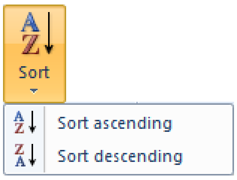
Step	Objective and explanation	Action
1.	**Importing** the datasets.	Click **Add data** and **import the** datasets to merge in SIMCA Import.
2.	**Initiating the merge** of two or more files in one single dataset.	On the **Edit** tab, in the **Merge** group, click **Merge spreadsheets**.
3.	Selecting the files to merge.	In the **Merge** dialog, clear spreadsheet check boxes so that only the files to merge are selected.
4.	Sorting the files.	Move the files using the arrows leaving the files in the desired order.
5.	Merging matching identifiers/index. When merging and matching by identifier, that identifier needs to be selected in the **Merge by** box. Selecting to merge by **Index** merges on row/column index.	In the **Merge by** box, select **Index** or **Primary ID**. If no primary ID has been specified, only **Index** is available.
6.	**Selecting direction to merge**. This option determines how the merging is done, positioning the datasets next to each other in **Side by side** or above and below in **Top / bottom**.	In the **Direction** box, select in which direction to merge, **Side by side** or **Top / bottom**.
7.	Selecting the form of the merged data. **Destination**: The destination file (first one in the dialog) specifies which observations/variables are included. **Intersection**: The observations/variables common to all selected datasets are included. **Union**: All observations/variables present in any of the datasets are included.	In the **Result** box select whether the result is variables/observations according to the **Destination** file, the **Intersection** or the **Union**.
8.	**Completing** the merge.	Click **OK** to merge the files as specified deleting the original spreadsheets.

6.5.3 Sort

Sort | Sort ascending and **Sort descending** are available when marking one column only

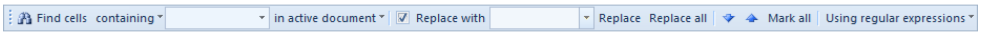
(click the column header).

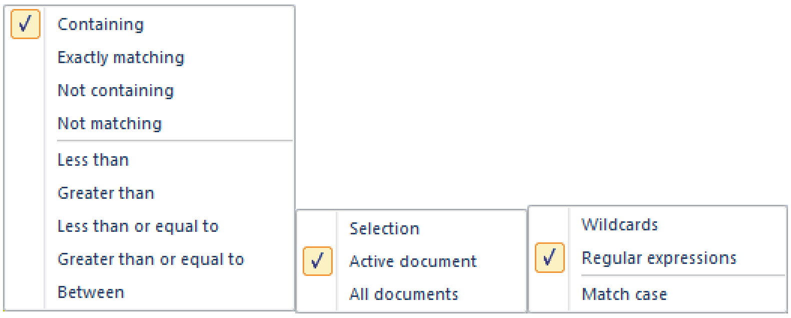
Clicking **Sort ascending/descending** results in that the entire dataset is sorted according to the marked variable.



6.5.4 Find toolbar

The **Find** toolbar opens when pressing CTRL+F or when clicking **Find and replace** on the **Edit** tab.





Using the **Find** toolbar you can find cells matching a certain expression, numerical or text.

To find:

1. In the first drop down menu select
   - **Containing** (default),
   - **Exactly matching**,
   - **Not containing**, or
   - **Not matching** that all apply to both text and values
   - **Less than**,
   - **Greater than**,
   - **Less than or equal to**,
   - **Greater than or equal to**, or
   - **Between** which all apply to values.
2. Enter the value or text in the first field.
3. In the second drop down menu select:
   - **Selection** - to only search in the current selection.
   - **Active document -** to search the current spreadsheet.
   - **All documents** - to search all spreadsheets open in SIMCA import.
4. If you want to replace, select the **Replace** check box and enter the new text/value in the **Replace with** field. When selecting the **Replace** check box two new buttons appear **Replace** and **Replace all**. Use these to replace once the items to replace have been found.
5. Click the arrows to find from top left to right going down (down arrow) or from bottom right to left going up.
6. Click the **Mark all** button to mark all cells that match.
7. In **Options** select:
   - **Wildcards** to be able to use the wild characters '?' to represent an unknown character or '*' to represent unknown beginning or ending of the expression.
   - **Regular expressions** to interpret the search string as a POSIX basic regular expression.
   - **Match case** to match character case.

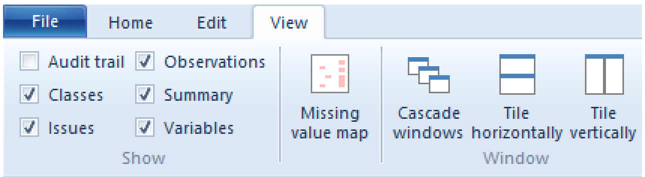
Note: **Wildcards** or **Regular expressions** can be selected, not both. **Match case** can be selected in combination with **Wildcards** and **Regular expressions**.

6.6 View

The information panes **Audit trail**, **Batch & phase**, **Classes**, **Issues**, **Observations**, and **Variables** can be shown or hidden from the **View** tab.

The Missing value map is also available here. See the Missing value map section.

Arranging windows cascaded or tiled is available by clicking **Cascade**, **Tile horizontally** and **Tile vertically**. All open spreadsheets are arranged accordingly.



☐ Audit trail ☑ Observations
☑ Classes ☑ Summary
☑ Issues ☑ Variables

6.6.1 Audit trail

The audit trail needs to be turned on before importing the first dataset to hold all information, see the Options subsection earlier in this section.

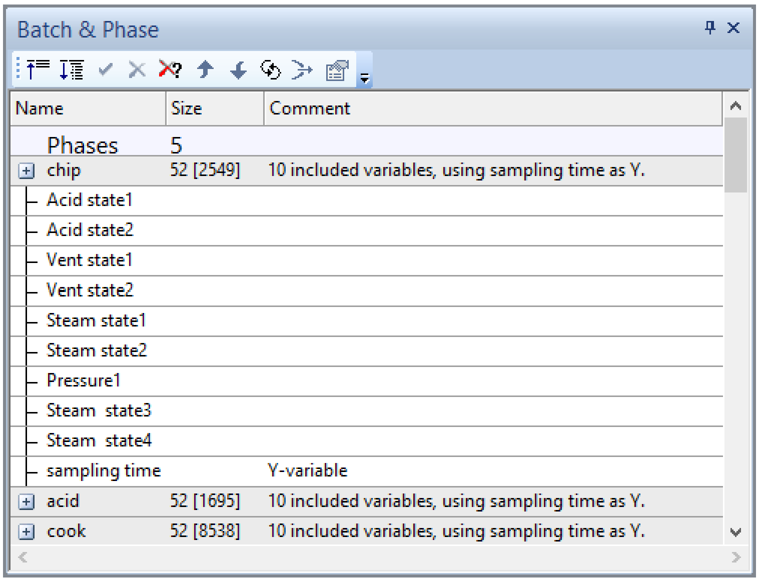
Note: The **Audit Trail** is empty until clicking **Finish** when the audit trail starts logging information later displayed in the Audit Trail pane in SIMCA.

For more, see the Audit trail section in Chapter 13, View.

6.6.2 Batch & Phase pane phase part

With a batch project with phases, the phase part of the **Batch & Phase** pane lists:

- Each phase.
- The number of batches containing that phase (batches do not have to include all phases).
- The number of variables in that phase (phases may have different variables).
- The roles of the variables.



Name	Size	Comment
Phases	5	
⊞ chip	52 [2549]	10 included variables, using sampling time as Y.
Acid state1		
Acid state2		
Vent state1		
Vent state2		
Steam state1		
Steam state2		
Pressure1		
Steam state3		
Steam state4		
sampling time		Y-variable
⊞ acid	52 [1695]	10 included variables, using sampling time as Y.
⊞ cook	52 [8538]	10 included variables, using sampling time as Y.

Note: When moving/deleting/rearranging phases in the Batch & Phase pane, nothing happens in the dataset spreadsheet until the dataset is imported to SIMCA.

6.6.2.1 Excluding variables

If the phases have different variables you can exclude variables in the following manner:

1. Expand the node in each phase to list the variables.
2. Mark the variables to exclude.
3. Click **Exclude**.

This excludes the variables in the default workset. You can also configure the variables for each phase, after import, in the Workset dialog.

6.6.2.2 Delete phases

Delete a phase in a certain batch by marking and clicking **Exclude**.

✕

Note: Deleting phases here will omit them in the import while excluding variables only exclude them in the default workset.

6.6.2.3 Switching the order of the phases

If phases are imported in the incorrect order, mark the phase and click the up or down arrow in the dialog.

↑ ↓

6.6.2.4 Rearranging phases automatically

Let SIMCA rearrange the phases automatically by clicking the **Rearrange phases** button. The phases will then be arranged in the order in the **Batch & Phase** pane.

6.6.2.5 Merging phases

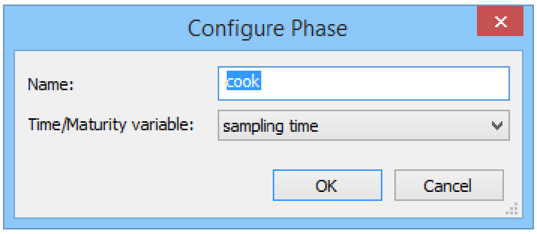
To merge phases, mark two or more phases and click the **Merge** button.

If you want to merge phases positioned in two different datasets, you first need to merge the datasets. See the Merging spreadsheets subsection for more.

Note: *You can merge consecutive phases by marking them (marking may be somewhat difficult to see) and clicking **Merge**.*

6.6.2.6 Assigning different time or maturity variable and renaming phases

If you want to assign different time/maturity variables to the different phases and/or rename a phase, mark a phase, click **Configure** (last button in the **Batch & Phase** pane), and select the desired time/maturity from the **Time/Maturity variable**-box, and/or type a new phase name.



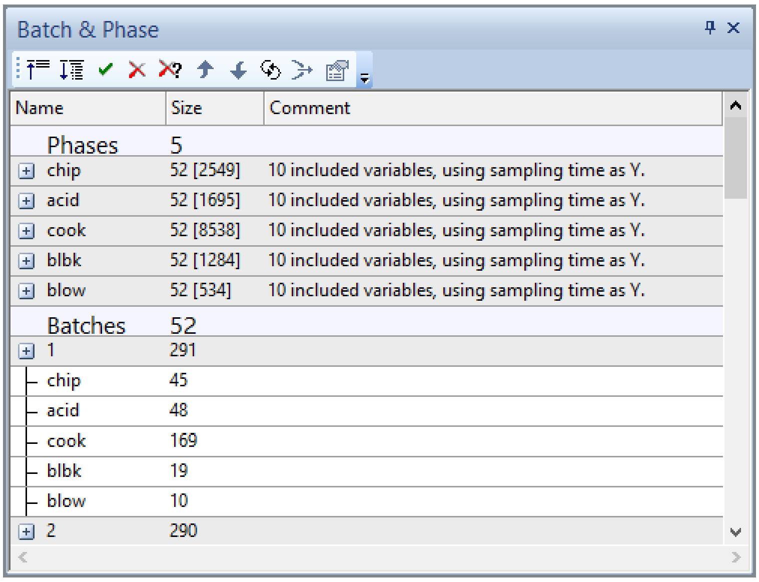
Configure Phase

Name: cook

Time/Maturity variable: sampling time

6.6.3 Batch & Phase pane batch part

The **Batch & Phase** pane **Batches** section displays batches, the phases present in each batch, and the number of observations in each phase for each batch.



Name	Size	Comment
Phases	5	
⊞ chip	52 [2549]	10 included variables, using sampling time as Y.
⊞ acid	52 [1695]	10 included variables, using sampling time as Y.
⊞ cook	52 [8538]	10 included variables, using sampling time as Y.
⊞ blbk	52 [1284]	10 included variables, using sampling time as Y.
⊞ blow	52 [534]	10 included variables, using sampling time as Y.
Batches	52	
⊞ 1	291	
chip	45	
acid	48	
cook	169	
blbk	19	
blow	10	
⊞ 2	290	

Expand the node to see all the phases in a batch with the number of observations in each phase.

6.6.3.1 Excluding batches or phases

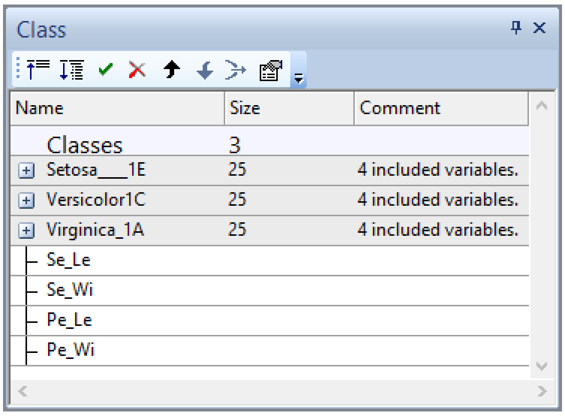
Exclude batches or a phase in a certain batch by marking and clicking **Exclude** ✕ .

6.6.4 Class pane

After specifying a Class ID, the **Class** pane is updated accordingly.

Use the Class pane to **Rename**, **Merge**, **Delete**, and switch the order of the classes or excluding variables in certain classes. For more about these actions, see the **Batch & Phase pane phase part** subsection later in this chapter.

Note: Deleting classes here will omit them in the import while excluding variables only exclude them in the default workset.



Name	Size	Comment
Classes	3	
⊞ Setosa___1E	25	4 included variables.
⊞ Versicolor1C	25	4 included variables.
⊞ Virginica_1A	25	4 included variables.
Se_Le		
Se_Wi		
Pe_Le		
Pe_Wi		

Note: When marking *classes, the marking may be somewhat difficult to see but is there.*

6.6.5 Issues pane

The **Issues** pane lists problems in individual sheets as well as between sheets. When there is an issue that the SIMCA import can resolve for you the **Select action** column displays what the action will be when **Resolve all** is clicked. Hover over the issue to display more information in a tooltip.

As long as there are unsolved issues, clicking **Finish** will not let you create a project.

6.6.5.1 Issues and actions in the Issues pane

The table lists some common issues, the reason for the issue, possible ways to resolve and the result from the selected resolution.

Note: Hover over the issue for more info.

Issue	Description	Actions available	Result after Resolve all
No primary Obs ID No primary Var ID	The ID has not been specified.		Clicking **Resolve all** or **Finish** both add unique primary IDs.
Missing observation ID Missing variable ID Missing batch name Missing phase name	There are missing values in the column/row specified as primary/batch/phase ID	rename auto rename exclude row/column	rename - opens a dialog allowing you to enter an ID. auto rename - adds a number to create unique IDs. exclude row - excludes the problem rows/columns.
Primary observation ID is not unique Primary variable ID is not unique	There is at least one duplicated primary ID.	rename auto generate exclude row/column	rename - opens a dialog allowing you to enter the new ID for the duplicate. auto generate - creates new observation/variable IDs for all. exclude row - excludes the rows/columns with duplicated IDs.
No batch ID	No batch ID was specified for the batch dataset.	auto generate	auto generate is available when a phase ID has been specified - creates batch ID using the phase ID.
No phase ID	No phase ID was specified for the batch dataset. Displayed when importing a dataset to a batch project with phases		This has to be resolved by specifying a phase ID.
Batch condition variable lacks primary variable ID	A variable specified as batch condition lacks primary variable ID.	rename auto rename exclude column	rename - opens a dialog allowing you to enter an ID. auto rename - suggests an ID. exclude column - excludes the problem columns.
More than one dataset have the name ...	Each dataset in a project needs to have a unique name. All datasets are by default named by the file name or sheet.	rename Note here that clicking **Rename** to the left of the issue allows you to specify the new dataset name	rename - adds a number making the dataset name unique.
Unrecognized qualitative setting in variable	For a project with one or more models, no new settings in a qualitative variable can be imported. To import a new setting, delete all models, including *unfitted* models before import.	treat as missing exclude row exclude column	treat as missing - replaces the new setting with missing. exclude row - excludes all rows with the new setting. exclude column - excludes the column.
Variable type mismatch	A variable must be of the same type in all datasets in a project. The *Variable type mismatch* warning appears when the same primary variable ID was specified for different variable types, e.g. quantitative/qualitative/date time.		

Issue	Description	Actions available	Result after Resolve all
Maturity is not specified. A variable called $Time will be generated	No y-variable has been specified.	None	Clicking **Resolve all** or **Finish** both add the $Time variable.
Non-continuous batch IDs	All data for a given batch must be continuous.	auto rename (default) exclude row sort	auto rename - adds a number to the batch IDs that are perceived to be out of order. exclude row - excludes the first row that appears out of order and continues until the batch IDs are in order. sort - sorts the batch IDs
Non-continuous phase IDs	All observations in a phase must be consecutive within every batch.	manual exclude (default) split batch exclude last in batch exclude first in batch	manual exclude - results in nothing when clicking **Resolve all**. You have to decide what to do yourself. split batch - adds number to all batch IDs following the observation with the problem in phase ID. exclude last in batch - excludes all rows following the problem phase ID in that phase. exclude first in batch - excludes all rows preceding the row with the problem phase ID.
Non-continuous phase iteration IDs	All observations in a phase iteration must be consecutive within every batch and phase.		manual corrections necessary.
Non-continuous Unit IDs	All observations in a phase must be consecutive within every batch and phase.		manual corrections necessary.
Existing batch variable combination	Datasets in the same project may only contain the same batches OR the same variables, not both.	rename batches (default) manual merge	rename batches - adds a number making the batch IDs unique. manual merge - results in nothing when clicking **Resolve all**. You have to decide what to do yourself.
Existing Var. Obs. combination	Datasets in the same project may only contain observations OR variables with the same primary IDs.	rename observations (default) rename variables exclude row exclude column	rename observations - adds a number to the primary IDs that are found matching, making them unique. rename variables - adds a number to the primary IDs that are found matching, making them unique. exclude row - excludes the rows with matching IDs. exclude column - excludes the columns with matching IDs.

Issue	Description	Actions available	Result after Resolve all
Conflicting batch ID Conflicting phase name Conflicting class name Conflicting phase iteration ID Conflicting unit ID	Identical primary observation IDs may not be associated with different batch/phase/class IDs. Identical primary observation IDs, in combination with batch/phase ID may not be associated wtih different phase iteration/unit IDs	auto rename exclude row	auto rename - adds a number making the IDs unique. exclude row - excludes the rows with matching IDs.
Phases out of order	The phases need to be in the same order for all batches.	reorder phases	reorder phases - orders the phases in the order of the phases in the **Batch & Phase** pane.
Phases not in the same order in all datasets	The phases need to be in the same order for all batches in all datasets.	manually reorder phases	The phases have to be reordered. You can do this easily for each dataset using the **Batch & Phase** pane.
Invalid value	String that is not in a row or column with identifiers or in a column defined as qualitative.	treat as missing exclude row exclude column	treat as missing - replaces the content of the cell with missing. exclude row - excludes all rows with the invalid values. exclude column - excludes the columns with the invalid values.
Variable IDs cannot contain any of the following characters: $ Observation IDs cannot contain any of the following characters: $	$ is reserved for SIMCA created vectors.	rename auto rename exclude column/row	rename - opens a dialog allowing you to enter an ID. auto rename - replaces $ with underscore. exclude row/column - excludes the problem rows/columns.
Incorrect date/time variable settings	The content of the cell cannot be formatted as date/time.	treat as missing exclude row exclude column	treat as missing - replaces the content of the cell with missing. exclude row - excludes all rows with the invalid values. exclude column - excludes the columns with the invalid values.
Unexpected phase ID Unexpected phase iteration ID	The first dataset in the project does not have phases, then other datasets may not either. Same goes for phase iteration IDs.	exclude	exclude - excludes the column.
Non printable character	ASCII characters 1 - 31.	exclude rename	exclude - excludes the row/column. rename - opens the rename dialog.

6.6.6 Observations pane

The **Observations** pane lists number of observations currently included, primary observation IDs of the currently included observations, and % missing.

Formatting and excluding observations can be done by marking one or more rows and right-clicking. The following commands are available: **Primary ID**, **Secondary ID**, **Exclude row**, and **Include row**.

All of these commands are available on the **Home** tab and are not described here.

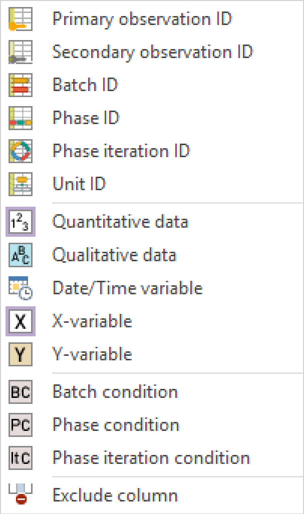
6.6.7 Variables pane

The **Variables** pane lists the number of variables currently included, primary variable IDs of the currently included variables, variable type and % missing.

Formatting columns, excluding, and merging can be done by marking one or more variables and right-clicking.

A menu opens with the following commands: **Primary observation ID**, **Secondary observation ID**, **Class ID** (regular projects only), **Batch ID** (batch projects only), **Phase ID** (batch), **Phase iteration ID** (batch), **Quantitative data**, **Qualitative data**, **Date/Time variable**, **Batch condition** (batch), **X-variable**, **Y-variable**, and **Exclude column**.

All of these commands are available on the **Home** tab and are not described here. The column menu for a batch dataset is displayed here.

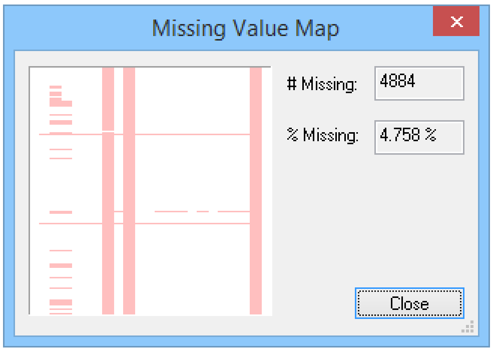


6.6.8 Missing value map

To display an overview of a dataset with respect to missing values:

- On the **Data** tab, in the **Summary** group, click **Missing value map** and then the desired dataset in SIMCA.
- In SIMCA import, on the **View** tab in the **Missing values** group, click **Missing value map**.

Missing values are colored while data present are white.



Missing: 4884

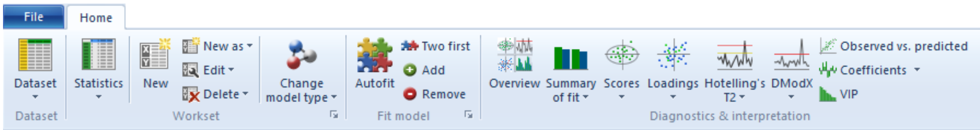
% Missing: 4.758 %

7 Home

7.1 Introduction

The **Home** tab holds the commands most commonly used when creating models and evaluating them. On the **Home** tab you can:

- View the imported datasets - **Dataset** spreadsheet
- View statistics and create a new model using the commands in the Workset group.
- Fit the model - using the Fit model group.
- View diagnostic and interpretation plots: **Summary of fit**, **Scores**, **Loadings**, **Hotelling's T2Range**, **DModX**, **Observed vs. predicted**, **Coefficients** and **VIP**.



Note: When the project window is not docked, **Project window** is found to the far left on the **Home** tab.

7.2 Workset

This section describes the features in the **Workset** group on the **Home** tab.

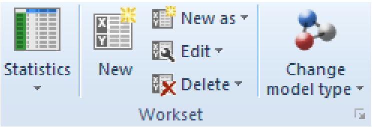
The workset is all or a subset of the selected datasets, with specifications for scaling, transformations, variable roles, lags and expansions of variables. Observations can be grouped in classes for SIMCA classification or discriminant analysis. In batch projects with phases the observations are grouped in phases.

When exiting the workset dialog, SIMCA creates an active model, linked to that workset. A workset is associated with every model.

7.2.1 Content

In the **Workset** group the following commands are available:

1. **Statistics** | **Workset statistics** displays the selected statistics for the current workset; **Correlation matrix** displays the correlations for the variables included in the current workset.
2. **New** opens the workset dialog with the settings of the default workset.
3. **New as** | **Mx** opens the workset dialog using the settings of the selected model.
4. **Edit** | **Mx** opens workset dialog of the selected model.
5. **Delete** | **Mx** deletes the selected model and workset.
6. **Change model type** lets the user select among the available model types.
7. The Model options dialog box launcher opens the Model Options dialog for the current workset, for editing and viewing.



7.2.2 Workset statistics

To display descriptive statistics for selected variables in the current workset, click **Statistics** | **Workset statistics**.

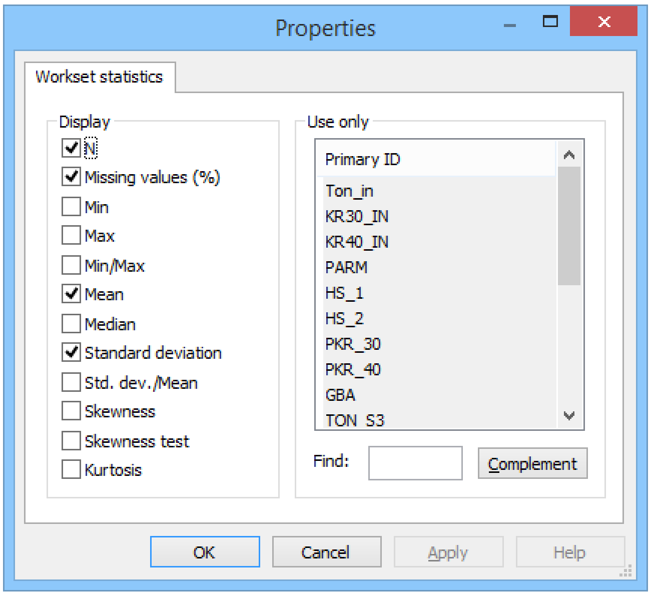
Note: When marking a CM, BEM or DA-model, the statistics are calculated over all classes/phases.

The default Workset statistics list displays N (number of observations), Missing values (%), Mean, and Standard deviation for the variables in the workset.

To view more than the default statistics, open **Properties** and select what to display. The **Properties** dialog is described next.

7.2.2.1 Properties

The Workset statistics Properties dialog has two sections: Display and Use only.



Display
☑ N
☑ Missing values (%)
□ Min
□ Max
□ Min/Max
☑ Mean
□ Median
☑ Standard deviation
□ Std. dev./Mean
□ Skewness
□ Skewness test
□ Kurtosis

Use only
Primary ID
Ton_in
KR30_IN
KR40_IN
PARM
HS_1
HS_2
PKR_30
PKR_40
GBA
TON_S3

7.2.2.1.1 Display

In the **Display** section, the statistics are listed.

The available statistics are: **N**, **Missing values (%)**, **Min**, **Max**, **Min/Max**, **Mean**, **Median**, **Standard deviation**, **Std. dev./Mean**, **Skewness**, **Skewness test**, and **Kurtosis**.

By default the **N**, **Missing values (%)**, **Mean**, and **Standard deviation** check boxes are selected.

To display other or more statistics, select the desired check boxes.

7.2.2.1.2 Use only

The statistics are computed on the included observations in the active model, for the variables selected in the **Use only** list. The statistics are displayed for the transformed and trimmed variables when specified in the workset.

By default all variables are included.

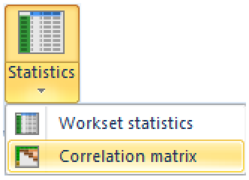
To view the statistics of a selection of variables, mark the variables in the **Use only** list.

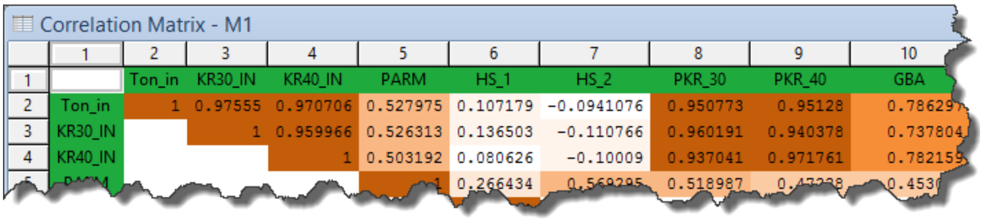
7.2.3 Correlation matrix

The correlation matrix is a spreadsheet that shows the pair-wise correlation between all variables (X and Y) in the current workset, scaled and transformed as the workset. Each variable is displayed on one row and one column in the correlation matrix, and the correlation between two variables is shown in the cell where the two variables intersect. By double-clicking a cell the corresponding scatter plot of the raw data is created. The value of the correlation coefficient represents the extent of the linear association between the two terms. The value of the correlation coefficient ranges from -1 to 1. When the correlation coefficient is close to zero there is no linear relationship between the terms.

Note: When marking a CM, BEM or DA-model, the correlations are calculated over all classes/phases.

To display the Correlation matrix for the current model, click **Statistics | Correlation matrix**.




Correlation Matrix - M1

	1	2	3	4	5	6	7	8	9	10
1		Ton_in	KR30_IN	KR40_IN	PARM	HS_1	HS_2	PKR_30	PKR_40	GBA
2	Ton_in	1	0.97555	0.970706	0.527975	0.107179	-0.0941076	0.950773	0.95128	0.78629
3	KR30_IN		1	0.959966	0.526313	0.136503	-0.110766	0.960191	0.940378	0.737804
4	KR40_IN			1	0.503192	0.080626	-0.10009	0.937041	0.971761	0.782159
5	PARM				1	0.266434	0.569295	0.518987	0.47228	0.453

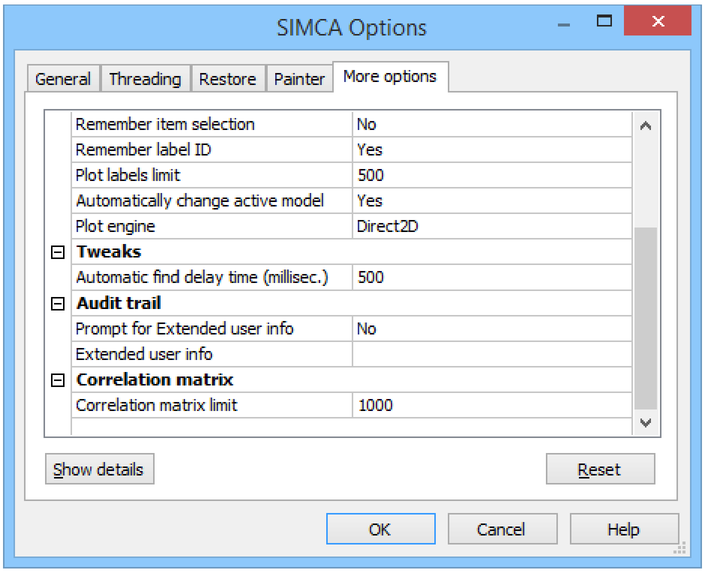
7.2.3.1 Coloring

SIMCA uses a coloring scheme in ten levels (from dark color to white) to assist in the interpretation of the correlation matrix. The darker the color, the higher the absolute correlation.

7.2.3.2 Limitation

By default the correlation matrix is restricted to 1000 variables, but this limit can be changed in the SIMCA Options dialog.

The calculations when creating the correlation matrix may become time consuming with many variables.



Remember item selection	No
Remember label ID	Yes
Plot labels limit	500
Automatically change active model	Yes
Plot engine	Direct2D
⊟ **Tweaks**	
Automatic find delay time (millisec.)	500
⊟ **Audit trail**	
Prompt for Extended user info	No
Extended user info	
⊟ **Correlation matrix**	
Correlation matrix limit	1000

7.2.4 New workset

To create a new workset from the settings of the default workset, click **New**. The Workset dialog opens.

For more about the Workset dialog, see the Workset dialog section later in this chapter.

7.2.4.1 Default workset

When exiting the SIMCA import the default workset is created according to specifications during the import. For batch projects all datasets imported when creating the project are by default included while only the first dataset is included when creating a regular project.

The properties that can be specified for the default workset are:

- Selected datasets.
- Variables as **X**, **Y**, or excluded.
- Variable scaling but only for the X respective Y variables as groups, not for individual variables.
- Observation class belonging.

Note: No lags, expansions, or transformations can be saved in the default workset.

7.2.4.1.1 Specifying the default workset

The default workset can be specified as follows:

- *Datasets included*: Select the desired datasets in the **Select data** page in the **Workset** dialog and click **Save as default workset**.
- *Y-variables*: Specify variables as Y in:
  - the SIMCA import or
  - the **Workset** dialog, **Variables** page, then click **Save as default workset**. Here the configuration of a batch project y-variable can also be saved.
- *Exclude variables*: Specify variables as **Excluded** in the **Workset** dialog, **Variables** page, and then click **Save as default workset**.
- *Scaling*: Specify X and Y variable scaling in **Project Options**, **Fit** tab, in the Default scaling section.
- *Classes*: Specify class belonging
  - by specifying **Class ID** in the SIMCA import or
  - by specifying classes in Dataset **Properties**, tab **Observations**.

7.2.5 New workset as model

To create a new workset copying the settings from a selected model, click **New as** and select the desired model.

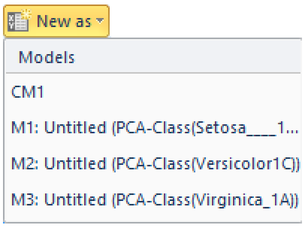
When the original model is a batch evolution model, BEM, and there are dependent batch level datasets, SIMCA offers to recreate these dependent datasets and models, when applicable. For details, see the Automatically recreate batch level datasets and models topic.

Note that switching which datasets are selected or the order of the selected datasets results in resetting the workset to default settings.

7.2.5.1 New as model with class models

To create a model identical to one that you already have, mark the model in the Project Window and click **New as**. The workset dialog opens a copy of all settings of the marked model.

With class models, the **New as** menu holds both wrapper CM and class models.

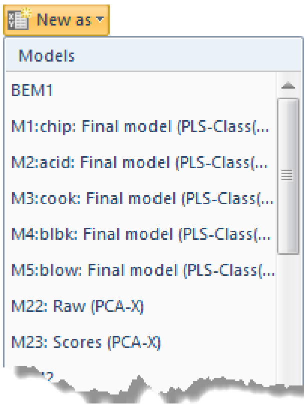

New as
Models
CM1
M1: Untitled (PCA-Class(Setosa___1...
M2: Untitled (PCA-Class(Versicolor1C))
M3: Untitled (PCA-Class(Virginica_1A))

Clicking **New as** |

- **CMxx** opens the workset dialog with the variables of all classes and the same specification as model CMxx. If a class model has been modified (scaling, transformations, etc.), these modifications are present (although not visible) for that specific class model, if no contradictory changes are introduced.
- **xx**, opens the workset dialog with only the observations and variables of the selected class and the same specifications as model xx. Any change to variables, scaling or transformation of variables affects only that class (model). Clicking **OK** creates an unfitted model for the selected class in a new CMxx wrapper.

7.2.5.2 New as model for batch projects with phases

For a batch project with phase models, the **New as** menu holds both wrapper BEM and phase models.


New as
Models
BEM1
M1:chip: Final model (PLS-Class(...
M2:acid: Final model (PLS-Class(...
M3:cook: Final model (PLS-Class(...
M4:blbk: Final model (PLS-Class(...
M5:blow: Final model (PLS-Class(...
M22: Raw (PCA-X)
M23: Scores (PCA-X)

Clicking **New as** |

- **BEMxx** opens the workset dialog with the variables of all phases (classes) and the same specification as model BEMxx. If a phase model has been modified (scaling, transformations, etc.), these modifications are present (although not visible) for that specific phase model, if no contradictory changes are introduced.
- **Mxx**, opens the workset dialog with only the observations and variables of the selected phase and the same specifications as model xx. Any change to variables, scaling or transformation of variables affects only that phase (model). Clicking **OK** creates an unfitted model for the selected phase in a new wrapper BEMxx.

7.2.6 Editing the workset

To edit the workset of a selected model, mark the model in the Project Window and click **Edit**. Alternatively, click the arrow to the right of Edit and select the desired workset. If the model is fitted, it is replaced by the edited unfitted model.

When the original model is a batch evolution model, BEM, and there are dependent batch level datasets, SIMCA offers to recreate these dependent datasets and models, when applicable. For details, see the Automatically recreate batch level datasets and models topic.

Editing a model is particularly useful when a transformation or scaling of a variable is necessary in one phase or one class only.

Note that switching which datasets are selected or the order of the selected datasets results in resetting the workset to default settings.

7.2.6.1 Editing models with class models

With class models, the **Edit** menu holds both wrapper CM and class models.

Clicking **Edit** |

- **CMxx** opens the workset dialog with the variables of all classes and the specification as model CMxx.
- **xx**, opens the workset dialog with only the observations and variables of the selected class (model). Any change to variables, scaling or transformation of variables affects only that class. Clicking **OK** replaces the previous model with an unfitted model.

7.2.6.2 Editing models for batch projects with phases

For a batch project with phase models, the **Edit** menu holds both wrapper BEM and phase models.

Clicking **Edit** |

- **BEMxx** opens the workset dialog with the variables of all phases (classes) and the specification as model BEMxx.
- **Mxx**, opens the workset dialog with only the observations and variables of the selected phase (model). Any change to variables, scaling or transformation of variables affects only that model. Clicking **OK** replaces the previous model with an unfitted model.

7.2.7 Automatically recreate batch level datasets and models

Automatic recreation of batch level datasets and models, after editing a BEM, is especially useful when updating a model that is running in SIMCA-online.

The option to automatically create batch level datasets and models is available provided;

- No observations, variables or batches are removed from any phase.
- No lags or expansions are added.

7.2.7.1 Edit/New as BEM

When editing or creating a new model as a BEM, you can select whether to automatically recreate batch level datasets and models connected to the original model, by selecting the appropriate option:

1. Yes, recreate all dependent datasets and models.
2. Yes, recreate all dependent datasets but no models.
3. No, delete old batch level datasets and models.

7.2.7.2 Recreate all datasets and models

When recreating all dependent batch level datasets and models, the alignments of the new models are taken from the original BEM. This means that if you have added batches that are much longer, the data representing batch duration longer than the original alignment will be discarded. Here a message is displayed stating how much longer the maturity of the added batches are, that is, how much longer the aligned maturity would have been, had the model been recreated with all batches included from the beginning.

Note that autofit is not used to fit any of the models when selecting this option, instead the objective is to extract the same number of components as the original model.

7.2.7.3 Recreate all datasets only

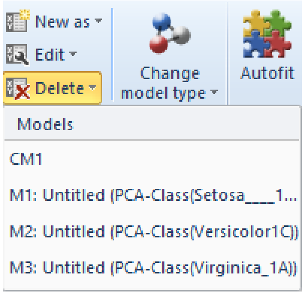
When recreating only the dependent datasets, the alignment is recomputed. This is preferable when newly added batches are significantly longer than the original batches, and when you do not want to recreate the batch level models.

7.2.7.4 Only create the BEM and no dependent datasets

Clicking **No** here results in the creation of the BEM only, with the alignment recomputed and autofit used.

7.2.8 Deleting the model

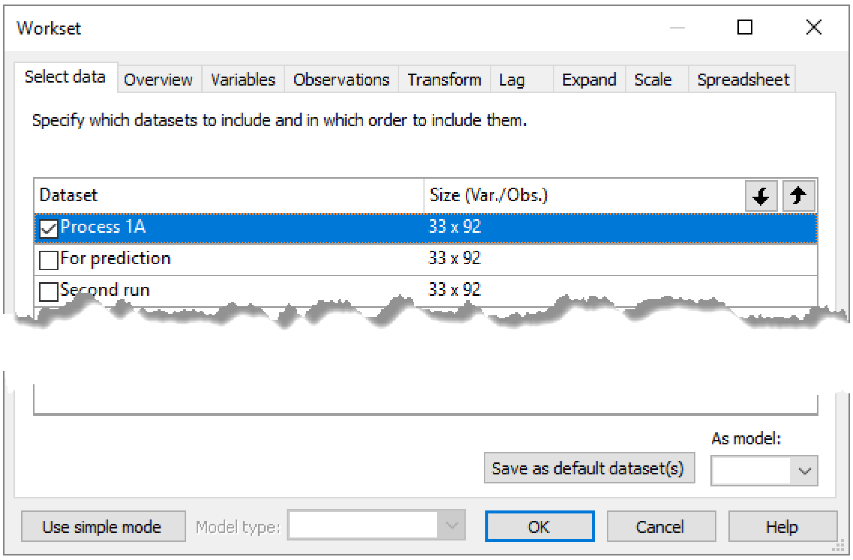
To delete a model, mark it in the Project window and click **Delete**. Alternatively, click the arrow beside **Delete** and click the model to delete in the menu. Both the workset and the model associated with it will be deleted.


New as
Edit
Delete
Change model type
Autofit
Models
CM1
M1: Untitled (PCA-Class(Setosa____1...
M2: Untitled (PCA-Class(Versicolor1C))
M3: Untitled (PCA-Class(Virginica_1A))

7.2.9 Workset dialog

After selecting to create a new workset, the **Workset** dialog opens with the current observations and variables and their attributes.

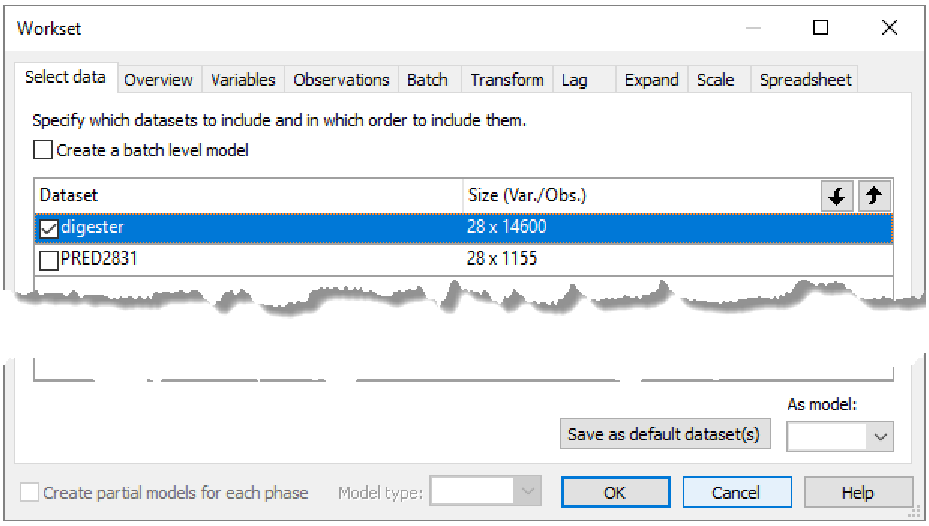
Regular project



Specify which datasets to include and in which order to include them.

Dataset	Size (Var./Obs.)
☑ Process 1A	33 x 92
□ For prediction	33 x 92
□ Second run	33 x 92

Batch project



Specify which datasets to include and in which order to include them.

□ Create a batch level model

Dataset	Size (Var./Obs.)
☑ digester	28 x 14600
□ PRED2831	28 x 1155

□ Create partial models for each phase

The Workset dialog is organized in tabs, each holding a page. Clicking through the tabs opens the desired pages to change the attributes of the observations or variables. The available tabs are Select data, Overview, Variables, Observations, Batch, Transform, Lag, Expand, Scale, and Spreadsheet. A description of each page follows later in this section.

Note: The list on each of the Workset dialog pages can be copied by selecting the items to copy and then pressing CTRL+C.

The first subsections describe features available on all or close to all pages. These features are:

- **Model type** box - described in the Model types in the Workset dialog subsection next.
- **Find** feature - described in the Find feature in workset dialog subsection. Available on all pages but the Select data, Overview and Spreadsheet pages.
- **As model** box - described in the As model subsection. Available on all pages but the Batch, Scale, and Spreadsheet pages.
- **Create partial models** check box - described in the Partial models for batch level subsection. Available for batch level models only.

The workset wizard, available for regular project, is described in the Simple mode workset wizard section later in this chapter.

Note: Pressing ENTER or clicking **OK**, at any time, exits the workset. To continue defining the workset dialog, click another tab.

Note: *When marking a variable in one page, it remains marked in all pages when clicking another tab.*

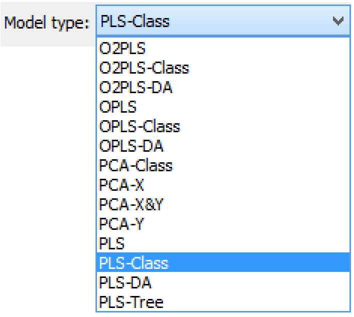
7.2.9.1 Model type in the Workset dialog

The default model type depends on the workset specifications.

Click the **Model type** box to change the model type.

7.2.9.1.1 Available model types in the Workset dialog

The possible model types, in the **Model type** box, are: **O2PLS**, **O2PLS-class**, **O2PLS-DA**, **O2PLS-hierarchical**, **OPLS**, **OPLS-class**, **OPLS-DA**, **OPLS-hierarchical**, **PCA-class**, **PCA-hierarchical**, **PCA-X**, **PCA-X&Y**, **PCA-Y**, **PLS**, **PLS-class**, **PLS-hierarchical**, **PLS-DA** and **PLS-Tree**.



Model type: PLS-Class

7.2.9.1.2 Default model type

The default model type is set as follows:

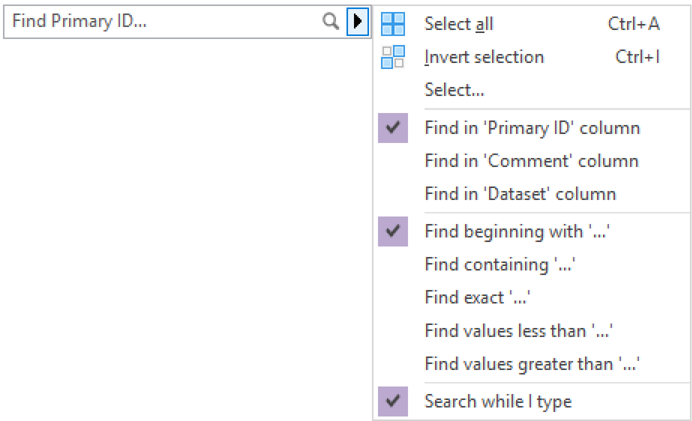
- **PLS** if there are continuous y-variables.
- **PLS-class** if there are continuous y-variables and observation classes defined.
- **PLS-DA** if there is one qualitative y-variable.
- **PLS-DA** if there are no y-variables and 6 or less classes.
- **PCA-class** if there are no y-variables and more than 6 classes.
- **PCA** if there are no y-variables and no classes.
- **PLS-hierarchical** if variables have been assigned to blocks and there are y-variables.
- **PCA-hierarchical** if variables have been assigned to blocks and there are no y-variables.

Note: The previously selected model type is default in new worksets with the same workset specification.

7.2.9.2 Find feature in workset dialog

The **Find** feature is available in all of the pages but the Select data, Overview and Spreadsheet pages of the Workset dialog, although with some variations.

There are two types of Find available from the arrow: searching independent of the Find field and the searching according to the entry in the **Find** field.

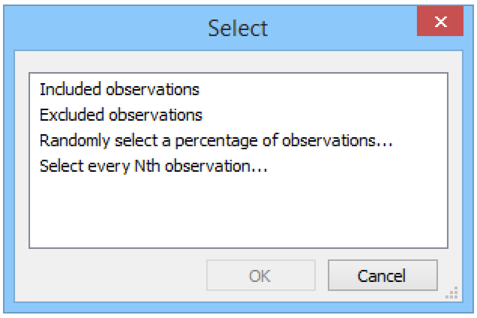


7.2.9.2.1 Select all, Complement selection, Select

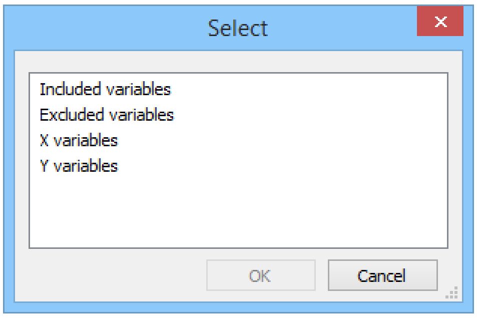
The first find options are independent of the **Find** field:

- **Select all** (CTRL+A) marks all items in the list.
- **Invert selection** (CTRL+I) marks all unmarked items and deselects the previously marked.
- **Select** opens a dialog with context sensitive options. Available in the **Variables** and **Observations** pages.

For observations:


Select
Included observations
Excluded observations
Randomly select a percentage of observations...
Select every Nth observation...
OK
Cancel

For variables



7.2.9.2.2 Find in column

The result from using **Find** starting with 'Find' depends on what is entered in the **Find** field.

In the first section all IDs are displayed, and for the **Transform** and **Scale** pages also the displayed statistics. Default is to **Find in ‘Primary ID’ column**.

The second section defines how the search is done: **Find beginning with**, **Find containing**, **Find exact**, **Find values less than**, and **Find values greater than**. Default is **Find beginning with**.

Note: In the Transform and Scale pages the Find utility can search in the statistics columns too.

7.2.9.2.3 **Find** while typing

When **Search while I type** is selected, the selection according to the current search string is continuously updated.

7.2.9.2.4 **Find** field

When typing in the **Find** field, the search is done according to the current settings, viewed by clicking the arrow.

Wild card symbols **'?'**, and **'*'** are allowed in specifying observations or variables IDs. For example “?LH*” selects observations or variables with IDs such as SLH2 or QLHSW, etc.

Note: *The Find utility in SIMCA is cASe inSensiTiVE.*

7.2.9.3 As model

The **As model** box is available on the Select data, Overview, Variables, Observations, Transform, Lag, and Expand pages. They allow selection of the same settings as another model according to the table:

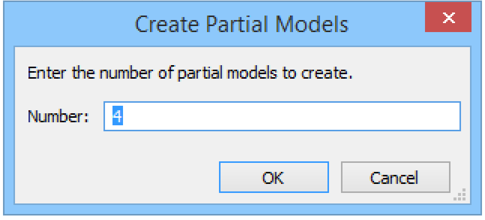
Page	Settings copied
Select data	Dataset selection.
Overview	Variable settings according to **Variables**, **Transform**, **Lag**, and **Expand** below. Observation settings according to **Observations** below.
Variables	Variables and roles as the selected model.
Observations	Observations with the same class structure as specified in the selected model.
Transform	The same transformations for the same variables as the selected model.
Lag	Lag structure of the selected model.
Expand	Expanded terms as in the selected model.

7.2.9.4 Partial models for batch level

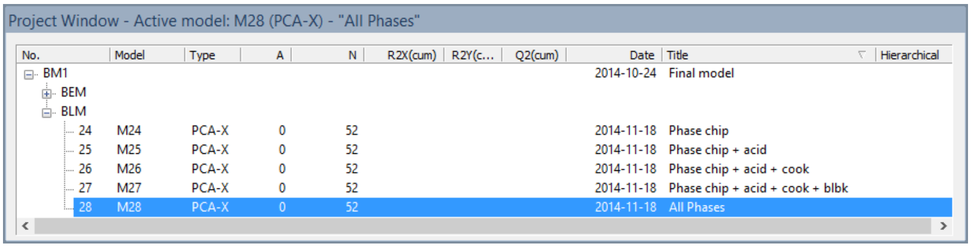
For batch level datasets, partial models can be generated to predict the quality of the batch, or classify the batch before completion, by selecting the **Create partial models…** check box found at the bottom of the **Workset** dialog.

☑ Create partial models for each phase

There are two types of partial models, one according to phases and one according to completion:

Steps	Description with and without phases
1. Select the **Create partial models...** check box in the **Workset** dialog.	**With phases** The check box just becomes selected.
	Without phases SIMCA opens the following dialog:  Create Partial Models Enter the number of partial models to create. Number: 4 In the **Number** field, type the number of partial models to create after Number. The variables are then parted according to maturity. Click **OK**.
2. Click **OK** to exit the **Workset** dialog.	**With phases** Automatically fits the models. The partial models are built sequentially from the phases.
	Without phases Automatically fits the models. The partial models are built from percent completion.
	With phases

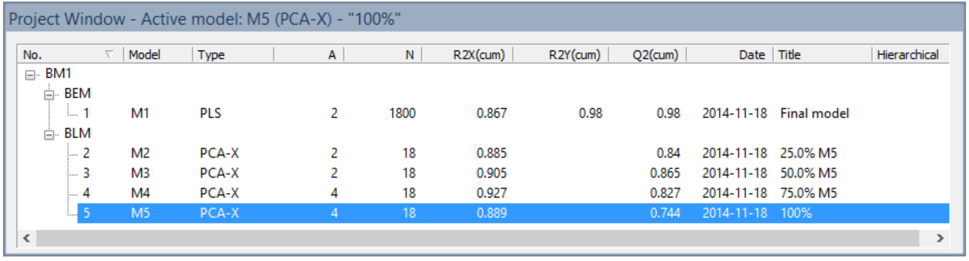
Steps	Description with and without phases
3. View the result.	



Project Window - Active model: M28 (PCA-X) - "All Phases"

No.	Model	Type	A	N	R2X(cum)	R2Y(c...	Q2(cum)	Date	Title	Hierarchical
⊟ BM1								2014-10-24	Final model	
⊞ BEM										
⊟ BLM										
24	M24	PCA-X	0	52				2014-11-18	Phase chip	
25	M25	PCA-X	0	52				2014-11-18	Phase chip + acid	
26	M26	PCA-X	0	52				2014-11-18	Phase chip + acid + cook	
27	M27	PCA-X	0	52				2014-11-18	Phase chip + acid + cook + blbk	
28	M28	PCA-X	0	52				2014-11-18	All Phases	

Without phases



Project Window - Active model: M5 (PCA-X) - "100%"

No.	Model	Type	A	N	R2X(cum)	R2Y(cum)	Q2(cum)	Date	Title	Hierarchical
⊟ BM1										
⊟ BEM										
1	M1	PLS	2	1800	0.867	0.98	0.98	2014-11-18	Final model	
⊟ BLM										
2	M2	PCA-X	2	18	0.885		0.84	2014-11-18	25.0% M5	
3	M3	PCA-X	2	18	0.905		0.865	2014-11-18	50.0% M5	
4	M4	PCA-X	4	18	0.927		0.827	2014-11-18	75.0% M5	
5	M5	PCA-X	4	18	0.889		0.744	2014-11-18	100%	

7.2.9.5 Select data page

The **Select data** page is available when there are more than one dataset available in the project.

The Select data page lists all datasets in the project for regular projects. For batch all batch evolution datasets are listed when the **Create a batch level model** check box is cleared and all batch level datasets are listed when the **Create a batch level model** check box is selected. When the **Create a batch level model** check box is selected, and one of the selected phase datasets has phase iterations, the Phase iteration options may be specified.

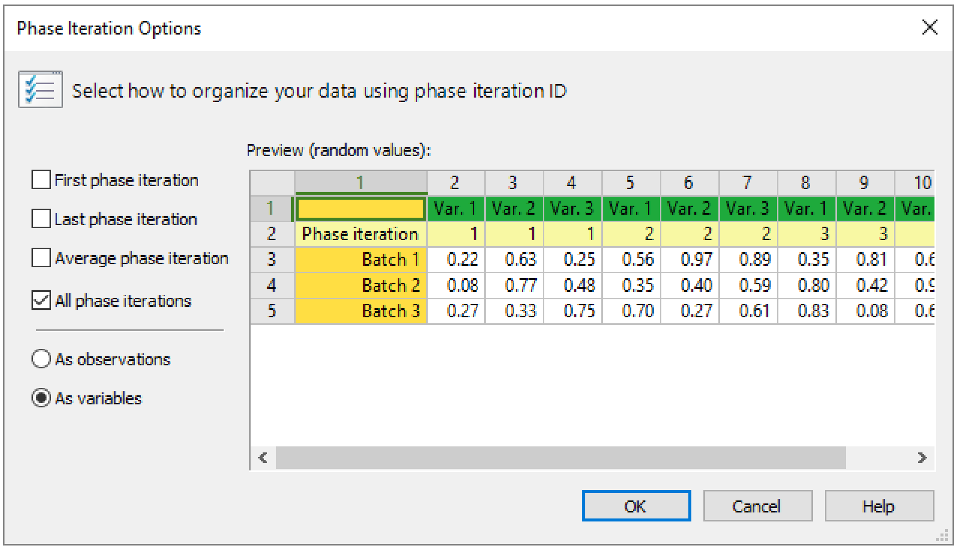
For each dataset the size dimensions are displayed in the Size (Var./Obs.) column.

When selecting more than one dataset, the datasets are merged by primary ID in the workset. The *Primary ID match* percentage is updated to indicate how well the primary IDs in the selected datasets correspond.

To see how the merged datasets will be arranged during the calculations, click the **Spreadsheet** tab. Select **workset as raw data** in the **View** box if you want to view the data in original units.

7.2.9.6 Phase iteration options

For batch level datasets, where phase iterations were specified for one or more phases, the desired organization of the data can be specified in order to support your investigation. The default is to arrange data such that the phase iterations show up **As variables**, with a variable ID named Phase iteration, that displays from which phase iteration the data originates.



Phase Iteration Options

Select how to organize your data using phase iteration ID

□ First phase iteration
□ Last phase iteration
□ Average phase iteration
☑ All phase iterations

○ As observations
● As variables

Preview (random values):

	1	2	3	4	5	6	7	8	9	10
1		Var. 1	Var. 2	Var. 3	Var. 1	Var. 2	Var. 3	Var. 1	Var. 2	Var.
2	Phase iteration	1	1	1	2	2	2	3	3	
3	Batch 1	0.22	0.63	0.25	0.56	0.97	0.89	0.35	0.81	0.6
4	Batch 2	0.08	0.77	0.48	0.35	0.40	0.59	0.80	0.42	0.9
5	Batch 3	0.27	0.33	0.75	0.70	0.27	0.61	0.83	0.08	0.6

7.2.9.6.1 First phase iteration

With **First phase iteration** selected, the data from the first phase iteration is included in the batch level model. This means that when using the batch level model in SIMCA-online, SIMCA-online displays only predictions for the first phase iteration, however many are imported.

7.2.9.6.2 Last phase iteration

With **Last phase iteration** selected, the data from the last phase iteration is included in the batch level model. This means that when using the batch level model in SIMCA-online, SIMCA-online displays the batch at batch level only after the batch has ended.

7.2.9.6.3 Average phase iteration

With **Average phase iteration** selected, the average over all phase iterations calculated and used in the batch level model. This means that when using the model in SIMCA-online, SIMCA-online displays the batch at batch level only after the batch has ended.

7.2.9.6.4 All phase iterations

With **All phase iterations** selected, all phase iterations are included in the batch level model. This means that when using the batch level model in SIMCA-online, SIMCA-online display predictions each of the phase iterations up until as many as the workset has. See also the Predictions subsection next.

7.2.9.6.5 Predictions for batch level models

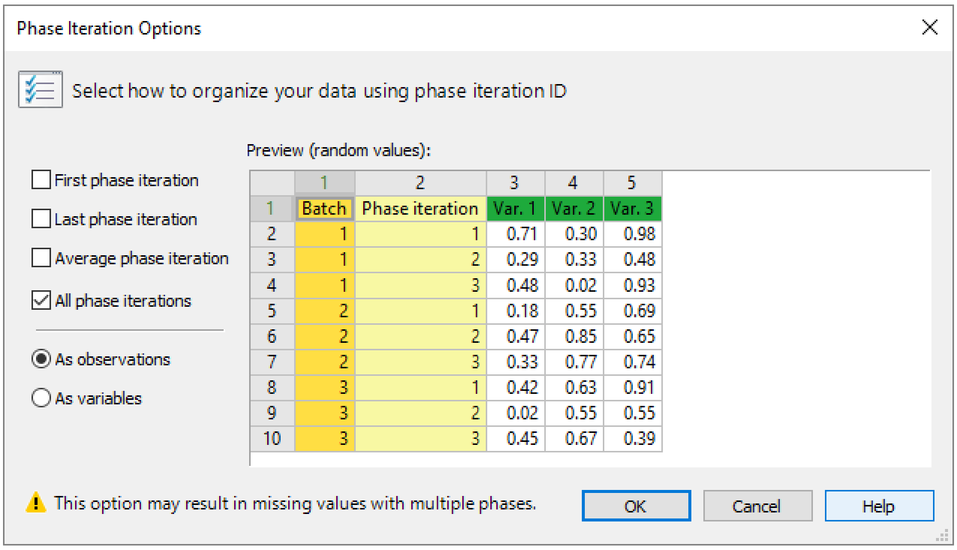
The prediction datasets are created using the phase iteration options specified for the batch level model. However, with **All phase iterations** selected, only the number of phase iterations available in the workset will be predicted, additional phase iterations will be ignored. This means for example that if there are two phase iterations in your batch level model for a specific phase, and the predictionset for that phase includes three iterations, the last phase iteration will not be used in the predictions in this case.

7.2.9.6.6 Special case for batch level model using All phase iterations As variables

Batches with fewer phase iterations than the batch with the most phase iterations in that phase, are filled up with the average of the phase iterations from the same batch and phase, when modeling and predicting. This means that for a batch with only one phase iteration, the data is repeated for as many phase iterations as the longest batch in that phase.

7.2.9.6.7 Batch level model using All phase iterations As observations

When you want to compare phase iterations within a phase, you can select to arrange your batch level data such that each batch and phase iteration in combination make up a row. This means that for each batch there are as many rows as there are phase iterations.


Phase Iteration Options

Select how to organize your data using phase iteration ID

□ First phase iteration
□ Last phase iteration
□ Average phase iteration
☑ All phase iterations

● As observations
○ As variables

Preview (random values):

	1	2	3	4	5
1	Batch	Phase iteration	Var. 1	Var. 2	Var. 3
2	1	1	0.71	0.30	0.98
3	1	2	0.29	0.33	0.48
4	1	3	0.48	0.02	0.93
5	2	1	0.18	0.55	0.69
6	2	2	0.47	0.85	0.65
7	2	3	0.33	0.77	0.74
8	3	1	0.42	0.63	0.91
9	3	2	0.02	0.55	0.55
10	3	3	0.45	0.67	0.39

⚠ This option may result in missing values with multiple phases.

7.2.9.7 Overview page

The **Overview** page displays the variables and observation lists with their respective attributes.

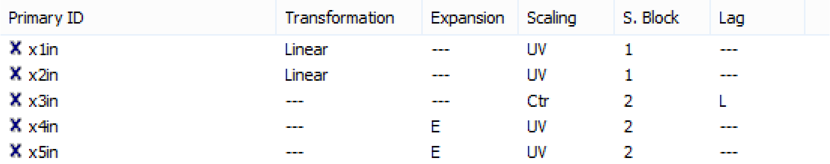
Available from the **Overview** page are:

- The variable list displaying the current role of each variable, X or Y, primary variable ID, transformations, expansions, scaling, scaling block, and lags.
- The observation list displaying primary observation ID and when available, Class IDs, Batch IDs, and Phase IDs.
- Shortcut menu both in the variable and observation lists with the same commands as in the **Variables** and **Observations** pages. For more, see the Variables page and Observations page subsections later in this chapter.
- **Missing value tolerance** – to specify accepted percentage of missing in variables and observations, and checking missing values.
- **As model** – for assigning X and Y etc. as another model. See the As model subsection, previously in this chapter for more.
- **Use simple mode** - see the Simple mode workset wizard subsection later in this chapter.

7.2.9.7.1 Variable list

The top part of the **Overview** page displays summarized variable information:

- **Variables**: Number of included variables in the workset, X and Y.
- **Expanded terms**: Number of expanded terms in the **Expand** page.
- **Lags**: Number of lags defined on the **Lag** page.



Primary ID	Transformation	Expansion	Scaling	S. Block	Lag
X x1in	Linear	---	UV	1	---
X x2in	Linear	---	UV	1	---
X x3in	---	---	Ctr	2	L
X x4in	---	E	UV	2	---
X x5in	---	E	UV	2	---

In the variable list, the X variables are listed first and Y variables last, and with the following information:

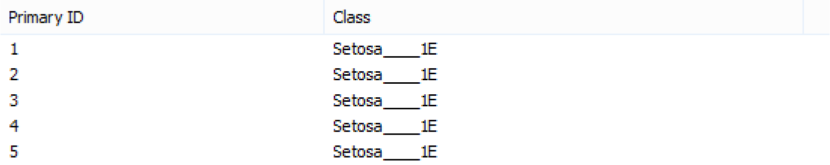
1. Variable role displayed as an X or a Y to left of the variable ID.
2. Primary Variable ID under **Primary ID**.
3. Defined transformations under **Transformation**.
4. **E** under **Expansion** indicates that the variable is expanded with cross, square, or cubic terms.
5. Type of scaling under **Scaling**.
6. Scaling block number, if the variable is part of block scaling under **S. Block**.
7. **L** indicating that the variable is lagged under **Lag**.

Lags and expansions appear at the bottom of the list.

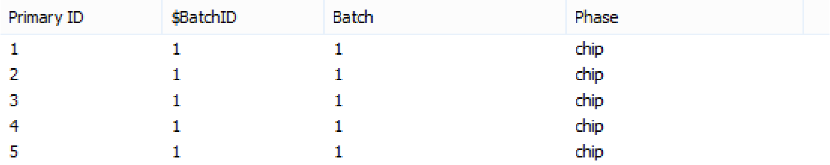
7.2.9.7.2 Observation list

Above the observation list the number of observations included is displayed.

The observation list holds the observation primary ID and class belonging, or for batch projects batch, and when available, phase IDs.



Primary ID	Class
1	Setosa____1E
2	Setosa____1E
3	Setosa____1E
4	Setosa____1E
5	Setosa____1E



Primary ID	$BatchID	Batch	Phase
1	1	1	chip
2	1	1	chip
3	1	1	chip
4	1	1	chip
5	1	1	chip

1. Primary Observation ID under **Primary ID**.
2. Class of the observations under **Class**, if the observations are grouped in classes.
3. Batch and phase IDs under **Batch** and **Phase** for batch projects.

7.2.9.7.3 Missing value tolerance

For the results of model fitting to be reliable, the workset should contain less than 50% missing values in observations or variables. This is the SIMCA default threshold for missing values for the workset and for predictions.

The **Missing value tolerance** section is positioned at the bottom of the **Overview** page. It contains the default missing value tolerance for **Variables** and **Observations** and a **Check missing values** button.

Missing values percentage exceeding tolerance

When clicking **Check missing values**, or **OK**, the observations and variables missing values percentage is checked versus the tolerance limits. When the missing values percentage of a variable or observation exceeds the specified tolerance limit, SIMCA prompts for including or excluding the variable or observation.

Changing the missing value tolerance limit

Change the tolerance limit displayed in the window of the workset by typing a new value in the **Variable** or **Observation** field. The new tolerance limit will only apply to the model generated by the current workset.

To change the tolerance limit of missing values for new worksets and models, see the Project options section in Chapter 5, File.

Variables with zero variance

Variables are also checked for zero variance when clicking **Check missing values** or **OK**. SIMCA issues a message for including or excluding the variable with zero variance. When selecting to include such a variable it is given scaling weight 1.

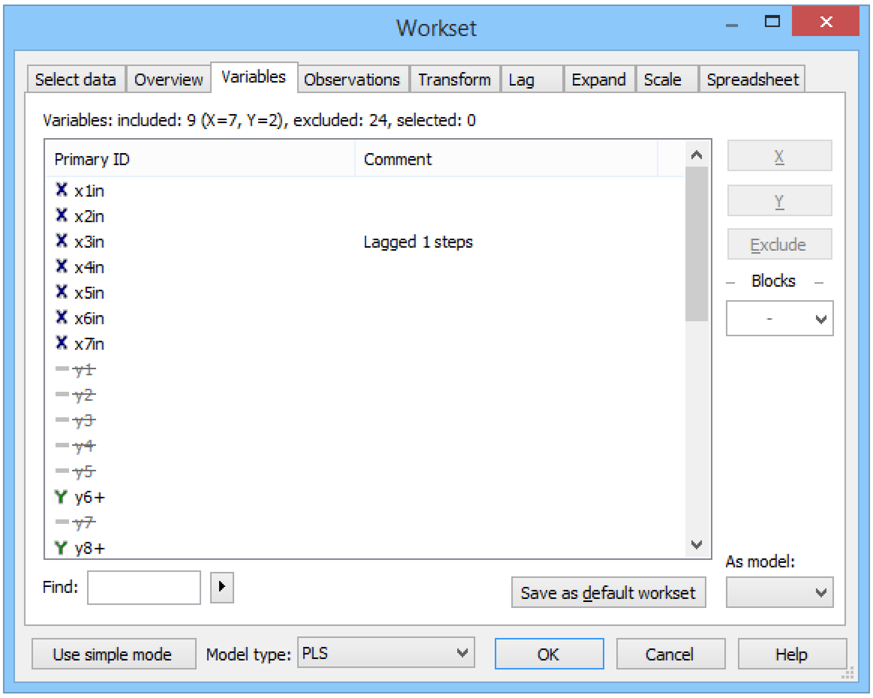
7.2.9.8 Variables page

Use the **Variables** page, to view and configure the roles of the variables.

Available from the Variables page are:

1. Summary row listing Variables:
   - **Included -** Number of variables included in the workset, number of variables defined as **X**, number of variables defined as **Y**.
   - **Excluded** - Number of excluded variables.
   - **Selected -** Number of currently selected variables in the dialog.
2. Variable list displaying the current role of each variable (X, Y, or -), primary variable ID, a **Comment** column, and a **Dataset** column when more than one dataset was selected in the **Select data** page.
3. Shortcut menu for selecting which variable IDs to display, **Switch X & Y**, and commonly used commands. For more about Switch X & Y, see the Switch X & Y subsection in the Change Model Type section later in this chapter.
4. **X** – for assigning variables to the X-block.
5. **Y** – for assigning variables to the Y-block.
6. **Exclude** – for excluding variables.
7. **Class** – for assigning variables to the classes specified in the Observations page.
8. **Blocks** – for assigning variables to blocks for hierarchical modeling.
9. **Phases** - for assigning variables to phases (batch evolution model only).
10. **Configure -** for configuring the y-variable for the batch evolution model.
11. **Find** – for finding variables. For more see the Find feature in Workset page subsection previously in this chapter.
12. **Save as default workset** – for saving the current specification as default workset.

13. **As model** – for assigning X and Y and excluding variables as another model. See the As model subsection, previously in this chapter for more.



Variables: included: 9 (X=7, Y=2), excluded: 24, selected: 0

Primary ID	Comment
X x1in	
X x2in	
X x3in	Lagged 1 steps
X x4in	
X x5in	
X x6in	
X x7in	
— ~~y1~~	
— ~~y2~~	
— ~~y3~~	
— ~~y4~~	
— ~~y5~~	
Y y6+	
— ~~y7~~	
Y y8+	

Model type: PLS

7.2.9.8.1 Selecting roles by specifying X and Y

To change the variable roles:

1. Select the variables.
2. Click the desired button **X**, **Y**, or **Exclude**. The list is updated accordingly.

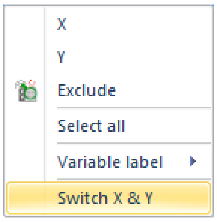
Note: Fitting a PLS, OPLS or O2PLS model with one qualitative Y is equivalent to fitting a PLS-DA, OPLS-DA or O2PLS-DA model with classes defined according to the qualitative variable.

7.2.9.8.2 Switch X & Y for O2PLS

Since O2PLS is bidirectional, it does not matter which variables are defined as X and which are defined as Y. But, in the model window the statistics are displayed in one direction.

To view the statistics for the other direction:

1. Click **New as | Mxx** and select the O2PLS-model.
2. On the **Variables** page, right-click and select **Switch X & Y**. Note that all variables previously defined as X are now defined as Y and vice versa.
3. Click **OK** and fit the new O2PLS-model.



7.2.9.8.3 Assigning variables to classes

When observations have been grouped in classes, by default all the X and Y variables belong to all the classes.

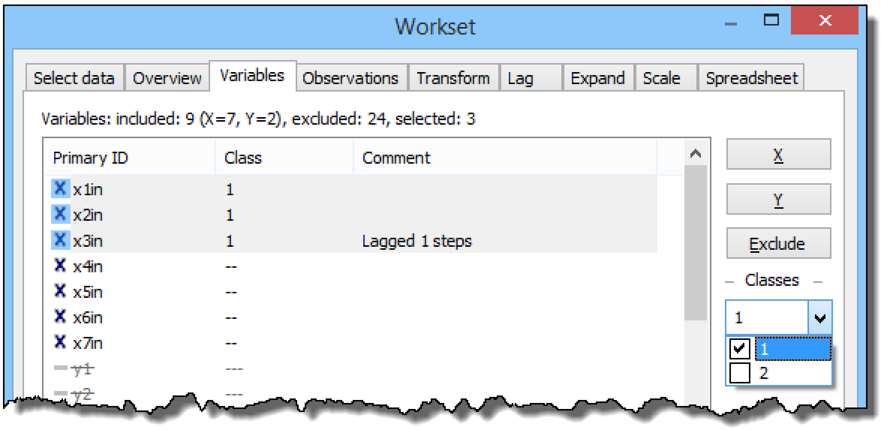
To assign variables to specific classes:

1. Mark the variables.

2. Select the class in the **Classes** box.

The class number is displayed near the variable in the **Class** column.

Note: -- in the Class column means that the variable is included for all classes.



Variables: included: 9 (X=7, Y=2), excluded: 24, selected: 3

Primary ID	Class	Comment
X x1in	1	
X x2in	1	
X x3in	1	Lagged 1 steps
X x4in	--	
X x5in	--	
X x6in	--	
X x7in	--	
~~y1~~	---	
~~y2~~	---	

Classes: 1
☑ 1
□ 2

7.2.9.8.4 Assigning variables to blocks resulting in hierarchical models

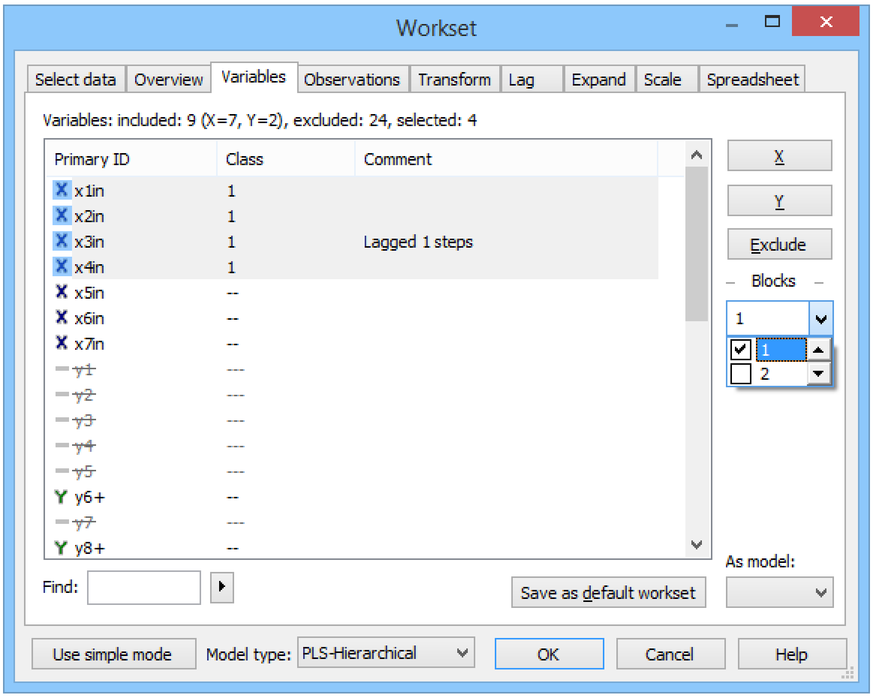
Variables can be assigned to variable blocks using the **Blocks** box.

To assign variables to blocks:

1. Mark the variables.
2. Select the block number from the **Blocks** box. After selecting the first block, the Blocks list is incremented to include the next block number.

The block number is displayed near the variable under the column **Class**.

After defining the blocks the additional model types **PCA-Hierarchical**, and if y-variables were specified, **PLS-Hierarchical**, **OPLS-Hierarchical**, and **O2PLS-Hierarchical** are available. For more, see the Model type in the Workset dialog subsection earlier in this section.



Variables: included: 9 (X=7, Y=2), excluded: 24, selected: 4

Primary ID	Class	Comment
X x1in	1	
X x2in	1	
X x3in	1	Lagged 1 steps
X x4in	1	
X x5in	--	
X x6in	--	
X x7in	--	
~~y1~~	---	
~~y2~~	---	
~~y3~~	---	
~~y4~~	---	
~~y5~~	---	
Y y6+	--	
~~y7~~	---	
Y y8+	--	

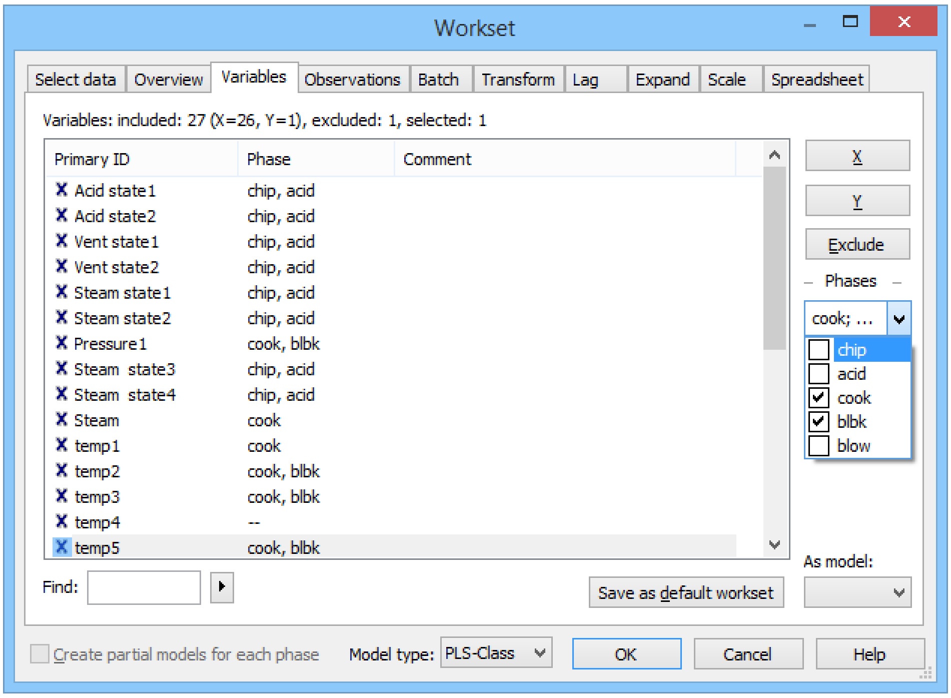
Blocks: 1
☑ 1
□ 2

Find:

Model type: PLS-Hierarchical

7.2.9.8.5 Assigning variables to phases

When batches have phases, by default the X and Y variables belong to the phases as specified at import.



Variables: included: 27 (X=26, Y=1), excluded: 1, selected: 1

Primary ID	Phase	Comment
X Acid state1	chip, acid	
X Acid state2	chip, acid	
X Vent state1	chip, acid	
X Vent state2	chip, acid	
X Steam state1	chip, acid	
X Steam state2	chip, acid	
X Pressure1	cook, blbk	
X Steam state3	chip, acid	
X Steam state4	chip, acid	
X Steam	cook	
X temp1	cook	
X temp2	cook, blbk	
X temp3	cook, blbk	
X temp4	--	
X temp5	cook, blbk	

Phases: cook; ...
□ chip
□ acid
☑ cook
☑ blbk
□ blow

□ Create partial models for each phase

Model type: PLS-Class

Note: -- in the Phase column means that the variable is included for all phases.

To assign a variable to different phases than specified by the default workset:

1. Mark the variable.
2. Select ALL the desired phases using the phase check boxes in the **Phases** box.

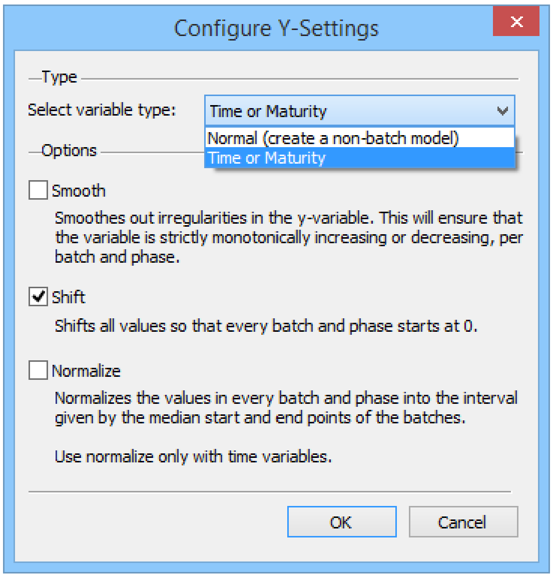
Hint: Do NOT mark all variables that belong to a certain phase and select the phase. Making another selection overlapping with the first will replace the first phase setting for the intersection variables.

7.2.9.8.6 Configuring y-variables

In a batch evolution model, the y-variable is a time or maturity variable. This time or maturity variable can be configured differently depending on batch and y-variable properties:

- **Smooth** - Smooth out noise in a maturity variable so that it is strictly monotonically increasing or decreasing.
- **Shift** - Shifts batches and phases to always start at 0.
- **Normalize** - Batches are time normalized within each phase, giving all batches in a model identical length.

To configure the y-variable, select it and click **Configure** under **Y-settings**. The following dialog opens:



Configure Y-Settings

Type

Select variable type: Time or Maturity

Normal (create a non-batch model)

Time or Maturity

Options

□ Smooth

Smoothes out irregularities in the y-variable. This will ensure that the variable is strictly monotonically increasing or decreasing, per batch and phase.

☑ Shift

Shifts all values so that every batch and phase starts at 0.

□ Normalize

Normalizes the values in every batch and phase into the interval given by the median start and end points of the batches.

Use normalize only with time variables.

Note: If the model should be used for on-line, NEVER select the **Normalize** check box in the **Configure Y-Settings** dialog.

Selecting variable type

When selecting to create a batch project, the y-variable type is **Time or maturity**.

In the case where the project has batches but you want to just fit regular PLS models, with Y not being time or maturity, select **Normal (create a non-batch project)** in the **Select variable type** box.

Selecting variable options

A combination or none of the three available options may be used for configuring y. In cases where a y-variable relating to Batch age, starting at 0 at batch start, is available no further y configuration is necessary. General recommendations for use of the three options are described in the table.

Option	Description	Technical details	Use	Do not use
Smooth	Smooths out irregularities in the y variable. This will ensure that the variable is strictly monotonically increasing or decreasing, per batch and phase.	Smoothing by fitting a constrained quadratic polynomial, using a piece wise least squares algorithm.	When the y-variable is a maturity.	When the y-variable is time.
Shift	Shifts all values so that every batch and phase starts at 0.	Shifting by subtracting the start value of each batch from all values.	Default setting, few exceptions.	When there is missing data at beginning of batches and the y variable is Batch age.
Normalize	Normalizes all batches to the same length. The y-values in every batch and phase are normalized into the interval given by the median start and endpoints of the batches.	Normalizing by applying a linear time warping function.	Rarely, when batch end is chemically or biologically driven.	For online monitoring models.

7.2.9.8.7 Save as default workset

To change the default workset roles of the variables, from what was specified at import, specify the X, Y or excluded as desired and click **Save as default workset**. This specification defines the default workset when clicking **New** in the **Workset** group on the **Home** tab.

Clicking **Save as default workset** saves the properties of the page. When clicked on the Select data tab, the datasets selected are saved, when clicked on the Variables tab the excluded and y-variables are saved.

Deleting a dataset or variable included in the default workset results in a default workset using the other included datasets and variables.

For more about specifying the default workset, see the Default workset subsection earlier in this chapter.

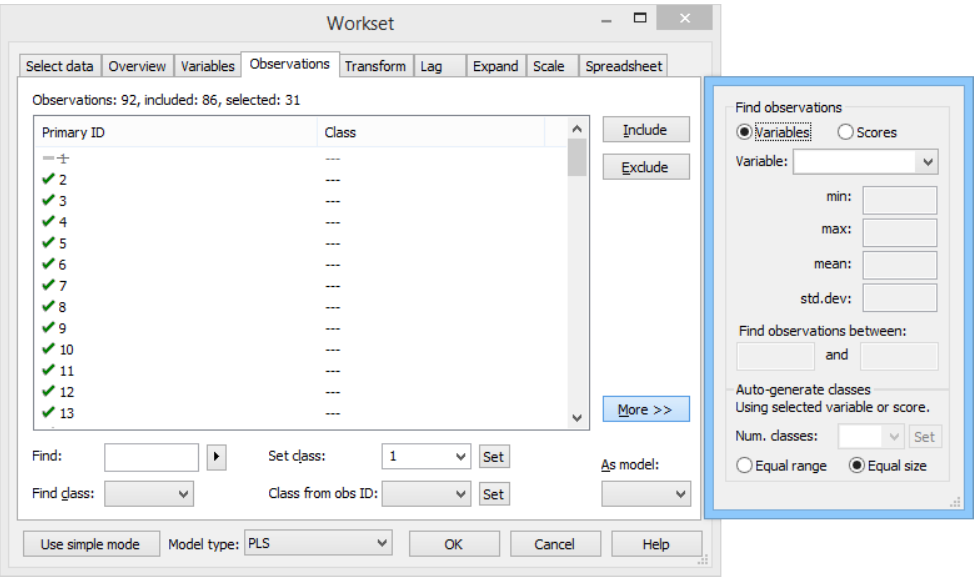
7.2.9.9 Observations page

The **Observations** page displays all observations for the current workset and is used for including and excluding observations and grouping observations in classes.

Available from the **Observations** page are:

1. Summary row listing:
   - **Observations**: Total number of observations in the project, both included and excluded.
   - **Included**: Number of included observations.
   - **Selected**: Number of currently selected observations in the dialog.
2. Observation list displaying ✓ for included and − for excluded observations, primary observation IDs, class number or name under **Class**, and for batch projects **Batch** and **Phase** numbers under the respective headers.
3. Shortcut menu – for selecting which observation IDs to display and the commands **Include**, **Exclude**, **Set class**, and **Select all**.
4. **Include** – for including excluded observations.
5. **Exclude** – for excluding included observations.
6. **Find** – for finding observations. For more see the Find feature in workset dialog subsection previously in this chapter.
7. **Find class** – for finding observations already assigned to a specific class.
8. **Set class** – for assigning observations to a class number or entered name.
9. **Class from obs ID** – for assigning classes from an available observation identifier.
10. **More** – for creating classes from variable or score values. For more, see the Creating classes from variables or scores values subsection later in this section.
11. **As model** – for including, excluding, and assigning classes according to an existing model. For more, see the As model subsection previously in this chapter.

Note: The observations have to be included to be assigned to and part of a class.



Observations: 92, included: 86, selected: 31

Primary ID	Class
− 1	---
✓ 2	---
✓ 3	---
✓ 4	---
✓ 5	---
✓ 6	---
✓ 7	---
✓ 8	---
✓ 9	---
✓ 10	---
✓ 11	---
✓ 12	---
✓ 13	---

Set class: 1

Model type: PLS

Find observations: ● Variables ○ Scores

Auto-generate classes
Using selected variable or score.

○ Equal range ● Equal size

7.2.9.9.1 Including and excluding observations

To include or exclude observations:

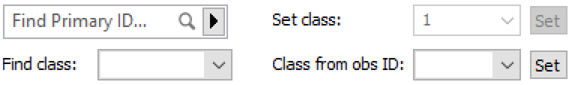
1. Select the observations.
2. Click **Include** or **Exclude**.

For more about including and excluding observations, see the Excluding marked items subsection in the Marked Items tab section in Chapter 14, Plot and list contextual tabs.

7.2.9.9.2 Grouping observations in classes using Set class

To group observations in classes using **Set class**:

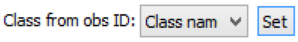
1. Select the observations by marking or by using **Find**.
2. Specify the class by using either of the following methods:
   - Clicking the **Set** button found after the **Set class** field. The class number is automatically incremented.
   - Typing the class name in the **Set class** field and clicking **Set**.
   - Selecting an observation ID in the **Class from obs ID** and clicking **Set**.



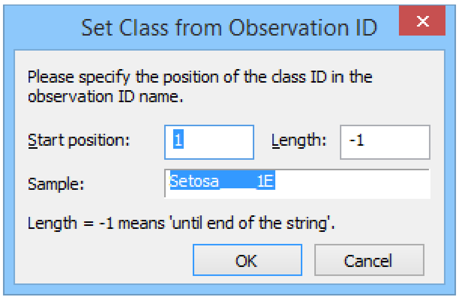
7.2.9.9.3 Automatic creation of classes from Observation ID

To automatically create classes from observations ID, primary or secondary:

1. Select the observation ID in the **Class from obs ID** box and click **Set**.



2. In the **Set Class from Observation ID** dialog, enter the starting position and length of the string (number of characters) to be used for the creation of classes.



Set Class from Observation ID

Please specify the position of the class ID in the observation ID name.

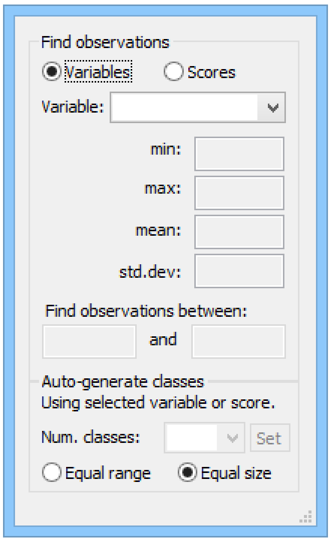
Start position: 1   Length: -1

Sample: Setosa   1E

Length = -1 means 'until end of the string'.

7.2.9.9.4 Creating classes from variables or scores values

To create classes from values of a variable or score vector from an existing model, click the **More** button. The following window opens:



● Variables ○ Scores

○ Equal range ● Equal size

After selecting a variable or a score vector, the **min**, **max**, **mean**, and **std. dev.** fields are automatically updated.

Find observations between section

To search for observations within a given range:

1. Click **Variables** or **Scores**.
2. Select the variable or score in the **Variable** or **Score** box.
3. Under **Find observations between**, type the limits defining the range for the variable or score vector.

To assign the selected observations to a class, use **Set class** arrow and click the **Set** button in the **Observations** page.

Auto-generate classes section

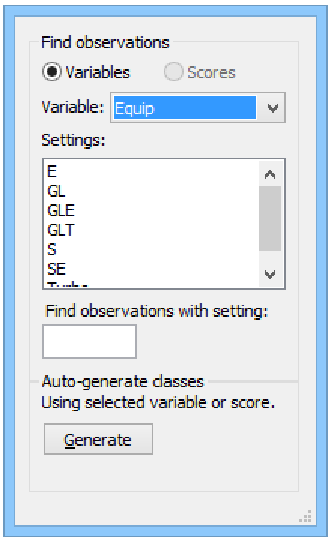
A set of classes can be generated automatically from variable or score values.

To generate classes automatically:

1. Click **Variables** or **Scores**.
2. Select the variable or score in the **Variable** or **Score** box.
3. Select number of classes from the **Num. classes** box.
4. Select **Equal**
    a. **range** – Splitting the range of the selected variable or scores in the desired number of classes. Note that this option may lead to different size classes.
    b. **size** – Splitting the group equally in the desired number of classes, after sorting the variable. Note that this option may lead to observations with identical values ending up in different classes.
5. Click the **Set** button in the **More** window.

Auto-generating classes according to qualitative setting

When selecting a qualitative variable in the **Variable** box, clicking the **Generate**-button automatically creates one class for each qualitative setting.


Find observations

● Variables ○ Scores

Variable: Equip

Settings:

E
GL
GLE
GLT
S
SE

Find observations with setting:

Auto-generate classes
Using selected variable or score.

7.2.9.9.5 Observations page for batch evolution models

For batch evolution models the **Observations** page is stripped of all class setting functionality. This means that observations belonging to one phase cannot be reassigned to a different phase.

The Observation page can be used for viewing the observations, searching for observations using the **More** or **Find** features, and to exclude or include single observations.

To exclude entire phases or batches, or crop the phases, use the Batch page.

7.2.9.10 Batch page

The **Batch** page displays all batches and phases, plus phase iterations if present, and is used for including, excluding, and cropping batches and phases for batch evolution models, BEM. For batch level models, BLM, the tab is there but no functionality is available.

Available from the **Batch** page are:

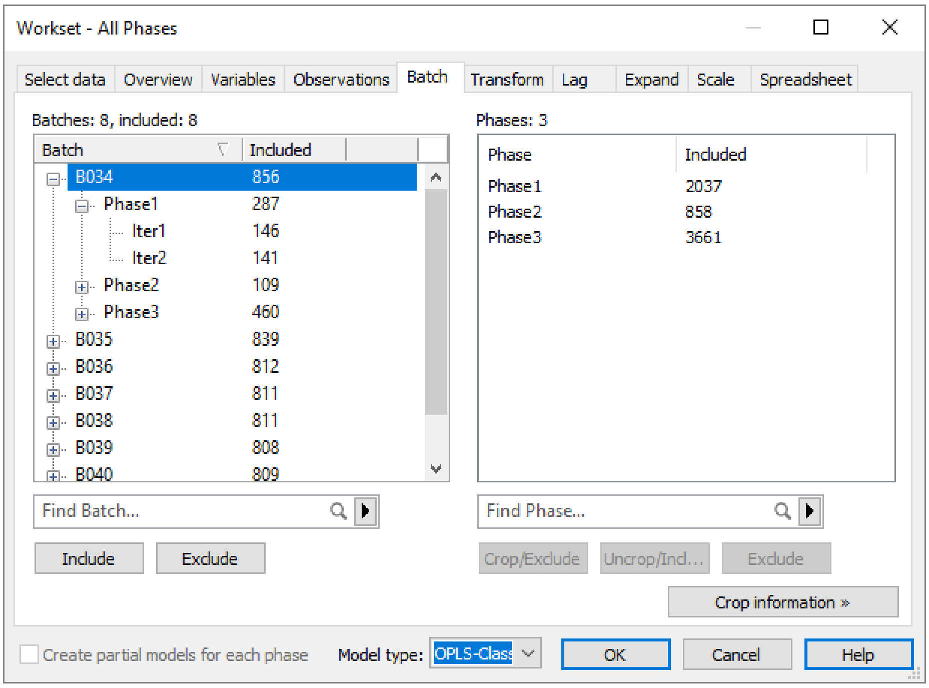
1. Summary row listing:
    - **Batches -** total number of batches in the project.
    - **Included** - Number of included batches in the current workset.
    - **Phases** - Number of phases in the project.
2. Batch and phase lists displaying batches and phases respectively.
    - In the Batch list, each batch displays the phases that batch has passed, and optionally passed phase iterations. The **Included** column displays number of included observations and is updated when that changes. If one or more observations was excluded, this also displays the total number of observations before anything was excluded.
    - In the Phases list, there is a **Status** column which states **Included** for included phases and the number of observations currently included in the phase. This column is updated when phases are cropped or excluded.
3. Shortcut menu with selected commands, also available as buttons.
4. **Find** – for finding batches or phases. For more see the Find feature in workset dialog subsection previously in this chapter.

Under **Batches**

5. **Include** – for including excluded batches, phases in a specific batch, or phase iterations in a specific batch and phase..
6. **Exclude** – for excluding batches, phases in a specific batch, or phase iterations in a specific batch and phase..

Under **Phases**

7. **Crop/Exclude** – for excluding observations phase-wise according to specified criteria.
8. **Uncrop/Include -** for reversing the cropping.
9. **Exclude –** for excluding phases.
10. **Crop information** – for viewing a summary of the performed cropping.



Batches: 8, included: 8

Batch	Included
B034	856
Phase1	287
Iter1	146
Iter2	141
Phase2	109
Phase3	460
B035	839
B036	812
B037	811
B038	811
B039	808
B040	809

Phases: 3

Phase	Included
Phase1	2037
Phase2	858
Phase3	3661

□ Create partial models for each phase

Model type: OPLS-Class

Note: When editing the workset (clicking **Edit** in the **Workset** group) and selecting a phase (class) model, the workset dialog displays only the selected model and the **Batch** page is not available.

7.2.9.10.1 Including and excluding batches

Below the batch list, find **Include** and **Exclude** enabling you to do just that.

To exclude or include a batch:

1. Select the batch in the **Batch** list.
2. Click the **Exclude** or **Include** button. The **Status** column is updated and states *Excluded* for the excluded batches and nothing for the included.

Note: Excluding batches excludes them from all phases.

7.2.9.10.2 Including and excluding entire phases

Below the phase list, find **Uncrop/Incl** and **Exclude** enabling you to include and exclude entire phases.

To exclude a phase:

1. Select the phase in the **Phase** list.
2. Click **Exclude**. The **Status** column is updated and states *Excluded* for the excluded phases.

To include all phases, mark all phases and click **Uncrop/Incl**. The **Status** column is updated and lists the number of observations in the respective phases.

Note: Excluding phase iterations can be done on the Observation page by using Find and the Phase iteration ID.

7.2.9.10.3 Cropping phases

Crop a phase by excluding as specified in the **Crop** dialog.

Note: Batches with no phases are treated as having one single phase and can be cropped in the **Batch** page.

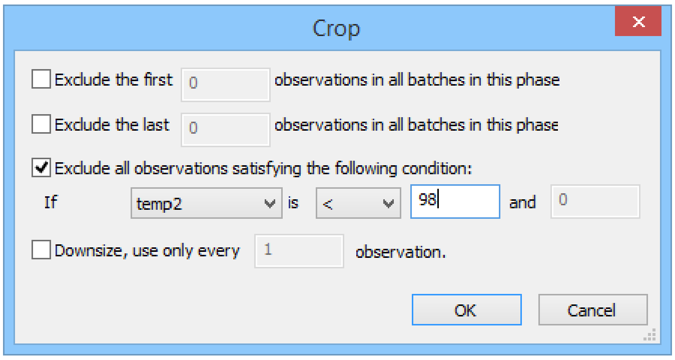
To crop a phase:

1. Select the phase in the **Phase** list.
2. Click the **Crop/Exclude**-button.
3. Specify the desired cropping according to the table.

The different cropping options are described in the table.

	Option	Description	Example and result
1.	Exclude the first x observations in all batches in this phase.	Excludes x observations, starting from the beginning of each batch, in the marked phase.	Entering '3' excludes the 3 first observations in all batches for the marked phase.
2.	Exclude the last x observations in all batches in this phase.	Excludes x observations, starting from the end of each batch, in the marked phase.	Entering '3' excludes the 3 last observations in all batches for the marked phase.
3.	Exclude all observations satisfying the following condition: If variable VAR1 is LOGICAL EXPRESSION VALUE1 and VALUE2.	Excludes the observations satisfying the condition defined by: • The variable. • The logical expression among '<', '>', '<=', '>=', and 'outside'. • The limiting value or for 'outside' values.	If variable 'bottom temp.', is '<', '60' excludes all observations with a value smaller than 60 in variable 'bottom temp.' Note that the result from cropping all phases with this type of cropping can be achieved with trimming too.
4.	Downsize, use only every x observation.	Downsizes the phase to only use every x observations.	Entering '3' excludes 2/3 of the observations in the phase, keeping observation number 1, 4, 7, 10, 13 etc.

Note: The check boxes can be selected independently and all together.



☐ Exclude the first 0 observations in all batches in this phase

☐ Exclude the last 0 observations in all batches in this phase

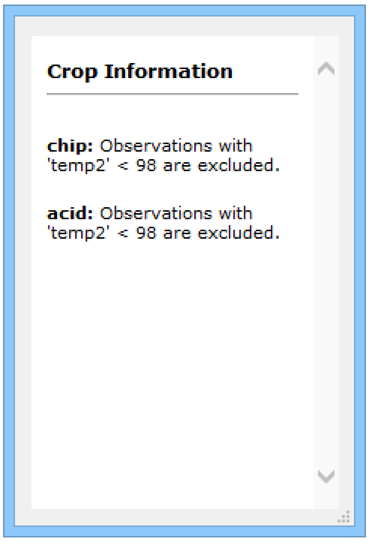
☑ Exclude all observations satisfying the following condition:

If temp2 is < 98 and 0

☐ Downsize, use only every 1 observation.

7.2.9.10.4 Crop information

After cropping, clicking **Crop information** displays a summary of the performed cropping per phase and per cropping. This means that for each time **OK** is clicked with cropping defined, the applied cropping details are displayed per phase in the **Crop information** window.



Crop Information

chip: Observations with 'temp2' < 98 are excluded.

acid: Observations with 'temp2' < 98 are excluded.

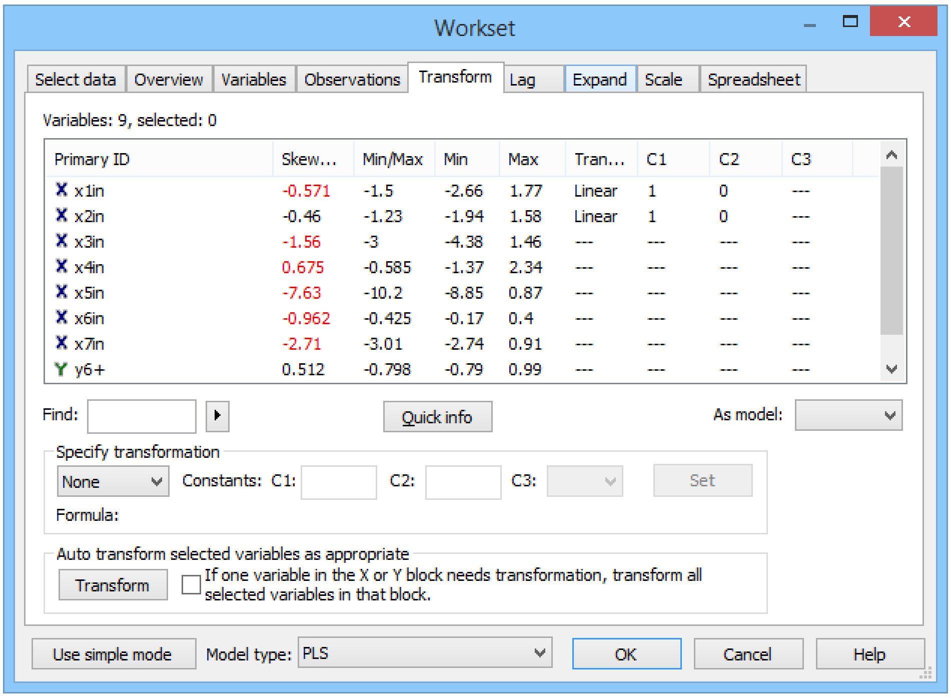
7.2.9.11 Transforming variables

The **Transform** page displays all variables with current transformation and statistics. The Transform page is used to apply transformations to selected variables.

Available from the Transform page are:

1. Summary row listing number of included variables and number of selected variables.
2. Variable list displaying variable role (X or Y), primary variable ID, **Skewness**, **Min/Max**, **Min**, **Max**, **Transform**, and the constants **C1**, **C2**, and **C3**. For more about the **Transform**, **C1**, **C2**, and **C3** columns see the Applying transformations subsection later in this section.
3. Shortcut menu with the commands for selecting which variable labels to display, **Set transform**, **Select all**, and **Quick info**.
4. **Find** – for finding variables. For more see the Find feature in workset dialog subsection previously in this chapter.
5. **Quick info** – for opening the **Quick Info** pane. For more see the Quick info subsection in Chapter 13, View.
6. **As model** – for transforming all variables as transformed in another model. See the As model subsection, previously in this chapter for more.
7. **Specify transformation** – for defining a transformation and applying it to the selected variables.
8. **Auto transform selected variables as appropriate** – to automatically transform the variables in need of logarithmic transformation.

Note: When batch data have phases, transformations of variables can be done for each phase by editing the phase model (edit by marking the phase model and on the **Home** tab, in the **Workset** group, clicking **Edit**).



Variables: 9, selected: 0

Primary ID	Skew…	Min/Max	Min	Max	Tran…	C1	C2	C3
X x1in	-0.571	-1.5	-2.66	1.77	Linear	1	0	---
X x2in	-0.46	-1.23	-1.94	1.58	Linear	1	0	---
X x3in	-1.56	-3	-4.38	1.46	---	---	---	---
X x4in	0.675	-0.585	-1.37	2.34	---	---	---	---
X x5in	-7.63	-10.2	-8.85	0.87	---	---	---	---
X x6in	-0.962	-0.425	-0.17	0.4	---	---	---	---
X x7in	-2.71	-3.01	-2.74	0.91	---	---	---	---
Y y6+	0.512	-0.798	-0.79	0.99	---	---	---	---

Specify transformation

None Constants: C1: C2: C3: Set

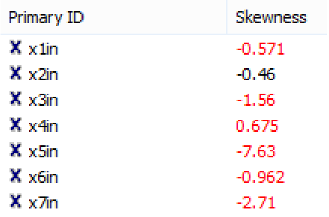
Formula:

Auto transform selected variables as appropriate

Transform ☐ If one variable in the X or Y block needs transformation, transform all selected variables in that block.

7.2.9.11.1 Skewness or Min/Max colored red

When the value in **Min/Max** or **Skewness** is colored in red, a transformation may be desired.



Primary ID	Skewness
X x1in	-0.571
X x2in	-0.46
X x3in	-1.56
X x4in	0.675
X x5in	-7.63
X x6in	-0.962
X x7in	-2.71

For more about the criteria used, see the Transform page criteria section in the Statistical appendix.

7.2.9.11.2 Quick info in Transform page

With the **Quick Info** pane open when applying transformations, the statistics and plots displayed in the **Quick Info** are updated. This enables you to view the before and after plots and statistics immediately.

To open the **Quick Info** pane, click the **Quick info** button.

For more about the **Quick Info** pane, see the Quick Info subsection in Chapter 13, View.

7.2.9.11.3 Applying transformations using Specify transformation

To apply a transformation:

1. Select the variables to transform in the list.
2. Select a transformation in the **Specify transformation** box. Under the selected transformation, the formula of the selected transformation appears to the right of *Formula*. The default values for the constants appear in the **C1**, **C2**, and **C3** fields.
3. Change from the default constants as appropriate.
4. Click **Set**. The columns **Transform**, **C1**, **C2**, and **C3** in the variable list are updated accordingly.
5. Repeat 1 - 4 as needed to transform all the desired variables.

Note: The transformation is applied when clicking **Set**. Clicking **OK** without having clicked **Set** does not apply the selected transformation.

Transformations available

The following transformations are available:

Transformation	Formula	Formula to back transform
None	Default	
Lin	$C_1 * Y + C_2$	$(x - C_2) / C_1$
Log	$Log_{10}(C_1 * Y + C_2)$	$1/C_1 * (b^x - C_2)$
Negative Log	$-Log_{10}(C_2 - C_1 * Y)$	$1/C_1 * (C_2 - b^{-x})$
Exp	$e^{(C1 * Y + C2)}$	$1/C_1 * (ln(x) - C_2)$
Logit	$Log_{10}((Y - C_1)/(C_2 - Y))$	$(10^x * C_2 + C_1) / (10x + 1)$
Power	$(C_1 * Y + C_2)^{C3}$ where $C_3 = [-2, -1, -0.5, -0.25, 0.25, 0.5, 1, 2]$.	$(x^{1/C3} - C_2) / C_1$

7.2.9.11.4 Automatic transformation

Automatic Log transformation according to certain criteria is available by following the steps:

1. Select the desired variables in the variable list.
2. Optionally select the **If one variable in the X or Y block needs transformation, transform all selected variables in that block** check box to have all variables in the same metric. In summary, when the check box is selected all variables are Log transformed if one meets the criteria for automatic transformation.
3. Click **Transform**. The software checks if any of the selected variables need a Log transformation and if so applies it.

The criteria used to decide if a log transform is needed is described in the Transform page criteria section in the Statistical appendix.

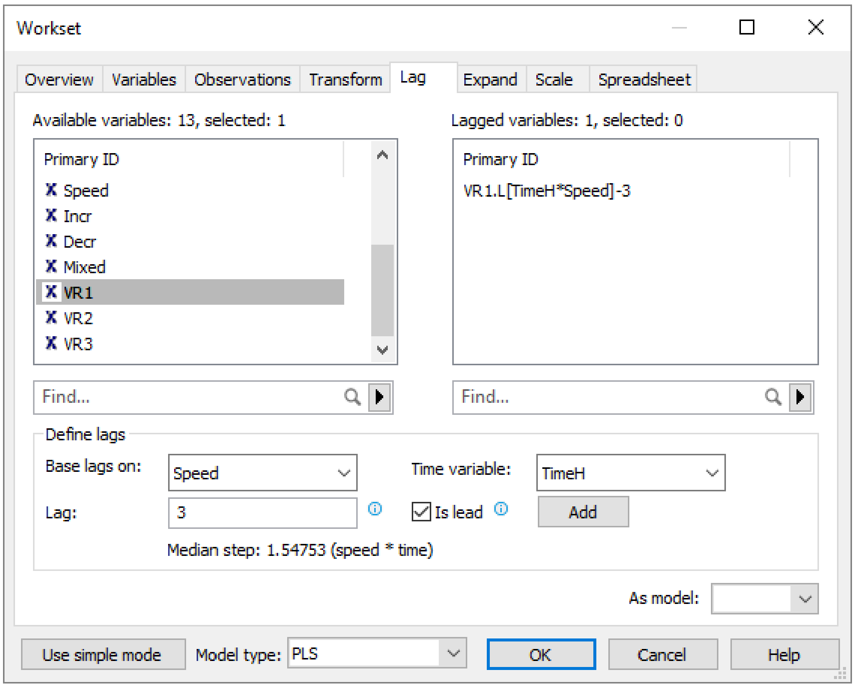
7.2.9.12 Lagging variables

When the X or Y-matrix is expanded with lagged variables, this allows the study of the influence of the process variables at **L** time units earlier in the process at time **t**.

All variables, included or excluded, can be lagged and included in the model.

Available from the **Lag** page are:

1. The lists displaying variable role and primary variable ID for **Available variables** and **Lagged variables**.
2. Shortcut menu with commonly used commands.
3. **Find** – for finding variables. For more, see the Find feature in workset dialog subsection previously in this chapter.
4. The Define lags section that is activated after marking a variable in the Available variables list. The marked variable can then be lagged based on Observation index (a. k. a. steps), Time variables or speed variables. For details about dynamic lags, see the Dynamic lags subsection later in this section.
5. **Lag** – to specify the lag specification. Depending on the selection in Base lags on and optionally Time variable, the format for entering the lag varies.
6. **Is lead** check box – for adding negative lags. Leads are automatically assigned to the Y-block.
7. **Add** to create the specified lag or lead and add it to the Lagged variables list.
8. **As model** – for adding lagged variables as in another model. For more, see the As model subsection previously in this chapter.



Available variables: 13, selected: 1

Primary ID
Speed
Incr
Decr
Mixed
VR1
VR2
VR3

Lagged variables: 1, selected: 0

Primary ID
VR1.L[TimeH*Speed]-3

Define lags

Base lags on: Speed

Time variable: TimeH

Lag: 3

☑ Is lead

Median step: 1.54753 (speed * time)

As model:

Model type: PLS

7.2.9.12.1 Lag specification

A variable can be lagged with several step lags and dynamic lags.

7.2.9.12.2 Adding the lagged variables

To create the lagged variables:

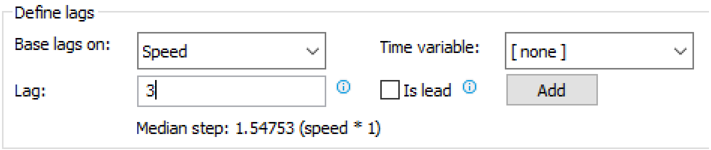
1. Mark the variable to lag in the **Available variables** list.
2. In **Base lags on**, select;
   a. **Observation index** to specify a lag by stepping a set number of observations.
   b. A variable under Time variables or Variables to specify a dynamic lag.
3. In the **Lag** field,
   a. With Observation index, specify a step wise lag by typing integers in the Lag field. Use '-' to specify a range, for example 1-5 means lags 1 to 5.
   b. With a Time variable selected, specify the time to lag the marked variable. Median step is listed below to indicate the current median time step between observations.
   c. With any other type of variable selected, specify a time variable in the **Time variable** field and specify the distance to lag the variable in the Lag field. Median step is listed below to indicate the current median step between observations for the calculated distance variable. To not select a time variable here ([none]) is a special case and treated as if time is 1.
4. If the lag is negative, select the **Is lead** check box.
5. Click **Add**. The lag variables are added in the **Lagged variables** list, according to the selected lag structure.

Note: Dynamic lags can only be based on monotonically increasing variables.

To remove any of the new lagged variables, mark it and press DELETE on your keyboard.

7.2.9.12.3 Dynamic lags

When the lag step is calculated based on a speed and/or time variable it is considered a "Dynamic lag". In the Workset Lag page such lags are specified in the **Base lags on** field by selecting something other than Observation index. Dynamic lags are useful when you know the distance between two sensors in your product line, for example 50 meters, but the speed for the process varies so you cannot lag for example 50 seconds or 50 observations.



Define lags

Base lags on: Speed

Time variable: [none]

Lag: 3

□ Is lead

Median step: 1.54753 (speed * 1)

From the selected speed and time variable SIMCA calculates the distance traveled for each observation and it is that distance you enter in the **Lag** field. If your speed variable is for example 5 m/s and the time variable has 2 seconds between each observation the distance will be 5 * 2 = 10 m. SIMCA also takes in account if the speed is not constant. The median step distance for the calculated distances is displayed in the workset wizard to help setting the correct lag.

If the distance between the points is 10 m and you lag 50 m it will have the same effect as lagging 50/10 = 5 steps.

If the lag is calculated to something uneven for example 1.5 step SIMCA interpolates the values to calculate the lag.

In the case where the lag is specified in time, the lag time for the created lag is displayed in the storing unit specified when importing the variable.

Gaps and boundaries

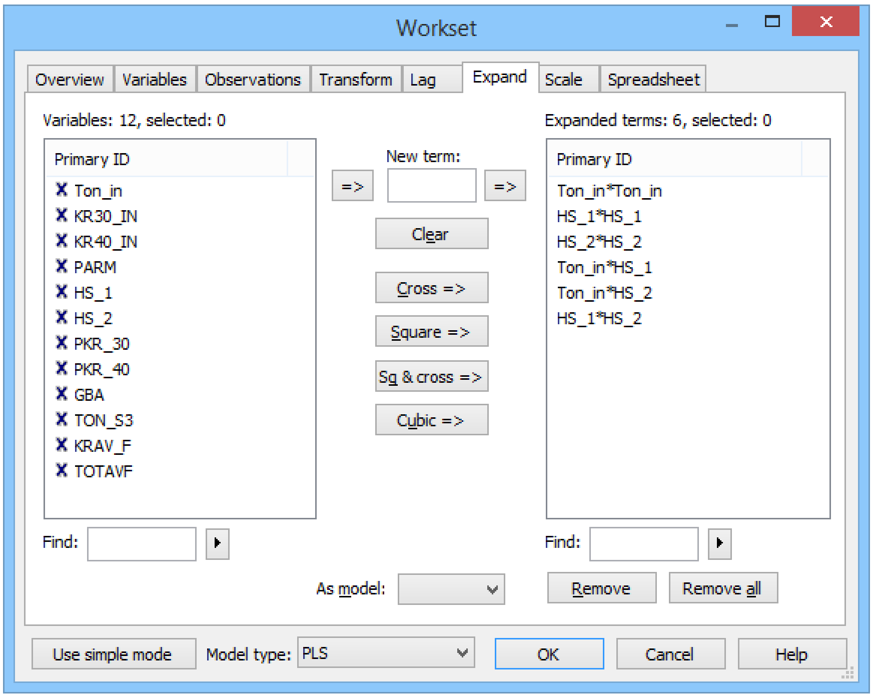
Dynamic lags are not calculated over batch or phase boundaries, and not over gaps in the process. Gaps in the process are identified when the step distance between 2 observations is greater than 3*(median step + 3 * interquartile range).

7.2.9.13 Expanding variables

The **Expand** page allows changing the default linear model by expanding the X matrix with squares, cross, and cubic terms.

Available from the Expand page are:

1. Summary row listing number of included variables, selected variables, expanded terms, and selected expansions.
2. **Variables** list displaying the included variables, including lag variables, and their roles.
3. **Expanded terms** list displaying the created expansions.
4. **New term** field and **=>** buttons for defining expansions. For more see the Adding expansions using the ‘New term’ field subsection later in this section.
5. Shortcut menu for selecting which variable IDs to display and commonly used commands.
6. **Cross**, **Square**, **Sq & cross**, and **Cubic**-buttons between the fields to add expansions. For more see the Adding terms using the buttons subsection later in this section.
7. **Find** – for finding variables. For more see the Find feature in workset dialog subsection previously in this chapter.
8. **Remove** and **Remove all** – for removing expansions.
9. **As model** – for adding expansions as in another model. See the As model subsection, previously in this chapter for more.



7.2.9.13.1 Term names

The names for expanded term are 'primary variable ID' x 'primary variable ID', i.e. x1*x1 for squares, x1*x2 for cross terms, and x1*x1*x1 for cubic terms. These names will appear on all plots and lists.

7.2.9.13.2 Scaling of expanded terms

All expanded terms are displayed in the **Scale** page. For more, see the Scaling of expanded terms subsection in the Statistical appendix.

7.2.9.13.3 Adding higher order terms

The x-variables, including lagged variables, are displayed in the **Variables** list.

To add an expansion, mark the desired variables and click:

Button	Result	Example
Cross	Adds all cross terms (2 factor interactions) possible for the marked variables.	With V1, V2, and V3 marked, clicking **Cross** adds V1*V2, V1*V3, and V2*V3.
Square	Adds all square (quadratic) terms possible for the marked variables.	With V1, V2, and V3 marked, clicking **Square** adds V1*V1, V2*V2, and V3*V3.
Sq & cross	Adds all square and cross terms possible for the marked variables.	With V1, V2, and V3 marked, clicking **Sq & cross** adds V1*V1, V2*V2, V3*V3, V1*V2, V1*V3, and V2*V3.
Cubic	Adds all cubic terms possible for the marked variables. If the squares were not added prior to clicking **Cubic**, the squares are added too.	With V1, V2, and V3 marked, clicking **Square** adds V1*V1*V1, V2*V2*V2, and V3*V3*V3. Additionally V1*V1, V2*V2, and V3*V3 if not already added.

7.2.9.13.4 Adding terms using the ‘New term’ field

Any term, including up to three of the available variables, can be added using **New term**.

To add three factor interactions:

1. Add a term (and see that it ends up in **New term**) by:
   a. Double-clicking a term OR
   b. Selecting a term and click the left arrow **=>**.
2. Repeat step 1 until the three factor interaction is displayed in **New term**.

3. Click the rightmost => arrow to add the term.

To empty the **New term** field, click the **Clear** button.

Note: The New term field is useful when the term you want to add includes three terms but is not cubic.

7.2.9.14 Scaling variables

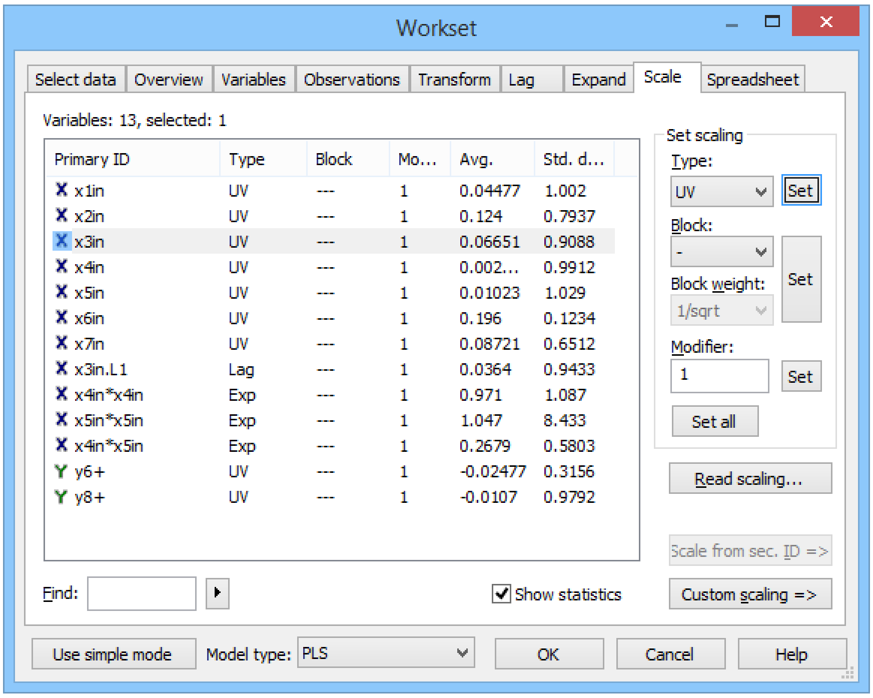
Usually with all variables of the same type or an assortment of different measurements, centering and auto scaling to unit variance is warranted. This is the SIMCA default and if this is your choice, no changes in the **Scale** page are necessary. The SIMCA default can be changed in Project options, see the Fitting options subsection in the Project options section in Chapter 5, File for more.

Customizing the scaling is available from the **Scale** page in 4 manners:

1. Using the Set scaling section.
2. Importing scaling weight and center values from file by clicking **Read scaling**.
3. Defining the scaling weight and center values from secondary variable ID by clicking **Scale from sec. ID**.
4. Defining the scaling weight and center values by entering them manually in the dialog by clicking **Custom scaling**.

When using customized scaling (2-4 above), variables with values left blank for the scaling weight use the calculated standard deviation from the data to calculate the weight. Similarly, variables with values left blank for the center use the calculated mean of the variable as center.

Note: To display the current scaling weight and center values after using **Read scaling** or **Scale from sec. ID**, click **Custom scaling**.



Variables: 13, selected: 1

Primary ID	Type	Block	Mo...	Avg.	Std. d...
X x1in	UV	---	1	0.04477	1.002
X x2in	UV	---	1	0.124	0.7937
X x3in	UV	---	1	0.06651	0.9088
X x4in	UV	---	1	0.002...	0.9912
X x5in	UV	---	1	0.01023	1.029
X x6in	UV	---	1	0.196	0.1234
X x7in	UV	---	1	0.08721	0.6512
X x3in.L1	Lag	---	1	0.0364	0.9433
X x4in*x4in	Exp	---	1	0.971	1.087
X x5in*x5in	Exp	---	1	1.047	8.433
X x4in*x5in	Exp	---	1	0.2679	0.5803
Y y6+	UV	---	1	-0.02477	0.3156
Y y8+	UV	---	1	-0.0107	0.9792

Set scaling
Type: UV
Block: -
Block weight: 1/sqrt
Modifier: 1

☑ Show statistics

Model type: PLS

7.2.9.14.1 Centering or not centering

Normally, variables are centered by subtracting their averages or other reference values. Centering by subtracting the average is the SIMCA default.

Occasionally, for example when working with difference data, you may be interested in the variation of the variables around zero (0), hence you do not want to center specific variables. Use one of the customization methods listed above to accomplish this.

Note: The scaling weights of all variables, except those with base type **Freeze** or **Frozen**, are recomputed when changing the selection of observations.

7.2.9.14.2 Show statistics

Selecting or clearing the **Show statistics** check box displays or hides the average and standard deviation of every variable.

Note: When using **Read scaling**, **Scale from sec. ID**, or **Custom scaling** the values displayed under **Avg** and **Std. dev.** are the calculated average and standard deviation values, not the values that will be used when scaling the variables.

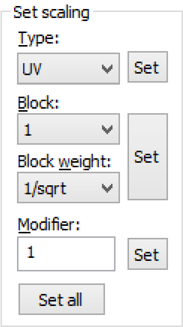
To read about the scaling of expanded terms, transformed variables, lagged variables, variables in classes, scaling after re-selecting observations, and calculation of the scaling weight, see the Scaling section in the Statistical appendix.

7.2.9.14.3 Scaling using the Set scaling section

To change the scaling base type from the **Set scaling** section:

1. Select the variables.
2. Select the base type in the **Type** box.
3. Click **Set** next to the **Type** box.

The new scaling type is displayed in the **Type** column.



Set scaling

Type: UV

Block: 1

Block weight: 1/sqrt

Modifier: 1

Scaling base weight types available

The following scaling base types are available from the **Type** box:

Base weight type	Description
None	No centering or scaling (ws = 1).
UV	Variable j is centered and scaled to "Unit Variance", i.e. the base weight is computed as $1/sd_j$, where sd_j is the standard deviation of variable j computed around the mean.
UVN	Same as UV, but the variable is not centered. The standard deviation is computed around 0.
Par	Variable j is centered and scaled to Pareto Variance, i.e. the base weight is computed as $1/\text{sqrt}(sd_j)$, where sd_j is the standard deviation of variable j computed around the mean. Pareto scaling is in between no scaling and UV scaling and gives the variable a variance equal to its standard deviation instead of unit variance.
ParN	Same as Par, but the variable is not centered The standard deviation is computed around 0.
Ctr	The variable is centered but not scaled (ws = 1)
Freeze	The scaling weight of the variable is frozen and will not be re-computed when observations in the workset change or the variable metric is modified after the freezing.

Block scaling

Block-wise scaling is warranted when a data table contains several types (blocks) of variables, with different numbers of variables in each block. Block-wise scaling allows each block to be thought of as a unit and to be given the appropriate variance, which is less than if each variable was auto scaled to unit variance.

Block scaling scales down the importance of the variables so that the whole block has $\sqrt{(Kblock)}$ variance, or unit variance, where Kblock is the number of variables in the block.

Defining the block scaling

To block scale:

1. Mark the variables in the first block.
2. Select the block weight.
3. Click the **Set** button found to the right of the blocking options.
4. Mark other variables.
5. Change the block number and optionally the block weight.
6. Click the **Set** button found to the right of the blocking options.
7. Repeat 4-6 until all blocks have been defined.

Block scaling types available

The following block scaling types are available:

Scaling	Description
1/√(KBlock)	The block weight is computed as 1/√(Block). This gives the whole block a variance equal to 1.
1/√(√(Kblock))	The block weight is computed as 1/(√(√((Block))). This gives the whole block a variance equal to square root of K.

where Block = number of variables in the block

Note: *X and Y variables cannot be grouped in the same scaling block.*

Modifier

Scaling variables up or down relative to their base weight is done using the **Modifier**.

To scale variables up or down relative to their base weight:

1. Mark the variables.
2. Enter the value in **Modifier**.
3. Click **Set**.

To reset the modifier to 1:

1. Mark the variables.
2. Enter ‘1’ in **Modifier**.
3. Click **Set**.

7.2.9.14.4 Reading scaling from file

Centers and scaling weights can be imported from file and used to scale the variables.

Importing scaling from file for regular projects

For regular projects, i.e. non batch data, the file must have the following rows:

- Variable IDs.
- Center values.
- Scaling weights.

Importing scaling from file for batch projects with phases

Specifying different scaling than the default for the variables in the different phases and applying them simultaneously to all phases, is available using **Read scaling**.

For batch projects with phases, centers and scaling weights for each phase can be defined in the **Import Scaling Data** wizard spreadsheet.

The imported file must have the following column and rows:

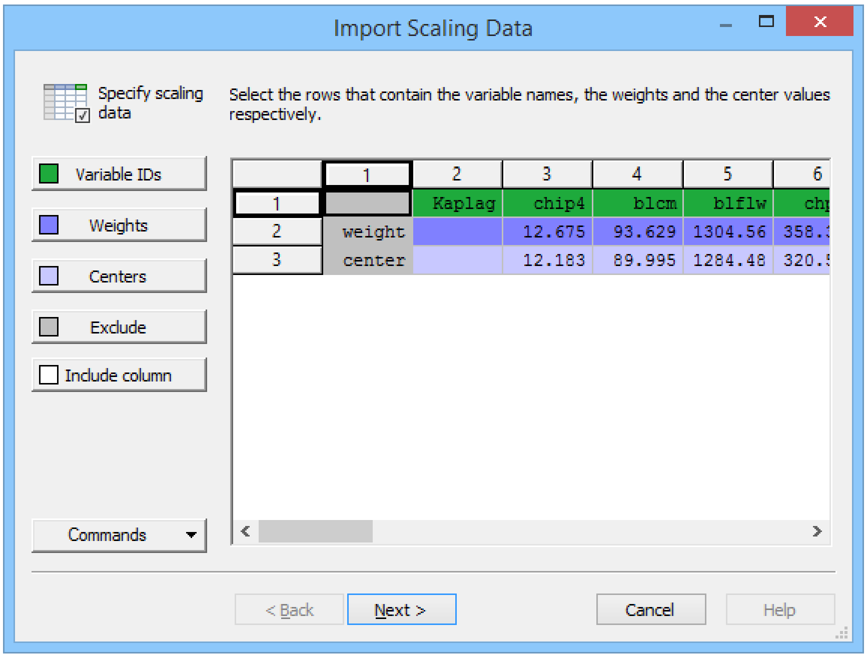
- Phase ID column.
- Variable names row.
- Center values rows, one for each phase.
- Scaling weights rows, one for each phase.

To see the different base weight types resulting from customized scaling, see the Scaling base weight types with customized scaling section later in this chapter.

Note: When using **Read scaling** to specify the scaling for all phases simultaneously, either click **Edit | BEMxx** or **New** in the **Workset** group. Using **Read scaling** when editing a phase will apply the scaling to that phase only. This is the case for class models too.

Import Scaling Data wizard

To import a file holding scaling weights and center values follow the steps that follow:

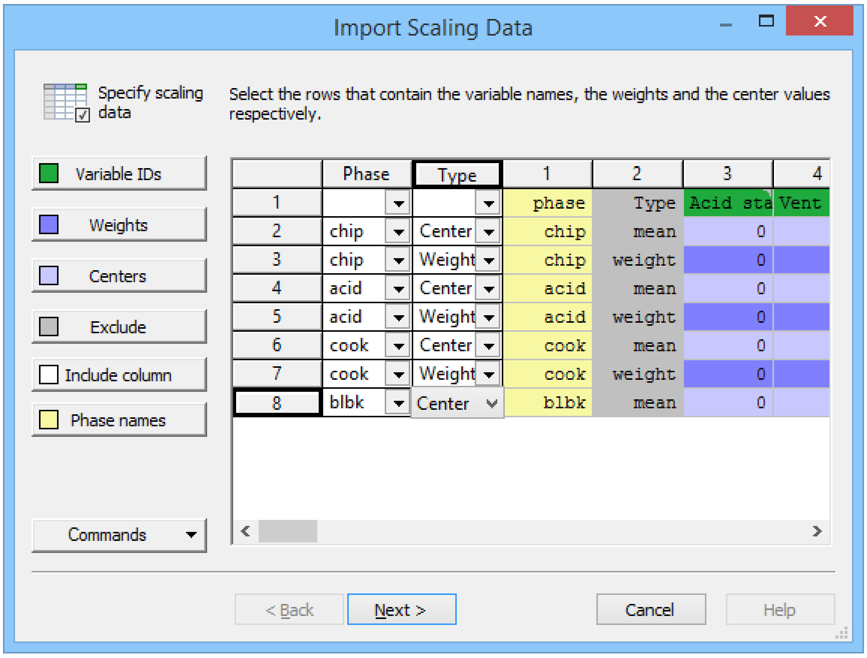
Step	Action and illustration
1. Select the scaling file.	Click **Read scaling** and select the file containing the weights and/or centers. Read scaling...
2. Specify weights and centers. For batch projects with phases, weights and centers need to be specified for each phase individually.	In the **Import Scaling Data** dialog, in turn mark the rows with primary variable IDs, weights, and centers and click **Variable IDs**, **Weights** and **Center**. SIMCA automatically recognizes the words 'mean' or 'center' and 'weight' when present in a column and marks these rows as center and weights. Variables that are not included in the list are centered and scaled UV. Variables with blank values for the center use as center the computed mean from the data and variables with blank for scaling weights are scaled UV. **Note**: When the batch project has phases, weights and centers have to be specified for each phase. Click **Next**. 

Import Scaling Data

Specify scaling data

Select the rows that contain the variable names, the weights and the center values respectively.

	1	2	3	4	5	6
1		Kaplag	chip4	blcm	blflw	chp
2	weight		12.675	93.629	1304.56	358.
3	center		12.183	89.995	1284.48	320.

Step	Action and illustration
	

Import Scaling Data

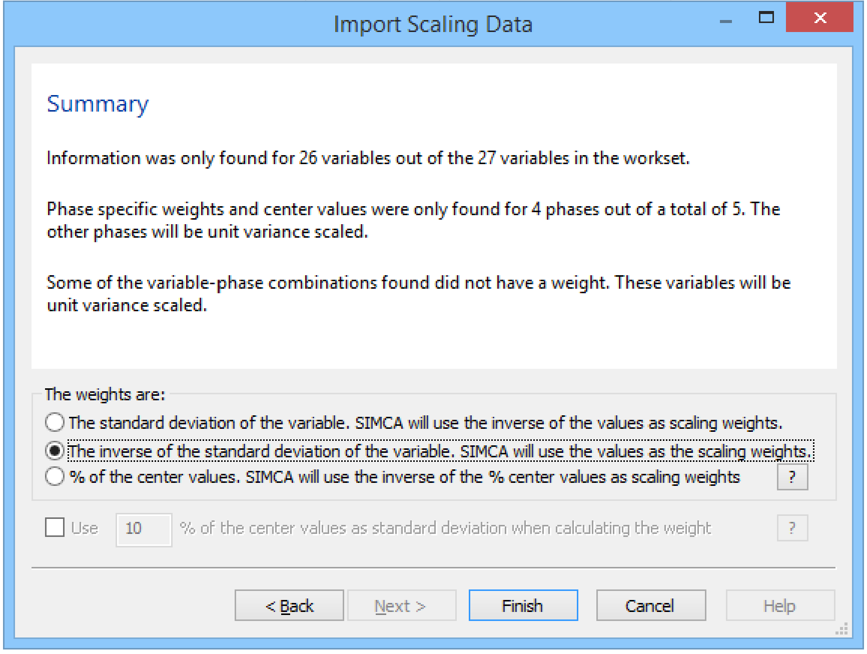
Specify scaling data

Select the rows that contain the variable names, the weights and the center values respectively.

- 🟩 Variable IDs
- ■ Weights
- □ Centers
- ■ Exclude
- □ Include column
- □ Phase names
- Commands

	Phase	Type	1	2	3	4
1			phase	Type	Acid sta	Vent
2	chip	Center	chip	mean	0	
3	chip	Weight	chip	weight	0	
4	acid	Center	acid	mean	0	
5	acid	Weight	acid	weight	0	
6	cook	Center	cook	mean	0	
7	cook	Weight	cook	weight	0	
8	blbk	Center	blbk	mean	0	

< Back | Next > | Cancel | Help

Step	Action and illustration
3. Specifying weight properties.	In the **Summary** page, specify how to use the weights and click **Finish**. View the table next for a description of the options in the **Summary** page. 

Import Scaling Data

Summary

Information was only found for 26 variables out of the 27 variables in the workset.

Phase specific weights and center values were only found for 4 phases out of a total of 5. The other phases will be unit variance scaled.

Some of the variable-phase combinations found did not have a weight. These variables will be unit variance scaled.

The weights are:

○ The standard deviation of the variable. SIMCA will use the inverse of the values as scaling weights.
● The inverse of the standard deviation of the variable. SIMCA will use the values as the scaling weights.
○ % of the center values. SIMCA will use the inverse of the % center values as scaling weights ?

□ Use 10 % of the center values as standard deviation when calculating the weight ?

< Back | Next > | Finish | Cancel | Help

Weight definition for imported scaling

This table describes the options in the **Import Scaling Data** wizard **Summary** page.

Weight selected	Description	Example
The standard deviation of the variable. SIMCA will use the inverse of the values as scaling weights.	The values specified as **Weights** in the spreadsheet are inverted and used as scaling weight.	**If the Weights** value for variable 'V1' in the spreadsheet is '3', then the scaling weight, ws = 1/3.

Weight selected	Description	Example
The inverse of the standard deviation of the variable. SIMCA will use the values as the scaling weights.	The values specified as **Weights** in the spreadsheet are used as scaling weight.	If the **Weights** value for variable 'V1' in the spreadsheet is '3', then the scaling weight, ws = 3.

% of the center values. SIMCA will use the inverse of the % center values as scaling weights.	The values specified as **Weights** in the spreadsheet are the percentage values that, multiplied with the center values, results in the standard deviation, SD (the inverse of the scaling weight).
	When **Centers** are specified in the spreadsheet, the SD used is the percent (weight value) of the center.
	For variables with the **Centers** left blank, the calculated mean is used as center and the standard deviation (SD) used is the specified percentage of the center or the calculated SD, whichever is greater.
	If the **Weights** are blank, this option defaults to using the SIMCA calculated weight.
		With center value: If the Weights value for variable 'V1' in the spreadsheet is '3' and the Centers value is '10', then the scaling weight, ws = 1/(0.03*10).
		Without center value: If the Weights value for variable 'V1' in the spreadsheet is '3' and the Centers value is blank, then the scaling weight used is the smaller of
		ws = 1/(0.03*calculated center)
		ws = 1/(the calculated SD).

Use xx % of the center values as standard deviation when calculating the weight.	The values defined as **Weights** in the spreadsheet are ignored. The entered percentage of the center values is used as standard deviation and inverted before used as standard deviation.	If xx entered is '5', the center value is '10'. The standard deviation, SD = 0.05*10. The scaling weight, ws = 1/SD = 2.

Note: When using **Read scaling** to specify the scaling for all phases simultaneously, either click **Edit | BEMxx** or **New** in the **Workset** group. Using **Read scaling** when editing a phase will apply the scaling to that phase only. This is the case for class models too.

7.2.9.14.5 Scaling from numerical secondary variable ID

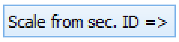
Scaling from secondary variable IDs is available when secondary variable IDs are numerical. The variable IDs must contain scaling weights or center values.

Note: When batch data have phases, scaling from secondary IDs can be done for each selected phases, by editing the phase model.

To see the different base weight types resulting from customized scaling, see the Scaling base weight types with customized scaling subsection later in this chapter.

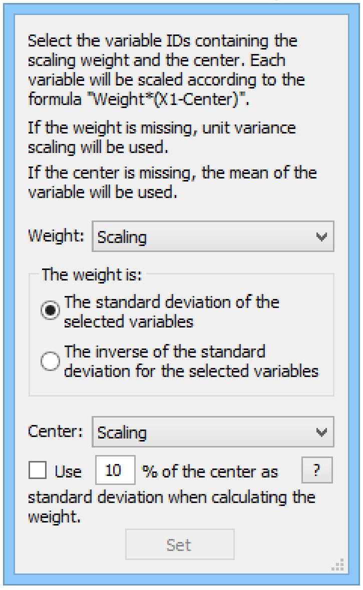
Scale from Sec. ID dialog

To scale and/or center from secondary variable IDs, follow the steps:

1. Select the variables to scale.
2. Click the **Scale from sec. ID** button. 

3. In the dialog that opens, select the secondary variable ID that contains the standard deviations or scaling weights in the **Weight** box. Selecting **1 (no scaling)** results in no scaling.
4. In **The weight is** section, the default is **The standard deviation of the selected variables**. This means that the inverted values in the variable ID will be used as scaling weights. To use the specified weight values in the secondary ID as scaling weight, select **The inverse of the standard deviation for the selected variables**.
5. In the **Center** box, select the secondary ID that holds the center values or **0 (center around zero)**.
6. Selecting the **Use x % of the center as standard deviation when calculating the weight** check box results in that the entered percentage of the center values is used as standard deviation and inverted before used as scaling weight. When selecting this check box the other **Weight** options are unavailable. For more details, see the second

table in the Import Scaling Data wizard subsection earlier in this chapter.



Select the variable IDs containing the scaling weight and the center. Each variable will be scaled according to the formula "Weight*(X1-Center)".

If the weight is missing, unit variance scaling will be used.

If the center is missing, the mean of the variable will be used.

Weight: Scaling

The weight is:

● The standard deviation of the selected variables

○ The inverse of the standard deviation for the selected variables

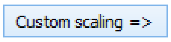
Center: Scaling

□ Use 10 % of the center as standard deviation when calculating the weight.

7.2.9.14.6 Custom scaling

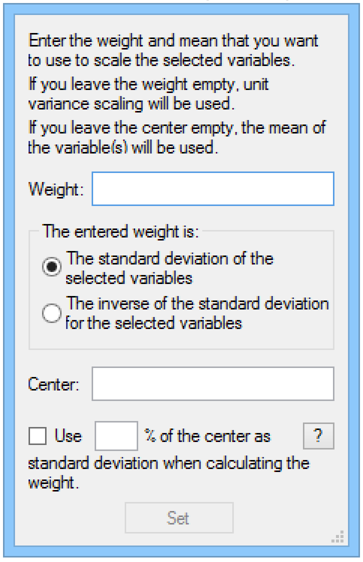
It is sometimes necessary to specify the center and the scaling weight of variables to be different than computed from the data. Using **Custom scaling** the scaling weight of the variables can be specified as follows:

1. Select the variables to scale.
2. Click **Custom scaling.**



3. In the window that opens, enter the standard deviation or scaling weight in the **Weight** field. Leaving blank results in using the calculated scaling weight.
4. In **The entered weight is** section, the default is **The standard deviation of the selected variables** option. This means that the inverted values in the variable ID will be used as scaling weights. To use the specified weight values in the secondary ID as scaling weight, select **The inverse of the standard deviation for the selected variables** option.
5. In the **Center** field, enter the center value to use. Leaving blank results in using the calculated mean as center.
6. Selecting the **Use x % of the center as standard deviation when calculating the weight** check box results in that the entered percentage of the center values is used as standard deviation and inverted before used as scaling weight. When selecting this check box the other **Weight** options are unavailable. For more details, see the second

table in the Reading scaling from file subsection earlier in this chapter.



Enter the weight and mean that you want to use to scale the selected variables.

If you leave the weight empty, unit variance scaling will be used.

If you leave the center empty, the mean of the variable(s) will be used.

Weight:

The entered weight is:

● The standard deviation of the selected variables

○ The inverse of the standard deviation for the selected variables

Center:

□ Use [ ] % of the center as standard deviation when calculating the weight.

7.2.9.14.7 Scaling base weight types with customized scaling

After changing the scaling using **Read scaling**, **Scale from sec. ID**, or **Custom scaling** the following scaling base types are available:

Base weight type	Description	Weight and center specification
Frozen	The center and the scaling weight of the variable are specified	**Weight** and **Center** values that are not weight=1 and center=0.
FrozenC	The scaling weight is specified, but not the center (value is left blank). The center is computed from the data.	**Weight** values (not=1) but **Center** is left empty. Not possible for **Scale from sec ID**.
FrozenN	The scaling weight is specified and no center is selected, (centering is done around 0).	**Weight** values (not=1) and **Center** = 0.
UVF	The center is specified, but not the scaling weight, the standard deviation is computed from the data and ws=1/standard deviation. UVF is UV scaled using a new center value.	**Weight** values left empty, **Center** values specified. Not possible for **Scale from sec ID**.
NoneF	The center is specified and no scaling is selected (ws=1)	**Weight** = 1, **Center** values specified.
%Mean	The center is not specified but the entered percentage of the center is used as standard deviation when calculating the weight.	No center or weight values specified. The **Use x % of the center as standard deviation when calculating the weight** check box selected and the desired percentage entered.
%Frozen	The center is specified and the entered percentage of the center is used as standard deviation when calculating the weight.	Center specified but not weight values. The **Use x % of the center as standard deviation when calculating the weight** check box selected and the desired percentage entered.

The calculation of the scaling weight is described in Scaling weight calculation subsection in the Statistical appendix.

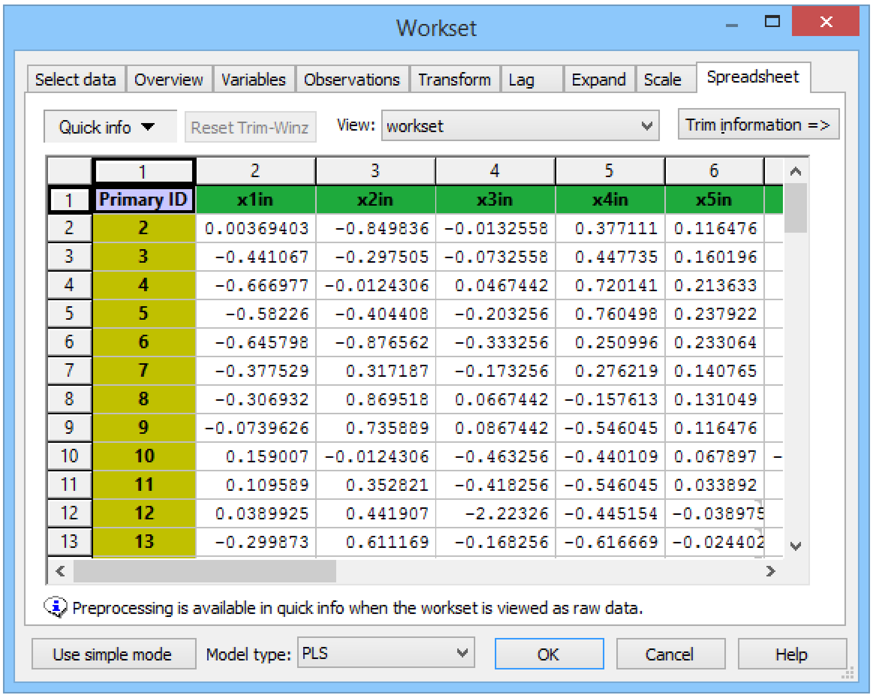
7.2.9.15 Spreadsheet

The **Spreadsheet** page, in the Workset dialog, displays the currently included variables and observations, including lagged and expanded variables.

Available in the Spreadsheet page are:

- **Quick info** – for viewing variables and observations.
- **Reset Trim-Winz** – for removing trimming and Winsorizing.

- **View** box – for selecting scaled or original units. When editing a batch model, average batch and aligned vectors are available.
- **Trim information** – for displaying the performed trimming.
- Workset list displaying all variable and observation IDs and values.
- Shortcut menu – for copying, locking columns, opening the **Quick Info**, zooming out, saving list to file, and printing.



View: workset

	1	2	3	4	5	6
1	Primary ID	x1in	x2in	x3in	x4in	x5in
2	2	0.00369403	-0.849836	-0.0132558	0.377111	0.116476
3	3	-0.441067	-0.297505	-0.0732558	0.447735	0.160196
4	4	-0.666977	-0.0124306	0.0467442	0.720141	0.213633
5	5	-0.58226	-0.404408	-0.203256	0.760498	0.237922
6	6	-0.645798	-0.876562	-0.333256	0.250996	0.233064
7	7	-0.377529	0.317187	-0.173256	0.276219	0.140765
8	8	-0.306932	0.869518	0.0667442	-0.157613	0.131049
9	9	-0.0739626	0.735889	0.0867442	-0.546045	0.116476
10	10	0.159007	-0.0124306	-0.463256	-0.440109	0.067897
11	11	0.109589	0.352821	-0.418256	-0.546045	0.033892
12	12	0.0389925	0.441907	-2.22326	-0.445154	-0.038975
13	13	-0.299873	0.611169	-0.168256	-0.616669	-0.024402

Preprocessing is available in quick info when the workset is viewed as raw data.

Model type: PLS

The Spreadsheet list displays the data and all variable and observation IDs of the currently included variables and observations.

7.2.9.15.1 Quick Info in the Workset dialog spreadsheet

The **Quick Info** pane displays overview information about the marked variables or observations, depending on whether selecting **Quick info | Variables** or **Quick info | Observations**.

Open the **Quick Info** pane by:

- Clicking **Quick info** and selecting **Variables** or **Observations**.
- Right-clicking the spreadsheet and selecting **Quick info | Variables** or **Observations**.

Trim-Winsorizing the workset

When trimming or Winsorizing the workset, it only affects the current workset and does not touch the dataset.

The **Trim-Winz var** and **Trim-Winz all** buttons are available in the **Quick Info Variables** pane when **workset as raw data** is selected in the **View** box, that is, when the variables are displayed in original units.

Trimming and Winsorizing is done on the selected variables across all phases and batches.

Note: When editing a phase model, trimming is unavailable.

For more about the **Quick Info** pane, see the Quick Info section in Chapter 13, View.

Removing the trimming and Winsorizing in the workset

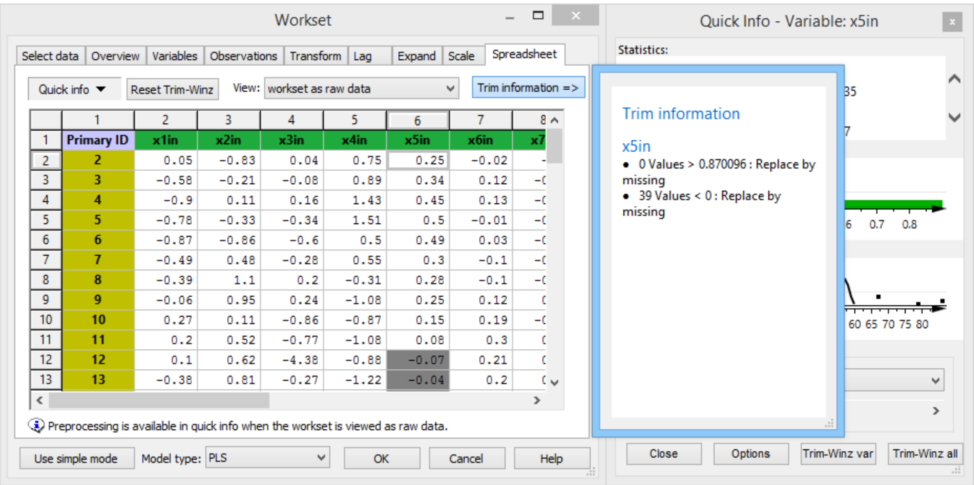
Removing the trimming or Winsorizing for the current workset can be done by:

- Clicking **Undo trimming** in one of the trimming Winsorizing dialogs.

- Clicking **Reset Trim-Winz** next to the **Quick info** button in the **Spreadsheet** tab.

7.2.9.15.2 Trimming and Winsorizing information

After trimming or Winsorizing, clicking **Trim information** displays a summary of the performed trimming/Winsorizing.



View: workset as raw data

	1	2	3	4	5	6	7	8
1	Primary ID	x1in	x2in	x3in	x4in	x5in	x6in	x7
2	2	0.05	-0.83	0.04	0.75	0.25	-0.02	-
3	3	-0.58	-0.21	-0.08	0.89	0.34	0.12	-0
4	4	-0.9	0.11	0.16	1.43	0.45	0.13	-0
5	5	-0.78	-0.33	-0.34	1.51	0.5	-0.01	-0
6	6	-0.87	-0.86	-0.6	0.5	0.49	0.03	-0
7	7	-0.49	0.48	-0.28	0.55	0.3	-0.1	-0
8	8	-0.39	1.1	0.2	-0.31	0.28	-0.1	-0
9	9	-0.06	0.95	0.24	-1.08	0.25	0.12	0
10	10	0.27	0.11	-0.86	-0.87	0.15	0.19	-0
11	11	0.2	0.52	-0.77	-1.08	0.08	0.3	0
12	12	0.1	0.62	-4.38	-0.88	-0.07	0.21	0
13	13	-0.38	0.81	-0.27	-1.22	-0.04	0.2	0

Preprocessing is available in quick info when the workset is viewed as raw data.

Model type: PLS

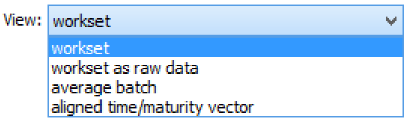
Trim information

x5in

- 0 Values > 0.870096 : Replace by missing
- 39 Values < 0 : Replace by missing

7.2.9.15.3 View workset in scaled or original units

The **View** box contains the options **workset** and **workset as raw data** and when editing a phase or batch model the additional options: **average batch** and **aligned time/maturity vector**.



View: workset

- workset
- workset as raw data
- average batch
- aligned time/maturity vector

By default, **workset** is selected in the **View** box, meaning that the variables are transformed, scaled, and centered according to the current workset specification.

To display all variables and observations in original units, select **workset as raw data**.

Average batch and aligned time/maturity

To view the average batch or aligned time or maturity vector for a BEM with phases, mark a *phase model* and click **Edit** in the **Workset** group. In the **Spreadsheet** page of the **Workset** dialog select **average batch** or **aligned time/maturity vector** in the **View** box. When editing a **BEM** (with phases) or **BLM** the additional batch options are unavailable.

Note: With phases, these calculations are done for every phase, since the alignment is done by phase.

7.2.9.16 Creating unfitted models

New unfitted models are created when exiting the **Workset** dialog by clicking **OK**.

7.2.9.16.1 Unfitted models in wrappers

When the **Model type** is **PCA/PLS/OPLS/O2PLS-class** SIMCA generates unfitted class models, one for each class with the wrapper CMxx. The numbering of the CM models is sequential.

For batch projects with phases, when clicking **OK** SIMCA generates unfitted PLS or OPLS class models, one for each phase with the wrapper BEMxx.

Note: Changes in the class or phase model are not remembered by the wrapper model CM respective BEM. This means that if you for instance exclude a batch in a phase model, that batch will be included if you click **Workset | New as model** and click the BEM.

7.2.10 Simple mode workset wizard

The workset dialog is opened in simple mode the very first time you open the **Workset** dialog in SIMCA. After that the dialog remembers whether to open in simple mode or advanced mode.

The simple mode workset wizard contains the following pages:

1. Start page – displays a short description of the workset wizard.
2. Select data page - displays the available datasets when there is more than one. See also the Select data subsection earlier in this chapter.
3. Variables page – for assigning roles and applying automatic transformation.
4. Observations page – for excluding, including, and assigning classes.
5. Summary page – displays a summary of the active model and allows changing from the default fitting type.

To switch between simple and advanced mode, click the **Use advanced mode** and **Use simple mode** respectively.

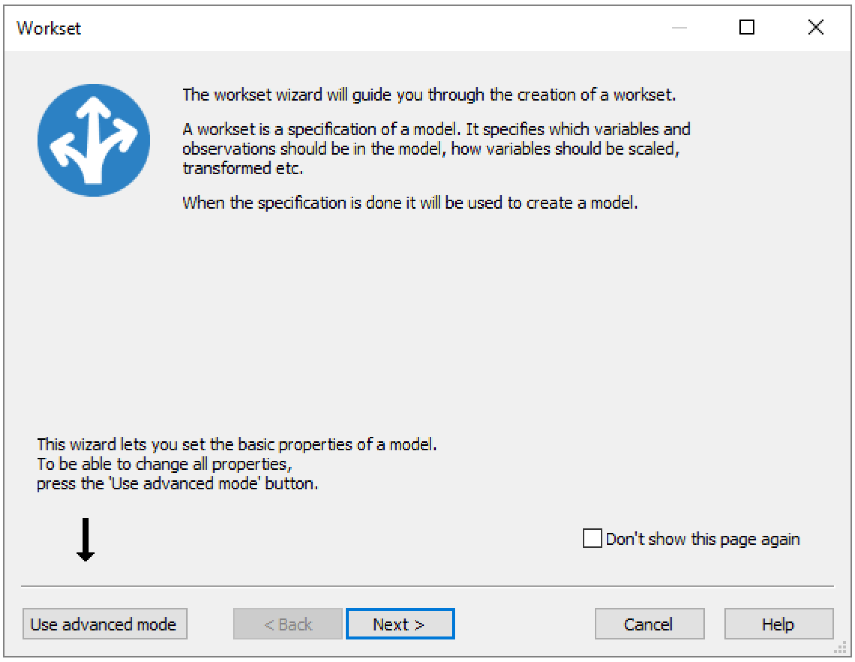
Note: Simple mode is unavailable for batch projects.

7.2.10.1 Simple mode start page

The first page of the workset wizard describes the features of the workset wizard.

To not display this introductory page the next time the simple mode workset opens for this project, select the **Don't show this page again** check box.

Click **Next**.



Workset

The workset wizard will guide you through the creation of a workset.

A workset is a specification of a model. It specifies which variables and observations should be in the model, how variables should be scaled, transformed etc.

When the specification is done it will be used to create a model.

This wizard lets you set the basic properties of a model.
To be able to change all properties,
press the 'Use advanced mode' button.

☐ Don't show this page again

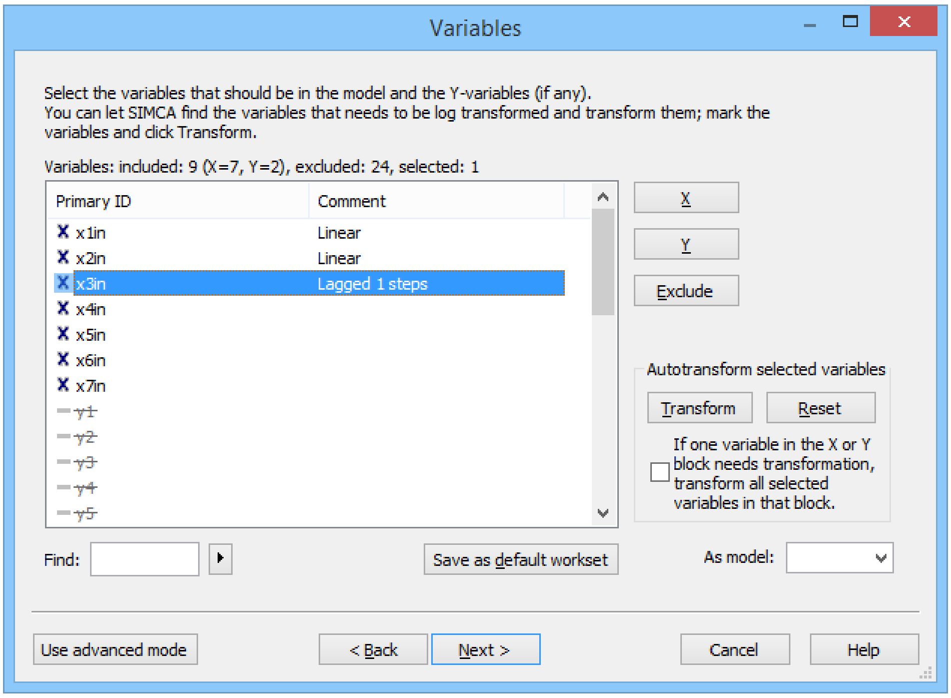
7.2.10.2 Variables page in simple mode

In the **Variables** page, the following is available:

1. A summary line displaying currently included and excluded variables.
2. The variable list displaying the current role of each variable (X, Y, or ' -'), variable IDs, and a **Comment** column.
3. X-button – for assigning variables to the X-block.
4. Y-button – for assigning variables to the Y-block.
5. **Exclude** – for excluding variables.
6. **Transform** - for autotransforming variables.
7. **Find and select** field – for finding variables. For more see the Find feature in Workset page previously in this chapter.
8. **Save as default workset** – for saving the current specification as default workset.

9. **As model** – for assigning X and Y and excluding variables as an existing model. See the As model section, previously in this chapter for more.

Clicking **Next** opens the **Observations** page of the wizard.



Variables

Select the variables that should be in the model and the Y-variables (if any).
You can let SIMCA find the variables that needs to be log transformed and transform them; mark the variables and click Transform.

Variables: included: 9 (X=7, Y=2), excluded: 24, selected: 1

Primary ID	Comment
X x1in	Linear
X x2in	Linear
X x3in	Lagged 1 steps
X x4in	
X x5in	
X x6in	
X x7in	
— ~~y1~~	
— ~~y2~~	
— ~~y3~~	
— ~~y4~~	
— ~~y5~~	

Autotransform selected variables

□ If one variable in the X or Y block needs transformation, transform all selected variables in that block.

Find:

As model:

7.2.10.2.1 Variable list

The variable list displays the current role, variable IDs, and **Comment**. The **Comment** column displays the current transformation. The only transformation available in Simple mode is the **Log** transform.

The following can be added in advanced mode and is then displayed in simple mode:

- Transformation other than Log displayed in Comment.
- Lagging displayed in Comment.
- Class belonging displayed in Class.

The context sensitive menu, opened by right-clicking the variables list, holds the following commands: **X**, **Y**, **Exclude**, **Select all (CTRL+A)**, and **Variable label**, where the last enables displaying the desired variable IDs.

7.2.10.2.2 Selecting roles by specifying X and Y

To change the variable roles:

1. Select the variables.
2. Click the desired button **X**, **Y**, or **Exclude**. The list is updated accordingly.

Note: Fitting a PLS, OPLS or O2PLS model with one qualitative Y is equivalent to fitting a PLS-DA, OPLS-DA or O2PLS-DA model with classes defined according to the qualitative variable.

7.2.10.2.3 Automatic transformation

Automatic Log transformation according to certain criteria is available by following the steps:

1. Select the desired variables in the variable list.
2. Optionally select the **If one variable in the X or Y block needs transformation, transform all selected variables in that block** check box to have all variables in the same metric. In summary, when the check box is selected all variables are Log transformed if one meets the criteria for automatic transformation.

3. Click **Transform**. The software checks if any of the selected variables need a Log transformation and if so applies it.

The criteria used to decide if a log transform is needed is described in the Transform page criteria section in the Statistical appendix.

7.2.10.2.4 Save as default workset

To change the default workset roles of the variables, from what was specified at import, specify the X, Y or excluded as desired and click **Save as default workset**. This specification defines the default workset when clicking **New** in the **Workset** group on the **Home** tab.

Clicking **Save as default workset** saves the properties of the page. When clicked on the Select data tab, the datasets selected are saved, when clicked on the Variables tab the excluded and y-variables are saved.

Deleting a dataset or variable included in the default workset results in a default workset using the other included datasets and variables.

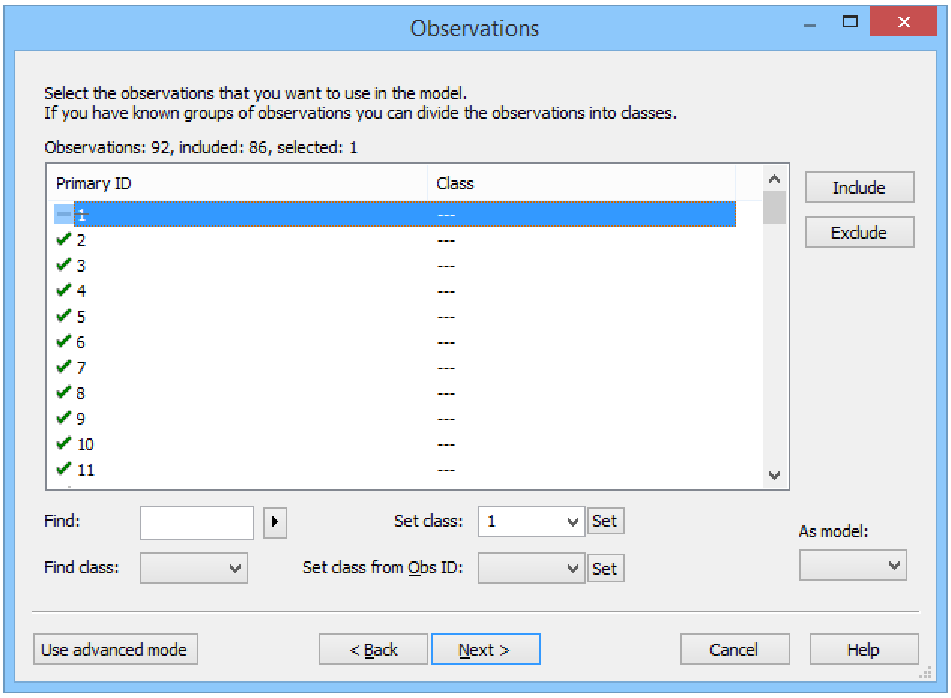
For more about specifying the default workset, see the Default workset subsection earlier in this chapter.

7.2.10.3 Observations page in simple mode

The **Observations** page functionality is identical to the **Observations** page in advanced mode with the following exception: there is no **More**-button so assigning classes from variables or scores is unavailable here.

For details about the **Observations** page, see the Observations page section previously in this chapter.

Click **Next** to open the **Summary** page.



Observations

Select the observations that you want to use in the model.
If you have known groups of observations you can divide the observations into classes.

Observations: 92, included: 86, selected: 1

Primary ID	Class
1	---
✓ 2	---
✓ 3	---
✓ 4	---
✓ 5	---
✓ 6	---
✓ 7	---
✓ 8	---
✓ 9	---
✓ 10	---
✓ 11	---

Find:

Find class:

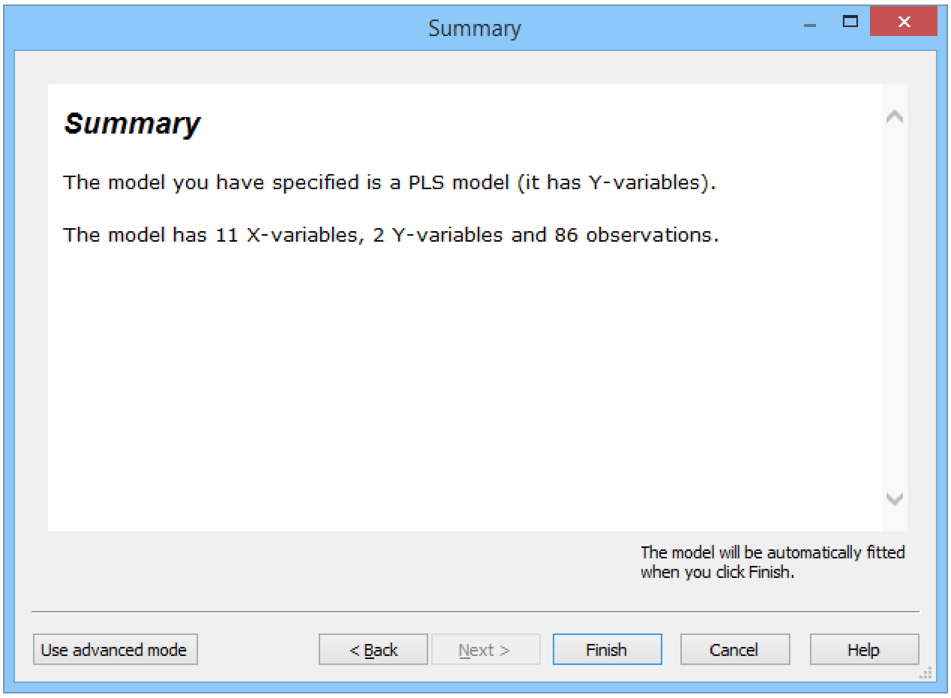
Set class: 1

Set class from Obs ID:

As model:

7.2.10.4 Summary page in simple mode

The **Summary** page displays a summary over the specification done in the workset wizard, including the model type that will be fitted.



Summary

The model you have specified is a PLS model (it has Y-variables).

The model has 11 X-variables, 2 Y-variables and 86 observations.

The model will be automatically fitted when you click Finish.

Click **Finish** to close the wizard and automatically fit the model or models.

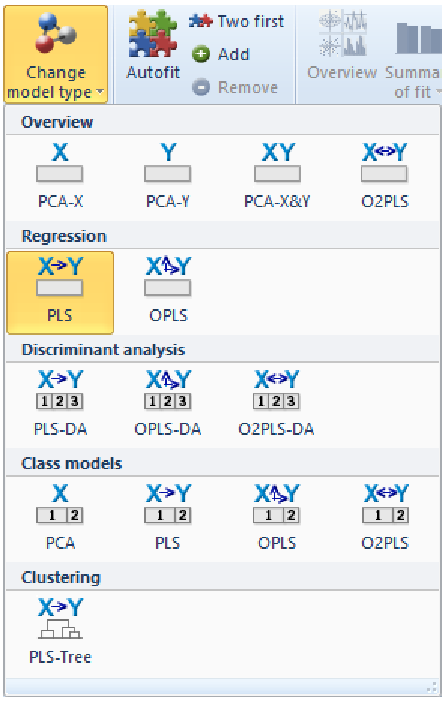
7.2.11 Change model type

The default model type after exiting the workset dialog is determined by the selected model type in the **Model type** box in the **Workset** dialog.

To change from the default model type, click **Change model type** and click a new model type in the gallery that opens.

For example after fitting a principal component model of the responses (**PCA-Y**), click **Change model type** and select **PLS** to fit a PLS model. SIMCA creates a new unfitted model, with type PLS.

Note: SIMCA creates a new unfitted model every time a new model type is selected.



Change model type is found in the **Workset** group on the **Home** tab.

7.2.11.1 Model types available

The available model types from **Change model type** are, in the order of the gallery:

Model type	Description
	Overview
PCA-X	Fits a PC to the X variables.
PCA-Y	Fits a PC to the Y (responses) variables.
PCA-X&Y	Fits a PC to all included variables (X and Y).
O2PLS	Fits an O2PLS model with the additional objective to model and interpret variation in X that is orthogonal to Y. The orthogonal variation can be further divided into two parts; the OPLS part and the PCA part. The PCA part consists of structured variation that does not affect the prediction but can be interesting to study to further improve the interpretation of complex multivariate data. Available when X and at least two Y variables were defined in the workset.
	Regression
PLS	Fits a PLS model. Available when both X and Y variables were defined in the workset.
OPLS	Fits an OPLS model with the additional objective to model and interpret variation in X that is orthogonal to Y, which needs to be modeled to achieve the best possible prediction and interpretation Available when both X and Y variables were defined in the workset.
	Discriminant analysis
PLS-DA	Fits a PLS model using SIMCA created dummy Y variables, one for each class. Available after grouping observations in two or more classes.
OPLS-DA	Fits an OPLS/O2PLS model using SIMCA created dummy Y variables, one for each class. See OPLS above. Available after grouping observations in two or more classes.
O2PLS-DA	Fits an O2PLS model using SIMCA created dummy Y variables, one for each class. See O2PLS above. Available after grouping observations in three or more classes.
	Class models
PCA-class	Fits PC models for the X block, one for each class, with a wrapper CM. Available after grouping observations in classes or variables in blocks.
PLS-class	Fits PLS models, one for each class, with a wrapper CM. Available after grouping observations in classes, or variables in blocks, and both X and Y variables are included.
OPLS-class	Fits OPLS models, one for each class, with a wrapper CM. See OPLS above. Available after grouping observations in classes, or variables in blocks, and both X and Y variables are included.
O2PLS-class	Fits O2PLS models, one for each class, with a wrapper CM. See O2PLS above. Available after grouping observations in classes, or variables in blocks, and both X and at least two Y variables are included.
	Clustering
PLS -Tree	Fits several PLS models grouped as branches in a tree.

Note: DA models are fitted to the X variables only. The Y-variables (responses), when present, are ignored.

Note: All results of the fit of a PC model (PCA-X and PCA-Y), such as SS explained are labeled as X (i.e. R2X).

Note: A PLS, OPLS or O2PLS model with one qualitative y-variable is equivalent to PLS-DA, OPLS-DA and O2PLS-DA respectively.

7.2.11.2 Model window for OPLS and O2PLS models

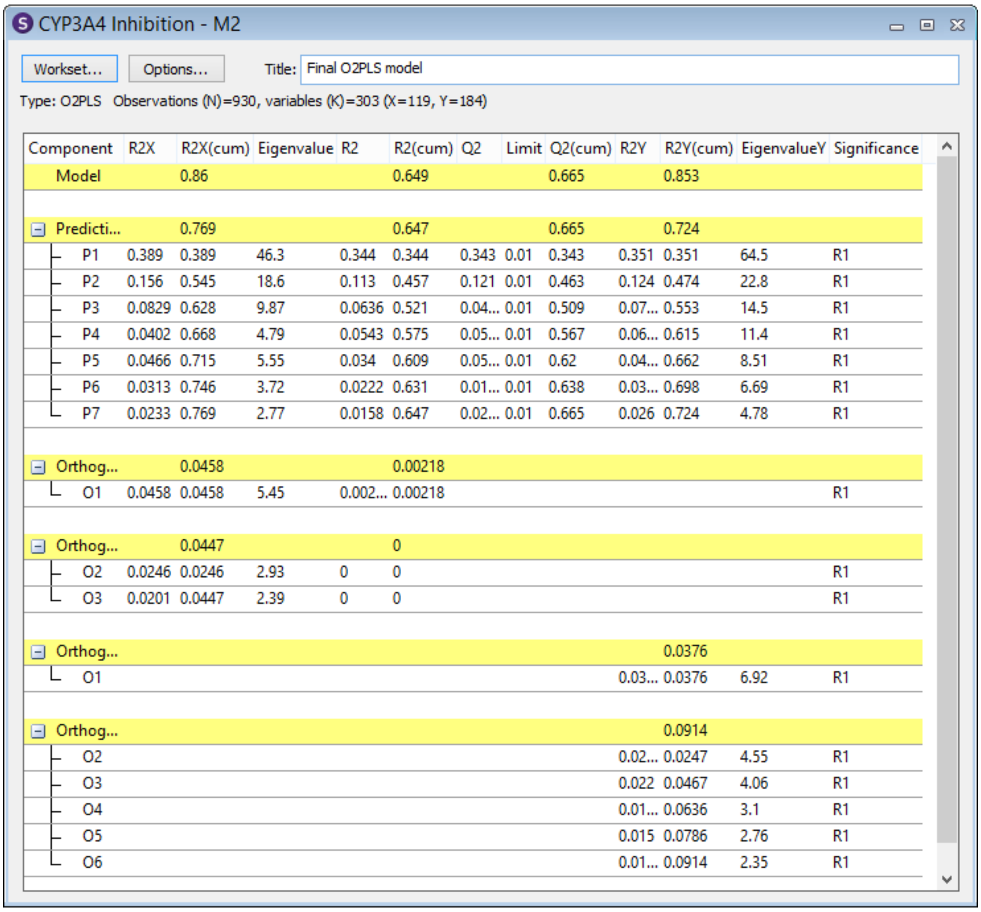
The **Model Window** corresponding to OPLS and O2PLS displays summary statistics related to the model. Components that capture variation found in both X and Y are denoted Predictive. Components that capture variation only found in X are denoted Orthogonal in X(OPLS). Components that capture variation only found in Y are denoted Orthogonal in Y(OPLS).

The OPLS model is based on the OPLS algorithm. The O2PLS model is based on the similar O2PLS algorithm, but in addition there is a PCA step. PCA is used after convergence of the O2PLS algorithm, to exhaust the E and F residual matrices from all remaining systematic variation. This yields the additional Orthogonal in X(PCA) and Orthogonal in Y(PCA) components.

The method underlying a certain orthogonal component is indicated in the name of the component in the **Model Window**.

Note: The model window for OPLS models displays, if existing, three types of components: Predictive, Orthogonal in X, Orthogonal in Y. Additionally, The model window for O2PLS displays, if existing, Orthogonal in X and Orthogonal in Y components estimated by PCA.

Figure 2. The Model Window for an O2PLS model with 7 predictive, 3 Orthogonal in X and 6 Orthogonal in Y components (a 7+3(1+2) +6(1+5) O2PLS model).



Title: Final O2PLS model

Type: O2PLS   Observations (N)=930, variables (K)=303 (X=119, Y=184)

Component	R2X	R2X(cum)	Eigenvalue	R2	R2(cum)	Q2	Limit	Q2(cum)	R2Y	R2Y(cum)	EigenvalueY	Significance
Model		0.86			0.649			0.665		0.853		
⊟ Predicti...		0.769			0.647			0.665		0.724		
P1	0.389	0.389	46.3	0.344	0.344	0.343	0.01	0.343	0.351	0.351	64.5	R1
P2	0.156	0.545	18.6	0.113	0.457	0.121	0.01	0.463	0.124	0.474	22.8	R1
P3	0.0829	0.628	9.87	0.0636	0.521	0.04...	0.01	0.509	0.07...	0.553	14.5	R1
P4	0.0402	0.668	4.79	0.0543	0.575	0.05...	0.01	0.567	0.06...	0.615	11.4	R1
P5	0.0466	0.715	5.55	0.034	0.609	0.05...	0.01	0.62	0.04...	0.662	8.51	R1
P6	0.0313	0.746	3.72	0.0222	0.631	0.01...	0.01	0.638	0.03...	0.698	6.69	R1
P7	0.0233	0.769	2.77	0.0158	0.647	0.02...	0.01	0.665	0.026	0.724	4.78	R1
⊟ Orthog...		0.0458			0.00218							
O1	0.0458	0.0458	5.45	0.002...	0.00218							R1
⊟ Orthog...		0.0447			0							
O2	0.0246	0.0246	2.93	0	0							R1
O3	0.0201	0.0447	2.39	0	0							R1
⊟ Orthog...										0.0376		
O1									0.03...	0.0376	6.92	R1
⊟ Orthog...										0.0914		
O2									0.02...	0.0247	4.55	R1
O3									0.022	0.0467	4.06	R1
O4									0.01...	0.0636	3.1	R1
O5									0.015	0.0786	2.76	R1
O6									0.01...	0.0914	2.35	R1

The **Model Window** displays:

Section	Description	Component types
Model	Summarizes the model, showing the cumulative R2X, R2, Q2, and R2Y.	

Section	Description	Component types
Predictive	The Predictive section where the first row summarizes the predictive components in the model followed by a listing of each predictive component.	The predictive loading vectors are *p* for the X-block and *q* for the Y- block. The predictive score vectors are *t* for the X-block and *u* for the Y-block. In the figure above there are 7 components for *p*, *q*, *t* and *u*.
Orthogonal in X (OPLS)	The Orthogonal in X(OPLS) section where the first row summarizes the orthogonal components in the X model followed by a listing of each orthogonal in X component. The orthogonal in X components show the variation in X that is uncorrelated to Y.	The orthogonal in X(OPLS) loading vectors are *po* for the X-block and *so* for the Y-block. The orthogonal in X (OPLS) score vector is *to* for the X-block. In the figure above there is one orthogonal in X(OPLS) component. This means that the po[1], so[1], and to[1] vectors are the orthogonal in X(OPLS) vectors.
Orthogonal in X (PCA)	The Orthogonal in X(PCA) sections where the first row summarizes the orthogonal components in the X model followed by a listing of each orthogonal in X component. The orthogonal in X components show the variation in X that is uncorrelated to Y	The orthogonal in X(PCA) loading vectors are *po* for the X-block and *so* for the Y-block. The orthogonal in X (PCA) score vector is *to.* The orthogonal in X(PCA) components are extracted after the orthogonal in X(OPLS) components, and their relational order is indicated through the shared nomenclature. In the figure above there are two orthogonal in X(PCA) components. This means that the po[2], po[3], so[2], so[3], to[2] and to[3] vectors are the orthogonal in X(PCA) vectors
Orthogonal in Y (OPLS)	The Orthogonal in Y (OPLS) sections where the first row summarizes the orthogonal components in the Y model followed by a listing of each orthogonal in Y component. The orthogonal in Y components show the variation in Y that is uncorrelated to X.	The orthogonal in Y(OPLS) loading vectors are *r* for the X-block and *qo* for the Y-block. The orthogonal in Y (OPLS) score vector is *uo* for the Y block. In the figure above there is one orthogonal in Y(OPLS) component. This means that the r[1], qo[1], and uo[1] vectors are the orthogonal in Y(OPLS) vectors.
Orthogonal in Y (PCA)	The Orthogonal in Y (PCA) sections where the first row summarizes the orthogonal components in the Y model followed by a listing of each orthogonal in Y component. The orthogonal in Y components show the variation in Y that is uncorrelated to X	The orthogonal in Y(PCA) loading vectors are *r* for the X-block and *qo* for the Y-block. The orthogonal in Y (PCA) score vector is *uo* for the Y block. The orthogonal in Y(PCA) components are extracted after the orthogonal in Y(OPLS) components and their relational order is indicated through the shared nomenclature. In the figure above there are five orthogonal in Y(PCA) components. This means that the r[2]-r[6], qo[2]-qo[6], and uo[2]-uo[6] vectors are the orthogonal in Y(PCA) vectors.

The table columns are:

- Component - Component index.

- R2X - Fraction of X variation modeled in that component, using the X model.
- R2X(cum) - Cumulative R2X up to the specified component.
- Eigenvalue - The minimum number of observations (N) and X-variables multiplied by R2X, that is, min(N,K)*R2X.
- R2 - Fraction of Y variation modeled in that component, using the X model.
- R2(cum) - Cumulative R2 up to the specified component.
- Q2 - Fraction of Y variation predicted by the X model in that component, according to cross-validation.
- Q2(cum) - Cumulative Q2 up to the specified component.
- R2Y - Fraction of the Y variation modeled in that component, using the Y model.
- R2Y(cum) - Cumulative R2Y up to the specified component
- EigenvalueY - The minimum number of observations (N) and Y-variables multiplied by R2Y, that is, min(N,M)*R2Y.
- Significance – Significance level of the model component.

For more, see the OPLS/O2PLS - Orthogonal PLS modeling section in the Statistical appendix.

7.2.12 Model Options

The **Model Options** hold model specific options. Most options are inherited from the **Project Options**.

Note: Model options cannot be changed for a wrapper model, only for the individual class or phase models.

To open the **Model Options** use one of these methods:

- Click the **Model Options** dialog box launcher in the bottom right corner of the **Workset** group, on the **Home** tab.
- Click the **Options** button in the **Model Window**.
- Right-click the model, either in the **Project Window** or in the **Model Window**, and click **Model options**.

Model Options includes the following pages:

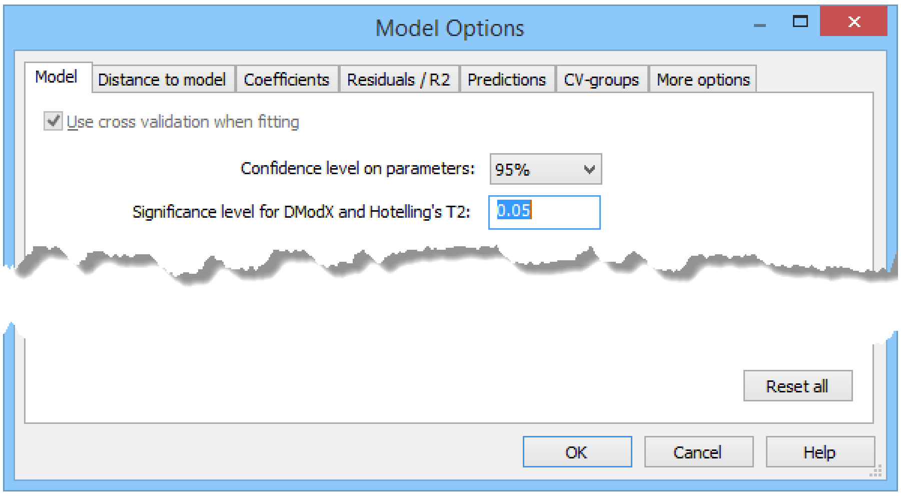
- **Model** – for setting confidence and significance levels, and selecting whether to use cross validation when fitting.
- **Distance to model** – for selecting in which domain the distance to model should be displayed.
- **Coefficients** – for selecting type of coefficient to display by default.
- **Residuals / R2** – for selecting residual and R2 type to display by default.
- **Predictions –** for selecting to display the predictions in scaled and transformed units and whether to trim the predictions as the workset.
- **CV-groups** – enables customized assignment of the cross validation groups.
- **More options** – displays and allows change of the used **T2 Center** and **Eigenvalue similarity level**.

Note: Changes in **Model Options** are only valid for the current model.

7.2.12.1 Model page

The **Model** page displays:

- **Use cross validation when fitting** box.
- **Confidence level on parameters** current setting.
- **Significance level for DModX and Hotelling's T2** current setting.
- **Reset all** button.



☑ Use cross validation when fitting

Confidence level on parameters: 95%

Significance level for DModX and Hotelling's T2: 0.05

7.2.12.1.1 Cross validation when fitting

By default, cross validation is used when fitting to decide whether a component is considered significant or not.

To fit components without cross validation, clear the **Use cross validation when fitting** check box.

Autofit is unavailable when the **Use cross validation when fitting** check box is cleared.

7.2.12.1.2 Confidence level on parameters

The confidence level used when computing confidence intervals on the parameters is by default **95%**.

To change from the default select **90%**, **99%**, or **None** in the **Confidence level on parameters** box.

7.2.12.1.3 Significance level for DModX and Hotelling’s T2

The significance level used when computing the critical limits for DModX and the Hotelling's T^2 ellipse is **0.05** (95% confidence).

To use a different significance level than 0.05, type a value between 0 and 1 (not exactly 0 or 1 but between) in the **Significance level for DModX and Hotelling's T2** field.

To not display the limits select ***None*** in the **Limits** page in **Properties**. For details, see the Limits subsection in Chapter 14, Plot and list contextual tabs.

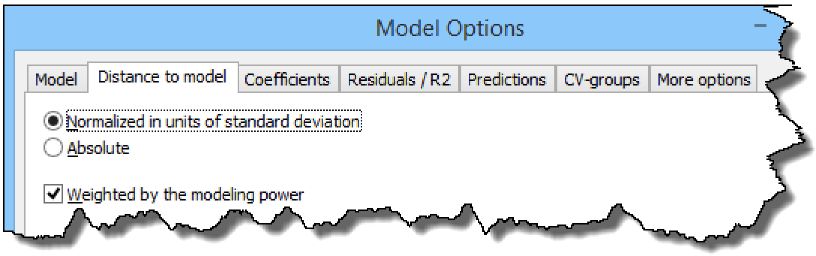
7.2.12.1.4 Reset all

To reset the options of the **Model**, **Distance to model**, **Coefficients**, **Residuals/R2**, and **Predictions** pages to the Project Options, click **Reset all**.

7.2.12.2 Distance to model page

The **Distance to model** page displays:

- **Normalized in units of standard deviation**.
- **Absolute**.
- **Weighted by the modeling power**.



● Normalized in units of standard deviation

○ Absolute

☑ Weighted by the modeling power

7.2.12.2.1 Normalized or absolute distances

The distance to the model (DModX and DModY) can be expressed as an **Absolute** or a **Normalized** value, where the normalized is in units of standard deviation of the pooled RSD of the model.

By default, the **Normalized in units of standard deviation** option is selected.

To change from the default, click **Absolute**.

7.2.12.2.2 Weighted by the modeling power

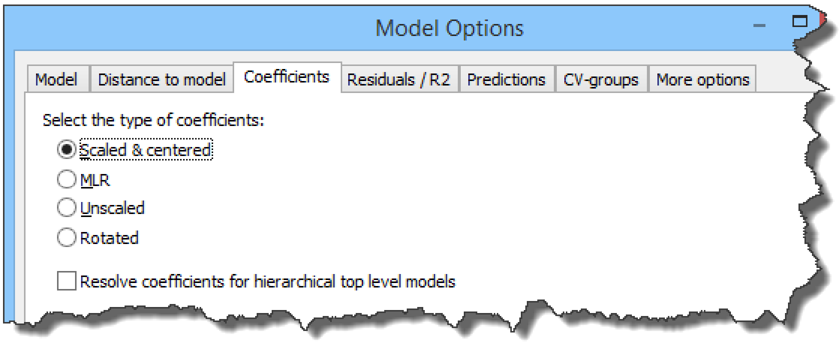
When computing the distance to the model (DModX), the residuals are by default weighted by the modeling power of the variables.

To change from the default, clear the **Weighted by the modeling power** check box.

For details, see the MPow weighted distance to the model section in the Statistical appendix.

7.2.12.3 Coefficients page

The **Coefficients** page displays the available types of coefficients: **Scaled & centered**, **MLR**, **Unscaled**, and **Rotated** and the **Resolve coefficients for hierarchical top level models** check box.


Model Options

Model | Distance to model | Coefficients | Residuals / R2 | Predictions | CV-groups | More options

Select the type of coefficients:

● Scaled & centered
○ MLR
○ Unscaled
○ Rotated

□ Resolve coefficients for hierarchical top level models

7.2.12.3.1 Scaled and centered

With **Scaled & centered** selected, the coefficients displayed are for scaled and centered X and scaled Y (as specified in the workset). This is the SIMCA default. Use these coefficients to interpret the influence of the x-variables on Y. Coefficients of different responses (y-variables) are also comparable as the y-variables are normalized (scaled).

7.2.12.3.2 MLR

With **MLR** selected, the coefficients displayed are the PLS coefficients when:

- Y is unscaled and uncentered,
- X is scaled and centered, and
- the second centering and scaling of the cross terms and squares has been removed.

7.2.12.3.3 Unscaled

With **Unscaled** selected, the coefficients displayed are the coefficients when X and Y are unscaled and uncentered.

7.2.12.3.4 Rotated

With **Rotated** selected, the coefficients are rotated so they correspond as much as possible to the pure spectral or other profiles. For more see the Coefficients rotated - CoeffRot subsection in the Statistical appendix.

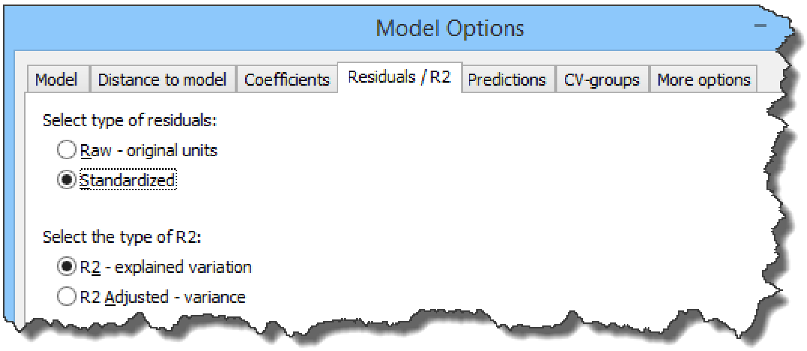
7.2.12.3.5 Resolve coefficients for hierarchical top level models

To automatically resolve coefficients of hierarchical top level models, select the **Resolve coefficients for hierarchical top level models** check box.

Note: For hierarchical models, **Resolve coefficients** is available from the **Tools** tab when the Coefficient plot or Coefficient overview plot is active.

7.2.12.4 Residuals / R2 page

The **Residuals / R2** page displays the available types of residuals and R2.



Select type of residuals:

○ Raw - original units

● Standardized

Select the type of R2:

● R2 - explained variation

○ R2 Adjusted - variance

7.2.12.4.1 Residuals

The **Standardized** residuals are displayed by default. The standardized residuals are the unscaled residuals divided by their standard deviation.

To display the residuals in original, unscaled units, click **Raw – original units**.

7.2.12.4.2 R^2

R2 – explained variation is selected by default. R^2 is the fraction of the Sum of Squares (SS) explained by the model.

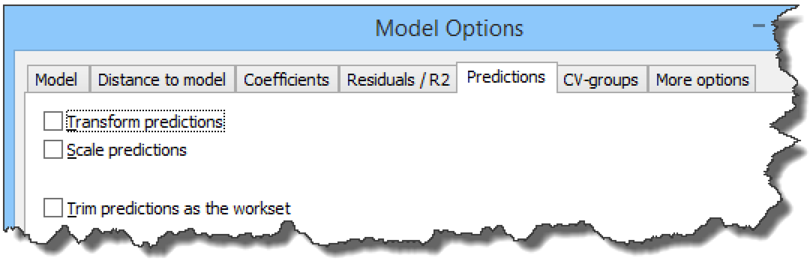
R^2 adjusted is the fraction of variance explained by the model (SS adjusted for the degrees of freedom).

To display the adjusted R^2, click **R2 Adjusted – variance**.

7.2.12.5 Predictions page

The **Predictions** page displays the following check boxes:

- **Transform predictions**
- **Scale predictions**
- **Trim predictions as the workset**



□ Transform predictions

□ Scale predictions

□ Trim predictions as the workset

7.2.12.5.1 Transform predictions

When the y-variables have been transformed, by default the predictions are back transformed to the original units.

To display the y-variables in transformed units, select the **Transform predictions** check box.

7.2.12.5.2 Scale predictions

When the y-variables have been scaled, by default the predictions are rescaled to the original units.

To display the y-variables in the same units as the workset, select the **Scale predictions** check box.

7.2.12.5.3 Trim predictions as the workset

When the workset has been trimmed or Winsorized, the predictionset can be trimmed or Winsorized in the same manner by selecting the **Trim predictions as the workset** check box.

By default the predictionset is not trimmed or Winsorized.

Note: When selecting the **Trim predictions as the workset** check box, all predictions found on the **Predict** tab are displayed trimmed.

7.2.12.6 CV-groups page

The default for regular projects is to assign every Nth observation to the same group, where the default N is defined in the **Fit** section on the **Project options** page in the **Options** dialog. The default for batch models evolution models is to group whole batches in the same group.

To change from the default, use the **Model Options**, **CV-groups** page to specify the assignment of cross validation groups.

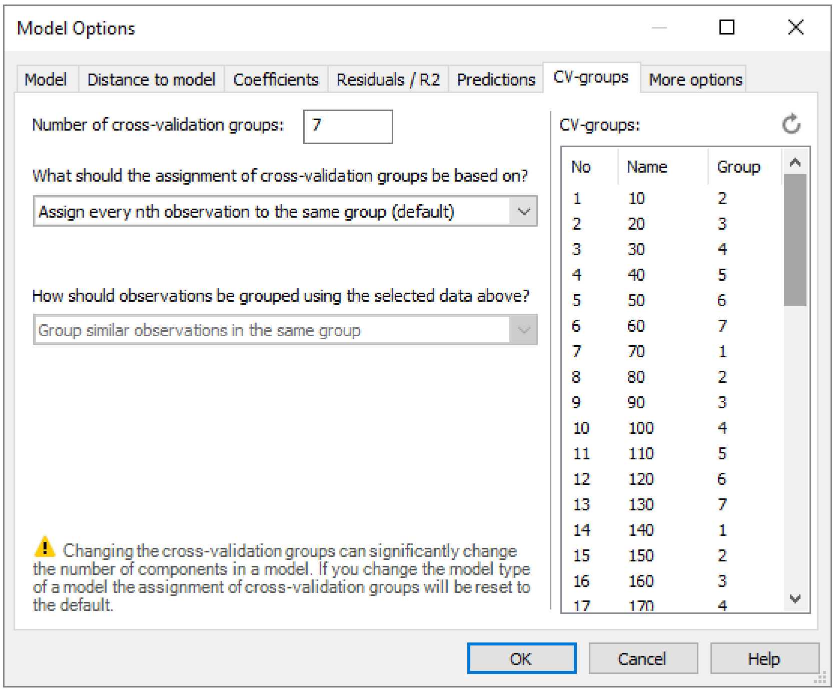
To access the **CV-groups** page, the model has to be unfitted. For fitted models, this page can be opened but all functionality is unavailable.

There are four sections in the **CV-groups** page:

- **Number of cross validation groups.**
- **What should the assignment of cross validation groups be based on?**
- **How should observations be grouped using the selected data above?**
- **CV groups** list.

All points are described in the subsections that follow.

Note: Clicking **Apply** updates the cross validation groups. Neglecting to click **Apply** before clicking **OK** will default back to the original cross validation groups.



Number of cross-validation groups: 7

What should the assignment of cross-validation groups be based on?
Assign every nth observation to the same group (default)

How should observations be grouped using the selected data above?
Group similar observations in the same group

Changing the cross-validation groups can significantly change the number of components in a model. If you change the model type of a model the assignment of cross-validation groups will be reset to the default.

CV-groups:

No	Name	Group
1	10	2
2	20	3
3	30	4
4	40	5
5	50	6
6	60	7
7	70	1
8	80	2
9	90	3
10	100	4
11	110	5
12	120	6
13	130	7
14	140	1
15	150	2
16	160	3
17	170	4

7.2.12.6.1 Number of cross validation groups

The number of cross validation groups decides the size of the excluded observation group during component computation. With the default number of cross validation groups (7) a 7th of the observations is excluded during each cross validation round.

To change from the default, type a number in the **Number of cross validation groups** field.

Note: When clicking **Apply** with the **Group observations with the same value in the same group** check box selected, the **Number of cross validation groups** field is automatically changed to the number of unique entries.

7.2.12.6.2 Cross validation group assignment

There are 4 types of assignments (5 for batch) available under **What should the assignment of cross validation groups be based on** for regular projects and 3 types of grouping options under **How should observations be grouped using the selected data above**.

In this table the options found under **What should the assignment of cross validation groups be based on?** are described:

In this table the options found under **How should observations be grouped using the selected data above?** are described:

Option	Description of assignment
Group similar observations in the same group	Groups observations with values numerically close by first sorting the selected vector (score, variable, or observation secondary ID), and then parting the vector in the number of cross validation groups and setting the first part as CV group 1, the second part as CV group 2 etc.
Group dissimilar observations in the same group	Groups observations with values numerically distant by sorting the selected vector and assigning groups as in **Assign every Nth observation to the same group (default)**.
Group observations with the same value in the same group	Groups observations with exactly the same value or text by sorting the selected vector, counting the number of unique entries, creating CV groups, one for each unique entry, and then assigning the observations to the respective groups. Note that when clicking **Apply** with this option, the **Number of cross validation groups** is automatically changed to the number of unique entries.
Divide the observations into blocks of equal range	Available when assigning cross validation groups using a variable. With a time variable, the variable range format is adjusted for time. When there are values exactly on the limit between two ranges, these observations are placed in the higher value range. Observations with missing in the variable that specifies the assignment are randomly assigned to all groups..

Note: Configuring cross validation groups must be done before the model is fitted.

7.2.12.6.3 Cross validation group examples

In this table the available combinations, with examples, are described:

No.	Assignment type	Grouping type	Example
1.	Assign every Nth observation to the same group (default)	No grouping type available.	With 7 cross validation groups, the first cross validation group will hold observations number 7, 14, 21 etc. The second CV group will hold observations 1, 8, 15, the third 2, 9, 16 etc.
2.	Divide the observations into equally sized blocks	No grouping type available.	With 7 cross validation groups, the first 7th of the observations are positioned in CV group 1, the second 7th in CV group 2 etc.
3.	Assign observations based on the score from model Mxx	Group similar observations in the same group	With 70 observations sorted according to the value in t[1], and 7 cross validation groups, the 10 observations with the smallest score values are assigned to CV group 1, etc.
4.		Group dissimilar observations in the same group	With 70 observations sorted according to the value in t[1], and 7 cross validation groups, the first CV group will hold observations with sort order number 7, 14, 21 etc. The second CV group will hold observations 1, 8, 15, the third 2, 9, 16 etc. as in 1.
5.		Group observations with the same value in the same group	The observations are sorted according to the value in t[1]. CV groups are created, one for each unique value. Generally this combination of options will lead to the leave-one-out solution.

No.	Assignment type	Grouping type	Example
6.	Assign observations based on variable V1	Group similar observations in the same group	With 70 observations sorted according to V1, and 7 cross validation groups, the 10 observations with the smallest values are assigned to CV group 1, etc.
7.		Group dissimilar observations in the same group	With 70 observations sorted according V1, and 7 cross validation groups, the first CV group will hold observations with sort order number 7, 14, 21 etc. The second CV group will hold observations 1, 8, 15, the third 2, 9, 16 etc. as in 1.
8.		Group observations with the same value in the same group	The observations are sorted according to V1. CV groups are created, one for each unique value.
9.		Divide the observations into blocks of equal range	The observations are sorted according to V1. With 7 cross validation groups, the range is parted in 7 equally sized ranges. The group with the smallest range are assigned to CV group 1, the next in line to CV group 2, etc.
10.	Assign observations based on observation ID	Group similar observations in the same group	The selected secondary observation ID is sorted. Then the entire vector is parted in the entered number of groups, for instance 7. This means that, with 70 observations and 7 cross validation groups, the 10 observations with the lowest ID values/text values are assigned to CV group 1, etc.
11.		Group dissimilar observations in the same group	With 70 observations sorted according to the selected observation ID, and 7 cross validation groups, the first CV group will hold observations with sort order number 7, 14, 21 etc. The second CV group will hold observations 1, 8, 15, the third 2, 9, 16 etc. as in 1.
12.		Group observations with the same value in the same group	The observations are sorted according to the selected observation ID. CV groups are created, one for each unique value.
13.	Group whole batches in the same group	Group observations with the same value in the same group	The observations are sorted according to batch ID. The batches are assigned to the number of CV groups listed first in this page. For instance, with 10 batches, the observations of the 1st and 8th batches are assigned to CV group 1, the observations of the 2nd and 9th batches are assigned to CV group 2 etc.

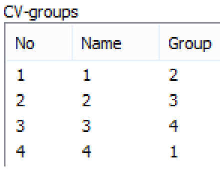
7.2.12.6.4 Cross validation group list

Under **CV-groups** all included observations are listed in the order of the dataset.

The **No** column lists the internal numbering, **Name** lists the primary observation ID, and **Group** lists the current cv group assignment.

Clicking the **Apply**-button updates the **CV-groups** list **Group** column according to the selected options.

Note: Configuring cross validation group must be done before the model is fitted.



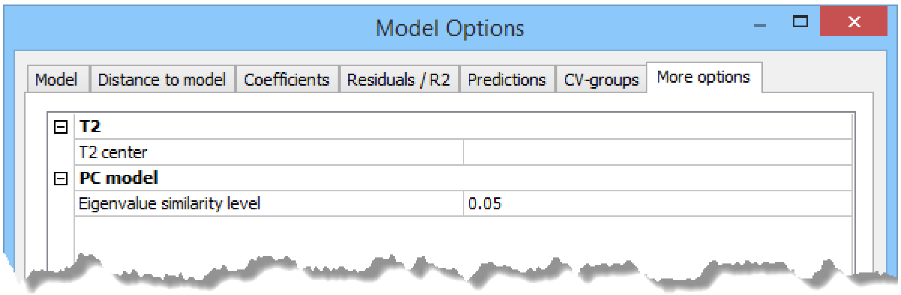
CV-groups

No	Name	Group
1	1	2
2	2	3
3	3	4
4	4	1

7.2.12.7 More options

The **More options** page contains advanced options that should generally not be altered. The page displays and allows change of the following:

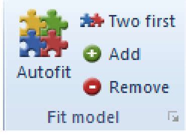
- **T2 center** - used when calculating T2Range and should only be changed to '0' when planning to import the model in MODDE. In all other cases it should remain at -99 to use the calculated center.
- **Eigenvalue similarity level** - is used in the autofit rules for PC modeling. The default is 0.05 and should generally not be changed.



T2	
T2 center	
PC model	
Eigenvalue similarity level	0.05

7.3 Fit model

You can fit the model using Autofit, Two first components, Add component, and Remove component in the **Fit model** group.



7.3.1 Autofit

SIMCA extracts as many components as considered significant when clicking **Autofit** in the **Fit model** group, on the **Home** tab.

When the active model is a wrapper model, BEM or CM, clicking **Autofit** opens the **Specify Autofit** dialog allowing you to autofit all models in the wrapper or a selection.

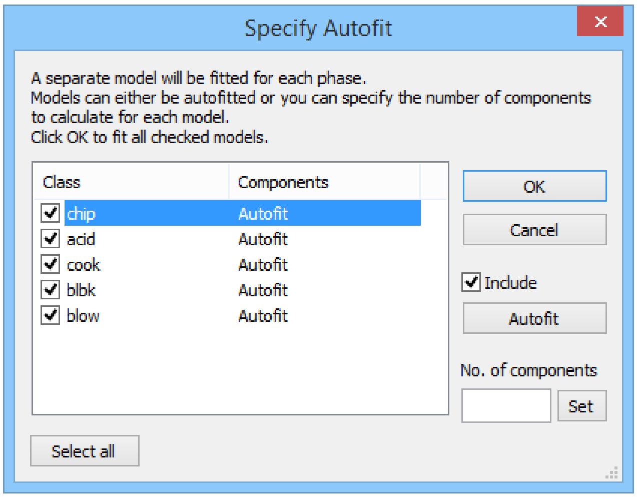
Autofit is only available when using cross validation.

7.3.1.1 Specifying how to fit the class or phase models

In the **Specify Autofit** dialog the list displays all class/phase models, all unfitted models default selected, and **Autofit** is the planned fit method. For fitted models, the current number of components is listed under **Components** and the models are not selected.

- To not fit a model, clear the corresponding check box by clicking it or selecting the row and clearing the **Include** check box.
- To fit a certain number of components, select the corresponding rows, enter the wanted number in the **No. of components** field and click **Set**.
- To autofit a model that has already been fitted, select the model and click the **Autofit** button.

Clicking **OK** closes the dialog and all the selected class models are fitted as specified.


Specify Autofit
A separate model will be fitted for each phase.
Models can either be autofitted or you can specify the number of components to calculate for each model.
Click OK to fit all checked models.

Class	Components
☑ chip	Autofit
☑ acid	Autofit
☑ cook	Autofit
☑ blbk	Autofit
☑ blow	Autofit

OK
Cancel
☑ Include
Autofit
No. of components
Set
Select all

7.3.1.2 Component significant according to cross validation rules

For regular (non-batch) PLS models, a component is significant if it is cross validated according to rule 1 or rule 2.

For PC models, a component is significant if it is cross validated according to rules 1, 2 or 3.

For OPLS model, a component is significant if it is cross validated according to rule 1 or rule 2.

For O2PLS models, a component is significant if it is cross validated according to rules 1, 2 or 3.

For details about the cross validation rules, see the Cross validation section in the Statistical appendix.

7.3.2 Two first components

To compute the two first components of the model, click **Two first** in the **Fit model** group, on the **Home** tab.

Two first is unavailable:

- after the two first components have been computed.
- for OPLS/O2PLS models with more than one y-variable.

Note: With a wrapper model marked, clicking **Two first** adds the two first components to all models in the wrapper.

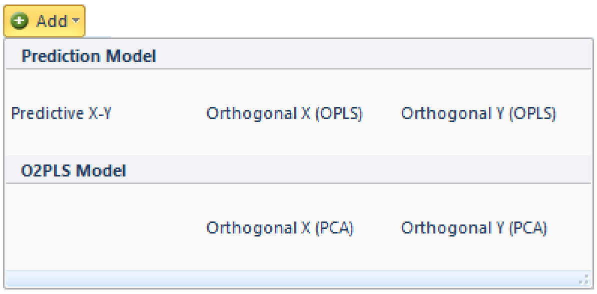
7.3.3 Add component

To compute the next model component, on the **Home** tab, in the **Fit model** group, click **Add**.

The component, irrespective of its significance, is added to the model if possible.

For OPLS and O2PLS models with more than one y-variable you can select which type of component to add from the respective galleries.

For OPLS the O2PLS specific PCA orthogonal components are unavailable.



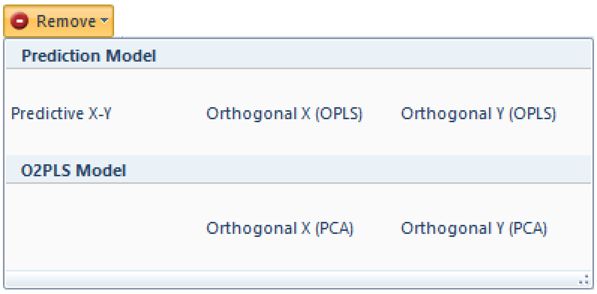
Note: With a wrapper model marked, clicking **Add** adds the next component to all models in the wrapper.

7.3.4 Remove component

When the model has been overfitted, removing components one by one is available by clicking **Remove** in the **Fit model** group on the **Home** tab.

Remove is available when the model has one or more components.

For OPLS and O2PLS models with more than one y-variable you can select which type of component to remove from the respective galleries.



Note: With a wrapper model marked, clicking **Remove** deletes the last component for all models in the wrapper.

7.4 Diagnostics & interpretation

The **Diagnostics & interpretation** group holds the plots and lists commonly used after fitting a model.

7.4.1 Overview plots

The first button in the **Diagnostics & interpretations** group is **Overview**. When clicked it opens the following plots and tiles them:

- X/Y overview
- Score scatter
- Loading scatter
- DModX

For BEM the following plots are displayed:

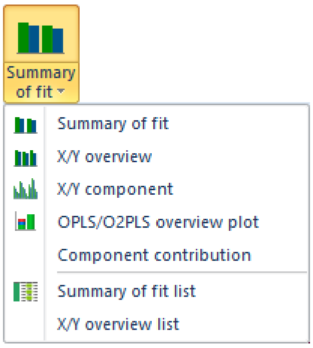
- X/Y overview
- Scores BCC
- Loadings column
- DModX BCC

For BLM the following plots are displayed:

- X/Y overview
- Score scatter
- Loadings Sources of variation Plot
- DModX

7.4.2 Summary of fit

The summary plots and lists are found by clicking the **Summary of Fit** button arrow. The available plots and lists are: **Summary of fit**, **X/Y overview**, **X/Y component**, **OPLS/O2PLS overview**, **Component contribution**, **Summary of fit list**, and **X/Y overview list**.



The summary plots by default display R2. To display R2 adjusted instead, click the plot and click **Properties** in the mini-toolbar. In the **Properties** dialog, click the **R2** tab, and change as desired.

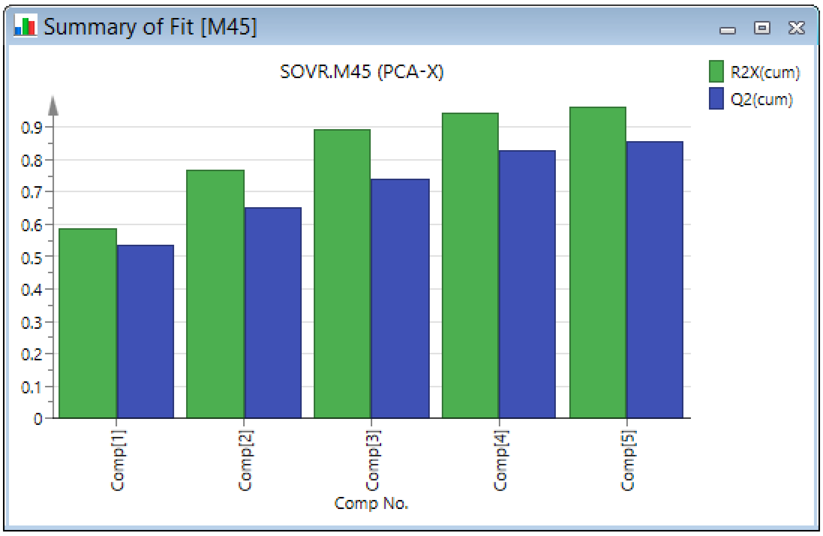
For more about the **Properties** dialog, see the Tools tab section in Chapter 14, Plot and list contextual tabs.

Note: For OPLS and O2PLS models, the summary plots and lists only display statistics for the predictive components for models with more than one predictive component.

For model statistics for the orthogonal components, see the Model window for OPLS and O2PLS models subsection earlier in this chapter.

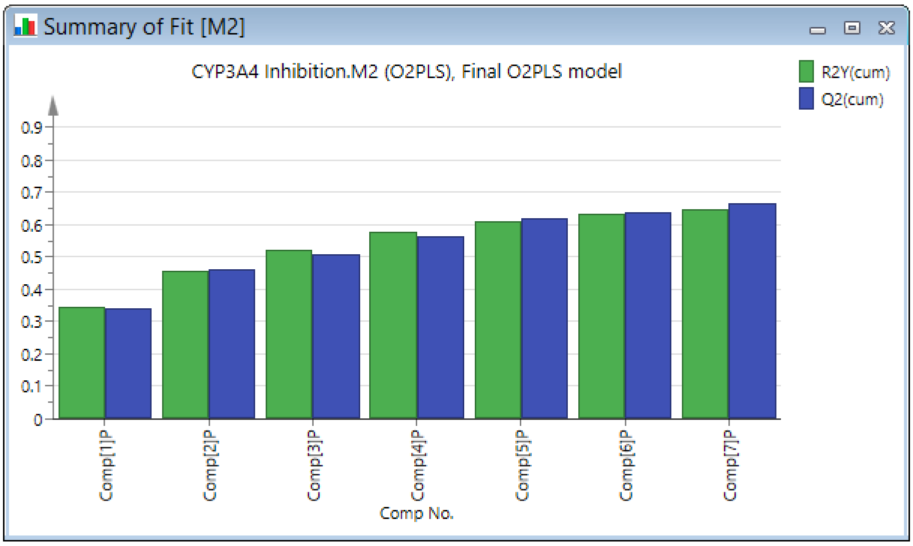
7.4.2.1 Summary of fit plot

The **Summary of Fit** plot displays the cumulative R^2 and Q^2 for the X-matrix for PCA and for the Y-matrix for PLS/OPLS/O2PLS, after each extracted component.

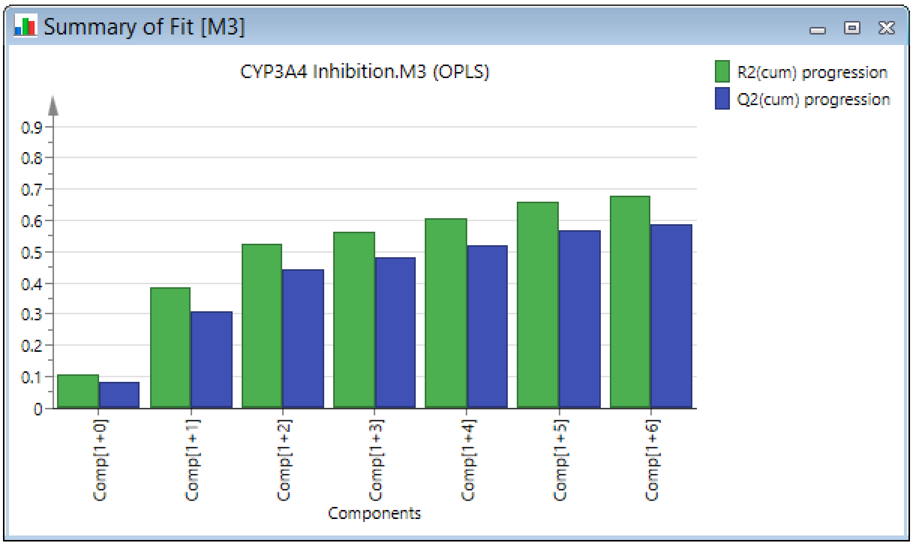


7.4.2.2 Summary of fit plot for OPLS

For an OPLS or O2PLS model with more than one predictive component, the **Summary of Fit** plot displays the cumulative R2 and Q2 for the Y-matrix modeled by X. For OPLS and O2PLS models the components are labeled P, for predictive.

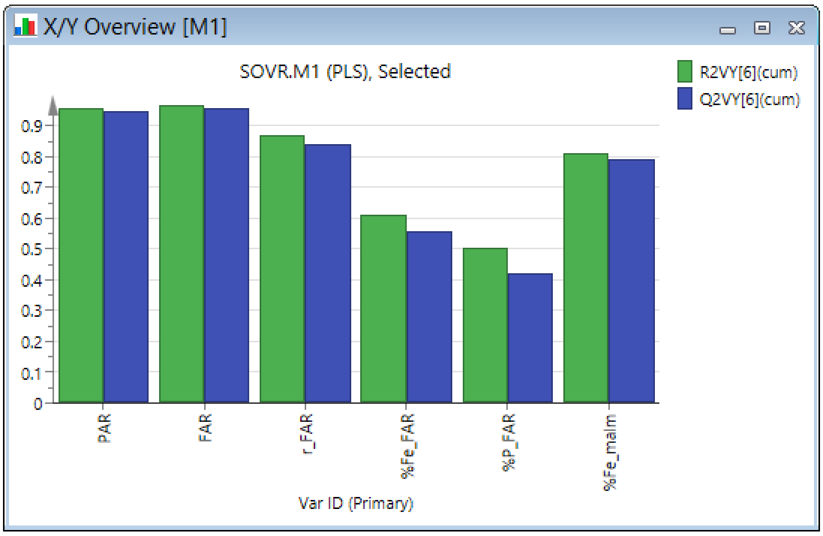


For a model with only one predictive component, the **Summary of Fit** plot displays how the R2 and Q2 for the Y-matrix evolve (progress) as 1+0, 1+1, 1+2 including the predictive component and each added orthogonal component to the overall explanation of the Y-variance.



7.4.2.3 X/Y overview plot

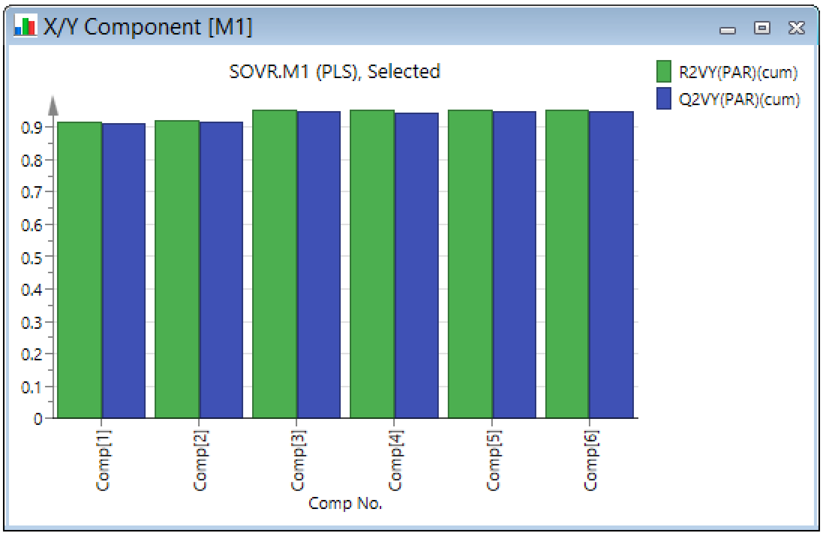
The **X/Y Overview** plot displays the individual cumulative R^2 and Q^2 for every X variable with a PCA model and every Y variable with a PLS model.



7.4.2.4 X/Y component plot

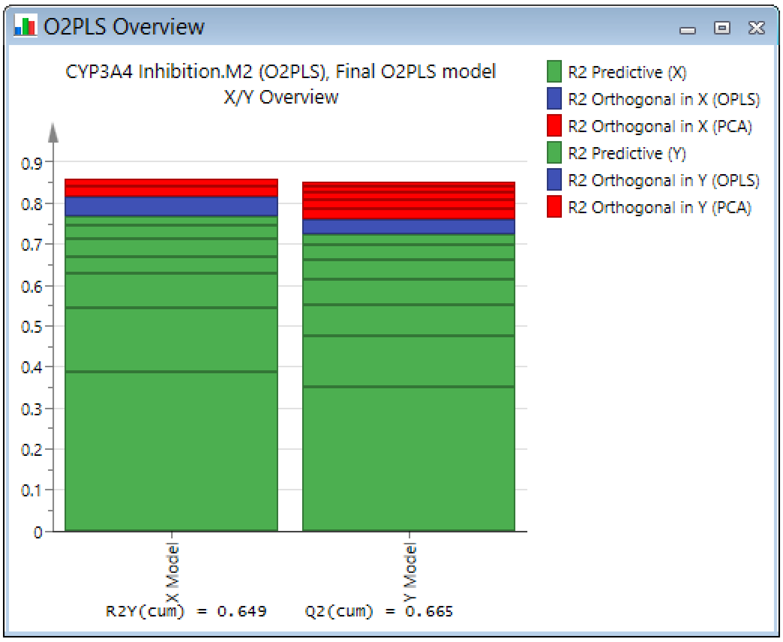
The **X/Y Component** plot displays the R²X or R²Y and Q²X or Q²Y cumulative, per component for the selected X variable with a PCA model or Y variable for a PLS model.

To switch which variable is displayed, on the **Tools** tab, in the **Properties** group, use the **Y-variable** box alternatively use open the **Properties** dialog. For more about the Properties dialog, see the Tools tab section in Chapter 14, Plot and list contextual tabs.



7.4.2.5 OPLS/O2PLS overview plot

The **OPLS/O2PLS overview** provides a graphical summary of the predictive and orthogonal sources of variation in the model. Being an extension of the conventional Summary of fit plot of SIMCA, this column plot is both stacked and color coded in accordance with the predictive and orthogonal variance structures (Figure 3).

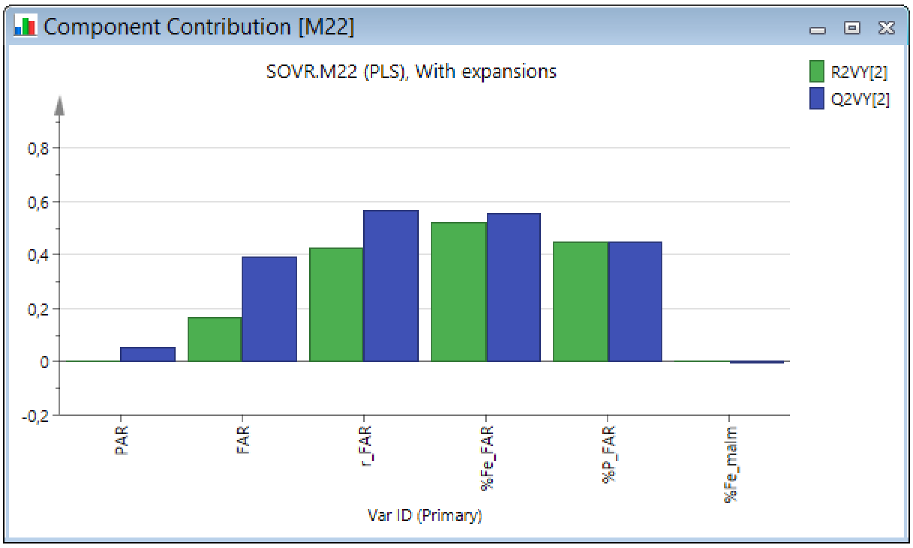


The green color corresponds to the joint X/Y variation. The blue color indicates orthogonal variations in X or Y respectively, estimated in terms of the OPLS/O2PLS algorithm. The red color represents orthogonal variations in X or Y, estimated by PCA subsequent to the convergence of the OPLS/O2PLS algorithm.

7.4.2.6 Component contribution plot

The **Component contribution** plot for every fitted X, with a PCA model, or Y, with a PLS model, the plot displays R^2X or R^2Y and Q^2 for a selected component. The selected component number is displayed in the legend.

To change component, on the **Tools** tab, in the **Properties** group, click the **Component** box. Alternatively open **Properties**, and click the **Component** tab. For more about the Properties dialog, see the Tools tab section in Chapter 14, Plot and list contextual tabs.



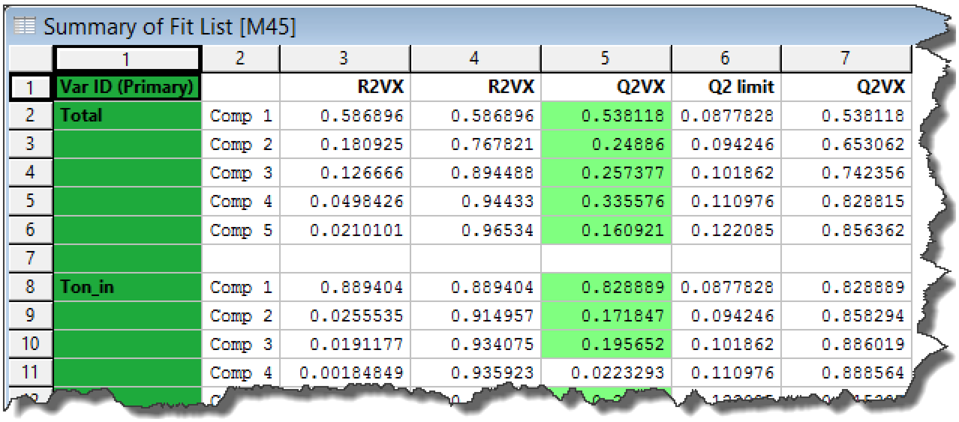
7.4.2.7 Summary of fit list

The **Summary of Fit List** displays, for each component and for the total X (PCA) or Y (PLS/OPLS/O2PLS) matrix:

- R2.
- R2 cumulative.
- Q2 – Significant components are colored green.
- Q2 limit.

- Q2 cumulative.

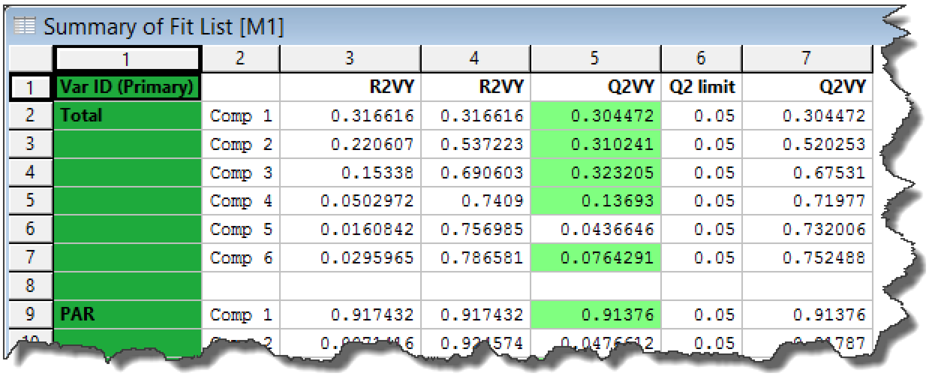
An example for a PCA model:



Summary of Fit List [M45]

	1	2	3	4	5	6	7
1	Var ID (Primary)		R2VX	R2VX	Q2VX	Q2 limit	Q2VX
2	Total	Comp 1	0.586896	0.586896	0.538118	0.0877828	0.538118
3		Comp 2	0.180925	0.767821	0.24886	0.094246	0.653062
4		Comp 3	0.126666	0.894488	0.257377	0.101862	0.742356
5		Comp 4	0.0498426	0.94433	0.335576	0.110976	0.828815
6		Comp 5	0.0210101	0.96534	0.160921	0.122085	0.856362
7							
8	Ton_in	Comp 1	0.889404	0.889404	0.828889	0.0877828	0.828889
9		Comp 2	0.0255535	0.914957	0.171847	0.094246	0.858294
10		Comp 3	0.0191177	0.934075	0.195652	0.101862	0.886019
11		Comp 4	0.00184849	0.935923	0.0223293	0.110976	0.888564

An example for a PLS model:



Summary of Fit List [M1]

	1	2	3	4	5	6	7
1	Var ID (Primary)		R2VY	R2VY	Q2VY	Q2 limit	Q2VY
2	Total	Comp 1	0.316616	0.316616	0.304472	0.05	0.304472
3		Comp 2	0.220607	0.537223	0.310241	0.05	0.520253
4		Comp 3	0.15338	0.690603	0.323205	0.05	0.67531
5		Comp 4	0.0502972	0.7409	0.13693	0.05	0.71977
6		Comp 5	0.0160842	0.756985	0.0436646	0.05	0.732006
7		Comp 6	0.0295965	0.786581	0.0764291	0.05	0.752488
8							
9	PAR	Comp 1	0.917432	0.917432	0.91376	0.05	0.91376

For details about the displayed vectors, see the tables in the **X/Y Overview List** section next.

Note: For OPLS models with one predictive component this list displays the progression vectors.

7.4.2.8 X/Y overview list

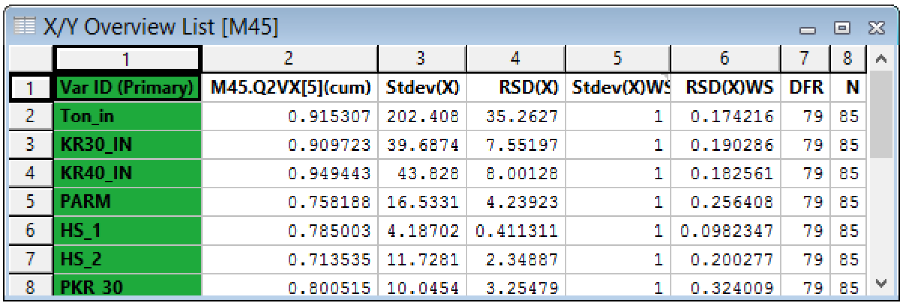
The **X/Y Overview List** displays a number of vectors. For PCA models the vectors are specific for the X-block and for PLS/OPLS/O2PLS models for the Y-block.

7.4.2.8.1 X/Y overview list for PCA models

For PCA models the **X/Y Overview List** displays the following for each X variable:

Vector	Description
Q^2VX(Cum)	The cumulative predicted fraction (cross-validation) of the variation of X.
Stdev(X)	Standard deviation of X in original units, and transformed if X is transformed.
RSD(X)	Residual standard deviation of X in original units (transformed if the variable is transformed)
Stdev(X)WS	Standard deviation of X scaled as specified in the workset (normally scaled to unit variance, UV).
RSD(X)WS	Residual Standard Deviation, scaled as specified in the workset (normally scaled to unit variance, UV).
DFR	Degrees of freedom of the X residuals.
N	Non missing observations in X.

An example for a PCA model:



X/Y Overview List [M45]

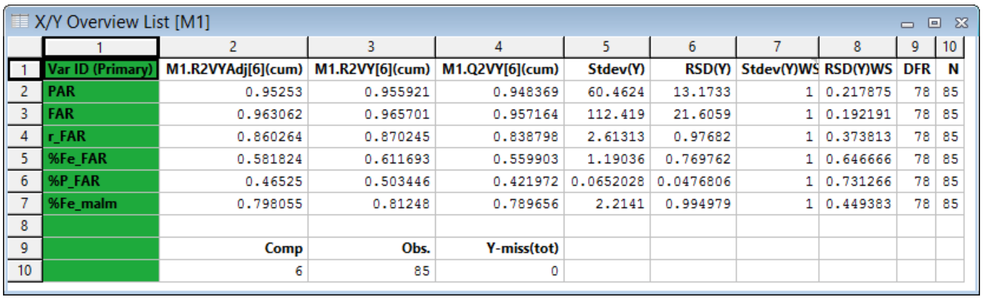
	1	2	3	4	5	6	7	8
1	Var ID (Primary)	M45.Q2VX[5](cum)	Stdev(X)	RSD(X)	Stdev(X)WS	RSD(X)WS	DFR	N
2	Ton_in	0.915307	202.408	35.2627	1	0.174216	79	85
3	KR30_IN	0.909723	39.6874	7.55197	1	0.190286	79	85
4	KR40_IN	0.949443	43.828	8.00128	1	0.182561	79	85
5	PARM	0.758188	16.5331	4.23923	1	0.256408	79	85
6	HS_1	0.785003	4.18702	0.411311	1	0.0982347	79	85
7	HS_2	0.713535	11.7281	2.34887	1	0.200277	79	85
8	PKR_30	0.800515	10.0454	3.25479	1	0.324009	79	85

7.4.2.8.2 X/Y overview list for PLS/OPLS/O2PLS models

For PLS models the **X/Y Overview List** displays the following for each y-variable:

Vector	Description
R2VYAdj(cum)	The cumulative fraction of the variation of the y-variable, adjusted for degrees of freedom, explained after the selected component (Cumulative Variance explained).
R2VY(cum)	The cumulative fraction of the variation of the y-variable explained after the selected component.
Q2VY(cum)	The cumulative predicted fraction (cross validation) of the variation of Y.
Stdev(Y)	Standard deviation of Y in original units, and transformed if Y is transformed).
RSD(Y)	Residual standard deviation of Y in original units (transformed if the variable was transformed).
Stdev(Y)WS	Standard deviation of Y scaled as specified in the workset (normally scaled to unit variance, UV).
RSD(Y)WS	Residual standard deviation scaled as specified in the workset (normally scaled to unit variance, UV).
DFR	Degrees of freedom of the Y residuals.
N	Non missing observations in Y.

An example for a PLS model:



X/Y Overview List [M1]

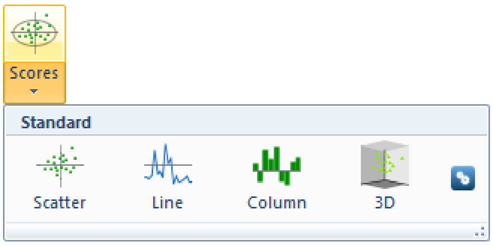
	1	2	3	4	5	6	7	8	9	10
1	Var ID (Primary)	M1.R2VYAdj[6](cum)	M1.R2VY[6](cum)	M1.Q2VY[6](cum)	Stdev(Y)	RSD(Y)	Stdev(Y)WS	RSD(Y)WS	DFR	N
2	PAR	0.95253	0.955921	0.948369	60.4624	13.1733	1	0.217875	78	85
3	FAR	0.963062	0.965701	0.957164	112.419	21.6059	1	0.192191	78	85
4	r_FAR	0.860264	0.870245	0.838798	2.61313	0.97682	1	0.373813	78	85
5	%Fe_FAR	0.581824	0.611693	0.559903	1.19036	0.769762	1	0.646666	78	85
6	%P_FAR	0.46525	0.503446	0.421972	0.0652028	0.0476806	1	0.731266	78	85
7	%Fe_malm	0.798055	0.81248	0.789656	2.2141	0.994979	1	0.449383	78	85
8										
9		Comp	Obs.	Y-miss(tot)						
10		6	85	0						

Note: For OPLS/O2PLS models, the **X/Y Overview List** only displays statistics for the predictive components.

7.4.3 Scores

The **tt** and **uu** plots of the X- and Y-scores of, for example, dimensions 1 and 2 (i.e. t_1 vs. t_2, and u_1 vs. u_2), can be interpreted as windows into the X- and Y-spaces, respectively. These show how the X space (X conditions) and response values are situated with respect to each other. These plots show the possible presence of outliers, groups, and other patterns in the data.

There are four types of score plots available from the **Scores** gallery on the Home tab: **Scatter**, **Line**, **Column**, and **3D**.



The **tu** plots (t_1 vs. u_1, t_2 vs. u_2, etc.) display the relation between X and Y. The degree of fit (good fit corresponds to small scatter around the straight line), indications of curvature, and outliers can also be seen.

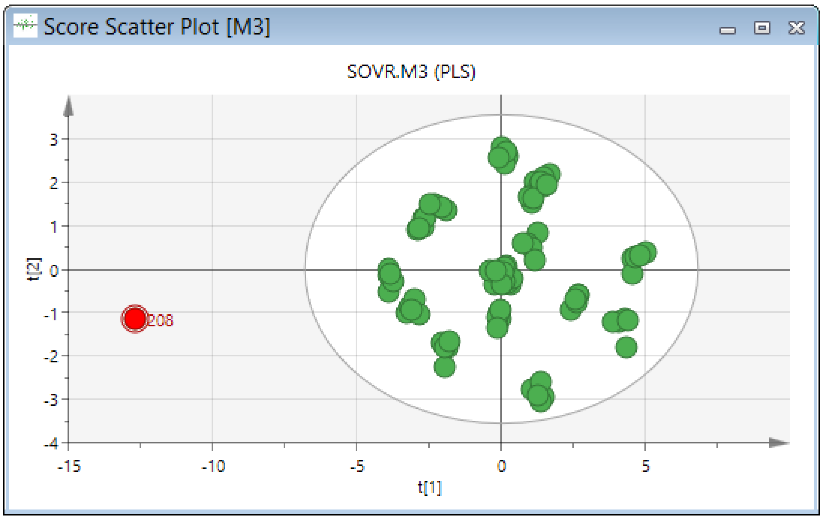
The tu plots are found on the **Analyze** tab, in the **Analysis** group, by clicking **Inner relation**.

7.4.3.1 Score scatter plot

To display the scores in a 2D scatter plot, on the **Home** tab, in the **Diagnostics & interpretation** group, click **Scores**.

The default scatter plot is displayed, t1 vs. t2 (PCA, PLS) or t1 vs. to1 (OPLS with 1+1).

When displaying a two-dimensional score plot displaying t, SIMCA draws the confidence ellipse based on Hotelling's T^2, by default at significance level 0.05. Observations situated outside the ellipse are considered to be outliers. For example, in the default score scatter plot displayed below it is evident that observation 208 is an outlier.



7.4.3.1.1 Ellipse modifications

To hide the ellipse, or change the confidence level of the ellipse, click the **Limits** tab in the **Properties** dialog and change as desired. For more see the Limits subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs.

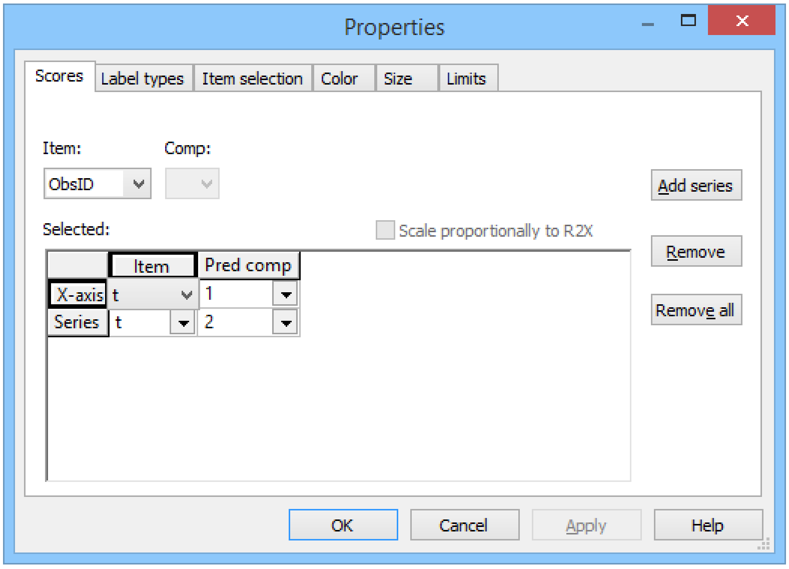
To change the default confidence level use **Model Options** or **Project Options**.

For more about the ellipse, see the Hotelling’s T2 subsection in the Statistical appendix.

7.4.3.1.2 Color by

To color by a variable, or scores etc., click **Color by** on the **Tools** tab or the **Color** tab in the **Properties** dialog. For more see the Color in the Properties dialog subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs.

7.4.3.1.3 Score plot Properties



Item: ObsID

Comp:

Selected:

□ Scale proportionally to R2X

	Item	Pred comp
X-axis	t	1
Series	t	2

In the **Scores** page of the **Properties** dialog you can select to:

- Display more or other series: make the selection in **Item** and **Comp** boxes, and click **Add series**.
- Modify the items on the axes.
- Clear the **Scale proportionally to R2X** check box for OPLS and O2PLS if warranted. For more about this option, see the R2X subsection in Chapter 12, Plot/List.

The other tabs are general and described in detail in the Properties dialog section in the Tools tab section in Chapter 14, Plot and list contextual tabs.

Note: When the dataset contains numerical IDs, they can be selected and plotted on either axis.

Removing ellipse in score plot

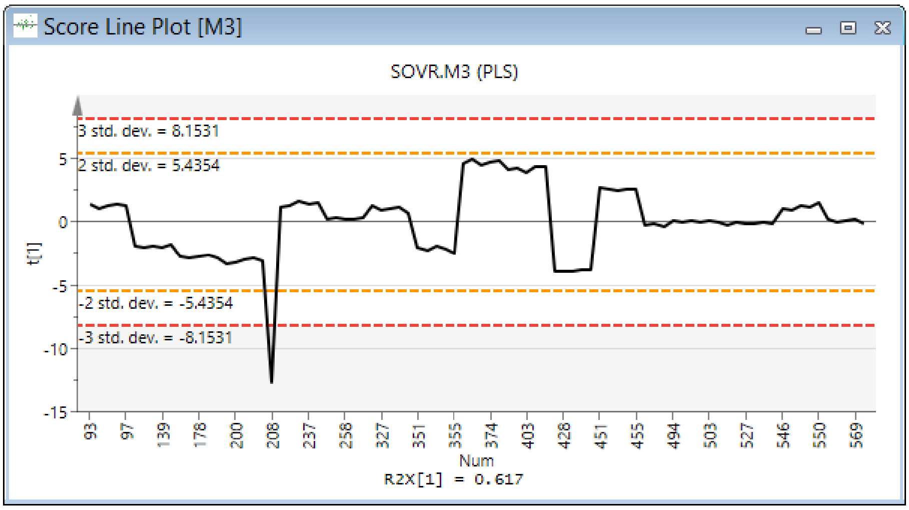
There are two ways to remove the ellipse in the **Score Scatter Plot**:

- Not display it by opening the **Format Plot** dialog and under the **Limits and regions** node, clicking **Ellipse** and selecting **Line style** *None* and **Fill type** *No fill*.
- Hide it in the **Limits** page in the **Properties** dialog. For more, see the Limits subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs.

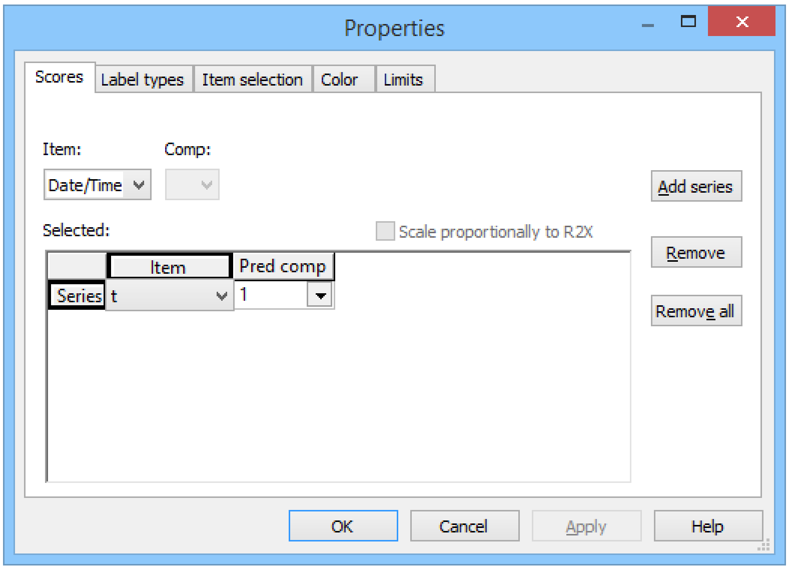
7.4.3.2 Score line plot

To display the scores in a line plot, on the **Home** tab, in the **Diagnostics & interpretation** group, click **Scores**, and then click **Line**.

The default line plot of t1 is displayed.



With a one-dimensional score line plot, e.g. t_a vs. Num, the score plot displays confidence intervals corresponding to the 2 and 3 sigma limits, i.e., 2 and 3 standard deviations of the vector are displayed by default. Here the plot is identical to the Shewhart control chart with no subgroups.



Item: Date/Time

Comp:

Selected:

□ Scale proportionally to R2X

	Item	Pred comp
Series	t	1

In the **Scores** page of the **Properties** dialog you can select to:

- Display more or other series: make the selection in **Item** and **Comp** boxes, and click **Add series**.
- Modify the items on the axes.
- Clear the **Scale proportionally to R2X** check box for OPLS and O2PLS if warranted. For more about this option, see the R2X subsection in Chapter 12, Plot/List.

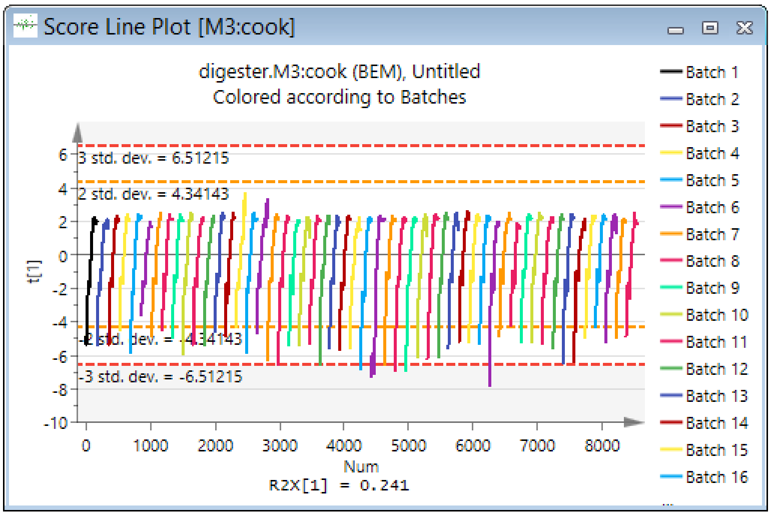
The other tabs are general and described in detail in the Properties dialog section in the Tools tab section in Chapter 14, Plot and list contextual tabs.

Note: When the dataset contains numerical IDs, they can be selected and plotted on either axis.

7.4.3.2.1 Score line plot for batch evolution models

Displaying the scores as a line plot in combination with DModX allows you to detect batches with upsets. These plots use the non-aligned batches.

The limits are computed from the variation of the t's as single vectors, as for steady state data. Batches outside the limits or different from the average behavior should be examined further, for example by displaying contribution plots. These batches should be removed from the workset if they are outlier batches.



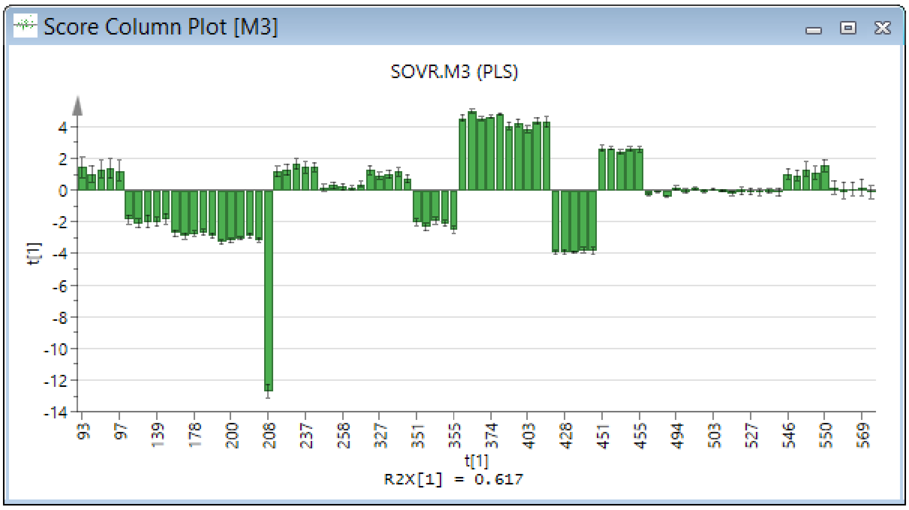
See also the DModX plot for BEM subsection later in this chapter.

For more, see the Limits topic in the Tools tab section in Chapter 14, Plot and list contextual tabs.

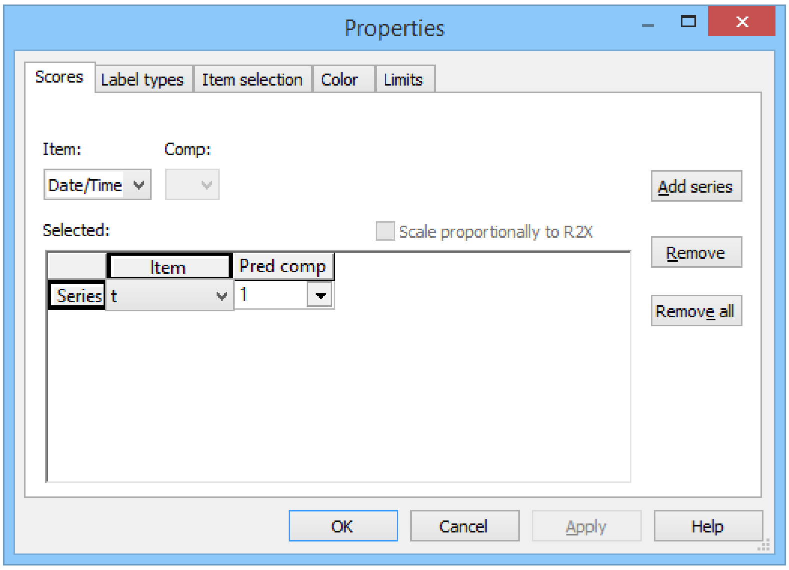
7.4.3.3 Score column plot

To display the scores in a column plot, on the **Home** tab, in the **Diagnostics & interpretation** group, click **Scores**, and then click **Column**.

The default column plot of t1 is displayed.



With a column plot displaying one vector, jack-knifing is used to calculate standard errors displayed as error bars at the end of each column.



Item: Date/Time

Comp:

Selected:

□ Scale proportionally to R2X

	Item	Pred comp
Series	t	1

In the **Scores** page of the **Properties** dialog you can select to:

- Display more or other series: make the selection in **Item** and **Comp** boxes, and click **Add series**.
- Modify the items on the axes.
- Clear the **Scale proportionally to R2X** check box for OPLS and O2PLS if warranted. For more about this option, see the R2X subsection in Chapter 12, Plot/List.

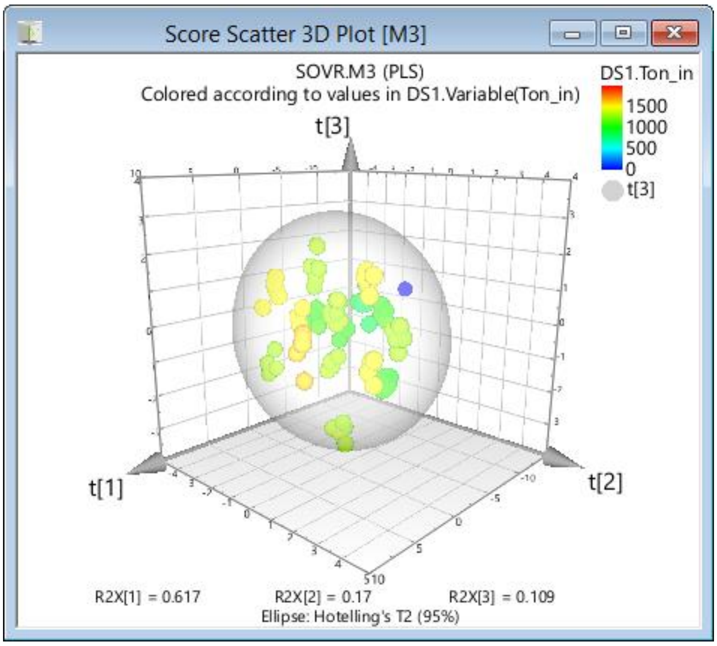
The other tabs are general and described in detail in the Properties dialog section in the Tools tab section in Chapter 14, Plot and list contextual tabs.

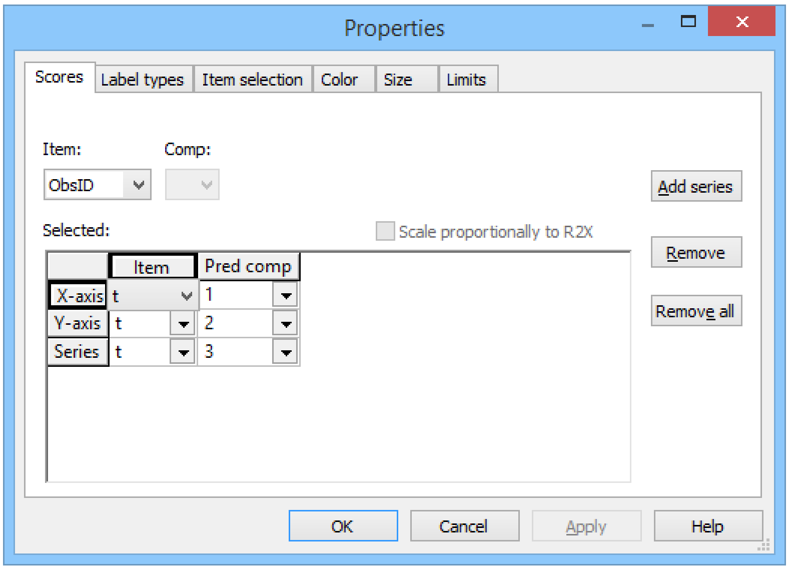
Jack-knifing is used to calculate standard errors displayed as error bars at the end of each column. The confidence level of the standard errors can be customized in the **Limits** page.

7.4.3.4 Score scatter 3D plot

To display the scores in a 3D scatter plot, on the **Home** tab, in the **Diagnostics & interpretation** group, click **Scores**, and then click **3D**.

The default scatter plot is displayed, t1 vs. t2 vs. t3 (PCA, PLS) or t1 vs. to1 vs to2 (OPLS with 1+2 for instance).





Item: ObsID

Comp:

Selected:

□ Scale proportionally to R2X

	Item	Pred comp
X-axis	t	1
Y-axis	t	2
Series	t	3

In the **Scores** page of the **Properties** dialog you can select to:

- Display more or other series: make the selection in **Item** and **Comp** boxes, and click **Add series**.
- Modify the items on the axes.
- Clear the **Scale proportionally to R2X** check box for OPLS and O2PLS if warranted. For more about this option, see the R2X subsection in Chapter 12, Plot/List.

The other tabs are general and described in detail in the Properties dialog section in the Tools tab section in Chapter 14, Plot and list contextual tabs.

Note: When the dataset contains numerical IDs, they can be selected and plotted on any axis.

7.4.3.4.1 Marking in 3D scatter plot

In the 3D plot, hold down the CTRL-button to mark several points.

To mark two groups, in order to create a group contribution plot, mark the first group then click a point after releasing the CTRL-button (so that the first group is *Previously Marked Values*) then mark the second group while pressing the CTRL-button. Open the **Marked Items** pane to see the observations included in each group.

Note: Avoid marking the single point again as it will then be unmarked.

7.4.3.4.2 Zooming in 3D plot

To zoom, scroll using the mouse wheel. Alternatively, press the CTRL-button while holding down the right mouse button and moving the mouse.

7.4.3.4.3 Rotating 3D plot

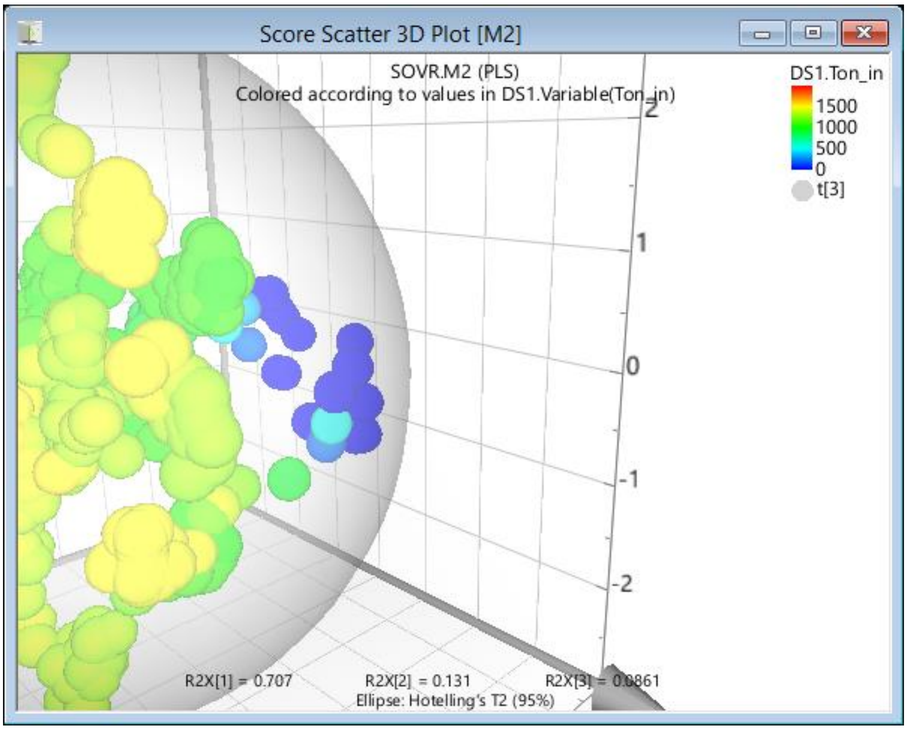
To rotate a 3D scatter plot or a Response Surface plot, hold down the left mouse button and move the mouse in the direction to turn it. To keep the plot rotating, release the mouse button while turning. To not have the plot continue rotating, stop turning before releasing the mouse button.

Resetting the rotation

To reset the rotation to default, right-click the plot and then click **Reset rotation**.

7.4.3.4.4 Moving the 3D plot in its window

To move the plot, hold down the right mouse button and move the mouse in the direction to move. Moving the plot is useful after having zoomed when wanting to see other areas of the plot.



7.4.3.5 OPLS specific score plots

There are four OPLS/O2PLS specific score plots, each displaying different components of the model.

If there are two or more of the score type in the model, the plots are scatter plots of the first two components. If there is only one component of the type available, the resulting plot is a column plot. By default the plotted score vectors are scaled proportionally to R2X, the variance explained by each component.

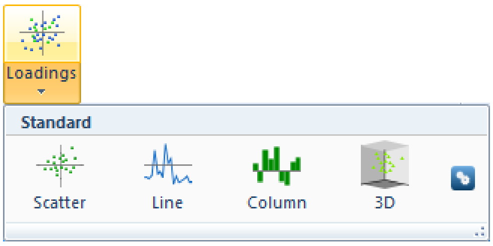
The OPLS/O2PLS specific score plots are:

- **Pred X** – X-score vectors t1 and t2 of the predictive components.
- **Pred Y** – Y-score vectors u1 and u2 of the predictive components.
- **Orth X** – X-score vectors to1 and to2 of the orthogonal in X components.
- **Orth Y** – Y-score vectors uo1 and uo2 of the orthogonal in Y components.

7.4.4 Loadings

Loading plots display the correlation structure of the variables. That is, they show the importance of the x-variables in the approximation of the X matrix.

There are four types of loading plots: **Scatter**, **Line**, **Column**, or **3D**.



Note: The score and loading plots complement each other. The position of objects in a given direction in a score plot is influenced by variables lying in the same direction in the loading plot.

The available loading vectors for PCA, PLS, OPLS and O2PLS models are described in the table in the Observations and Loadings vectors subsection in the Statistical appendix.

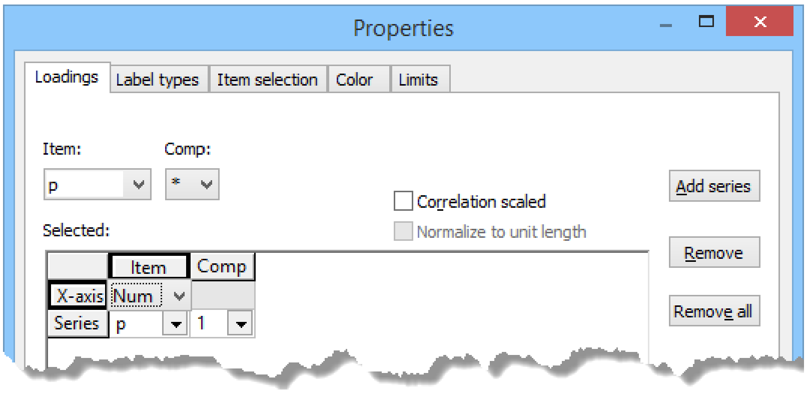
Loading vector	Short description
c	PLS only. Displays the correlation between the Y variables and the X scores T(X). Weights that combine the Y variables with the scores **u**, so as to maximize their correlation with X. Y variables with large c's are highly correlated with T(X).
p	Displays the importance of a variable in approximating X as TP'.
pc	PLS only. Combination of the p and c vectors.
c(corr)	PLS only. Available after selecting the **Correlation scaled** check box in the loading dialog. c scaled as correlations resulting in all points falling inside the circle with radius 1.
p(corr)	Available after selecting the **Correlation scaled** check box in the loading dialog. p scaled as correlations resulting in all points falling inside the circle with radius 1.
pc(corr)	PLS only. Available after selecting the **Correlation scaled** check box in the loading dialog. Combination of the p(corr) and c(corr) vectors.
w	PLS only. Weights that combine the X variables (first dimension) or the residuals of the X variables (subsequent dimensions) to form the scores t.
w*	PLS only. Weights that combine the original X variables (not their residuals as with w) to form the scores t.
w*c	PLS only. Combination of the w* and c vectors. Plotting both the X-weights, w*, and Y-weights, c, in the same plot displays the correlation structure between X and Y. Interpretation of how the X and Y variables combine in the projections, and how the X variables relate to the Y variables, is possible.

7.4.4.1 Loading scatter plot

To display the loadings in a 2D scatter plot, on the **Home** tab, in the **Diagnostics & interpretation** click **Loadings**, and then click **Line**.

The default scatter plot is displayed, p1 vs. p2 (PCA), w*c1 vs. w*c2 (PLS) or pq1 vs. poso1 (OPLS with 1+1 for instance).

To change what is displayed, open the Properties dialog by clicking the plot and then **Properties** in the mini-toolbar.



Item: p

Comp: *

□ Correlation scaled

□ Normalize to unit length

Selected:

	Item	Comp
X-axis	Num	
Series	p	1

In the **Loadings** page of the **Properties** dialog you can select to:

- Display more or other series: make the selection in **Item** and **Comp** boxes, and click **Add Series**.
- Modify the items on the axes.
- Display loadings vectors p, c, pc, pq, po, poso, scaled as correlations: select the **Correlation scaled** check box. The correlation scaling done is the same as in the **Biplot**. For more, see the Biplot subsection in Chapter 10, Analyze.

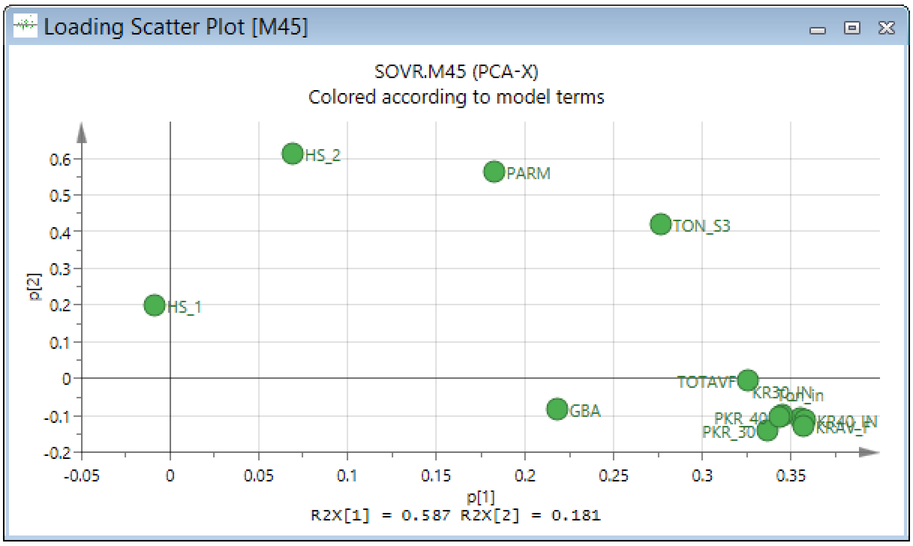
- Clear the Normalize to unit length check box. **Normalize to unit length** check box is default selected for OPLS and O2PLS. For more about this transformation, see the Normalize subsection in Chapter 12, Plot/List.

The other tabs are general and described in detail in the Properties dialog subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs.

Note: When the dataset contains numerical IDs, they can be selected and plotted on either axis.

7.4.4.1.1 Loading scatter plot PCA

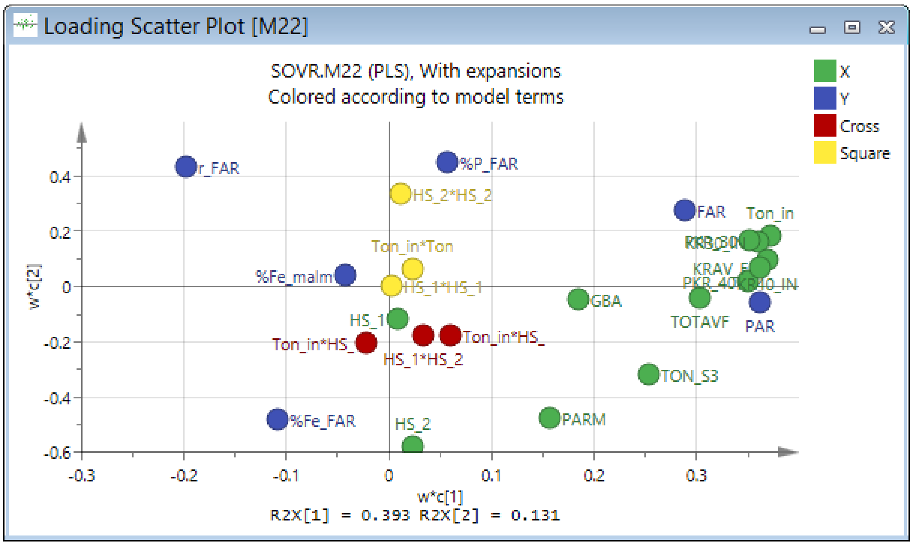
Variables with the largest absolute values of p1 or/and p2 dominate the projection. Variables near each other are positively correlated; variables opposite to each other are negatively correlated.



7.4.4.1.2 Loading scatter plot PLS

Variables with large w* or c values are situated far away from the origin (on the positive or negative side) in the plot.

X variables with large values in w* (positive or negative) are highly correlated with U (Y).



The default coloring of the loading scatter plot is by **Terms**.

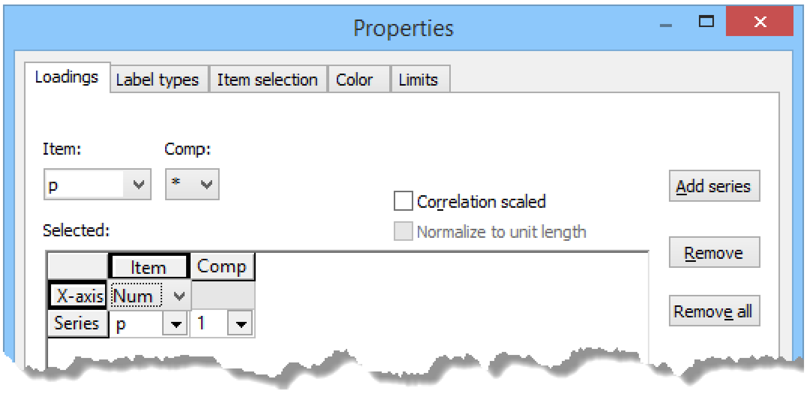
7.4.4.2 Loading line plot

To display the loadings in a line plot, on the **Home** tab, in the **Diagnostics & interpretation** group, click **Loadings**, and then click **Line**.

The default line plot is displayed, p1 (PCA), w*c1 (PLS) or pq1 (OPLS).

To change what is displayed, open the Properties dialog by clicking the plot and then **Properties** in the mini-toolbar.

The Properties dialog opens.



In the **Loadings** page of the **Properties** dialog you can select to:

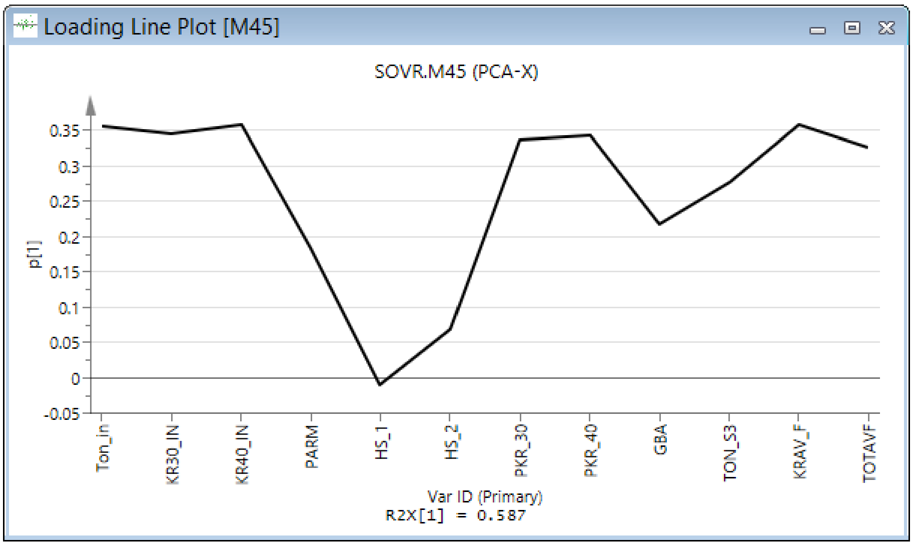
- Display more or other series: make the selection in **Item** and **Comp** boxes, and click **Add Series**.
- Modify the items on the axes.
- Display loadings vectors p, c, pc, pq, po, poso, scaled as correlations: select the **Correlation scaled** check box. The correlation scaling done is the same as in the **Biplot**. For more, see the Biplot subsection in Chapter 10, Analyze.
- Clear the Normalize to unit length check box. **Normalize to unit length** check box is default selected for OPLS and O2PLS. For more about this transformation, see the Normalize subsection in Chapter 12, Plot/List.

The other tabs are general and described in detail in the Properties dialog subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs.

Note: When the dataset contains numerical IDs, they can be selected and plotted on either axis.

7.4.4.2.1 Loading Line Plot PCA

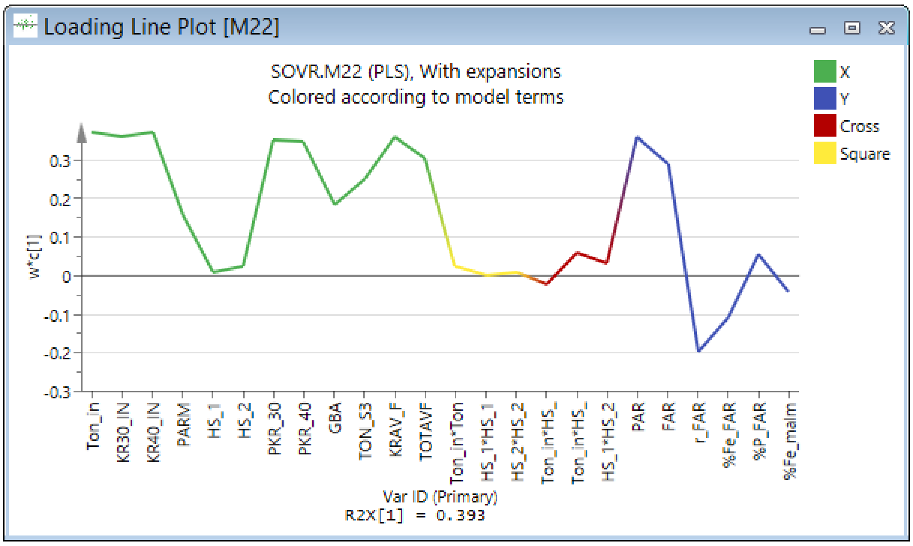
Variables with the largest absolute values of p1 dominate the projection.



7.4.4.2.2 Loading Line Plot PLS

Variables with large w* or c values are situated far away from the origin (on the positive or negative side) in the plot.

X variables with large values in w* (positive or negative) are highly correlated with U (Y).

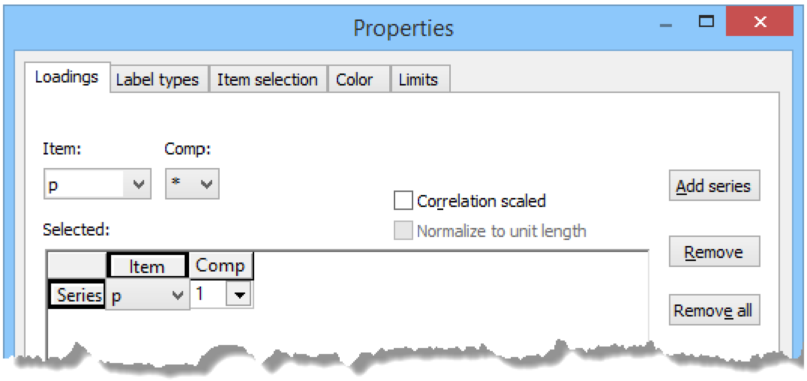


7.4.4.3 Loading column plot

To display the loadings in a column plot, on the **Home** tab, in the **Diagnostics & interpretation** group, click **Loadings** and then **Column**.

The default column plot is displayed, p1 (PCA), w*c1 (PLS) or pq1 (OPLS).

To change what is displayed, open the Properties dialog by clicking the plot and then **Properties** in the mini-toolbar.



Item: p

Comp: *

☐ Correlation scaled

☐ Normalize to unit length

Selected:

	Item	Comp
Series	p	1

In the **Loadings** page of the **Properties** dialog you can select to:

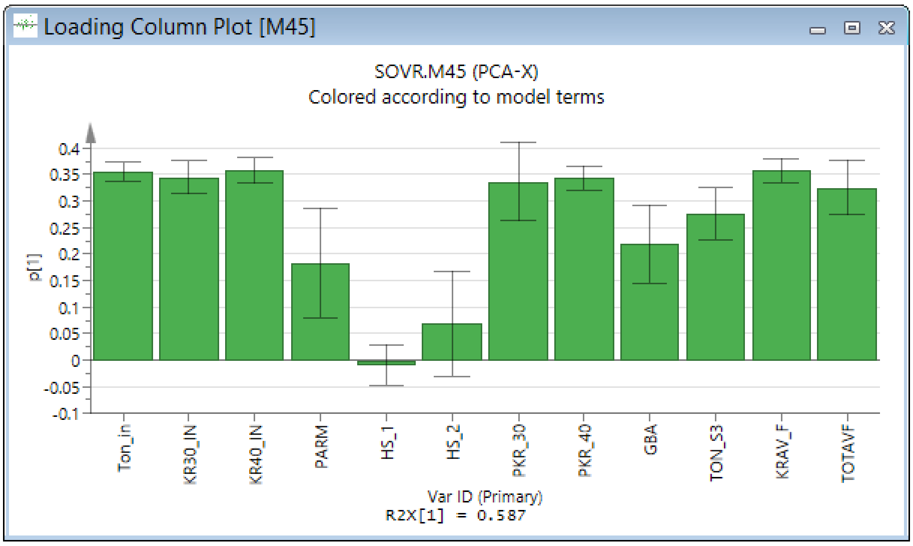
- Display more or other series: make the selection in **Item** and **Comp** boxes, and click **Add Series**.
- Modify the items on the axes.
- Display loadings vectors p, c, pc, pq, po, poso, scaled as correlations: select the **Correlation scaled** check box. The correlation scaling done is the same as in the **Biplot**. For more, see the Biplot subsection in Chapter 10, Analyze.
- Clear the Normalize to unit length check box. **Normalize to unit length** check box is default selected for OPLS and O2PLS. For more about this transformation, see the Normalize subsection in Chapter 12, Plot/List.

The other tabs are general and described in detail in the Properties dialog subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs.

With a column plot, jack-knifing is used to calculate standard errors displayed as error bars at the end of each column. The confidence level of the standard errors can be customized in the Limits page.

7.4.4.3.1 Loading column plot PCA

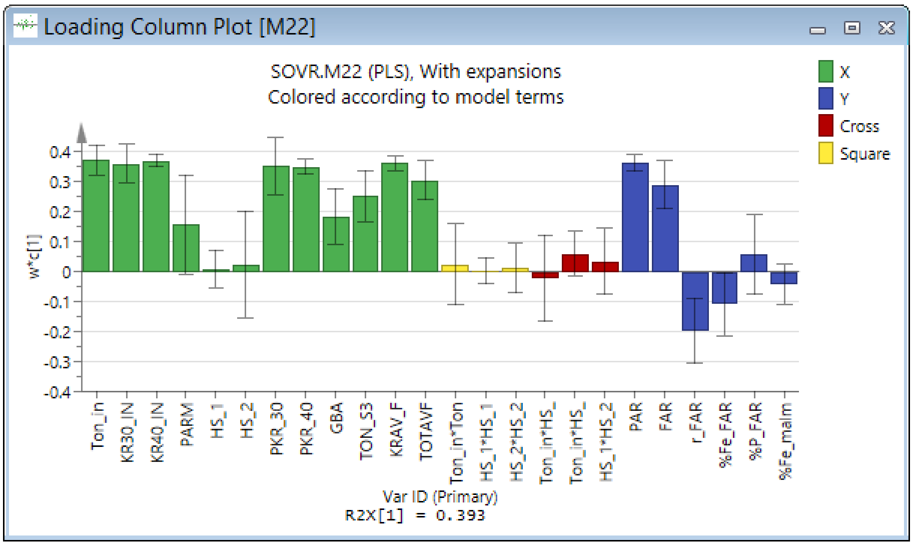
Variables with the largest absolute values of p1 dominate the projection.



7.4.4.3.2 Loading column plot PLS

Variables with large w* or c values are situated far away from the origin (on the positive or negative side) in the plot.

X variables with large values in w* (positive or negative) are highly correlated with U (Y).

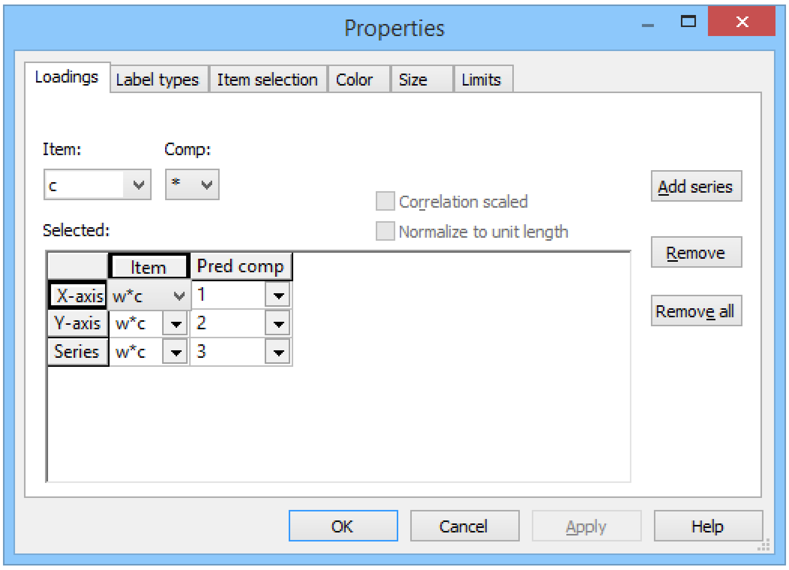


7.4.4.4 Loading scatter 3D plot

To display the loadings in a 3D scatter plot, on the **Home** tab, in the **Diagnostics & interpretation** group, click **Loadings**, and then click **3D**.

The default 3D scatter plot is displayed, p1 vs. p2 vs. p3 (PCA), w*c1 vs. w*c2 vs. w*c3 (PLS) or pq1 vs. poso1 vs. poso2 (OPLS with 1+2 components for instance).

To change what is displayed, open the **Properties** dialog by clicking the plot and then **Properties** in the mini-toolbar.



Item: c

Comp: *

☐ Correlation scaled

☐ Normalize to unit length

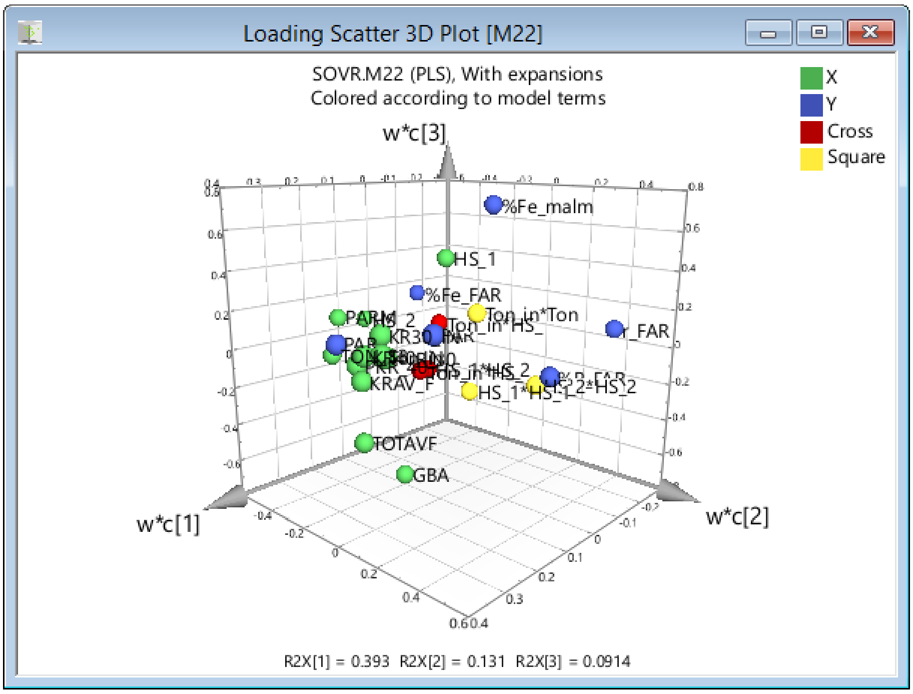
Selected:

	Item	Pred comp
X-axis	w*c	1
Y-axis	w*c	2
Series	w*c	3

Note: When the dataset contains numerical IDs, they can be selected and plotted on any axis.

7.4.4.4.1 Loading scatter 3D plot example

Variables with the largest absolute loading values dominate the projection. Variables near each other are positively correlated; variables opposite to each other are negatively correlated.



For how to mark, zoom, rotate, move the plot in its window, color and size the 3D plot, see the Score Scatter 3D Plot section earlier in this chapter.

7.4.4.5 OPLS specific loadings

There are three OPLS and O2PLS specific loading plots, each displaying different components of the model.

If there are two or more components for the loading type to display, the displayed plot is a scatter plot. If there is only one component, the resulting plot is a column plot.

By default the plotted loading vectors are scaled to unit length.

- **Pred X-Y**: X-Y-loading vectors pq1 and pq2 of the predictive components.

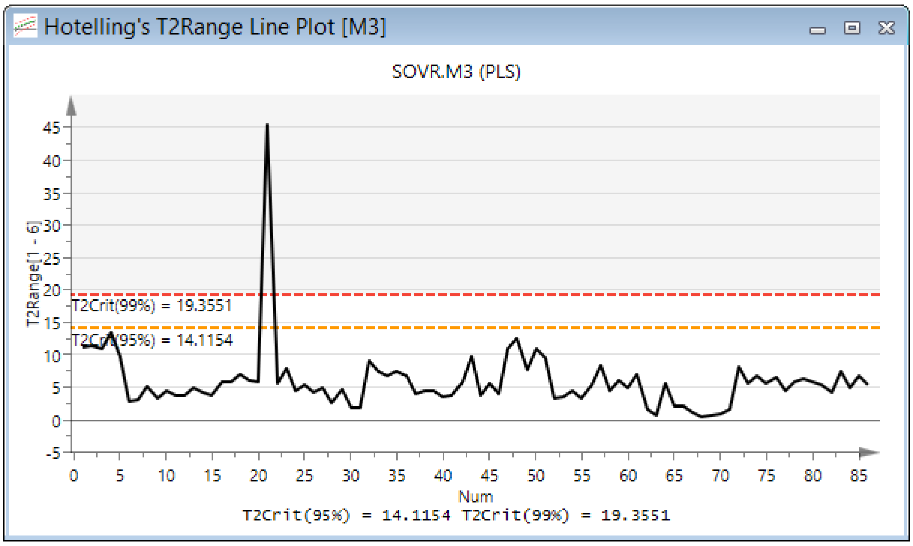
- **Orth X**: X-loading vectors poso1 and poso2 of the orthogonal in X components.
- **Orth Y**: Y-loading vectors qor1 and qor2 of the orthogonal in Y components.

7.4.5 Hotelling's T2Range

The Hotelling's T2Range can be displayed as two plot types, **Line** and **Column**, by clicking **Hotelling's T2** in the **Diagnostics & interpretation** group on the **Home** tab.

The Hotelling's T^2Range plot displays the distance from the origin in the model plane (score space) for each selected observation. The plot shows the T^2 calculated for the range of selected components, i.e., 1 to 7, or 3 to 6.

Default is to display from the first to the last component. For OPLS and O2PLS models the range is locked to from the first predictive to the last orthogonal in X. To change the range of components, right-click the plot and select **Properties**, and then click the **Component** tab. y



For all other pages in Properties, see the Properties dialog subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs.

The Hotelling's T2 subsection in the Statistical appendix describes how the Hotelling's T2 is calculated.

7.4.5.1 Limits in Hotelling's T2Range

Values larger than the yellow limit are suspect (0.05 level), and values larger than the red limit (0.01 level) can be considered serious outliers.

A large T^2-range value for a given observation, i.e., a value far above the critical limits, indicates that the observation is far from the other observations in the selected range of components in the score-space. Hence, this is likely to be an outlying observation that, if included the workset, may pull the model in a detrimental way.

7.4.6 Distance to model

Distance to model is an estimate of how far from the model plane, in the X or Y space, the observation is positioned.

The distance to the model can be displayed in absolute and normalized units. By default the distance to model plot is displayed in normalized units after the last component with limit for significance level 0.05. To change from the defaults, use **Model Options** or **Project Options**. The significance level can be changed in the **Limits** page in the **Properties** dialog. For more, see the Limits subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs.

There are two plots displaying the distance to the model, **DModX** and **DModY**, available on the **Home** tab in the **DModX** gallery:

- Under the **DModX** header, click **Line** or **Column** to display DModX in that plot type.
- Under the **DModY** header, click **Line** or **Column** to display DModY in that plot type.

7.4.6.1 Overview of calculation of distance to the model

The RSD of an observation in the X or Y space, is proportional to the observation distance to the hyper plane of the model in the X or Y space. SIMCA computes the observation distances to the model, in the X space (DModX) or Y space (DModY).

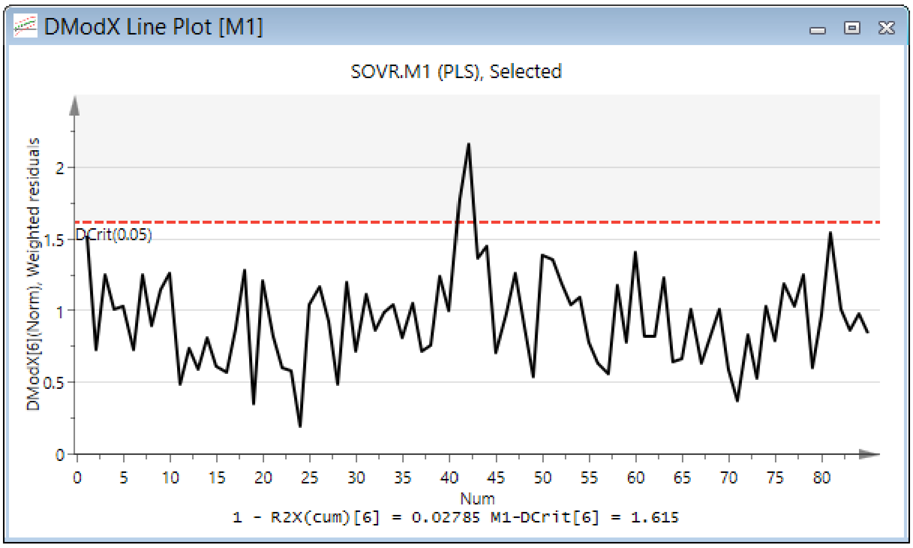
DModX can also be weighted by the modeling power by selecting the **Weighted by the modeling power** check box in the **Distance to model** page in **Model Options** or **Project Options**.

For details about the calculations of the distance to the model, see the Distance to model section in the Statistical appendix.

7.4.6.2 Distance to the model in the X-block

The distance to the model in the X space, DModX, is by default displayed in normalized units.

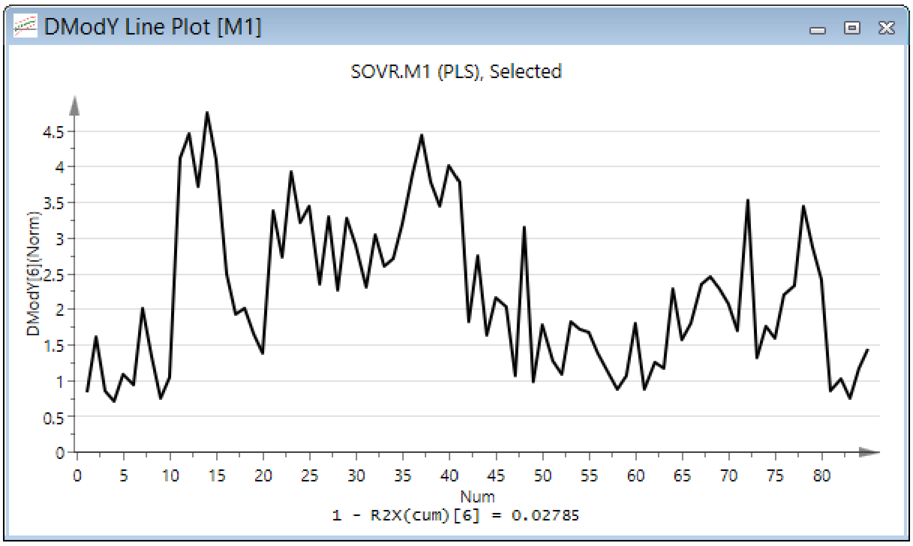
Larger DModX than the critical limit indicates that the observation is an outlier in the X space.



7.4.6.3 Distance to the model in the Y-block

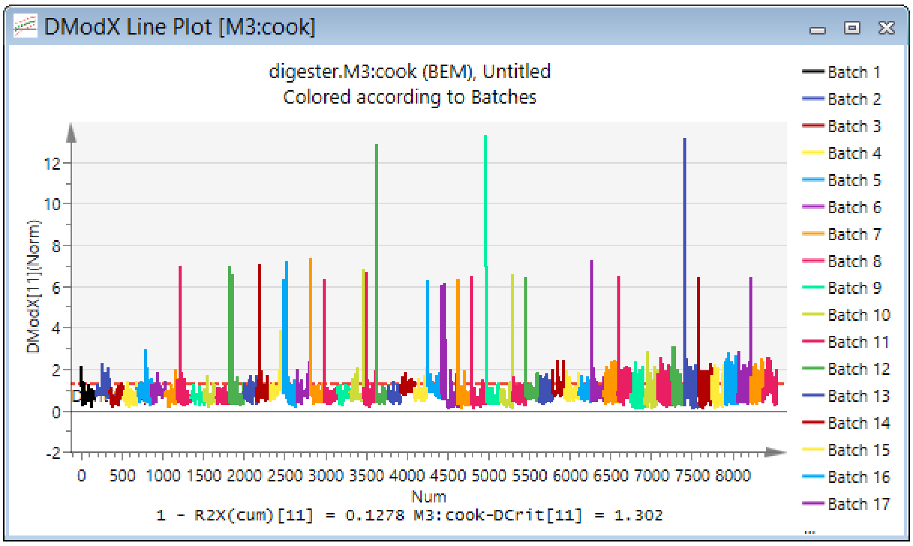
The distance to the model in the Y space, DModY, is by default displayed in normalized units.

A large DModY value indicates that the observation is an outlier in the Y space.



7.4.6.4 DModX plot for batch evolution models

The DCrit is computed as for steady state data and from an F distribution. Hence it is very sensitive to tails. Batch data are usually dynamic, and some variables increase or decrease with time. Hence, batches will often be outside the DModX limit at the beginning or the end of the evolution. To detect abnormal batches, look for batches far above the average of the high points.



To exclude batches in a plot, first select the batch using **Batch marking mode**, the whole batch will be marked, then use the **Exclude** tool (red arrow), on the **Marked items** tab, to exclude the batch.

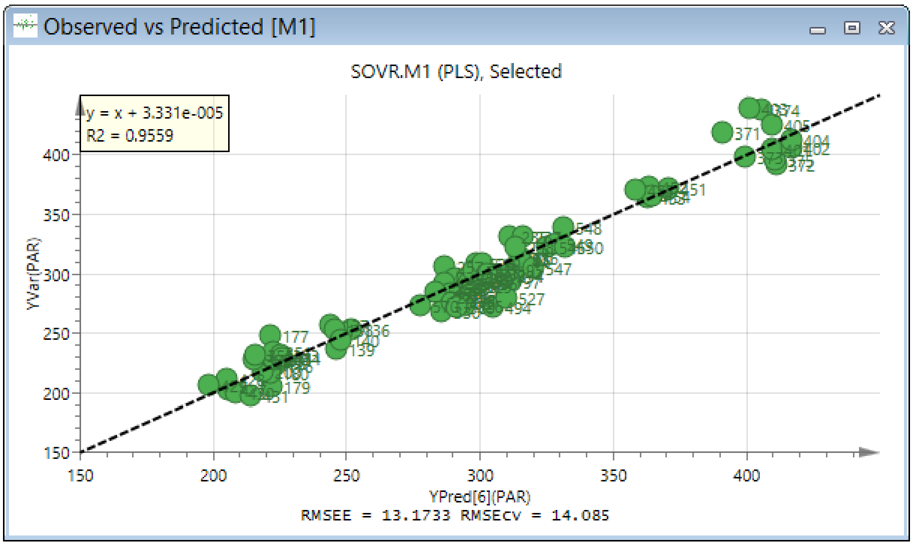
When batches have phases, the batch will be excluded from all the class (phase) models and a new unfitted batch model, with all class models, generated. You can mark several batches holding the CTRL key, and then exclude them.

See also the Batch control charts section later in this chapter.

7.4.7 Observed vs. predicted

The Observed vs. predicted plot, displayed by clicking **Observed vs. predicted** in the **Diagnostics & interpretation** group, on the **Home** tab, displays the observed values vs. the fitted or predicted values for the selected response, after the last component.

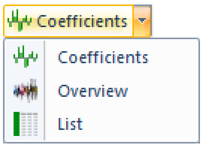
To switch to another y-variable use the Tools tab (**X-Axis YVar** box in the **Properties** group) or the Properties dialog (**Select y-variable** tab). For more, see the Switching components, batches, and models subsection respective the Select y-variable subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs.



7.4.8 Coefficients

For each y-variable SIMCA computes regression coefficients. These express the relation between the Y-variables and all the terms in the model. By default, the regression coefficients relate to the centered and scaled data, CoeffCS, and are computed from all extracted components.

Note: All coefficients are cumulative.



For PLS/OPLS/O2PLS models two plots and one list are available on the **Home** tab by clicking **Coefficients**:

- Plot - column plot displayed with uncertainty bars for the selected y-variable.
- Overview - column plot displaying all y-variables.
- List - displayed for all y-variables with uncertainty estimates.

For hierarchical top models, the Resolve coefficients check box is available on the **Tools** tab when the Coefficient plot or Coefficient overview plot is active.

7.4.8.1 Coefficient types

The coefficient plots can be displayed for **Scaled and centered**, **MLR**, **Unscaled**, and **Rotated** coefficients. The confidence intervals are only available for coefficients of scaled and centered data.

Displaying the **Rotated** coefficients is relevant when the X block is spectral data. The rotated coefficients express the pure spectra as it relates to each y-variable.

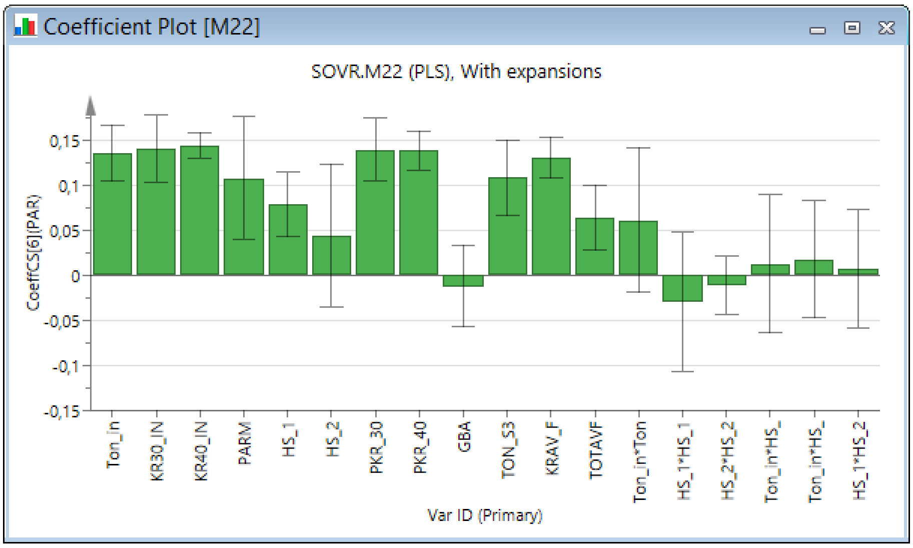
To switch coefficient type, click the plot and in the mini-toolbar click **Properties**. Click the **Coefficients** tab, and then click the desired coefficient type.

For all other pages in **Properties**, see the Properties dialog subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs.

For details about the different coefficient types, see the Coefficients section in Appendix A: Statistics.

7.4.8.2 Coefficient plot

The **Coefficient plot** by default displays the coefficients referring to scaled and centered data for a given response, with confidence intervals derived from jack-knifing. The confidence level of these limits can be modified in the **Properties** dialog. For more, see the Limits subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs.



Note: For hierarchical top models, the Resolve coefficients check box is available on the Tools tab when the Coefficient plot or Coefficient overview plot is active.

Use the **Properties** dialog to switch coefficient type.

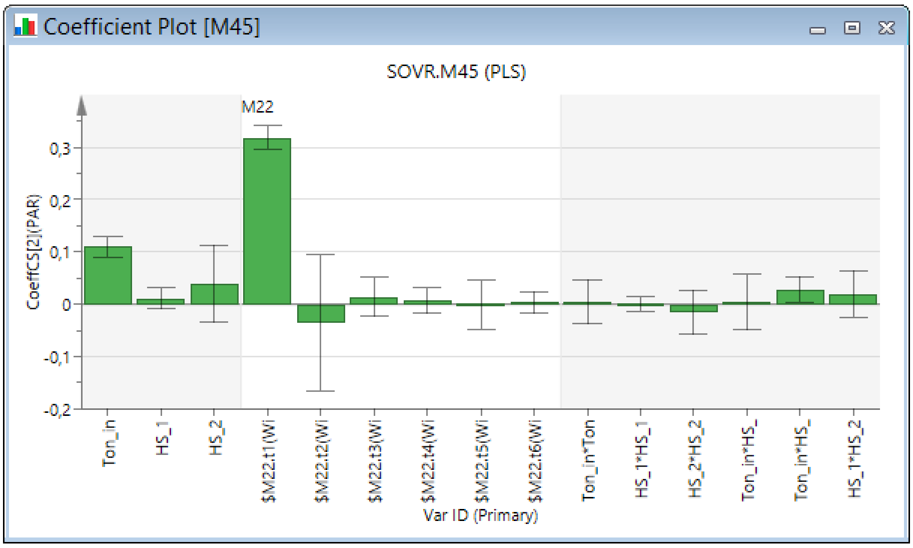
7.4.8.3 Coefficient plot for hierarchical top level models

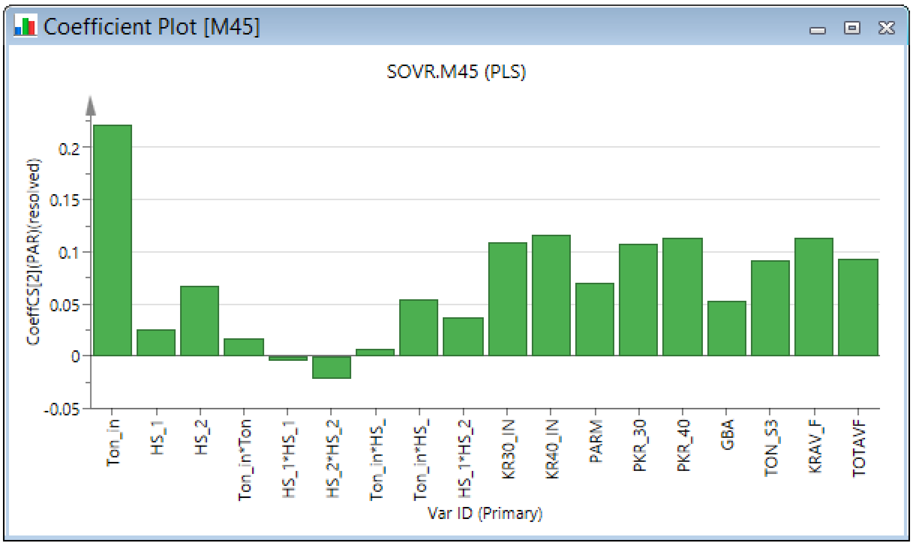
In hierarchical top level models, coefficients refer to the upper level variables, usually scores of the base level models. For the interpretation of the upper level model, it is desirable to be able to translate the upper level coefficients to coefficients of the individual variables of the base models.

For hierarchical top models the **Coefficient plot** by default displays the top level coefficients. To resolve to the base model coefficients, on the **Tools** tab, in the **Properties** group, select the **Resolve coefficients** check box.

To change this default to display the resolved coefficients, see the Coefficients page in Model Options subsection in the Workset section earlier in this chapter.

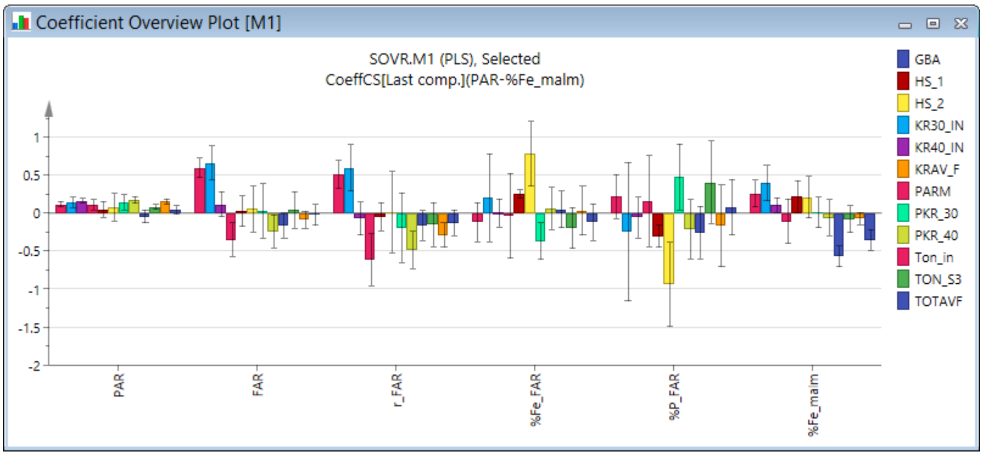
Note: Only linear terms are resolved. If the top model contains expanded terms (interaction, squares etc.) these terms are not resolved.





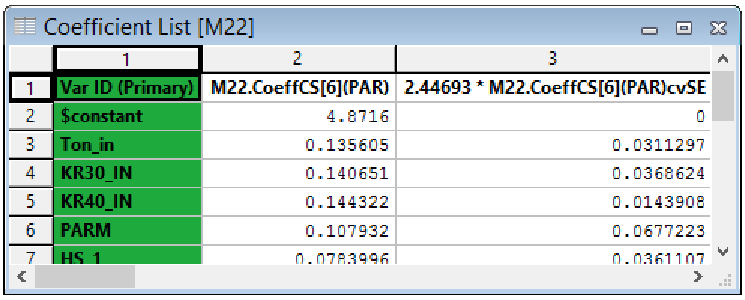
7.4.8.4 Coefficient overview plot

The Coefficient overview plot displays the coefficients, referring to scaled and centered data, for every response as bar graphs side by side.



7.4.8.5 Coefficient list

The Coefficient list default displays the coefficients referring to scaled and centered data for all responses, with confidence interval derived from jack-knifing.



	1	2	3
1	Var ID (Primary)	M22.CoeffCS[6](PAR)	2.44693 * M22.CoeffCS[6](PAR)cvSE
2	$constant	4.8716	0
3	Ton_in	0.135605	0.0311297
4	KR30_IN	0.140651	0.0368624
5	KR40_IN	0.144322	0.0143908
6	PARM	0.107932	0.0677223
7	HS_1	0.0783996	0.0361107

7.4.9 VIP

Interpreting a PLS or OPLS model with many components and a multitude of responses can be a complex task. A parameter which summarizes the importance of the X-variables, both for the X- and Y-models, is called the variable influence on projection, VIP.

For PLS, VIP is a weighted sum of squares of the PLS weights, w*, taking into account the amount of explained Y-variance in each dimension. Its attraction lies in its intrinsic parsimony; for a given model and problem there will always be only one VIP-vector, summarizing all components and Y-variables. One can compare the VIP of one term to the others. Terms with large VIP, larger than 1, are the most relevant for explaining Y.

The VIP values reflect the importance of terms in the model both with respect to Y, i.e. its correlation to all the responses, and with respect to X (the projection). With designed data, i.e. close to orthogonal X, the VIP values mainly reflect the correlation of the terms to all the responses. VIP values are computed, by default, from all extracted components.

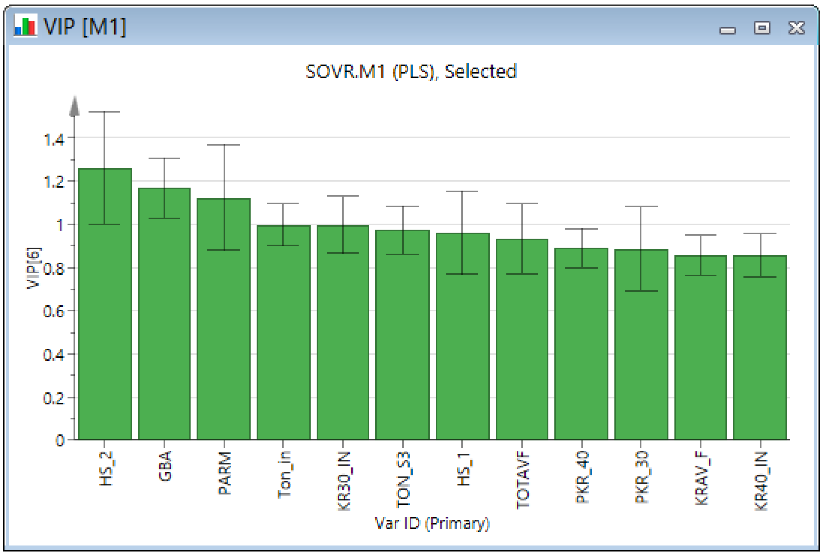
To take advantage of the interpretational clarity of OPLS, VIP for OPLS consists of three vectors, VIP for the predictive components (VIP predictive), VIP for the orthogonal components (VIP orthogonal), and VIP for the total model (VIP total). In each one of these three vectors, the VIP values are regularized such that if all X-variables would have the same importance for the model they would all have the value 1. Consequently, terms with VIP values larger than 1 in either VIP total, VIP predictive or VIP orthogonal, point to variables with large importance for that part of the model.

The VIP plots are available on the **Home** tab, in the **Diagnostics & interpretation** group, by clicking **VIP**. For OPLS and O2PLS models there are three VIP plots available, **VIP total**, **VIP predictive** and **VIP orthogonal**.

Note: The VIP plots are cumulative.

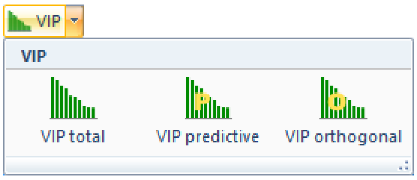
7.4.9.1 VIP Plot

The **VIP** plot displays the VIP values as a column plot sorted in descending order with confidence intervals derived from jack-knifing.



The plot is displayed with jack-knife uncertainty bars. The confidence level of these limits can be modified in the **Properties** dialog. For more, see the Limits subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs.

For OPLS models there are three VIP plot types;



Uncertainty bars are displayed for VIP total only.

For more about the OPLS specific VIP total, VIP predictive, and VIP orthogonal see the Variable importance, VIP subsection in the Statistical appendix.

7.4.9.1.1 Unsorted VIP plot

To display an unsorted VIP plot (useful in spectroscopy and chromatography)

1. Open the VIP plot.
2. On the **Tools** tab, click **Change type | Column**.

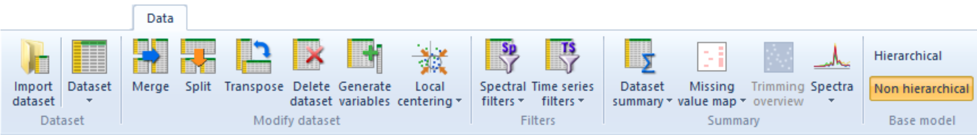
8 Data

8.1 Introduction

This chapter describes all commands on the **Data** tab.

On the **Data** tab the following commands are available:

1. **Import dataset** to the current project.
2. **Dataset** spreadsheet to view and open the available datasets. For more about the Dataset spreadsheet, see that section in Chapter 7, Home.
3. **Merge** datasets observation or variable wise.
4. **Split** the selected dataset variable wise.
5. **Transpose** dataset making the current columns rows and vice versa.
6. **Delete dataset** to remove datasets from the project.
7. **Generate variables** from variables in the dataset or from results of fitted models.
8. **Local centering** allowing importing local centering and then viewing it.
9. **Spectral filters**: Derivative, MSC, SNV, Row center, Savitzky-Golay, EWMA, Wavelet compression, Wavelet denoising, OSC, etc. as individual filters, or chained in any combination.
10. **Time series filters**: Wavelet compression and Wavelet denoising/decimation of PLS Time series.
11. **Dataset summary** displaying the properties of the selected dataset including **Filter** tab after filtering.
12. **Missing value map** displaying an overview of the distribution of the missing data in the selected dataset.
13. **Trimming overview** available after trimming or Winsorizing illustrating the result.
14. **Spectra** plot displaying XObs for all observations in the selected dataset.
15. **Hierarchical** base model resulting in hierarchical dataset according to selection.



8.2 Import

To import more data to the current project, click **Data | Import dataset**. See Chapter 6, SIMCA import for how to continue.

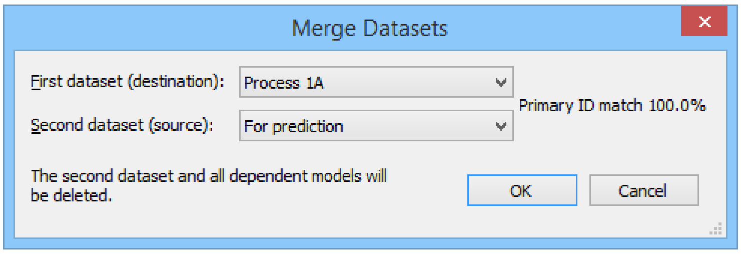
For batch projects batch condition data can be imported at the same time as the batch evolution data or later using **Import dataset**.

Merging with another dataset while importing is not necessary as all relevant datasets can be selected in the **Workset** dialog and merged by primary ID on the fly when creating the workset.

8.3 Merge

Merging of two datasets is available by clicking **Merge** in the **Modify dataset** group on the **Data** tab.

In this dialog, datasets can only be merged by matching primary IDs. The resulting file will include the union of the available variables and observations.



First dataset (destination): Process 1A

Second dataset (source): For prediction

Primary ID match 100.0%

The second dataset and all dependent models will be deleted.

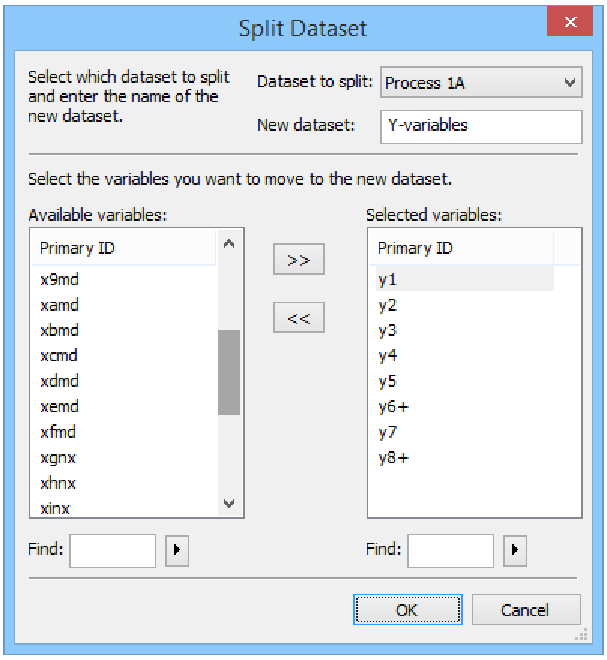
To merge:

1. In the **First dataset (destination)** box select the dataset that should end up on top or to the left.
2. In the **Second dataset (source)** box select the dataset that should end up at the bottom or to the right.

Note: Datasets created by SIMCA (filtered datasets, batch level datasets etc.) cannot be merged.

8.4 Split dataset

Datasets can be split in two by clicking **Split** in the **Modify dataset** group on the **Data** tab.



Select which dataset to split and enter the name of the new dataset.

Dataset to split: Process 1A

New dataset: Y-variables

Select the variables you want to move to the new dataset.

Available variables:	Selected variables:
Primary ID	Primary ID
x9md	y1
xamd	y2
xbmd	y3
xcmd	y4
xdmd	y5
xemd	y6+
xfmd	y7
xgnx	y8+
xhnx	
xinx	

In the **Split Dataset** dialog:

1. Select the **Dataset to split**.
2. Enter a dataset name in the **New dataset** field.
3. In the **Available variables** mark the variables to split out to the new dataset and click the **>>**-button.
4. Click **OK** to create the new dataset splitting the specified variables from the original dataset.

Note: Datasets created by SIMCA (filtered datasets, batch level datasets etc.) cannot be split.

Note: This feature is also available last in the **Spectral Filters** wizard after excluding some variables.

8.5 Transpose

Transposing of datasets is available by clicking **Transpose** in the **Modify dataset** group on the **Data** tab.

When clicking **Transpose** a message is displayed stating that when transposing the dataset the following changes happens:

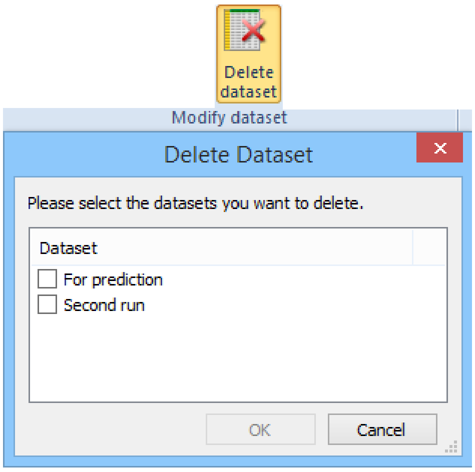
- All dependent datasets will be deleted.
- The current predictionset will be deleted.

- All dependent models will be deleted.
- Qualitative variables will lose their descriptors, that is, will no longer be qualitative variables but the descriptors will be replaced by integers according to their order.

Note: Datasets created by SIMCA (filtered datasets, batch level datasets etc.) cannot be transposed, nor can batch evolution datasets.

8.6 Delete dataset

Delete datasets by clicking **Delete dataset** in the **Modify dataset** group on the **Data** tab. Any dependent datasets, predictionsets and models are automatically deleted.



Please select the datasets you want to delete.

Dataset

□ For prediction

□ Second run

OK Cancel

Note: The first imported dataset cannot be deleted.

8.7 Generate variables

New variables can be generated by using a function, an expression with operators, or model results, in the formula field on the first page of the **Generate Variables** wizard. Function names are case *insensitive* and the result of a function can be passed as an argument to other functions. The result of an expression must yield a matrix with one or more columns where the columns will become new variables.

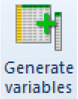
Note: To generate new observations, first transpose the dataset, then use the **Generate variables** feature, and finally transpose the dataset again.

In the subsections that follow, the **Generate Variables** wizard, creation of new variables from other datasets, and generating variables in batch projects are covered.

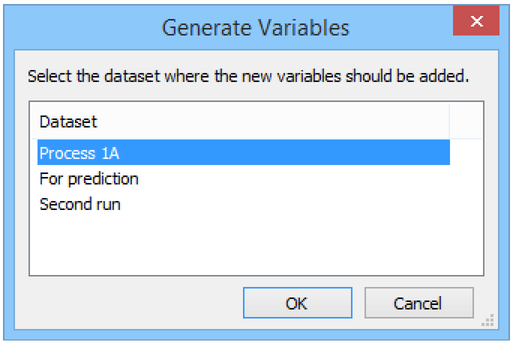
8.7.1 Generate Variables wizard

Creating new variables as functions of existing ones, or from the results of fitted models, is available on the **Data** tab, in the **Modify dataset** group, by clicking **Generate variables**. All new variables are appended to the right of the last column of the selected dataset.

To add generated variables:

Step	Description and illustration
1.	Start generating variables by clicking **Generate variables**. 
2.	Select dataset, in the dialog listing the available datasets. When only one dataset is available, this dialog is not opened.

Step **Description and illustration**



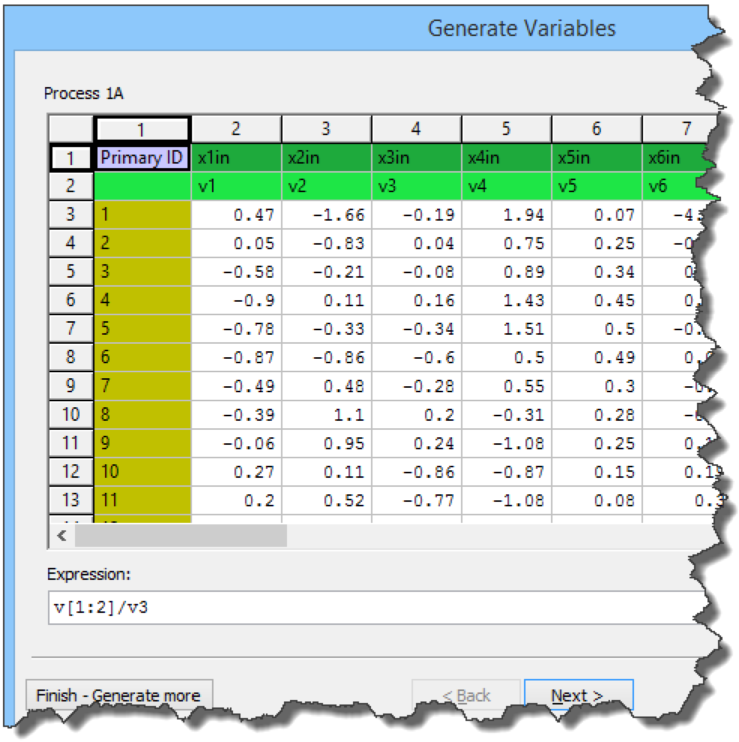
Generate Variables

Select the dataset where the new variables should be added.

Dataset
Process 1A
For prediction
Second run

3. In the **Generate Variables** wizard enter the expression defining the new variable(s). Click the question mark button ? to read about the operators and functions available. Click **Next**.

Note: Power, multiplication, and division cannot be applied to a set of variables and another set of variables. The first operand can be a constant, a variable or a set of variables, but the second and following operands must be a single variable or a constant.



Generate Variables

Process 1A

	1	2	3	4	5	6	7
1	Primary ID	x1in	x2in	x3in	x4in	x5in	x6in
2		v1	v2	v3	v4	v5	v6
3	1	0.47	-1.66	-0.19	1.94	0.07	-4
4	2	0.05	-0.83	0.04	0.75	0.25	-0
5	3	-0.58	-0.21	-0.08	0.89	0.34	0
6	4	-0.9	0.11	0.16	1.43	0.45	0.
7	5	-0.78	-0.33	-0.34	1.51	0.5	-0.
8	6	-0.87	-0.86	-0.6	0.5	0.49	0.
9	7	-0.49	0.48	-0.28	0.55	0.3	-0
10	8	-0.39	1.1	0.2	-0.31	0.28	-
11	9	-0.06	0.95	0.24	-1.08	0.25	0.
12	10	0.27	0.11	-0.86	-0.87	0.15	0.1
13	11	0.2	0.52	-0.77	-1.08	0.08	0.

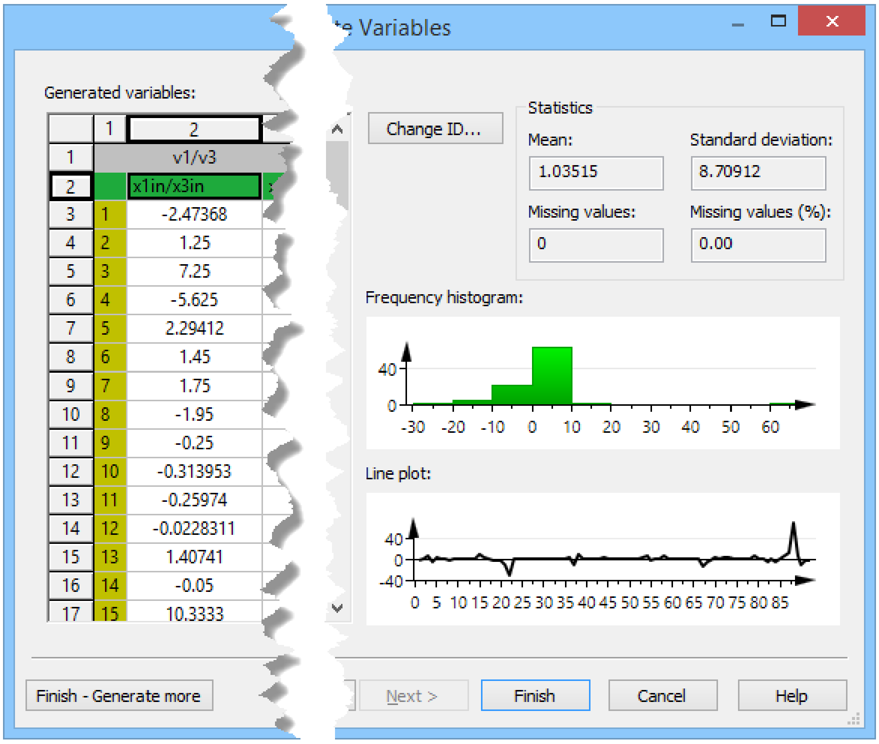
Expression:

```
v[1:2]/v3
```

4. The new variables are displayed with their formula, statistics and Quick info plots.

By default the new variables are named according to their recipe. To change the names, see point 5, otherwise go to point 6.

Step **Description and illustration**



Variables

Generated variables:

	1	2
1		v1/v3
2		x1in/x3in
3	1	-2.47368
4	2	1.25
5	3	7.25
6	4	-5.625
7	5	2.29412
8	6	1.45
9	7	1.75
10	8	-1.95
11	9	-0.25
12	10	-0.313953
13	11	-0.25974
14	12	-0.0228311
15	13	1.40741
16	14	-0.05
17	15	10.3333

Statistics

Mean: 1.03515

Standard deviation: 8.70912

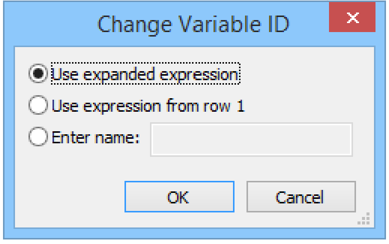
Missing values: 0

Missing values (%): 0.00

Frequency histogram:

Line plot:

5. Change the IDs as desired, either manually or by clicking the **Change ID** button available when marking the current variable ID.
In the Change Variable ID dialog select Use expanded expression, Use expression from row 1 or Enter name.
When selecting **Enter name** a sequential number is automatically added after the name specified in the field.



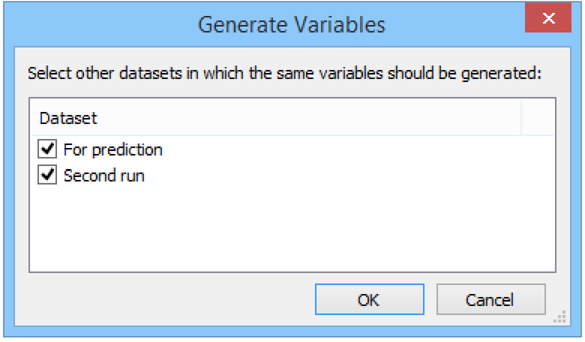
Change Variable ID

● Use expanded expression

○ Use expression from row 1

○ Enter name:

6. Click **Finish** to exit the wizard or **Finish - generate more** to reopen the **Generate Variables** wizard and continue at point 3.
When clicking **Finish** after adding variables to the dataset, if there are more datasets, SIMCA will display a dialog enabling adding the variables to other datasets also. If you don't want to add the variables to any other datasets, click **Cancel**.



Generate Variables

Select other datasets in which the same variables should be generated:

Dataset

☑ For prediction

☑ Second run

8.7.2 New variables from other dataset

You can generate new variables from any existing SIMCA datasets.

SIMCA accepts the following syntax:

D*int1*: v[*int2: int3*]
Variables number *int2* to *int3* in dataset *int1*.
This expression is only valid if the current dataset has the same number of observations as dataset number *int1*

Examples:

D2:v[3,6,8:11]
Generates variables 3,6,8,9,10,11 from dataset 2.

Note: *Dataset number 1 is the first dataset. New variables are always appended at the end of the selected dataset.*

Hint: More syntax details are available when you click the ?-mark to the right of the Expression field in the Generate Variables wizard.

8.7.2.1 Finding the dataset number

When creating new variables from another dataset, the DS-number can be seen in the **Data** box in any of the dialogs opened from the **Plot/List** tab, for instance **Scatter**.

The **Dataset** menu on the **Home** tab lists the datasets, but not their number. Dataset numbers are not reused for hierarchical which means that if you create a hierarchical dataset (specify a hierarchical base model), and then remove the dataset (specify the model as non hierarchical), the dataset numbering is no longer consecutive.

8.7.3 Generating variables in batch projects

With batches all functions operating on the whole vector (variable) are implemented batch by batch within a phase. When batches have phases, the default is to apply the function to all phases. If you want the function to operate on a variable in only selected phases, you must use the phase function and specify the desired phases.

Note: For batch level datasets, **Generate variables** can only add variables to batch condition datasets, not to the dataset created by SIMCA.

8.7.3.1 Batch specific syntax

The syntax is as follows:

Function Phase (*set-of-variables, integer-set*)

Where:

- **Function** is the selected function to apply.
- **Phase** signifies that the function should be applied phase wise
- *Set-of-variables* is any matrix resulting from other functions or a set of variables.
- *Integer-set* is a set of one or more numbers, representing the phase numbers. Enclose the numbers with square brackets if you want to specify more than one phase. For example: [1, 3, 5:10] means phases 1, 3 and 5 to 10.

8.7.3.2 Applying a function to some phases

When the function operates on some phases only, the default is to leave the values of the variables as they are for the omitted phases.

If you want to have missing values for the variable in the omitted phases, or a specific value for example 0, you must add the text *misval* or the *fvalue* at the end of the function.

For example:

Function Phase (*set-of-variables, integer-set, misval*) will set the variable to missing in the omitted phases.

While **Function Phase** (*set-of-variables, integer-set, 0*) will set the variable to 0 in the omitted phases.

Setting the values to 0 in the omitted phases, allows you to apply different functions to the same variable in different phases,

For example:

Low Pass (Phase (v1, 2, 0)) + HiPass (Phase (v1, [1,3], 0)) will generate a new variable by applying a Low Pass filter to variable v1 in phase 2 and a Hi Pass filter to variable v1 in phase 1 and 3.

8.7.3.3 Generate Variables for batch level without batch conditions

When you have no batch condition datasets but want to generate variables built on the batch level dataset you first need to create a batch condition dataset. Create this batch condition dataset as follows:

1. Copy the batch ID of the batch level dataset.
2. **Data | Import dataset**.
3. Select an empty spreadsheet (in SIMCA import click **Add data | Blank** on the **Home** tab).
4. Paste the batch ID and specify it as batch ID.
5. Type a variable name and leave all cells blank.
6. Specify the first row as primary variable ID:
7. Verify that the **Issues** pane will exclude all rows and columns that lack batch ID or primary variable ID and click **Resolve all**.
8. Click **Finish** to import the dataset. Now use this dataset to add the generated variables to by selecting the dataset in the **Generate Variables** dialog. Note that you have to use the dataset number to refer to the other dataset. See dataset numbers in the **Plot/List** dialogs.

Hint: More syntax details are available when you click the ?-mark to the right of the Expression field in the Generate Variables wizard.

8.8 Local centering

Local centering is useful when applying run-to-run control and changing set points.

With local centering one models the variation of the:

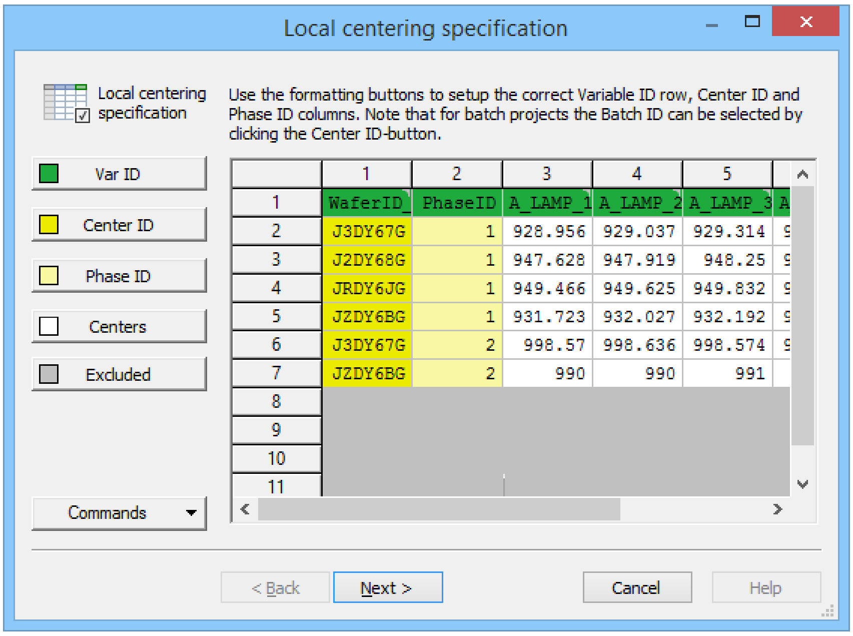
- Batch around its specified center in a phase for batch projects.
- Variable, or part of variable with for instance classes, around the specified center.

The imported local centering values are applied to all selected datasets when fitting the model and when making predictions.

8.8.1 Importing local centering

To import local centering:

1. On the **Data** tab, in the **Modify dataset** group, click **Local centering | Import**.
2. Select the file containing the specifications for local centering of the variables.
3. In the dialog, format according to the below:
   - **Var ID** is the primary variable as a row, specifying the variables to center.
   - **Center ID** is the Secondary observation ID/Class ID/Batch ID/Phase iteration ID as a column, specifying the observations to center. Using a secondary observation ID to specify which observations to center together can be useful when the dataset has classes. When using the **Batch ID** as center ID, the column may hold each batch ID only once, or once per phase. Specifying batch ID is necessary for batch evolution datasets where you want to specify the local centering per batch.
   - **Phase ID** as a column with each phase ID only available once per batch. Specifying Phase ID is necessary for batch projects with phases.
   - **Centers**, used for the subtraction, as data in the spreadsheet.

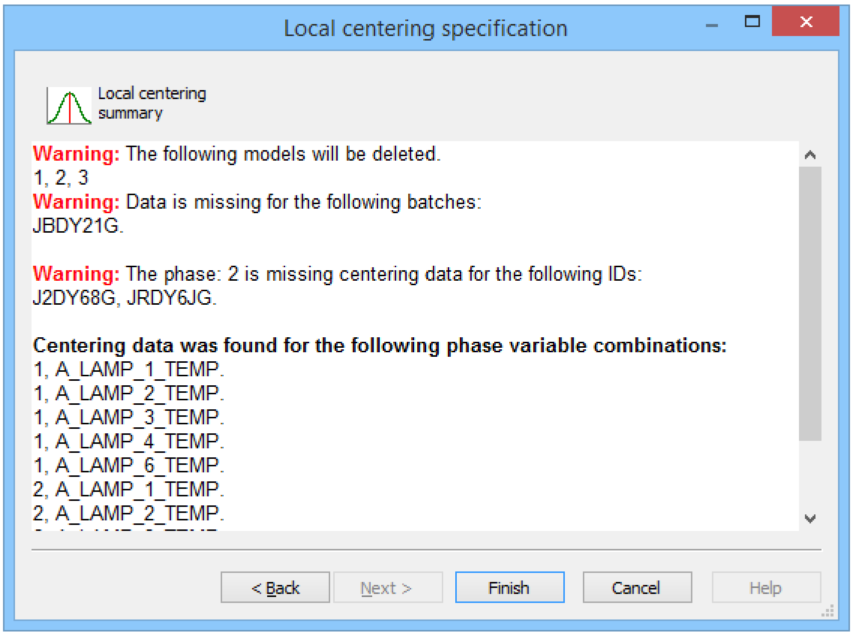


Use the formatting buttons to setup the correct Variable ID row, Center ID and Phase ID columns. Note that for batch projects the Batch ID can be selected by clicking the Center ID-button.

	1	2	3	4	5	
1	WaferID_	PhaseID	A_LAMP_1	A_LAMP_2	A_LAMP_3	A
2	J3DY67G	1	928.956	929.037	929.314	9
3	J2DY68G	1	947.628	947.919	948.25	9
4	JRDY6JG	1	949.466	949.625	949.832	9
5	JZDY6BG	1	931.723	932.027	932.192	9
6	J3DY67G	2	998.57	998.636	998.574	9
7	JZDY6BG	2	990	990	991	
8						
9						
10						
11						

Note: The local centering specification specifies the values to subtract from the selected variables.

Clicking **Next** opens the **Local Centering Summary** page.



Warning: The following models will be deleted.
1, 2, 3
Warning: Data is missing for the following batches:
JBDY21G.

Warning: The phase: 2 is missing centering data for the following IDs:
J2DY68G, JRDY6JG.

Centering data was found for the following phase variable combinations:
1, A_LAMP_1_TEMP.
1, A_LAMP_2_TEMP.
1, A_LAMP_3_TEMP.
1, A_LAMP_4_TEMP.
1, A_LAMP_6_TEMP.
2, A_LAMP_1_TEMP.
2, A_LAMP_2_TEMP.

8.8.2 Local centering of the predictionset

The predictionset dataset uses the imported local centering when available.

See also the Local centering missing subsection.

8.8.3 Local centering missing

After local centering has been imported, variables that lack local centering value are treated as follows:

8.8.3.1.1 Batch project

When the local centering was applied according to **Batch ID**, but no local centering is available for some batches, the locally centered variables of that batch are locally centered using the average of the local centering values of all batches included in the workset.

If you want to import the original values for a certain batch, specify local centering as '0' for that batch/variable combination.

When local centering is missing for predictions, the average of the workset batches for that variable is used in the local centering.

8.8.3.1.2 Regular project

When the local centering was applied according to **Center ID**, but no local centering is available for some classes, the observations are not centered at all; their original value is used.

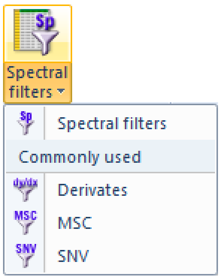
8.8.4 View imported local centering

The imported local centering values can be displayed by clicking **Local centering | View**. If **View** is unavailable, no local centering has been imported.

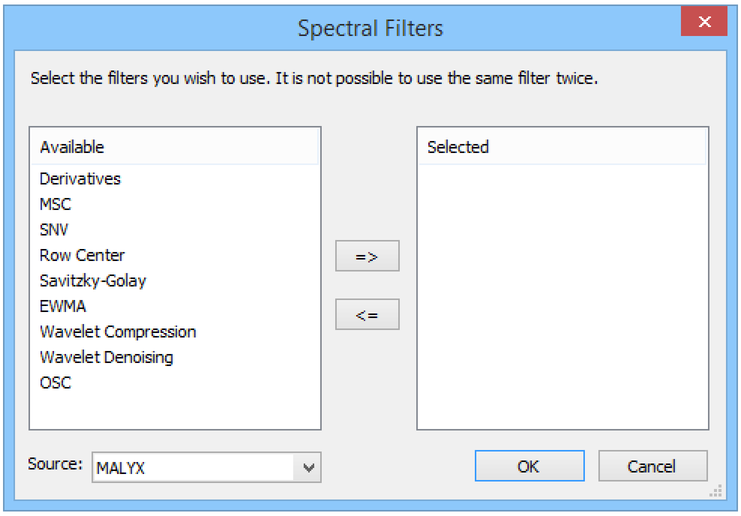
Note: Local centering is only saved if the variable is available in one of the imported datasets.

8.9 Spectral filters

To apply spectral filters observation wise, on the **Data** tab, in the **Filters** group, click **Spectral filters**. The three filter methods **Derivatives**, **MSC** and **SNV** are available by clicking the arrow.



Clicking **Spectral filters** opens the following dialog:



Select the filters you wish to use. It is not possible to use the same filter twice.

Source: MALYX

The filters listed in this dialog are described in the subsections that follow. A short background is available in the Preprocessing appendix.

To specify which filter or chain of filters to use:

1. Click the desired filter in the **Available** list.
2. Click the **=>** button.
3. Repeat 1-2 until the **Selected** list displays the desired filters.
4. If there are more than one dataset in the project, select the desired dataset in the **Source** box.

5. Click **OK** and the wizard of each filter opens successively and the filters are applied in the order specified in the **Spectral Filters** dialog.

6. After completed filtering, a new filtered dataset is created, leaving all original variables in the original dataset. Optionally excluded variables can be split out to a separate dataset by selecting the **Split out new variables to a new dataset** check box on the last page of the wizard. For more about splitting datasets, see the Split subsection previously in this chapter.

SIMCA also supports user written filters. For more information, contact your Sartorius Stedim Data Analytics sales office.

8.9.1 Filtering limitations

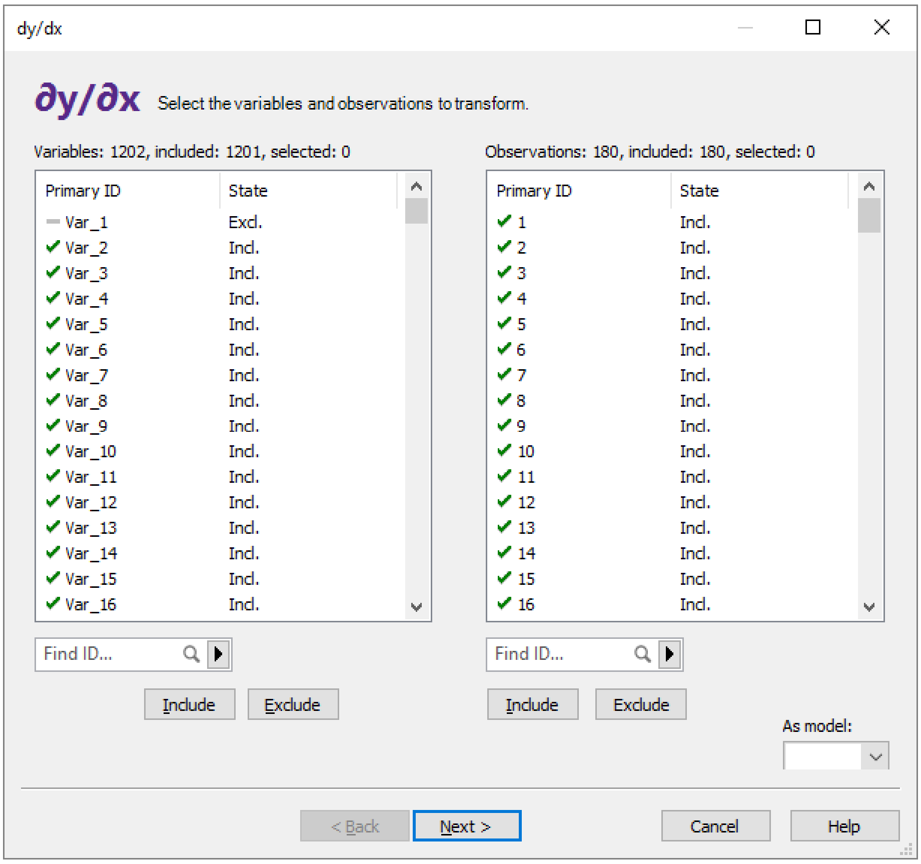
The following limitations are present for filtering:

- Only one of the wavelet filters can be included in a chain. All other filters can be applied in any order or combination.
- No filtering is available for filtered converted projects.
- Qualitative variables cannot be filtered and are automatically excluded and cannot be included.
- Projects with local centering data cannot be filtered.
- Only one dataset at a time can be filtered. To filter two datasets, first Merge them.

8.9.2 First, second, and third derivatives

Applying derivatives transforms the dataset from the original domain to the first, second, or third derivate. For more, see the Derivatives section in the Preprocessing appendix.

When selecting **Derivatives**, the first page of the derivatives wizard displays lists of variables and observations.



Select the variables and observations to transform.

Variables: 1202, included: 1201, selected: 0

Primary ID	State
Var_1	Excl.
✓ Var_2	Incl.
✓ Var_3	Incl.
✓ Var_4	Incl.
✓ Var_5	Incl.
✓ Var_6	Incl.
✓ Var_7	Incl.
✓ Var_8	Incl.
✓ Var_9	Incl.
✓ Var_10	Incl.
✓ Var_11	Incl.
✓ Var_12	Incl.
✓ Var_13	Incl.
✓ Var_14	Incl.
✓ Var_15	Incl.
✓ Var_16	Incl.

Observations: 180, included: 180, selected: 0

Primary ID	State
✓ 1	Incl.
✓ 2	Incl.
✓ 3	Incl.
✓ 4	Incl.
✓ 5	Incl.
✓ 6	Incl.
✓ 7	Incl.
✓ 8	Incl.
✓ 9	Incl.
✓ 10	Incl.
✓ 11	Incl.
✓ 12	Incl.
✓ 13	Incl.
✓ 14	Incl.
✓ 15	Incl.
✓ 16	Incl.

8.9.2.1 Selecting the variables and observations to transform

To apply the filter to the dataset, on the first page of the wizard:

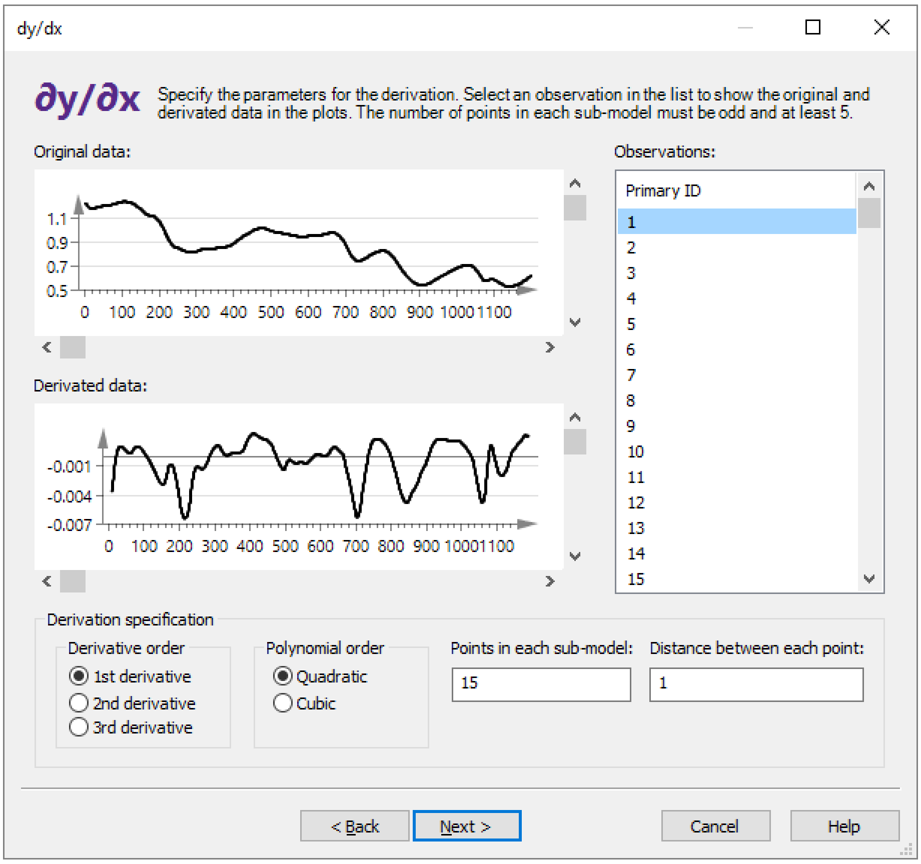
1. In the **Variables** list, mark and **Exclude** unwanted variables. All variables specified as X in the default workset are by default included, while those specified as Y are by default excluded. Qualitative variables cannot be filtered.
2. In the **Observations** list, mark and **Exclude** the observations to exclude from the filtering. All observations are by default included.
3. To specify variables and observations according to a fitted model, select the model in the **As model** box. Variables in the model specified as Y are automatically excluded.
4. Click **Next**.

8.9.2.2 Specifying parameters for derivation

Specify the parameters for the derivation in the **Derivation specification** section by following the steps described here. Note that marking an observation updates the graphs displaying the **Original data** (spectra) and the **Derivated data** with the current settings.

1. Select **Derivative order**: **1st derivative**, **2nd derivative**, or **3rd derivative**.
2. Select **Polynomial order**: **Quadratic** or **Cubic**.
3. Enter the number of points to include in the sub-models in the **Points in each sub-model** field. This number is default 15 and has to be odd and >5.
4. Optionally enter the **Distance between each point**.
5. Click **Next**.

Note: The filtered dataset is created without the edge effects leaving the first and last window size/2 variables empty (default first and last 7 variables).



Specify the parameters for the derivation. Select an observation in the list to show the original and derivated data in the plots. The number of points in each sub-model must be odd and at least 5.

Derivation specification

Derivative order: ● 1st derivative ○ 2nd derivative ○ 3rd derivative

Polynomial order: ● Quadratic ○ Cubic

Points in each sub-model: 15

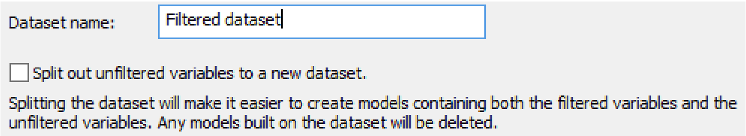
Distance between each point: 1

8.9.2.3 Creating the filtered dataset

The last page completes the creation of the filtered dataset.

- Enter the **Dataset name**.

- Select to split out unfiltered variables to a new dataset by selecting the **Split out unfiltered variables to a new dataset** check box if desired.
- Click **Finish**.



Dataset name: Filtered dataset

□ Split out unfiltered variables to a new dataset.

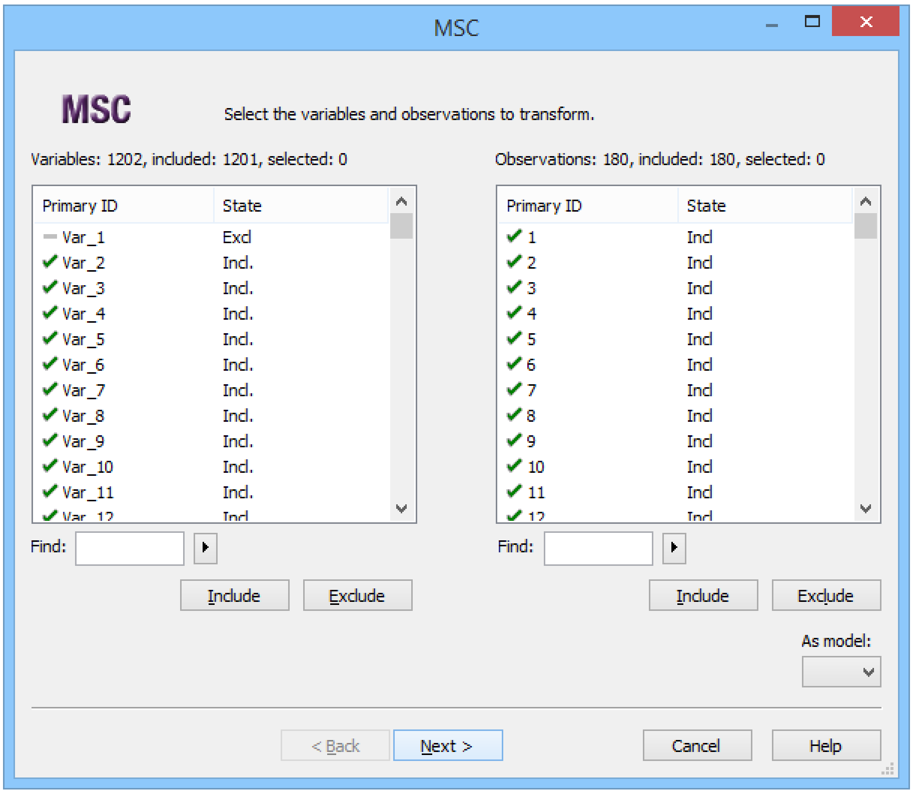
Splitting the dataset will make it easier to create models containing both the filtered variables and the unfiltered variables. Any models built on the dataset will be deleted.

Note: To create a model using both filtered and original data, both datasets have to be selected in the **Select data** page in the **Workset** dialog.

8.9.3 Multiplicative Signal Correction – MSC

When applying **Multiplicative Signal Correction**, each observation (spectra) $\mathbf{x}_i$ is "normalized" by regressing it against the average spectrum.

When selecting **MSC**, the first page of the **MSC** wizard displays lists of variables and observations.



Select the variables and observations to transform.

Variables: 1202, included: 1201, selected: 0

Primary ID	State
Var_1	Excl
✓ Var_2	Incl.
✓ Var_3	Incl.
✓ Var_4	Incl.
✓ Var_5	Incl.
✓ Var_6	Incl.
✓ Var_7	Incl.
✓ Var_8	Incl.
✓ Var_9	Incl.
✓ Var_10	Incl.
✓ Var_11	Incl.
✓ Var_12	Incl.

Observations: 180, included: 180, selected: 0

Primary ID	State
✓ 1	Incl
✓ 2	Incl
✓ 3	Incl
✓ 4	Incl
✓ 5	Incl
✓ 6	Incl
✓ 7	Incl
✓ 8	Incl
✓ 9	Incl
✓ 10	Incl
✓ 11	Incl
✓ 12	Incl

For more see <u>Multiplicative Signal Correction (MSC)</u> in the

<u>Multiplicative Signal Correction (MSC)</u>

8.9.3.1 Selecting the variables and observations to transform

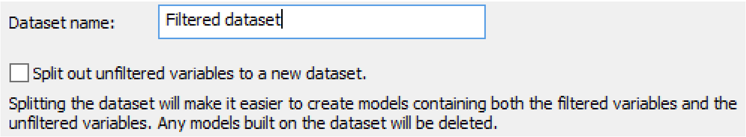
To apply the filter to the dataset, on the first page of the wizard:

1. In the **Variables** list, mark and **Exclude** unwanted variables. All variables specified as X in the <u>default workset</u> are by default included, while those specified as Y are by default excluded. Qualitative variables cannot be filtered.
2. In the **Observations** list, mark and **Exclude** the observations to exclude from the filtering. All observations are by default included.
3. To specify variables and observations according to a fitted model, select the model in the **As model** box. Variables in the model specified as Y are automatically excluded.
4. Click **Next**.

8.9.3.2 Creating the filtered dataset

The last page completes the creation of the filtered dataset.

- Enter the **Dataset name**.
- Select to split out unfiltered variables to a new dataset by selecting the **Split out unfiltered variables to a new dataset** check box if desired.
- Click **Finish**.



Dataset name: Filtered dataset

□ Split out unfiltered variables to a new dataset.

Splitting the dataset will make it easier to create models containing both the filtered variables and the unfiltered variables. Any models built on the dataset will be deleted.

Note: To create a model using both filtered and original data, both datasets have to be selected in the **Select data** page in the **Workset** dialog.

8.9.4 Standard Normal Variate – SNV

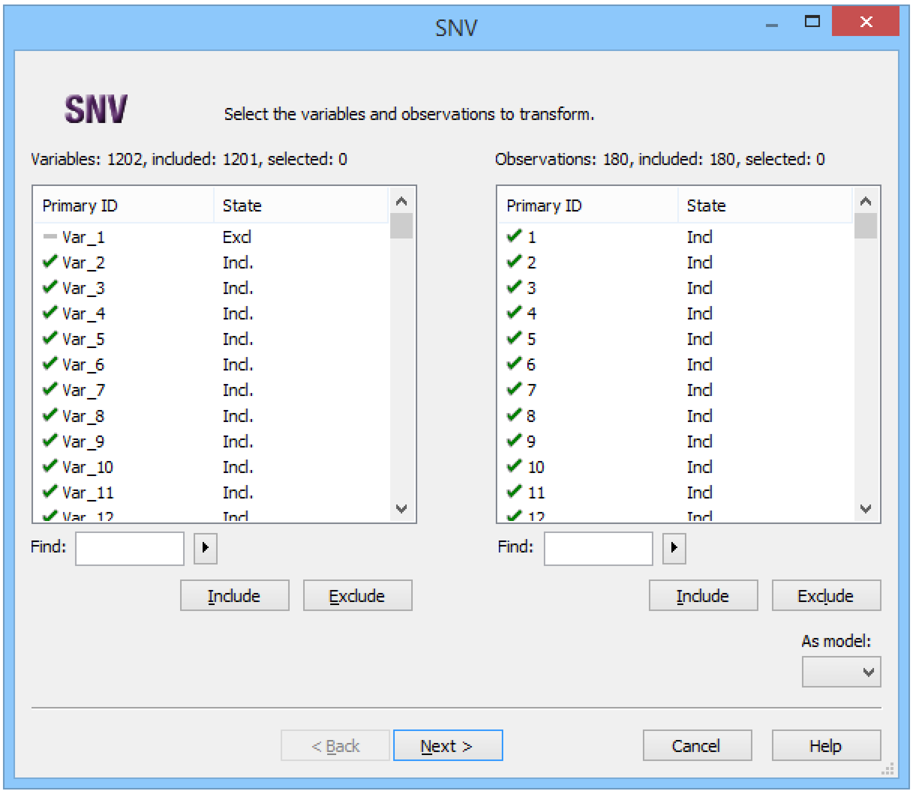
When applying the **SNV** filter, each observation (spectra) is “normalized” by subtracting the mean and dividing with the standard deviation.

For more, see the Standard Normal Variate (SNV) section in the Preprocessing appendix.

Hint: In the **Workset** dialog, first select the filtered dataset and then specify the workset for the calibration model.

8.9.4.1 SNV wizard

When selecting **SNV**, the first page of the **SNV** wizard displays lists of variables and observations.



Select the variables and observations to transform.

Variables: 1202, included: 1201, selected: 0

Primary ID	State
Var_1	Excl
✓ Var_2	Incl.
✓ Var_3	Incl.
✓ Var_4	Incl.
✓ Var_5	Incl.
✓ Var_6	Incl.
✓ Var_7	Incl.
✓ Var_8	Incl.
✓ Var_9	Incl.
✓ Var_10	Incl.
✓ Var_11	Incl.
✓ Var_12	Incl.

Observations: 180, included: 180, selected: 0

Primary ID	State
✓ 1	Incl
✓ 2	Incl
✓ 3	Incl
✓ 4	Incl
✓ 5	Incl
✓ 6	Incl
✓ 7	Incl
✓ 8	Incl
✓ 9	Incl
✓ 10	Incl
✓ 11	Incl
✓ 12	Incl

8.9.4.2 Selecting the variables and observations to transform

To apply the filter to the dataset, on the first page of the wizard:

1. In the **Variables** list, mark and **Exclude** unwanted variables. All variables specified as X in the default workset are by default included, while those specified as Y are by default excluded. Qualitative variables cannot be filtered.

2. In the **Observations** list, mark and **Exclude** the observations to exclude from the filtering. All observations are by default included.

3. To specify variables and observations according to a fitted model, select the model in the **As model** box. Variables in the model specified as Y are automatically excluded.

4. Click **Next**.

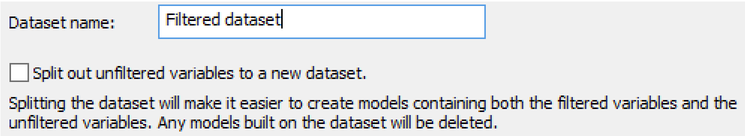
8.9.4.3 Creating the filtered dataset

The last page completes the creation of the filtered dataset.

- Enter the **Dataset name**.

- Select to split out unfiltered variables to a new dataset by selecting the **Split out unfiltered variables to a new dataset** check box if desired.

- Click **Finish**.



Dataset name: Filtered dataset

□ Split out unfiltered variables to a new dataset.

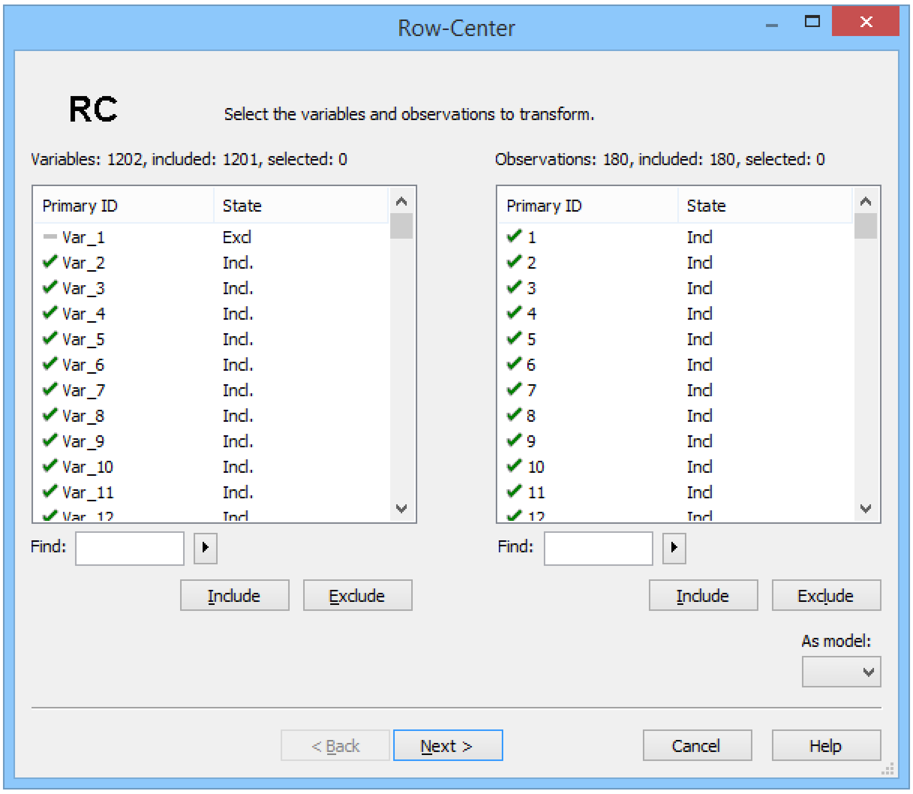
Splitting the dataset will make it easier to create models containing both the filtered variables and the unfiltered variables. Any models built on the dataset will be deleted.

Note: To create a model using both filtered and original data, both datasets have to be selected in the **Select data** page in the **Workset** dialog.

8.9.5 Row Center

Applying the **Row Center** filter subtracts the row mean from each row value.

When selecting **Row Center** in the **Spectral Filters** dialog and clicking **Next**, the first page of the **Row Center** wizard opens displaying lists of variables and observations.



Row-Center

RC

Select the variables and observations to transform.

Variables: 1202, included: 1201, selected: 0

Primary ID	State
Var_1	Excl
✓ Var_2	Incl.
✓ Var_3	Incl.
✓ Var_4	Incl.
✓ Var_5	Incl.
✓ Var_6	Incl.
✓ Var_7	Incl.
✓ Var_8	Incl.
✓ Var_9	Incl.
✓ Var_10	Incl.
✓ Var_11	Incl.
✓ Var_12	Incl

Observations: 180, included: 180, selected: 0

Primary ID	State
✓ 1	Incl
✓ 2	Incl
✓ 3	Incl
✓ 4	Incl
✓ 5	Incl
✓ 6	Incl
✓ 7	Incl
✓ 8	Incl
✓ 9	Incl
✓ 10	Incl
✓ 11	Incl
✓ 12	Incl

8.9.5.1 Selecting the variables and observations to transform

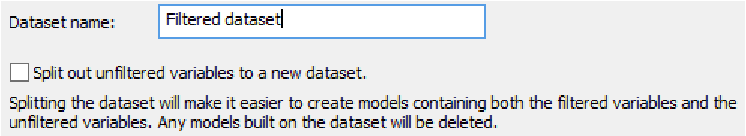
To apply the filter to the dataset, on the first page of the wizard:

1. In the **Variables** list, mark and **Exclude** unwanted variables. All variables specified as X in the default workset are by default included, while those specified as Y are by default excluded. Qualitative variables cannot be filtered.
2. In the **Observations** list, mark and **Exclude** the observations to exclude from the filtering. All observations are by default included.
3. To specify variables and observations according to a fitted model, select the model in the **As model** box. Variables in the model specified as Y are automatically excluded.
4. Click **Next**.

8.9.5.2 Creating the filtered dataset

The last page completes the creation of the filtered dataset.

- Enter the **Dataset name**.
- Select to split out unfiltered variables to a new dataset by selecting the **Split out unfiltered variables to a new dataset** check box if desired.
- Click **Finish**.



Dataset name: Filtered dataset

□ Split out unfiltered variables to a new dataset.

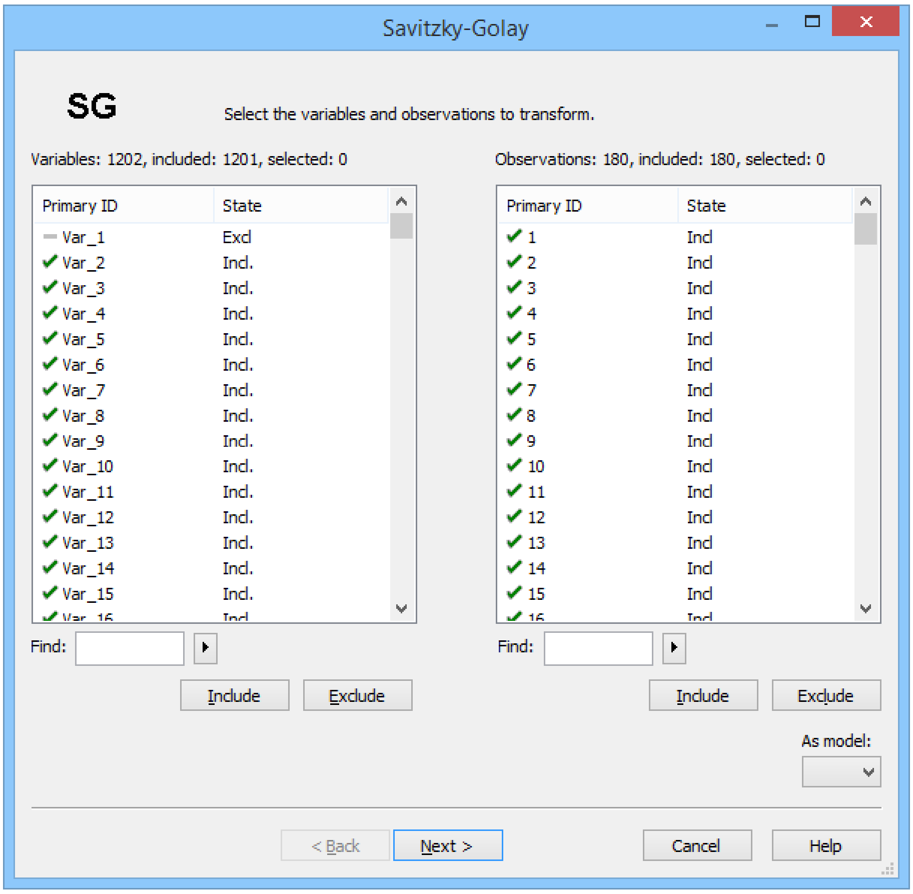
Splitting the dataset will make it easier to create models containing both the filtered variables and the unfiltered variables. Any models built on the dataset will be deleted.

Note: To create a model using both filtered and original data, both datasets have to be selected in the **Select data** page in the **Workset** dialog.

8.9.6 Savitzky-Golay

Applying the **Savitzky-Golay** filter removes noise by applying a moving polynomial to the data. For more, see the Derivatives section in the Preprocessing appendix.

When selecting **Savitzky-Golay** in the **Spectral Filters** dialog and clicking **Next**, the first page of the Savitzky-Golay wizard opens displaying lists of variables and observations.



SG

Select the variables and observations to transform.

Variables: 1202, included: 1201, selected: 0

Primary ID	State
Var_1	Excl
✓ Var_2	Incl.
✓ Var_3	Incl.
✓ Var_4	Incl.
✓ Var_5	Incl.
✓ Var_6	Incl.
✓ Var_7	Incl.
✓ Var_8	Incl.
✓ Var_9	Incl.
✓ Var_10	Incl.
✓ Var_11	Incl.
✓ Var_12	Incl.
✓ Var_13	Incl.
✓ Var_14	Incl.
✓ Var_15	Incl.
✓ Var_16	Incl

Find:

Observations: 180, included: 180, selected: 0

Primary ID	State
✓ 1	Incl
✓ 2	Incl
✓ 3	Incl
✓ 4	Incl
✓ 5	Incl
✓ 6	Incl
✓ 7	Incl
✓ 8	Incl
✓ 9	Incl
✓ 10	Incl
✓ 11	Incl
✓ 12	Incl
✓ 13	Incl
✓ 14	Incl
✓ 15	Incl
✓ 16	Incl

Find:

As model:

8.9.6.1 Selecting the variables and observations to transform

To apply the filter to the dataset, on the first page of the wizard:

1. In the **Variables** list, mark and **Exclude** unwanted variables. All variables specified as X in the default workset are by default included, while those specified as Y are by default excluded. Qualitative variables cannot be filtered.

2. In the **Observations** list, mark and **Exclude** the observations to exclude from the filtering. All observations are by default included.

3. To specify variables and observations according to a fitted model, select the model in the **As model** box. Variables in the model specified as Y are automatically excluded.

4. Click **Next**.

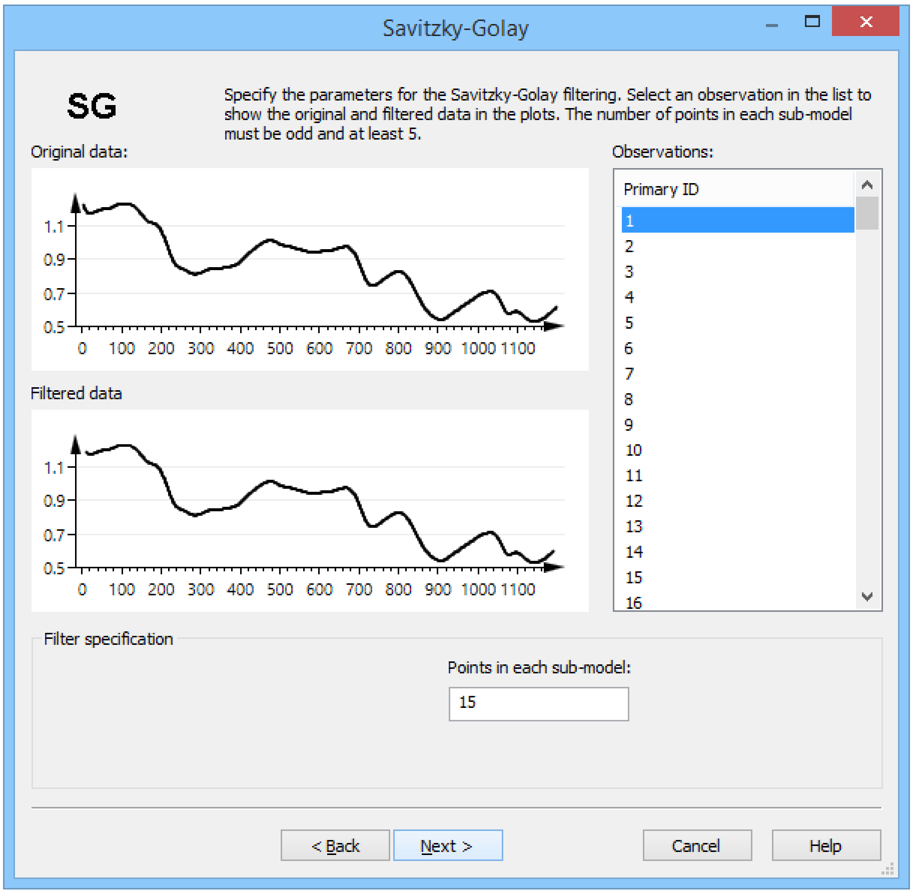
8.9.6.2 Specifying parameters for Savitzky-Golay

Specify the parameters for the filtering in the **Filter specification** section by following the steps described here. Note that marking an observation updates the graphs displaying the **Original data** (spectra) and the **Filtered data** with the current settings.

1. Enter number of points to include in the sub-models in the **Points in each sub-model** field. This number is default 15 and has to be odd and ≥5.

2. Click **Next**.

Note: The filtered dataset is created without the edge effects leaving the first and last window size/2 variables empty (default first and last 7 variables).



Specify the parameters for the Savitzky-Golay filtering. Select an observation in the list to show the original and filtered data in the plots. The number of points in each sub-model must be odd and at least 5.

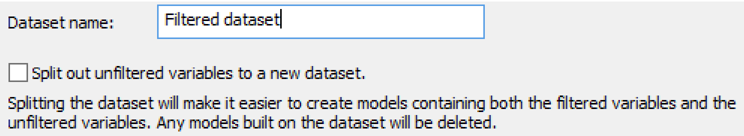
Filter specification

Points in each sub-model: 15

8.9.6.3 Creating the filtered dataset

The last page completes the creation of the filtered dataset.

- Enter the **Dataset name**.
- Select to split out unfiltered variables to a new dataset by selecting the **Split out unfiltered variables to a new dataset** check box if desired.
- Click **Finish**.



Dataset name: Filtered dataset

□ Split out unfiltered variables to a new dataset.

Splitting the dataset will make it easier to create models containing both the filtered variables and the unfiltered variables. Any models built on the dataset will be deleted.

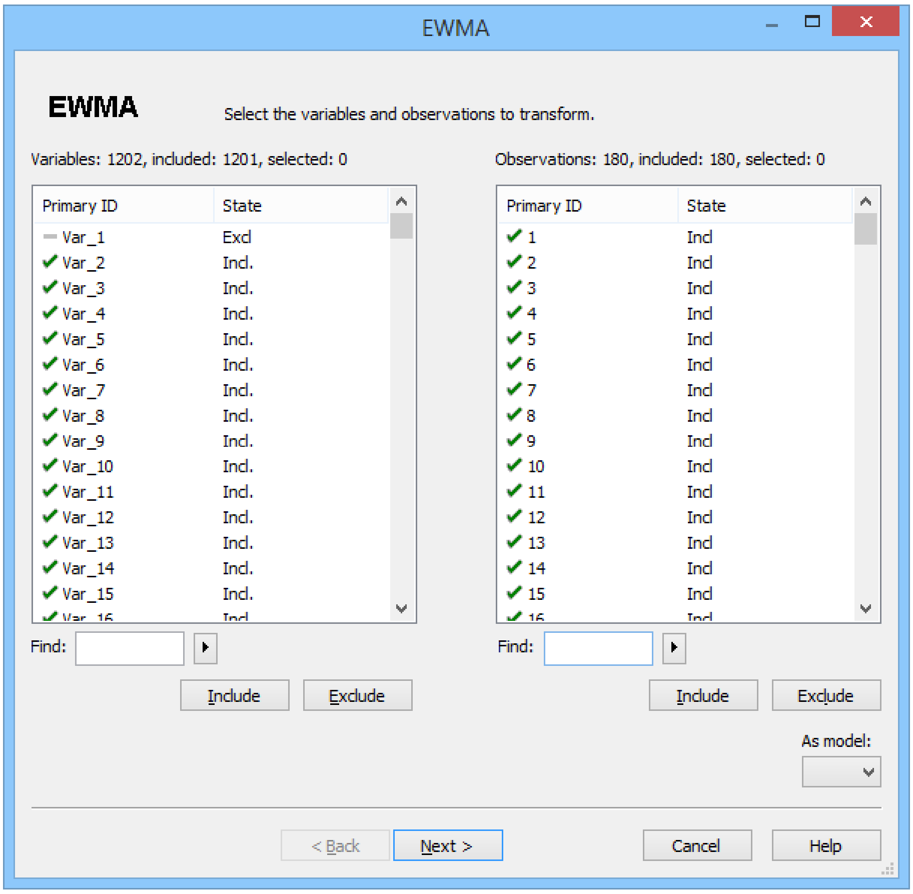
Note: To create a model using both filtered and original data, both datasets have to be selected in the **Select data** page in the **Workset** dialog.

8.9.7 EWMA

Filter removing noise by applying an exponentially weighted moving average to the data.

To change from the default EWMA type (Filter), click File | Options | SIMCA options, and the **Plot** section.

When selecting **EWMA** in the **Spectral Filters** dialog and clicking **Next**, the first page of the **EWMA** wizard opens displaying lists of variables and observations.



EWMA Select the variables and observations to transform.

Variables: 1202, included: 1201, selected: 0

Primary ID	State
— Var_1	Excl
✓ Var_2	Incl.
✓ Var_3	Incl.
✓ Var_4	Incl.
✓ Var_5	Incl.
✓ Var_6	Incl.
✓ Var_7	Incl.
✓ Var_8	Incl.
✓ Var_9	Incl.
✓ Var_10	Incl.
✓ Var_11	Incl.
✓ Var_12	Incl.
✓ Var_13	Incl.
✓ Var_14	Incl.
✓ Var_15	Incl.
✓ Var_16	Incl

Observations: 180, included: 180, selected: 0

Primary ID	State
✓ 1	Incl
✓ 2	Incl
✓ 3	Incl
✓ 4	Incl
✓ 5	Incl
✓ 6	Incl
✓ 7	Incl
✓ 8	Incl
✓ 9	Incl
✓ 10	Incl
✓ 11	Incl
✓ 12	Incl
✓ 13	Incl
✓ 14	Incl
✓ 15	Incl
✓ 16	Incl

8.9.7.1 Selecting the variables and observations to transform

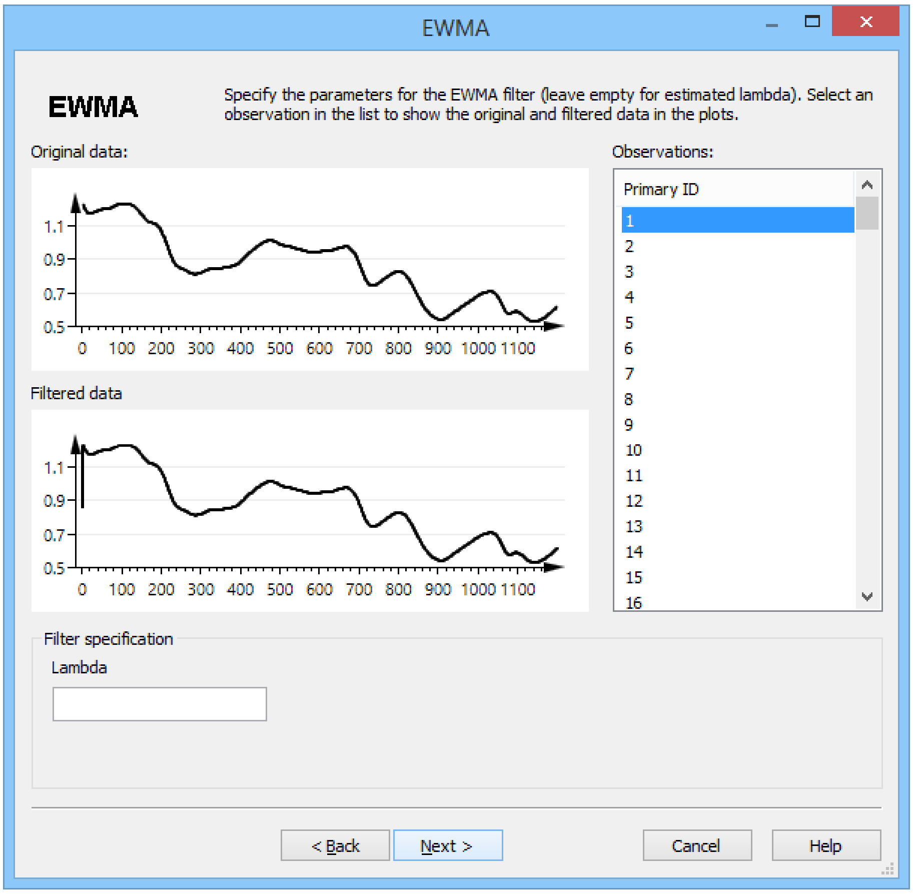
To apply the filter to the dataset, on the first page of the wizard:

1. In the **Variables** list, mark and **Exclude** unwanted variables. All variables specified as X in the default workset are by default included, while those specified as Y are by default excluded. Qualitative variables cannot be filtered.
2. In the **Observations** list, mark and **Exclude** the observations to exclude from the filtering. All observations are by default included.
3. To specify variables and observations according to a fitted model, select the model in the **As model** box. Variables in the model specified as Y are automatically excluded.
4. Click **Next**.

8.9.7.2 Specifying lambda for EWMA

Enter the desired lambda for the filtering in the **Lambda** field. Leaving the **Lambda** field empty results in using the estimated lambda.

Note that marking an observation updates the graphs displaying the **Original data** (spectra) and the **Filtered data** with the current settings.



EWMA

Specify the parameters for the EWMA filter (leave empty for estimated lambda). Select an observation in the list to show the original and filtered data in the plots.

Original data:

Filtered data

Observations:

Primary ID: 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16

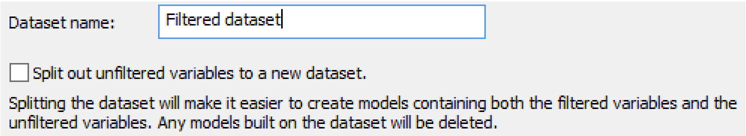
Filter specification

Lambda

8.9.7.3 Creating the filtered dataset

The last page completes the creation of the filtered dataset.

- Enter the **Dataset name**.
- Select to split out unfiltered variables to a new dataset by selecting the **Split out unfiltered variables to a new dataset** check box if desired.
- Click **Finish**.



Dataset name: Filtered dataset

□ Split out unfiltered variables to a new dataset.

Splitting the dataset will make it easier to create models containing both the filtered variables and the unfiltered variables. Any models built on the dataset will be deleted.

Note: To create a model using both filtered and original data, both datasets have to be selected in the **Select data** page in the **Workset** dialog.

8.9.8 Wavelet Compression Spectral – WCS

The wavelet transform of a signal x(t) decomposes the signal x(t) into sets of coefficients by frequency band. These bands are on a logarithmic scale, and decrease by the power of 2 from the Nyquist frequency to the lowest frequency in the signal. To compress the signal, all small coefficients are removed and the transformed signal compressed. To denoise the signal, all small coefficients are removed and the data is transformed back to the original domain.

For more, see the Wavelet compression or de-noising of signals section in the Preprocessing appendix.

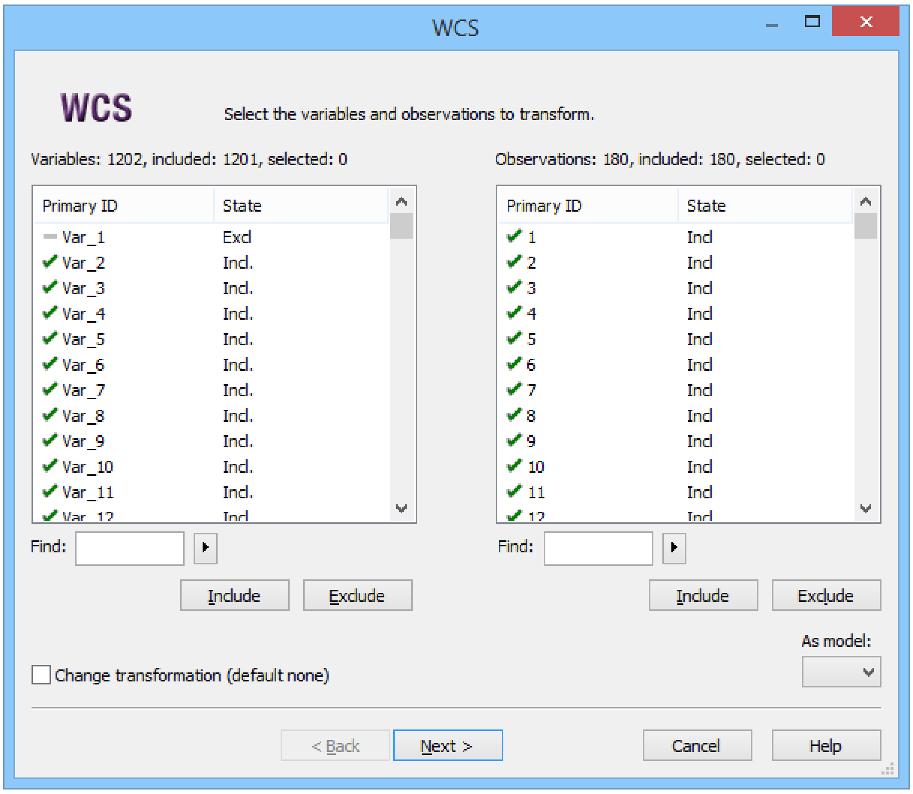
Note: With compression, reconstruct is done when the **Reconstruct wavelets** check box is selected in the Fit page of **Project Options**. This is the SIMCA default.

8.9.8.1 Digitized spectra

When the dataset consist of digitized spectra (i.e. NIR, NMR, and Raman etc.) each observation in the X matrix is the spectrum of a sample, and the wavelet transform and denoising of the matrix X is done row wise.

8.9.8.2 WCS wizard

When selecting **Wavelet Compression** in the **Spectral Filters** dialog and clicking **Next**, the first page of the WCS wizard opens displaying lists of variables and observations.



Select the variables and observations to transform.

Variables: 1202, included: 1201, selected: 0

Primary ID	State
Var_1	Excl
✓ Var_2	Incl.
✓ Var_3	Incl.
✓ Var_4	Incl.
✓ Var_5	Incl.
✓ Var_6	Incl.
✓ Var_7	Incl.
✓ Var_8	Incl.
✓ Var_9	Incl.
✓ Var_10	Incl.
✓ Var_11	Incl.
✓ Var_12	Incl

Observations: 180, included: 180, selected: 0

Primary ID	State
✓ 1	Incl
✓ 2	Incl
✓ 3	Incl
✓ 4	Incl
✓ 5	Incl
✓ 6	Incl
✓ 7	Incl
✓ 8	Incl
✓ 9	Incl
✓ 10	Incl
✓ 11	Incl
✓ 12	Incl

□ Change transformation (default none)

8.9.8.3 Selecting variables, observations, transform - WCS

To apply the filter to the dataset, on the first page of the wizard:

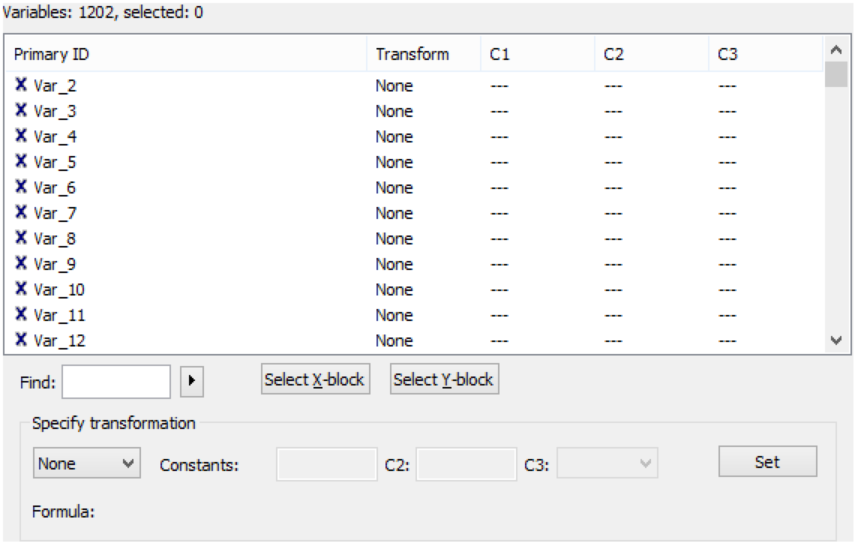
1. In the **Variables** list, mark and **Exclude** unwanted variables. All variables are specified according to the default workset.
2. In the **Observations** list, mark and **Exclude** the observations to exclude from the filtering. All observations are by default included.
3. To transform variables prior to the wavelet transformation, select the **Change transformation** check box. By default the variables are not transformed. See the Selecting variable transformations in spectral filtering subsection next.
4. To specify variables and observations according to a fitted model, select the model in the **As model** box. Variables in the model specified as Y are automatically excluded.
5. Click **Next**.

8.9.8.4 Selecting variable transformations in spectral filtering

With the **Change transformation** check box selected, clicking **Next** opens the **Select transformations** page.

Apply transformations before the compression by:

1. Marking the variables to transform.
2. Selecting the transformation: **Linear**, **Log**, **NegLog**, **Logit**, **Exponential**, or **Power** and then clicking **Set**.
3. Clicking **Next**.



Variables: 1202, selected: 0

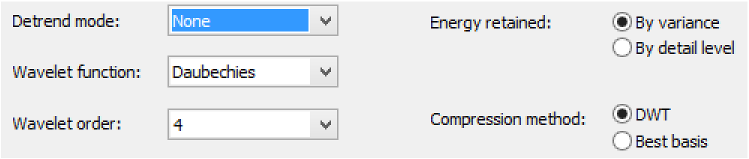
Primary ID	Transform	C1	C2	C3
✗ Var_2	None	---	---	---
✗ Var_3	None	---	---	---
✗ Var_4	None	---	---	---
✗ Var_5	None	---	---	---
✗ Var_6	None	---	---	---
✗ Var_7	None	---	---	---
✗ Var_8	None	---	---	---
✗ Var_9	None	---	---	---
✗ Var_10	None	---	---	---
✗ Var_11	None	---	---	---
✗ Var_12	None	---	---	---

None
Constants:
C2:
C3:

For details about the transformations available, see the Applying transformations section in the Workset section in Chapter 7 Home.

8.9.8.5 Selecting wavelet options

The page for wavelet options holds options for detrending, wavelet function, wavelet order, exclusion criteria, and compression method. This page is the same for WDS and WCS.



Detrend mode: None

Wavelet function: Daubechies

Wavelet order: 4

Energy retained: ● By variance ○ By detail level

Compression method: ● DWT ○ Best basis

In the page for selecting wavelet options:

1. In the **Detrend mode** box the default is **None**. Click the box to select **Mean** or **Linear**. **Mean** signifies removing the mean while **Linear** signifiers removing the best linear fit.
2. In the **Wavelet function** box the default is **Daubechies**. Click the box to select **Beylkin**, **Coiflet**, **Symmlet**, **Biorthogonal1**, **Biorthogonal2**, **Biorthogonal3**, **Biorthogonal4**, **Biorthogonal5**, or **Biorthogonal6**. For details about the wavelet functions, see the Wavelet families section in the Preprocessing appendix.
3. In the **Wavelet order** box, select the wavelet order. The default is the lowest available. The wavelet order differs depending on the wavelet function selected. Find the orders available for each wavelet function in the wavelet table.
4. Select the method of exclusion of wavelets coefficients by selecting **Energy retained** to be **By variance** or **By detail level**.
5. Click the desired decomposition and **Compression method**, **DWT** or **Best basis**. **DWT**, discrete wavelet transform, is recommended for low frequency signals and Best basis for high frequency signals. With **By detail level**, **DWT** is the only available compression method.
6. Click **Next**.

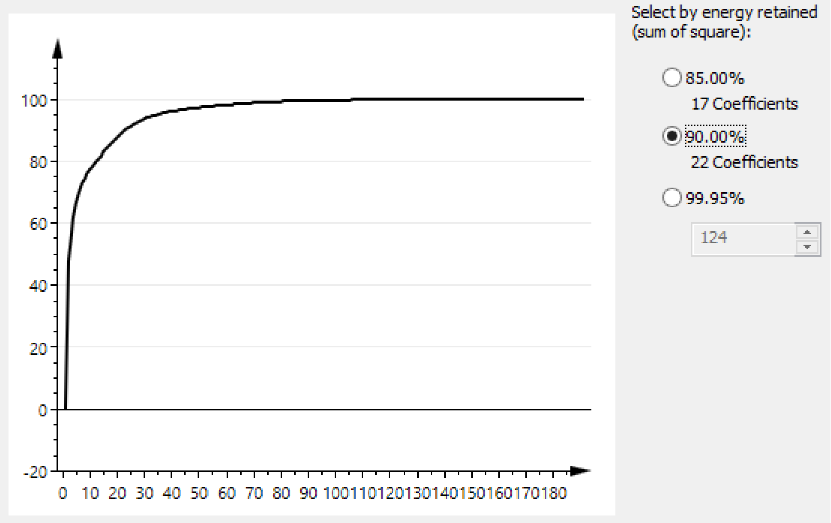
Wavelet function	Wavelet order
Beylkin	N/A
Coiflet	2, 3, 4, 5
Daubechies	4, 6, 8, 10, 12, 20, 50
Symmlet	4, 6, 8, 10
Biorthogonal1	1, 3, 5

Wavelet function	Wavelet order
Biorthogonal2	2, 4, 6, 8
Biorthogonal3	1, 3, 5, 7, 9
Biorthogonal4	4
Biorthogonal5	5
Biorthogonal6	8

8.9.8.6 Wavelet compression/denoising By variance

When compressing/denoising the signal by the percent of variance explained, SIMCA computes and displays the percentage of the variance explained by the wavelet coefficients of the target vector, sorted in order of importance.

1. Use the plot to decide the number of coefficients to keep. The default is to keep the coefficients that accounts for 99.5% of the variance.
2. Optionally change from the default by clicking another option under **Select by energy retained (sum of squares)**.
3. Click **Next**.



Select by energy retained (sum of square):

○ 85.00%
17 Coefficients

● 90.00%
22 Coefficients

○ 99.95%
124

Compression/denoising **By variance** is done either using compression method **DWT** or **Best basis**. For details about DWT and best basis, see the Wavelet compression or de-noising of signals section in the Preprocessing appendix.

8.9.8.7 Wavelet compression/denoising By detail level

The compression/denoising **By detail level** is performed by excluding all the detail coefficients corresponding to selected scales (levels) of the target vector. **DWT** is the only available compression method.

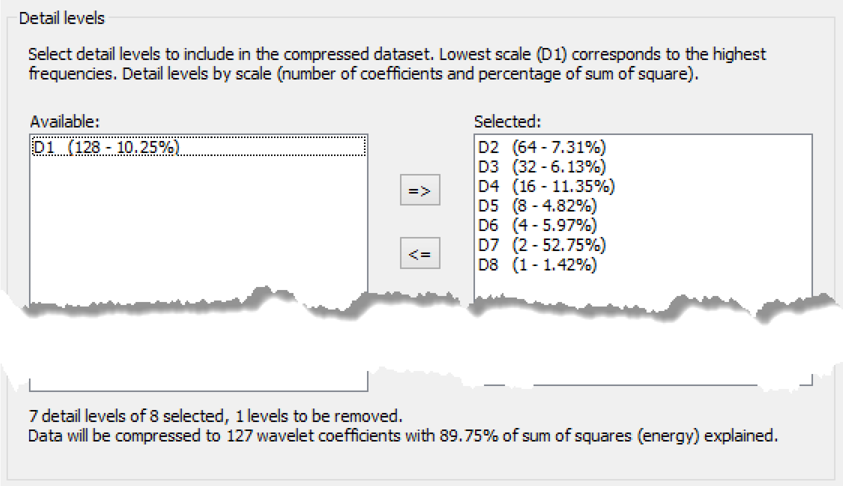
The wavelet transform is first done on the target vector and the results are displayed as a table. After selecting the wavelets coefficients or the scales to be removed, the same transformation is performed on each X observation vector.

8.9.8.8 Selecting wavelet coefficients

When selecting **By detail level** to compress/denoise the X block by removing detail levels, SIMCA decomposes the target X to its detail coefficients at every scale. The left table displays for every detail level (scale) the number of coefficients and the percentage of the sum of square (energy), not including the DC component.

To exclude levels from the denoised X-block:

1. Select the undesired levels in the **Selected** list.
2. Click <= to remove.
3. Click **Next**.



Detail levels

Select detail levels to include in the compressed dataset. Lowest scale (D1) corresponds to the highest frequencies. Detail levels by scale (number of coefficients and percentage of sum of square).

Available:

D1 (128 - 10.25%)

Selected:

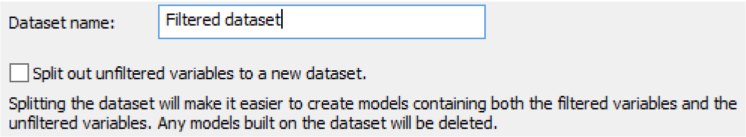
D2 (64 - 7.31%)
D3 (32 - 6.13%)
D4 (16 - 11.35%)
D5 (8 - 4.82%)
D6 (4 - 5.97%)
D7 (2 - 52.75%)
D8 (1 - 1.42%)

7 detail levels of 8 selected, 1 levels to be removed.
Data will be compressed to 127 wavelet coefficients with 89.75% of sum of squares (energy) explained.

8.9.8.9 Creating the filtered dataset

The last page completes the creation of the filtered dataset.

- Enter the **Dataset name**.
- Select to split out unfiltered variables to a new dataset by selecting the **Split out unfiltered variables to a new dataset** check box if desired.
- Click **Finish**.



Dataset name: Filtered dataset

□ Split out unfiltered variables to a new dataset.

Splitting the dataset will make it easier to create models containing both the filtered variables and the unfiltered variables. Any models built on the dataset will be deleted.

Note: To create a model using both filtered and original data, both datasets have to be selected in the **Select data** page in the **Workset** dialog.

8.9.8.10 WCS dataset properties

When variables have been compressed, the new variables are linear combinations of the original ones. Loading, coefficients, VIP or any plots displaying variables is difficult to interpret in the wavelet domain. A property of the wavelet transform is the fact that it is possible to reconstruct not only the original variables, but also individual vectors such as loadings, coefficients, VIP etc.

By default the **Reconstruct wavelets** check box is selected (in **Project Options**), and all plots, including quick info plots observation wise, are displayed in the domain of the original dataset.

Use the **Workset** commands, as usual, to specify the workset for the model.

8.9.9 Wavelet Denoise Spectral – WDS

Wavelet Denoise Spectral, WDS, is similar to **Wavelet Compression Spectral**, WCS. The difference is that after the removal of the wavelet coefficients, the X block is transformed back to the original domain for WDS while WCS remains in the transformed domain but can be reconstructed.

Note: The denoised dataset is transformed back to the original domain. Therefore reconstruction is not available.

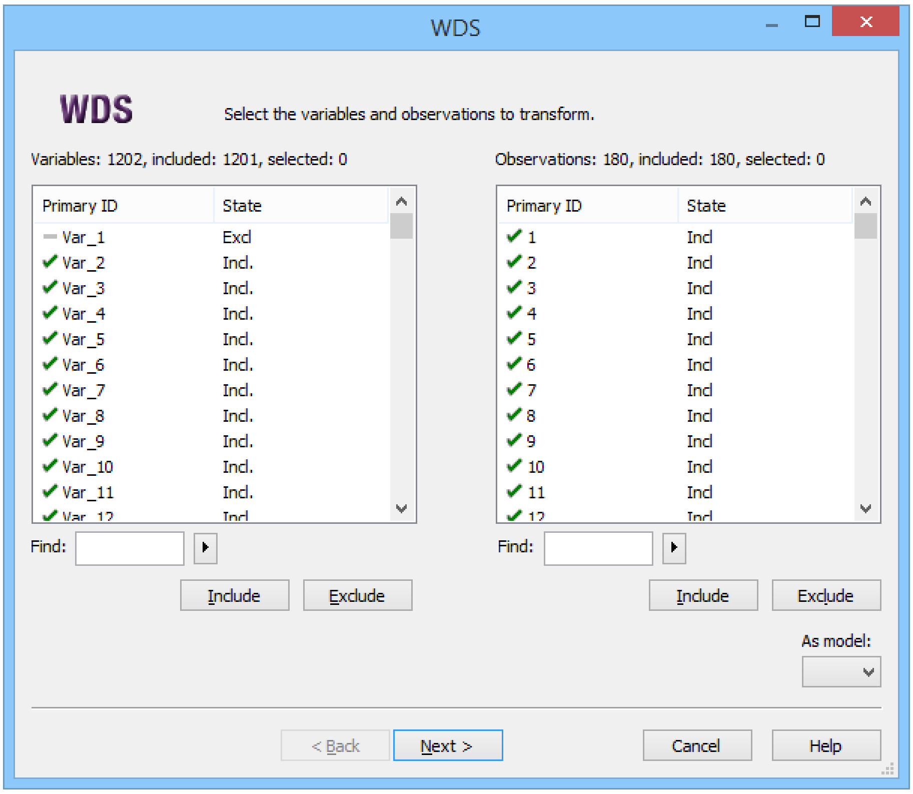
Note: In a WDS transformed dataset, use the **Workset** commands, as usual, to specify the workset for the model.

8.9.9.1 Digitized spectra

When the dataset consist of digitized spectra (i.e. NIR, NMR, and Raman etc.) each observation in the X matrix is the spectrum of a sample, and the wavelet transform and denoising of the matrix X is done row wise.

8.9.9.2 WDS wizard

When selecting **Wavelet Denoising** in the **Spectral Filters** dialog and clicking **Next**, the first page of the **WDS** wizard opens displaying lists of variables and observations.



Select the variables and observations to transform.

Variables: 1202, included: 1201, selected: 0

Primary ID	State
Var_1	Excl
✓ Var_2	Incl.
✓ Var_3	Incl.
✓ Var_4	Incl.
✓ Var_5	Incl.
✓ Var_6	Incl.
✓ Var_7	Incl.
✓ Var_8	Incl.
✓ Var_9	Incl.
✓ Var_10	Incl.
✓ Var_11	Incl.
✓ Var_12	Incl

Observations: 180, included: 180, selected: 0

Primary ID	State
✓ 1	Incl
✓ 2	Incl
✓ 3	Incl
✓ 4	Incl
✓ 5	Incl
✓ 6	Incl
✓ 7	Incl
✓ 8	Incl
✓ 9	Incl
✓ 10	Incl
✓ 11	Incl
✓ 12	Incl

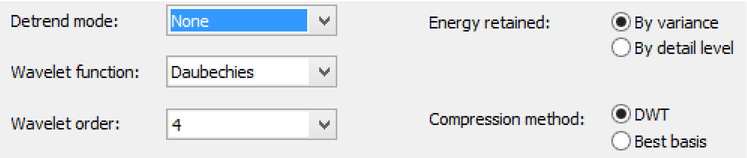
8.9.9.3 Selecting the variables and observations to transform

To apply the filter to the dataset, on the first page of the wizard:

1. In the **Variables** list, mark and **Exclude** unwanted variables. All variables specified as X in the default workset are by default included, while those specified as Y are by default excluded. Qualitative variables cannot be filtered.
2. In the **Observations** list, mark and **Exclude** the observations to exclude from the filtering. All observations are by default included.
3. To specify variables and observations according to a fitted model, select the model in the **As model** box. Variables in the model specified as Y are automatically excluded.
4. Click **Next**.

8.9.9.4 Selecting wavelet options

The page for wavelet options holds options for detrending, wavelet function, wavelet order, exclusion criteria, and compression method. This page is the same for WDS and WCS.



Detrend mode: None

Wavelet function: Daubechies

Wavelet order: 4

Energy retained: ● By variance ○ By detail level

Compression method: ● DWT ○ Best basis

In the page for selecting wavelet options:

1. In the **Detrend mode** box the default is **None**. Click the box to select **Mean** or **Linear**. **Mean** signifies removing the mean while **Linear** signifiers removing the best linear fit.
2. In the **Wavelet function** box the default is **Daubechies**. Click the box to select **Beylkin**, **Coiflet**, **Symmlet**, **Biorthogonal1**, **Biorthogonal2**, **Biorthogonal3**, **Biorthogonal4**, **Biorthogonal5**, or **Biorthogonal6**. For details about the wavelet functions, see the Wavelet families section in the Preprocessing appendix.

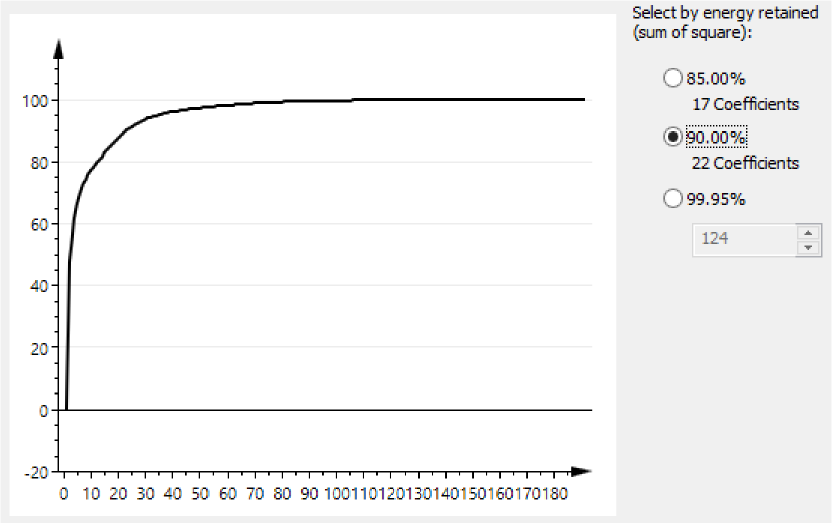
3. In the **Wavelet order** box, select the wavelet order. The default is the lowest available. The wavelet order differs depending on the wavelet function selected. Find the orders available for each wavelet function in the wavelet table.
4. Select the method of exclusion of wavelets coefficients by selecting **Energy retained** to be **By variance** or **By detail level**.
5. Click the desired decomposition and **Compression method**, **DWT** or **Best basis**. **DWT**, discrete wavelet transform, is recommended for low frequency signals and Best basis for high frequency signals. With **By detail level**, **DWT** is the only available compression method.
6. Click **Next**.

Wavelet function	Wavelet order
Beylkin	N/A
Coiflet	2, 3, 4, 5
Daubechies	4, 6, 8, 10, 12, 20, 50
Symmlet	4, 6, 8, 10
Biorthogonal1	1, 3, 5
Biorthogonal2	2, 4, 6, 8
Biorthogonal3	1, 3, 5, 7, 9
Biorthogonal4	4
Biorthogonal5	5
Biorthogonal6	8

8.9.9.5 Wavelet compression/denoising By variance

When compressing/denoising the signal by the percent of variance explained, SIMCA computes and displays the percentage of the variance explained by the wavelet coefficients of the target vector, sorted in order of importance.

1. Use the plot to decide the number of coefficients to keep. The default is to keep the coefficients that accounts for 99.5% of the variance.
2. Optionally change from the default by clicking another option under **Select by energy retained (sum of squares)**.
3. Click **Next**.



Select by energy retained
(sum of square):

○ 85.00%
17 Coefficients

● 90.00%
22 Coefficients

○ 99.95%

124

Compression/denoising **By variance** is done either using compression method **DWT** or **Best basis**. For details about DWT and best basis, see the Wavelet compression or de-noising of signals section in the Preprocessing appendix.

8.9.9.6 Wavelet compression/denoising By detail level

The compression/denoising **By detail level** is performed by excluding all the detail coefficients corresponding to selected scales (levels) of the target vector. **DWT** is the only available compression method.

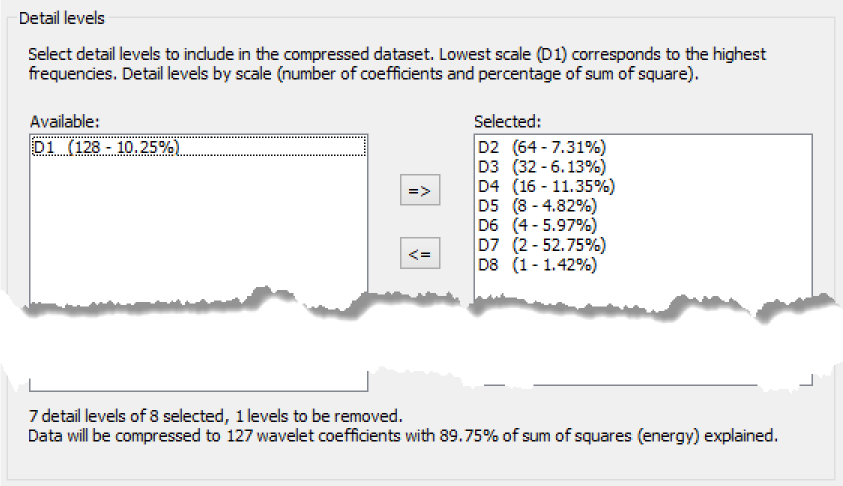
The wavelet transform is first done on the target vector and the results are displayed as a table. After selecting the wavelets coefficients or the scales to be removed, the same transformation is performed on each X observation vector.

8.9.9.7 Selecting wavelet coefficients

When selecting **By detail level** to compress/denoise the X block by removing detail levels, SIMCA decomposes the target X to its detail coefficients at every scale. The left table displays for every detail level (scale) the number of coefficients and the percentage of the sum of square (energy), not including the DC component.

To exclude levels from the denoised X-block:

1. Select the undesired levels in the **Selected** list.
2. Click <= to remove.
3. Click **Next**.


Detail levels

Select detail levels to include in the compressed dataset. Lowest scale (D1) corresponds to the highest frequencies. Detail levels by scale (number of coefficients and percentage of sum of square).

Available:
D1 (128 - 10.25%)

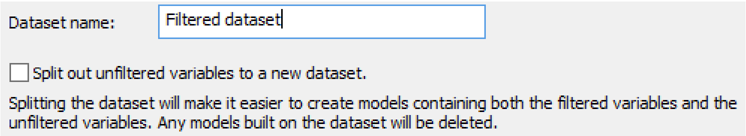
Selected:
D2 (64 - 7.31%)
D3 (32 - 6.13%)
D4 (16 - 11.35%)
D5 (8 - 4.82%)
D6 (4 - 5.97%)
D7 (2 - 52.75%)
D8 (1 - 1.42%)

7 detail levels of 8 selected, 1 levels to be removed.
Data will be compressed to 127 wavelet coefficients with 89.75% of sum of squares (energy) explained.

8.9.9.8 Creating the filtered dataset

The last page completes the creation of the filtered dataset.

- Enter the **Dataset name**.
- Select to split out unfiltered variables to a new dataset by selecting the **Split out unfiltered variables to a new dataset** check box if desired.
- Click **Finish**.


Dataset name: Filtered dataset

□ Split out unfiltered variables to a new dataset.

Splitting the dataset will make it easier to create models containing both the filtered variables and the unfiltered variables. Any models built on the dataset will be deleted.

Note: To create a model using both filtered and original data, both datasets have to be selected in the **Select data** page in the **Workset** dialog.

8.9.10 Orthogonal Signal Correction – OSC

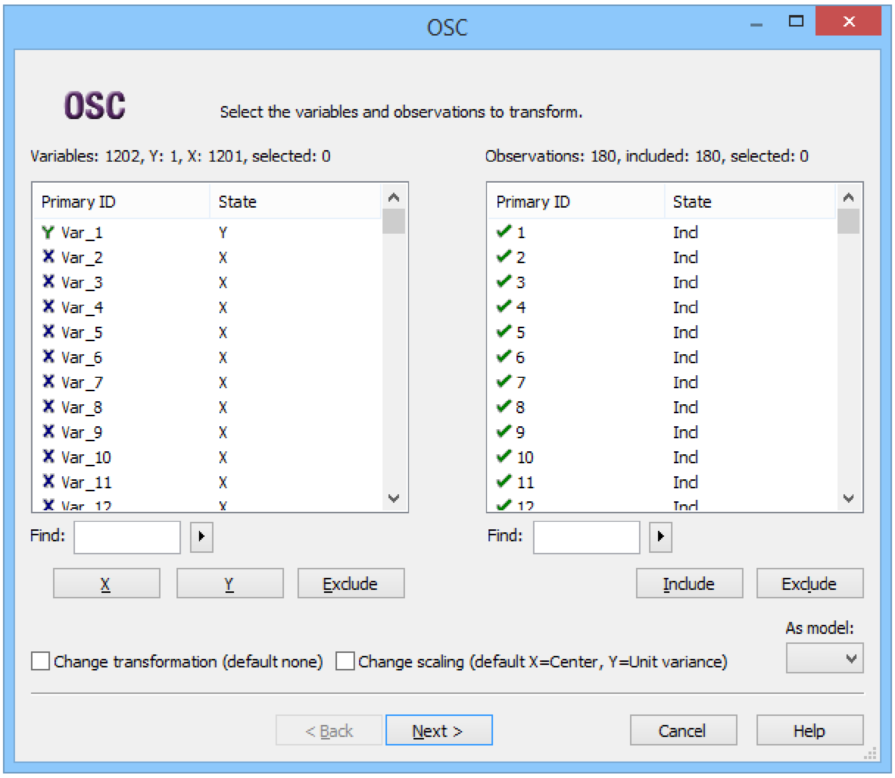
OSC uses a PLS model, to remove from X, information that is orthogonal to Y. Results are displayed as ordinary PLS plots, i.e. scores, loading. These plots are interpreted as regular PLS plots, with the difference that the patterns displayed are orthogonal to, rather than correlated to, Y.

Note: The OSC filter is prone to overfit and may give results that are too optimistic. The OPLS/O2PLS approach provides more realistic results and separates orthogonal variation from predictive variation in a single model.

When selecting **OSC** in the **Spectral Filters** dialog and clicking **Next**, the first page of the **OSC** wizard opens displaying lists of variables and observations.

***Note**: Serious outliers in the score plot need to be removed before OSC, as they may bias the corrected data X.*

8.9.10.1



Select the variables and observations to transform.

Variables: 1202, Y: 1, X: 1201, selected: 0

Primary ID	State
Y Var_1	Y
X Var_2	X
X Var_3	X
X Var_4	X
X Var_5	X
X Var_6	X
X Var_7	X
X Var_8	X
X Var_9	X
X Var_10	X
X Var_11	X
X Var_12	X

Observations: 180, included: 180, selected: 0

Primary ID	State
✓ 1	Ind
✓ 2	Ind
✓ 3	Ind
✓ 4	Ind
✓ 5	Ind
✓ 6	Ind
✓ 7	Ind
✓ 8	Ind
✓ 9	Ind
✓ 10	Ind
✓ 11	Ind
✓ 12	Ind

□ Change transformation (default none) □ Change scaling (default X=Center, Y=Unit variance)

8.9.10.2 Selecting variables, observations, transform, scale - OSC

To apply the filter to the dataset, on the first page of the wizard:

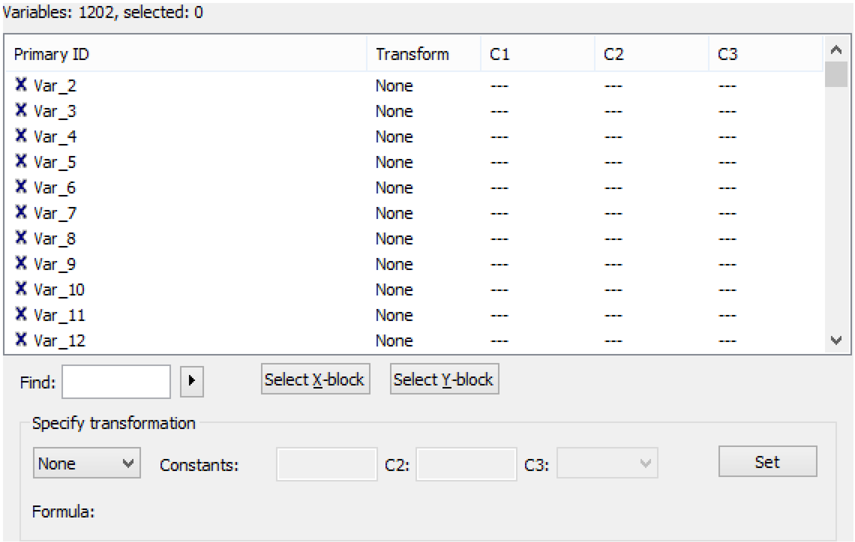
1. In the **Variables** list, specify the **Y** variables and mark and **Exclude** unwanted variables. All variables are specified according to the default workset.
2. In the **Observations** list, mark and **Exclude** the observations to exclude from the filtering. All observations are by default included.
3. To transform variables prior to the OSC, select the **Change transformation** check box. For more, see the Selecting variable transformations in spectral filtering subsection next.
4. To change the scaling of the variables, select the **Change scaling** check box. By default, all the X variables are centered and the Y variables are centered and scaled to unit variance UV. For more, see the Selecting scaling in spectral filtering subsection later in this chapter.
5. To specify variables and observations according to a fitted model, select the model in the **As model** box.
6. Click **Next**.

8.9.10.3 Selecting variable transformations in spectral filtering

With the **Change transformation** check box selected, clicking **Next** opens the **Select transformations** page.

Apply transformations before the compression by:

1. Marking the variables to transform.
2. Selecting the transformation: **Linear**, **Log**, **NegLog**, **Logit**, **Exponential**, or **Power** and then clicking **Set**.
3. Clicking **Next**.



Variables: 1202, selected: 0

Primary ID	Transform	C1	C2	C3
X Var_2	None	---	---	---
X Var_3	None	---	---	---
X Var_4	None	---	---	---
X Var_5	None	---	---	---
X Var_6	None	---	---	---
X Var_7	None	---	---	---
X Var_8	None	---	---	---
X Var_9	None	---	---	---
X Var_10	None	---	---	---
X Var_11	None	---	---	---
X Var_12	None	---	---	---

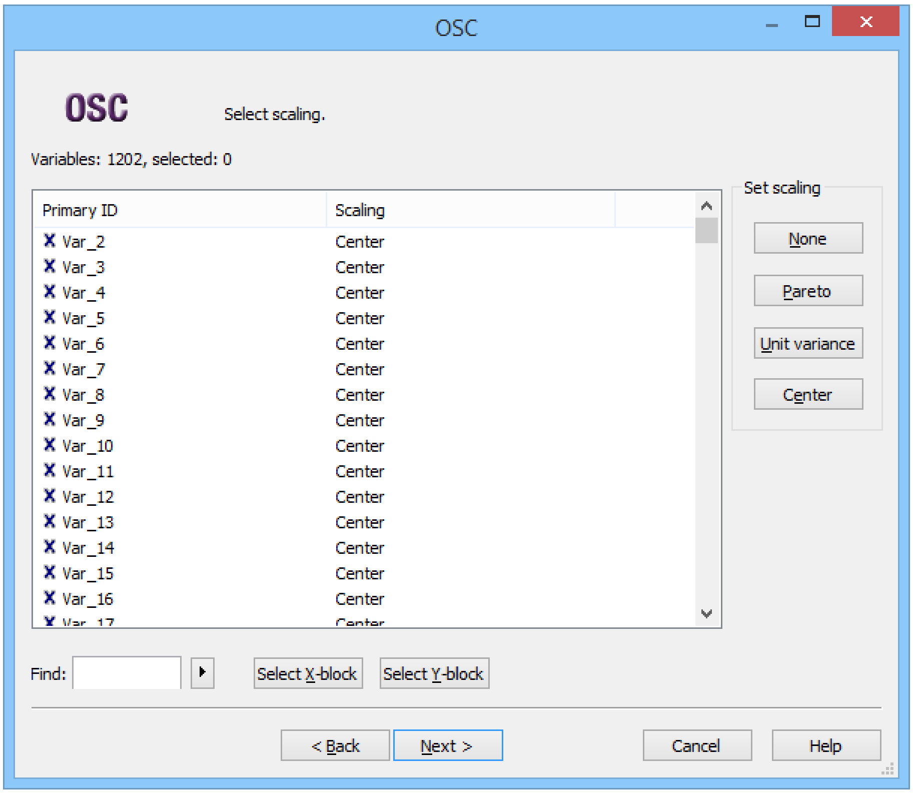
For details about the transformations available, see the Applying transformations section in the Workset section in Chapter 7 Home.

8.9.10.4 Selecting scaling in spectral filtering

With the **Change scaling** check box selected, clicking **Next** opens the **Select scaling** page.

To change scaling:

1. Mark the variables.
2. Click the desired scaling button: **None**, **Pareto**, **Unit variance**, or **Center**.
3. Click **Next**.



Select scaling.

Variables: 1202, selected: 0

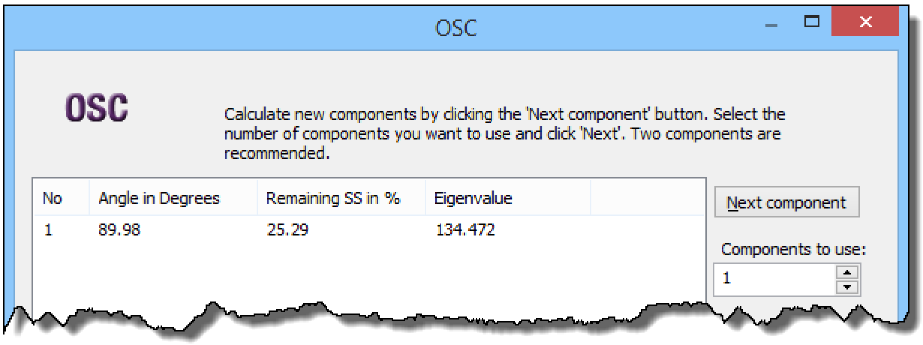
Primary ID	Scaling
X Var_2	Center
X Var_3	Center
X Var_4	Center
X Var_5	Center
X Var_6	Center
X Var_7	Center
X Var_8	Center
X Var_9	Center
X Var_10	Center
X Var_11	Center
X Var_12	Center
X Var_13	Center
X Var_14	Center
X Var_15	Center
X Var_16	Center
X Var_17	Center

8.9.10.5 Computing the OSC model

SIMCA computes the first component of the OSC model, and displays the angle between t and Y for that component, the Sum of Squares (SS) remaining in the X block, and the **Eigenvalue**.

When the angle is 90 degree, OSC has reached orthogonality.

- To compute the next component, click **Next component**. Usually two components are recommended.
- When done, select the number of components to retain in the **Components to use** field.
- Click **Next**.



Calculate new components by clicking the 'Next component' button. Select the number of components you want to use and click 'Next'. Two components are recommended.

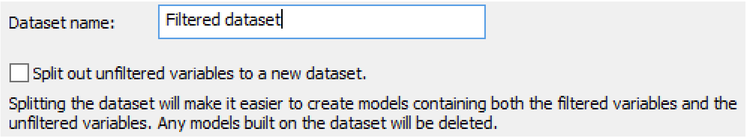
No	Angle in Degrees	Remaining SS in %	Eigenvalue
1	89.98	25.29	134.472

Components to use: 1

8.9.10.6 Creating the filtered dataset

The last page completes the creation of the filtered dataset.

- Enter the **Dataset name**.
- Select to split out unfiltered variables to a new dataset by selecting the **<u>Split out unfiltered variables to a new dataset</u>** check box if desired.
- Click **Finish**.



Dataset name: Filtered dataset

□ Split out unfiltered variables to a new dataset.

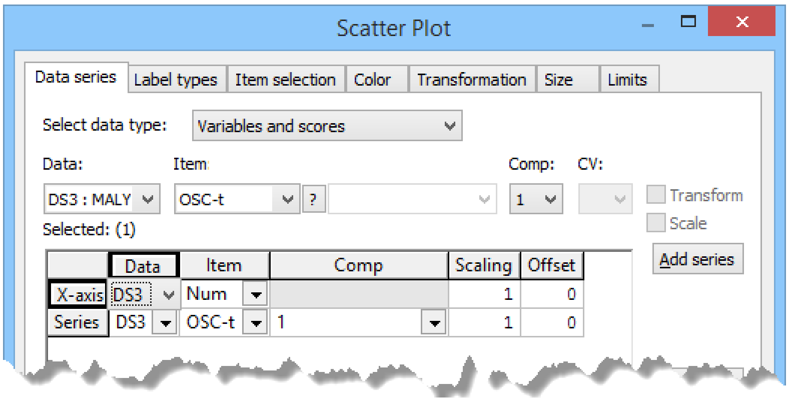
Splitting the dataset will make it easier to create models containing both the filtered variables and the unfiltered variables. Any models built on the dataset will be deleted.

Note: To create a model using both filtered and original data, both datasets have to be selected in the **Select data** page in the **Workset** dialog.

8.9.10.7 OSC dataset

With an OSC dataset, use the menu **Plot/List** to examine the OSC model by:

1. Selecting a plot type.
2. Selecting the OSC-dataset in the **Data** box.
3. Selecting **Variable and scores** or **Observations and loadings** in the **Select data type** box.
4. Adding the series to plot.



Select data type: Variables and scores

Data: DS3 : MALY Item: OSC-t ? Comp: 1 CV:

□ Transform
□ Scale

Selected: (1)

	Data	Item	Comp	Scaling	Offset
X-axis	DS3	Num		1	0
Series	DS3	OSC-t	1	1	0

Vector	Description
OSC-p	Loadings of the X variables in the OSC model. These best approximate X together with scores that are orthogonal to Y.
OSC-t	X scores t of the OSC model. They summarize X and are the best combination of the X's that are orthogonal to Y.
OSC-w	Loading weights of the X variables or their residuals (higher dimensions) in the OSC model. These weights are selected to make t orthogonal to u.
OSC-w*	Loading weights of the X variables (not their residuals) in the OSC model. X variables with large w* are little correlated with u and (Y).

8.9.10.7.1 Fitting a calibration model

To fit a calibration model, create a new workset and select both the OSC dataset and the original dataset, or the split dataset, to access the y-variables. Any scaling or transformation specified during the filtering needs to be specified in the workset.

To fit the PLS calibration model to the OSC data, click **Autofit**.

8.9.10.8 Using OSC with a batch level dataset

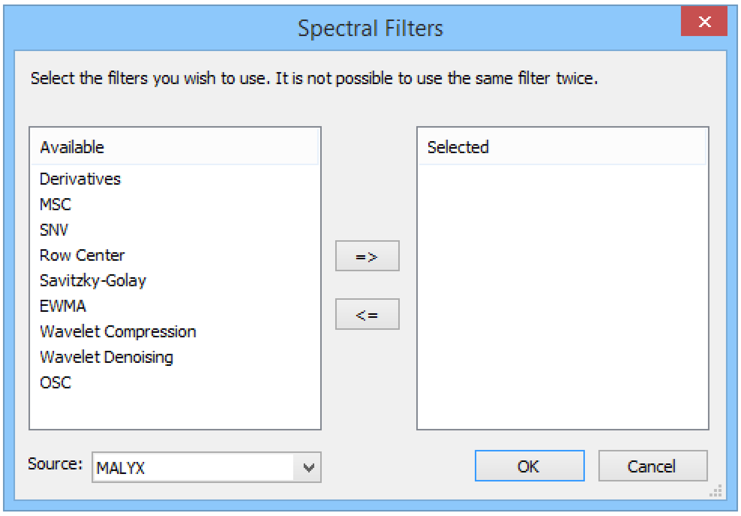
When you have quality variables in a batch level dataset, and want to use a PLS model, you may want to use OSC to preprocess your data. After using OSC, SIMCA creates a new OSCed batch level dataset.

To OSC preprocess the predictionset, select the batch evolution predictionset. Preprocessing is then done automatically.

8.9.11 Chaining filters

Apply several filters in combination by clicking **Spectral filters** on the **Data** tab and adding the desired filters. The filters can be applied in any order although each filter can be applied only once.

Note: If wavelet compression is performed before OSC filtering, the former usually needs to keep 99.9 of the variance.



Spectral Filters

Select the filters you wish to use. It is not possible to use the same filter twice.

Available: Derivatives, MSC, SNV, Row Center, Savitzky-Golay, EWMA, Wavelet Compression, Wavelet Denoising, OSC

Selected

Source: MALYX

To define the chain of filters:

1. Click a filter in the **Available** list.
2. Click the **=>** button.
3. Repeat 1-2 until the desired chain of filters is displayed in the **Selected** list.
4. Click **OK** and the wizard of each filter opens successively and the filters are applied in the order specified.

8.9.12 Predictionsets and filtered datasets

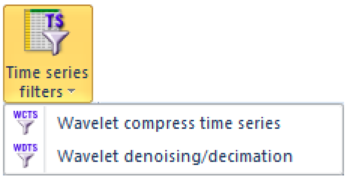
When the model is built on a filtered dataset, the predictionset may not be filtered. The predictionset is automatically signal corrected/denoised as the filtered dataset.

Use the **Predict** tab commands, as usual.

Note: The predictionset needs to include all variables of the original dataset the filtered dataset was created from.

8.10 Time series filters

The following time series filters are available by clicking **Time series filters** on the **Data** tab: **Wavelet compress time series** (WCTS) and **Wavelet denoising/decimation** (WDTS). These filters are applied variable wise.



A short background is available in the PLS wavelet compression of time series section in the Preprocessing appendix.

8.10.1 Wavelet Compress Time Series – WCTS

With continuous process data (time series), you may want to compress the data to reduce the number of observations.

The wavelet transform of time series focuses on the selected target response Y, with the objective to achieve a parsimonious representation of the signal Y, while keeping all the information.

Note: The dataset must hold at least one y-variable to wavelet compress time series, as the compression is designed for PLS *models.*

The *Wavelet Compress Time Series* differs from *Wavelet Compress Spectral* in that compression is done variable wise and not observation wise and that WCTS requires a y-variable.

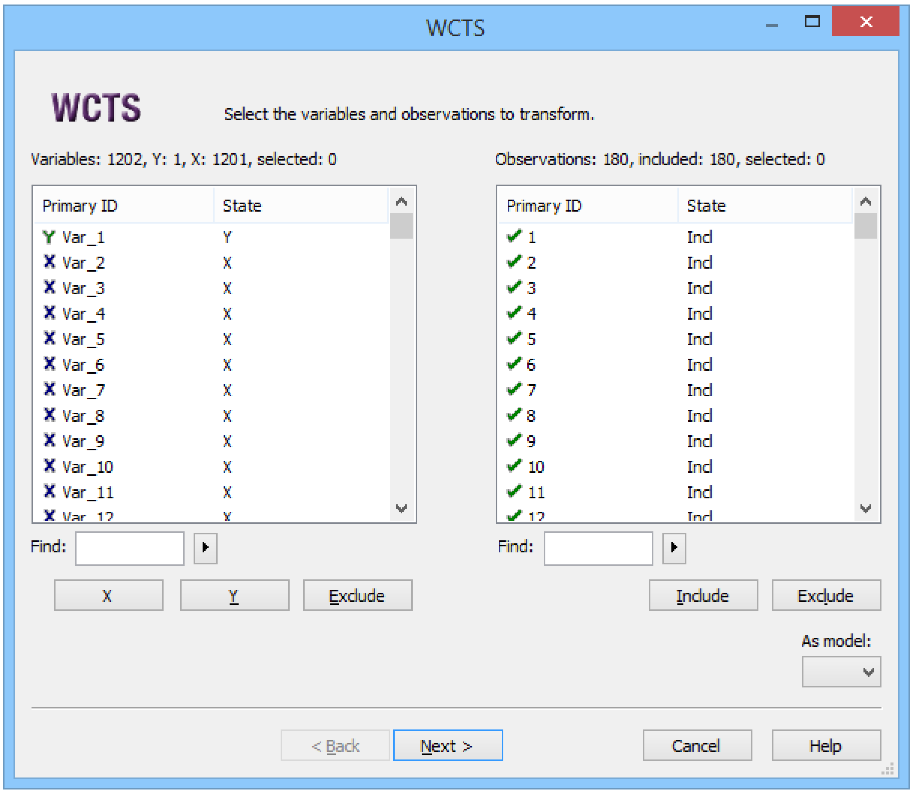
Note: With compression, reconstruct is done when the **Reconstruct wavelets** check box is selected in the **Fit** page of the **File | Options | Project**. This is the SIMCA default.

8.10.1.1 Compression method

The X and Y blocks are first mean centered and scaled to UV and then transformed, using **DWT** or **Best basis**, to the wavelet domain. After compression the mean of every variable and original variance are added back to the wavelet coefficients of that variable.

8.10.1.2 WCTS wizard

To compress the data by reducing the number of observations, in the **Dataset** tab, click **Time series filters | Wavelet compress time series**. The first page of the WCTS wizard opens displaying lists of variables and observations.


WCTS

Select the variables and observations to transform.

Variables: 1202, Y: 1, X: 1201, selected: 0

Primary ID	State
Y Var_1	Y
X Var_2	X
X Var_3	X
X Var_4	X
X Var_5	X
X Var_6	X
X Var_7	X
X Var_8	X
X Var_9	X
X Var_10	X
X Var_11	X
X Var_12	X

Observations: 180, included: 180, selected: 0

Primary ID	State
✓ 1	Incl
✓ 2	Incl
✓ 3	Incl
✓ 4	Incl
✓ 5	Incl
✓ 6	Incl
✓ 7	Incl
✓ 8	Incl
✓ 9	Incl
✓ 10	Incl
✓ 11	Incl
✓ 12	Incl

8.10.1.3 Selecting y-variables and observations - WCTS

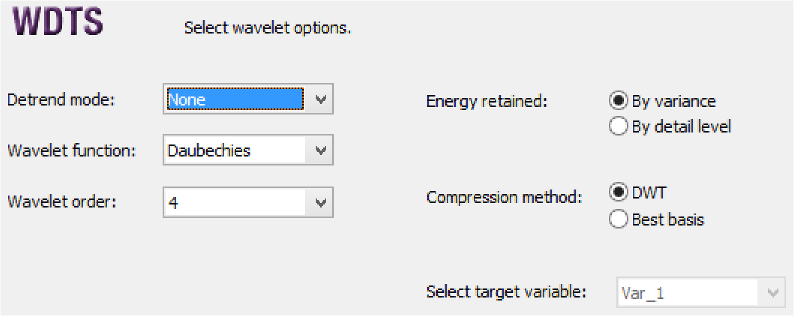
To apply the filter to the dataset, on the first page of the wizard:

1. In the **Variables** list, specify the **Y** variables and mark and **Exclude** unwanted variables. With many y-variables they must be positively correlated, and the most important one should be selected as target on the next page. All variables are specified according to the default workset.
2. In the **Observations** list, mark and **Exclude** the observations to exclude from the filtering. All observations are by default included.
3. To specify variables and observations according to a fitted model, select the model in the **As model** box.
4. Click **Next**.

Note: Specifying several uncorrelated y-variables or anti-correlated y-variables as Y will give poor results. In such cases first do a PCA and select only a group of positively correlated y-variables to be compressed together.

8.10.1.4 Selecting wavelet options

The page for wavelet options holds options for detrending, wavelet function, wavelet order, exclusion criteria, compression method, and target variable. This page is the same for WCTS and WDTS.


WDTS

Select wavelet options.

Detrend mode: None

Wavelet function: Daubechies

Wavelet order: 4

Energy retained: ● By variance ○ By detail level

Compression method: ● DWT ○ Best basis

Select target variable: Var_1

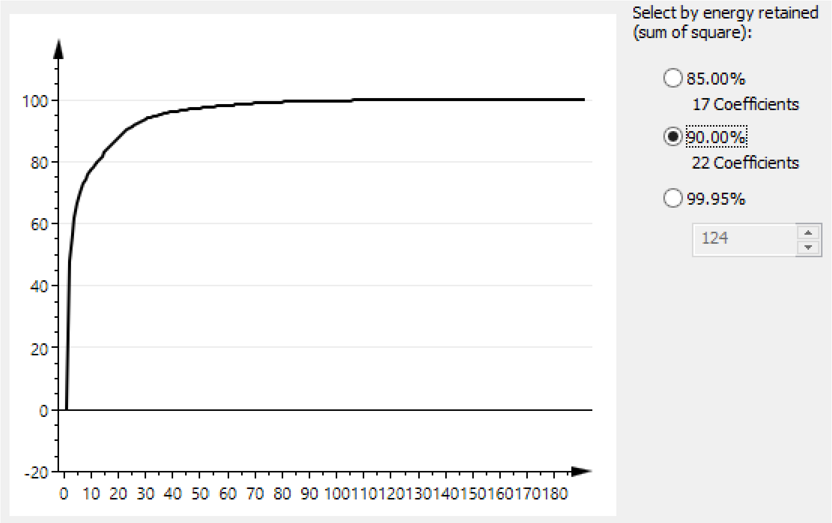
In the page for selecting wavelet options:

1. In the **Detrend mode** box the default is **None** for WDTS. Click the **Detrend mode** box to select **Mean** or **Linear**. **Mean** signifies removing the mean while **Linear** signifiers removing the best linear fit. For WCTS the **Detrend mode** box is unavailable and the selected detrending mode is **Mean**.
2. In the **Wavelet function** box the default is **Daubechies**. Click the **Wavelet function** box to select **Beylkin**, **Coiflet**, **Symmlet**, **Biorthogonal1**, **Biorthogonal2**, **Biorthogonal3**, **Biorthogonal4**, **Biorthogonal5**, or **Biorthogonal6**. For details about the wavelet functions, see the Wavelet families section in the Preprocessing appendix.
3. In the **Wavelet order** box, select the wavelet order. The default is the lowest available. The wavelet order differs depending on the wavelet function selected. Find the orders available for each wavelet function in the table in the Selecting wavelet options - WCS subsection earlier in this chapter.
4. Select the method of exclusion of wavelets coefficients by selecting **Energy retained** type **By variance** or **By detail level**.
5. Click the desired decomposition and **Compression method**, **DWT** or **Best basis**. **DWT**, discrete wavelet transform, is recommended for low frequency signals and **Best basis** for high frequency signals. With **By detail level**, **DWT** is the only available compression method.
6. In the **Select target variable** box select which of the variables to use as target variable.
7. Click **Next**.

8.10.1.5 Wavelet compression By variance - WCTS

When compressing the signal by the percent of variance explained, SIMCA computes and displays the percentage of the variance explained by the wavelet coefficients of the target vector, sorted in order of importance.

1. Use the plot to decide the number of coefficients to keep. The default is to keep the coefficients that account for 90% of the variance. The same coefficients are kept for all y-variables.
2. Optionally change from the default under **Select by energy retained (sum of squares)**.
3. Click **Next**.



Select by energy retained (sum of square):

○ 85.00%
17 Coefficients

● 90.00%
22 Coefficients

○ 99.95%

124

Compression/denoising **By variance** is done either using compression method **DWT** or **Best basis**. For details about DWT and best basis, see the Wavelet transformations section in the Preprocessing appendix.

8.10.1.6 Creating the new dataset

On the last page of the WCTS wizard:

1. Enter the **Dataset name**.
2. Click **Finish**.

8.10.1.7 WCTS dataset properties

The X and Y matrices are compressed by extracting only the selected number of significant coefficients, or detail level coefficients, in both the X and Y block, column wise.

8.10.1.7.1 Observation identifiers with Best basis

With **Best basis** selected, the observations in the new project are labeled $ WTS-*Scale*–*Position* (e.g., $WTS-6-15).

Scale is the block index of the packet table. It represents the frequency resolution of the signal, i.e., the number of times it has passed through the Low pass and Hi pass filters. This means that when the scale value equals 1 the signal has passed once through the filters. The scale ranges from 1 to log2 (N), where N=length of the signal (padded if N was not power of 2). Frequency resolution and time resolutions are the inverse of each other.

Position is the position of the coefficient within the block. The position index ranges from 1 to N, and is related to the frequencies in the signal. Here 1 is the lowest and N is the highest frequency.

8.10.1.7.2 Predictionset

Predictionsets will not be wavelet transformed, and can be used as they are in the original domain.

8.10.2 Wavelet Denoising/Decimation – WDTS

The *Wavelet Denoising/Decimation* differs from *Wavelet Denoise Spectral* in that compression is done variable wise and not observation wise.

After the removal of the wavelet coefficients, the X variables are transformed back to the original domain.

After transforming all the variables to the wavelet domain, the denoising is done by performing the inverse wavelet transform with either the selected coefficients or the coefficients from the selected details. All other coefficients are set to 0.

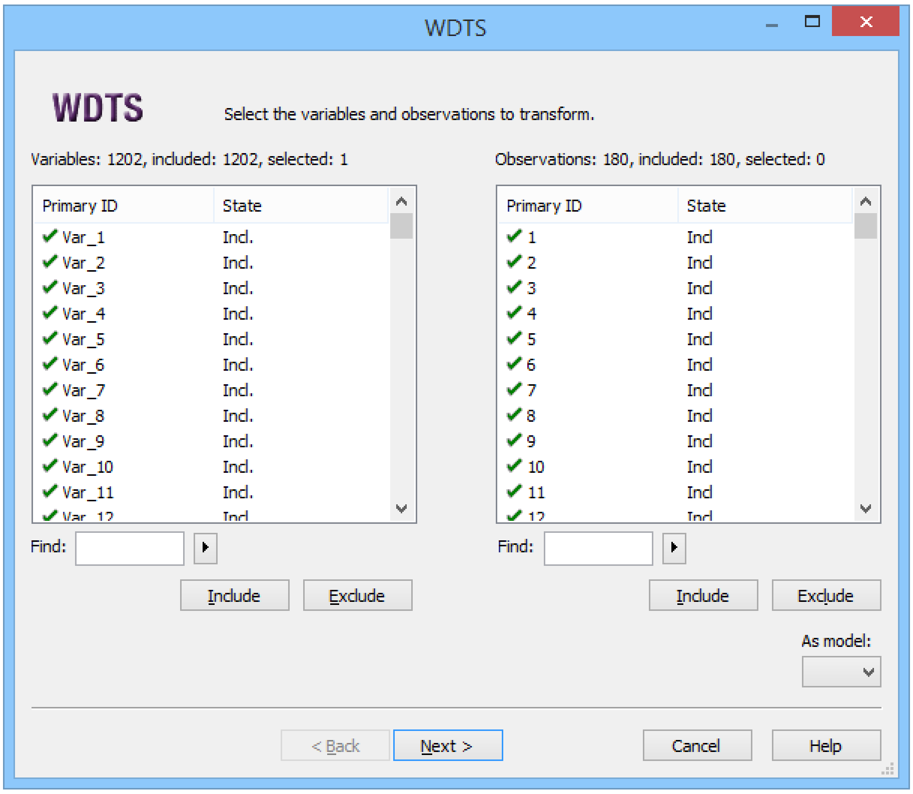
8.10.2.1 Decimation

Decimation is a re-sampling of data after removal of the high frequencies, by selecting every second or fourth or eighth, etc. observations. This is useful when the sampling interval is much faster than the time constant of the system.

The decimation is performed on the dataset after it is transformed back to original units. Decimation is only available by a value that is power of 2.

8.10.2.2 WDTS wizard

To compress the data by reducing the number of observations, on the **Data** tab, in the **Filters** group, click **Time series filters | Wavelet denoising/decimation**. The first page of the WDTS wizard opens displaying lists of variables and observations.



WDTS

WDTS Select the variables and observations to transform.

Variables: 1202, included: 1202, selected: 1

Primary ID	State
✓ Var_1	Incl.
✓ Var_2	Incl.
✓ Var_3	Incl.
✓ Var_4	Incl.
✓ Var_5	Incl.
✓ Var_6	Incl.
✓ Var_7	Incl.
✓ Var_8	Incl.
✓ Var_9	Incl.
✓ Var_10	Incl.
✓ Var_11	Incl.
✓ Var_12	Incl

Observations: 180, included: 180, selected: 0

Primary ID	State
✓ 1	Incl
✓ 2	Incl
✓ 3	Incl
✓ 4	Incl
✓ 5	Incl
✓ 6	Incl
✓ 7	Incl
✓ 8	Incl
✓ 9	Incl
✓ 10	Incl
✓ 11	Incl
✓ 12	Incl

Find:

As model:

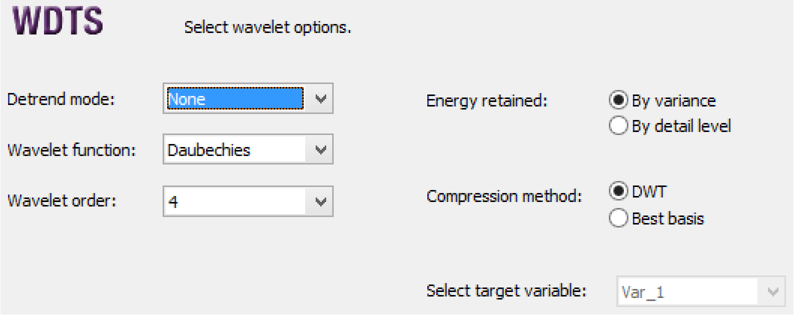
8.10.2.3 Selecting the variables and observations to transform

To apply the filter to the dataset, on the first page of the wizard:

1. In the **Variables** list, mark and **Exclude** unwanted variables. All variables specified as X in the default workset are by default included, while those specified as Y are by default excluded. Qualitative variables cannot be filtered.
2. In the **Observations** list, mark and **Exclude** the observations to exclude from the filtering. All observations are by default included.
3. To specify variables and observations according to a fitted model, select the model in the **As model** box. Variables in the model specified as Y are automatically excluded.
4. Click **Next**.

8.10.2.4 Selecting wavelet options

The page for wavelet options holds options for detrending, wavelet function, wavelet order, exclusion criteria, compression method, and target variable. This page is the same for WCTS and WDTS.



WDTS Select wavelet options.

Detrend mode: None

Wavelet function: Daubechies

Wavelet order: 4

Energy retained: ● By variance ○ By detail level

Compression method: ● DWT ○ Best basis

Select target variable: Var_1

In the page for selecting wavelet options:

1. In the **Detrend mode** box the default is **None** for WDTS. Click the **Detrend mode** box to select **Mean** or **Linear**. **Mean** signifies removing the mean while **Linear** signifiers removing the best linear fit. For WCTS the **Detrend mode** box is unavailable and the selected detrending mode is **Mean**.

2. In the **Wavelet function** box the default is **Daubechies**. Click the **Wavelet function** box to select **Beylkin**, **Coiflet**, **Symmlet**, **Biorthogonal1**, **Biorthogonal2**, **Biorthogonal3**, **Biorthogonal4**, **Biorthogonal5**, or **Biorthogonal6**. For details about the wavelet functions, see the Wavelet families section in the Preprocessing appendix.

3. In the **Wavelet order** box, select the wavelet order. The default is the lowest available. The wavelet order differs depending on the wavelet function selected. Find the orders available for each wavelet function in the table in the Selecting wavelet options - WCS subsection earlier in this chapter.

4. Select the method of exclusion of wavelets coefficients by selecting **Energy retained** type **By variance** or **By detail level**.

5. Click the desired decomposition and **Compression method**, **DWT** or **Best basis**. **DWT**, discrete wavelet transform, is recommended for low frequency signals and **Best basis** for high frequency signals. With **By detail level**, **DWT** is the only available compression method.

6. In the **Select target variable** box select which of the variables to use as target variable.

7. Click **Next**.

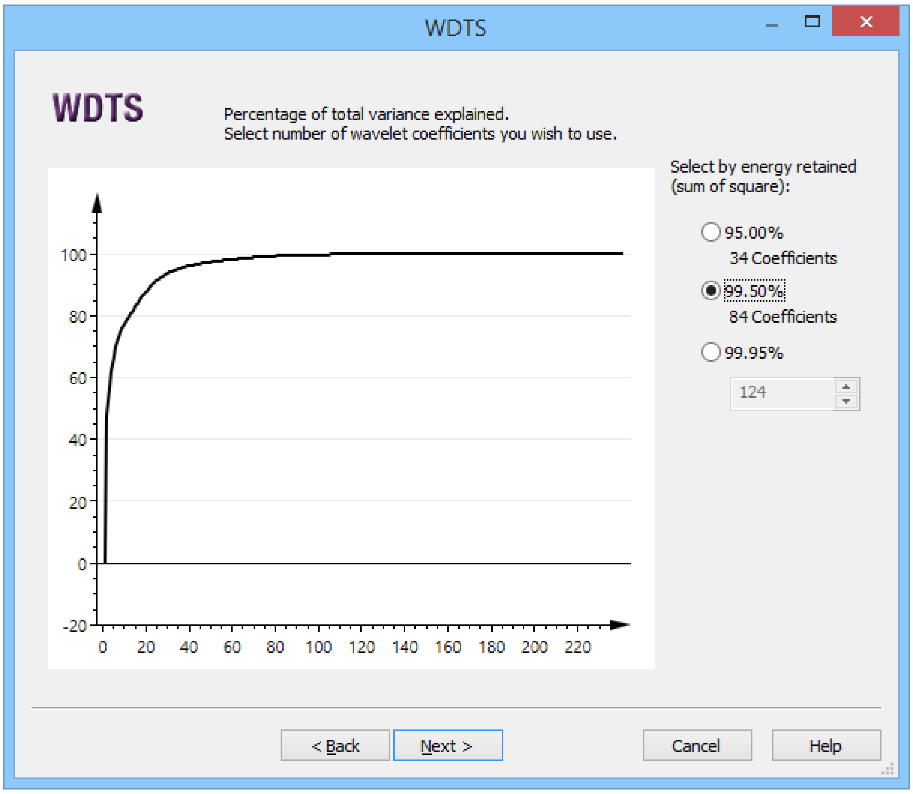
8.10.2.5 Wavelet denoising By variance – WDTS

When denoising the signal by the percent of variance explained, SIMCA computes and displays the percentage of the variance explained by the wavelet coefficients of the target vector, sorted in order of importance.

1. Use the plot to decide the number of coefficients to keep. The default is to keep the coefficients that accounts for 99.5% of the variance.

2. Optionally change from the default under **Select by energy retained (sum of squares)**.

3. Click **Next**.



WDTS

WDTS

Percentage of total variance explained.
Select number of wavelet coefficients you wish to use.

Select by energy retained (sum of square):

○ 95.00%
34 Coefficients

● 99.50%
84 Coefficients

○ 99.95%

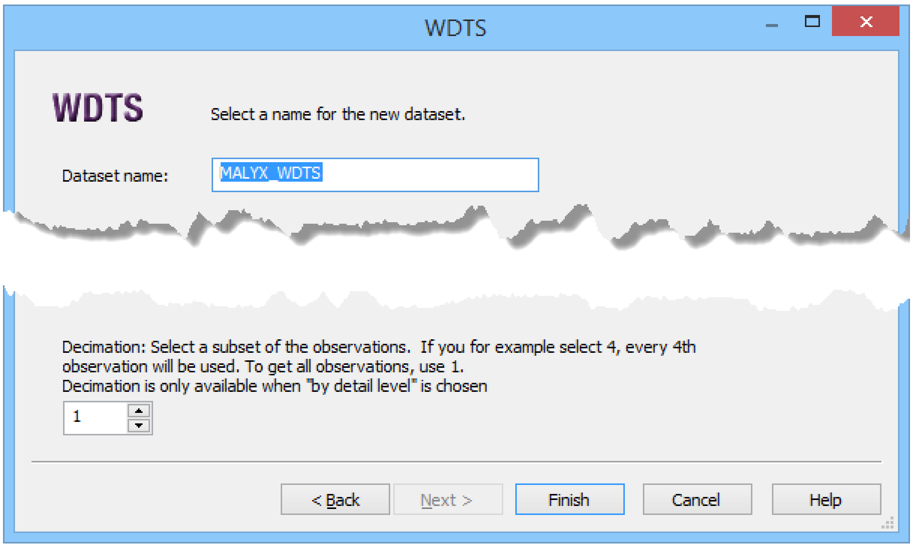
124

Compression/denoising **By variance** is done either using compression method **DWT** or **Best basis**. For details about DWT and best basis, see the Wavelet transformations section in the Preprocessing appendix.

8.10.2.6 Creating the new dataset - WDTS

On the last page of the WDTS wizard:

- Enter the **Dataset name**.
- Optionally enter the number to decimate. This option is available when **By detail level** was selected in the **Selecting wavelet options** page. For more, see the Applying decimation subsection next.
- Click **Finish**.



Select a name for the new dataset.

Dataset name: MALYX_WDTS

Decimation: Select a subset of the observations. If you for example select 4, every 4th observation will be used. To get all observations, use 1.
Decimation is only available when "by detail level" is chosen

1

8.10.2.7 Applying decimation

Decimation is available when using **By detail level**. The objective is to select a subset of the observations by keeping every second or fourth or eighth etc. observation.

Decimation is only available by a value that is power of 2. For example select 4, every 4th observation will be used. Leaving the decimation = 1 will include all observations.

The following decimation is recommended:

- After removing D1, decimate by 2.
- After removing D1 and D2, decimate by 4
- After removing D1, D2, and D3, decimate by 8 etc.

Note: Decimation is done after the WDTS transformation.

8.10.2.8 WDTS dataset properties

The dataset is compressed by extracting only the selected number of significant coefficients, or detail level coefficients, column wise.

In the WDTS transformed project, use the **Workset** commands, as usual, to specify the workset for the model.

8.10.2.8.1 Predictionset

Predictionsets will not be wavelet transformed, and can be used as they are in the original domain.

8.11 Dataset summary

The **Dataset summary** (Properties dialog) holds information about the selected dataset including number of variables and observations, where the data was imported from, missing values, variable types etc.

To open the dialog:

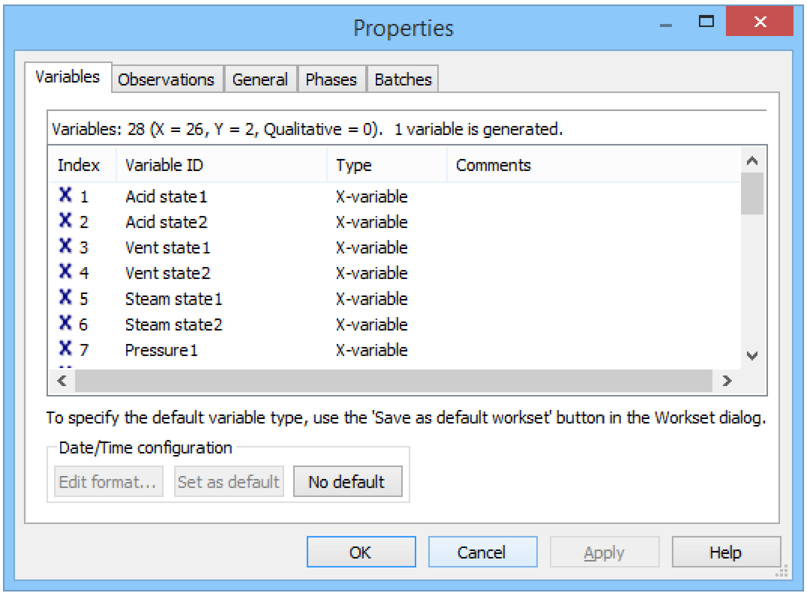
- On the **Data** tab, in the **Summary** group, click **Dataset summary**.
- Right-click the open dataset spreadsheet and click **Properties**.

In the dataset properties dialog there are always three tabs **Variables**, **Observations** and **General**.

For batch evolution datasets the following tabs are additionally available:

- **Batches** tab – always.
- **Phases** tab – when there are phases.

For filtered datasets the **Filter** tab is additionally available.



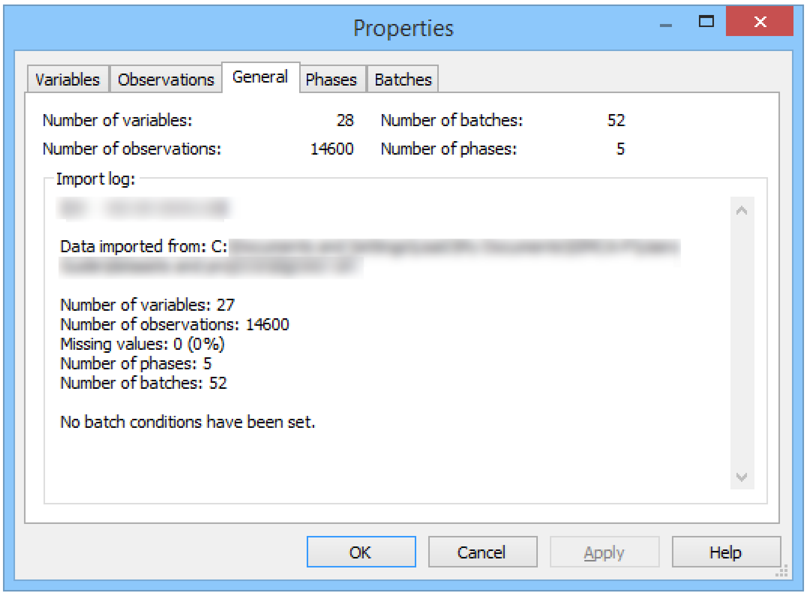
Variables: 28 (X = 26, Y = 2, Qualitative = 0). 1 variable is generated.

Index	Variable ID	Type	Comments
X 1	Acid state1	X-variable	
X 2	Acid state2	X-variable	
X 3	Vent state1	X-variable	
X 4	Vent state2	X-variable	
X 5	Steam state1	X-variable	
X 6	Steam state2	X-variable	
X 7	Pressure1	X-variable	

To specify the default variable type, use the 'Save as default workset' button in the Workset dialog.

8.11.1 General page in dataset Properties

The **General** page displays the number of variables and observations, number of batches and phases for batch projects, and the **Import log**.



Number of variables: 28 Number of batches: 52

Number of observations: 14600 Number of phases: 5

Import log:

[redacted]

Data imported from: C:[redacted]

Number of variables: 27
Number of observations: 14600
Missing values: 0 (0%)
Number of phases: 5
Number of batches: 52

No batch conditions have been set.

8.11.2 Observations page

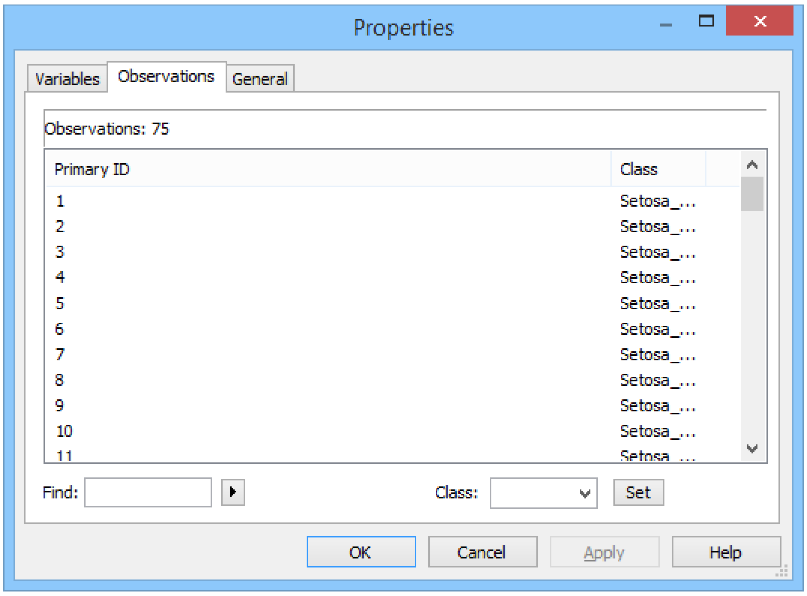
To display the observations and assigning them to classes for the default workset, click the **Observations** tab. After assigning classes in here, the classes are by default assigned in all new worksets.

To view secondary IDs, right-click the list, and select the desired ID.

To assign observations to a class:

1. Mark the observations manually or using **Find**.

2. Type the class name in the **Class** field or use class numbers.
3. Click **Set**.
4. Repeat 1-3 until done.
5. Click **Apply** or **OK**.



Observations: 75

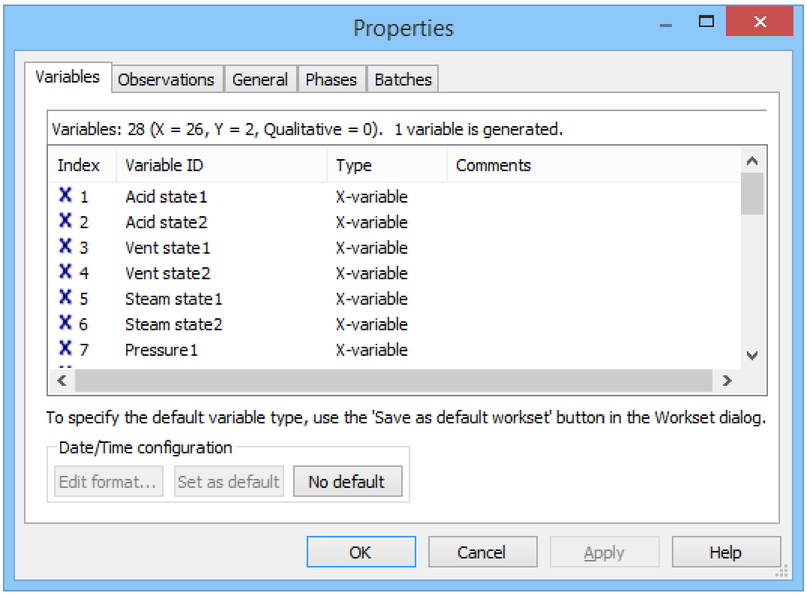
Primary ID	Class
1	Setosa_...
2	Setosa_...
3	Setosa_...
4	Setosa_...
5	Setosa_...
6	Setosa_...
7	Setosa_...
8	Setosa_...
9	Setosa_...
10	Setosa_...
11	Setosa_...

Note: Assigning classes is unavailable in batch projects.

8.11.3 Variables page

To display the variables and their roles (i.e. what's X and what's Y), click the **Variable** tab.

To change the variable type, open the **Workset** dialog, modify as desired, and then click the **Save as default workset** button.



Variables: 28 (X = 26, Y = 2, Qualitative = 0). 1 variable is generated.

Index	Variable ID	Type	Comments
X 1	Acid state1	X-variable	
X 2	Acid state2	X-variable	
X 3	Vent state1	X-variable	
X 4	Vent state2	X-variable	
X 5	Steam state1	X-variable	
X 6	Steam state2	X-variable	
X 7	Pressure1	X-variable	

To specify the default variable type, use the 'Save as default workset' button in the Workset dialog.

8.11.3.1 Date/Time configuration in dataset Properties

A variable that has been specified as **Y Date/Time variable** or **Date/Time variable** can be reformatted by right-clicking the variable in the dataset spreadsheet, and then clicking **Format date/time**. See step 4 in the table.

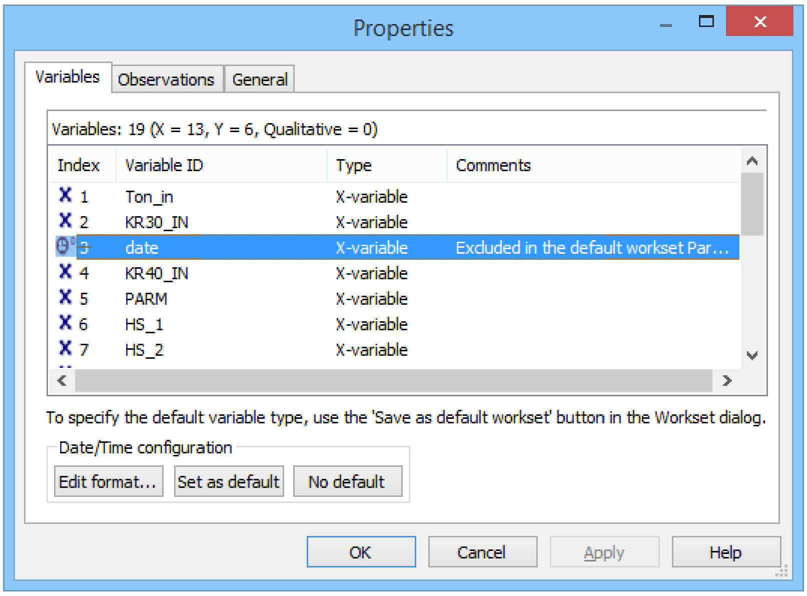
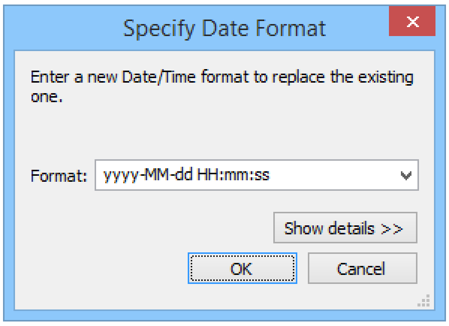
Reformatting can also be done, as well as other **Date/Time** variable settings, in the Dataset **Properties** dialog described in the table, opened by clicking **Dataset summary** in the **Summary** group on the **Data** tab.

In the **Date/Time configuration** section there are three buttons. The **No default** button is always available while the **Edit format** (described in the table) and **Set as default**, buttons are available when a date/time formatted variable is selected in the list.

Clicking the **Set as default**-button sets the selected Date/Time variable as the default variable to display in line plots and scatter plots with one series.

Clicking the **No default**-button will revert to using **Num** in the places where Date/Time is by default displayed when available.

Note: Editing the format only affects how the variable is displayed, not how it is saved.

Step	Dialog
1. Open the dataset **Properties** dialog and click the **Variables** tab. 2. Mark the date/time variable. 3. Click Edit format in the Date Time configuration section.	
4. In the **Specify Date Format** dialog, enter the new format.	

Properties

Variables: 19 (X = 13, Y = 6, Qualitative = 0)

Index	Variable ID	Type	Comments
X 1	Ton_in	X-variable	
X 2	KR30_IN	X-variable	
3	date	X-variable	Excluded in the default workset Par…
X 4	KR40_IN	X-variable	
X 5	PARM	X-variable	
X 6	HS_1	X-variable	
X 7	HS_2	X-variable	

To specify the default variable type, use the 'Save as default workset' button in the Workset dialog.

Date/Time configuration

Specify Date Format

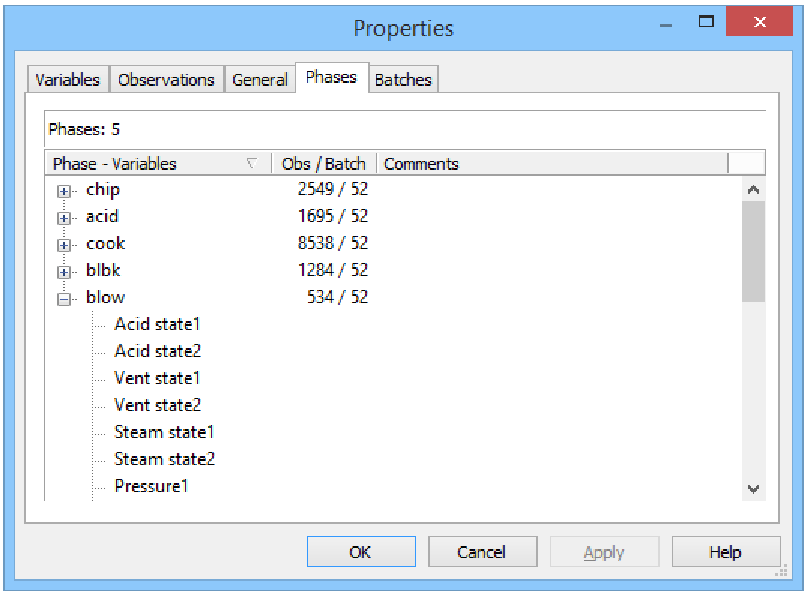
Enter a new Date/Time format to replace the existing one.

Format: yyyy-MM-dd HH:mm:ss

8.11.4 Phases

The **Phases** page displays all phases in the dataset with the number of observations and batches in that phase. Under **Comments**, view the current y-variable for each phase.

Clicking the + sign displays the variables included in the respective phases.

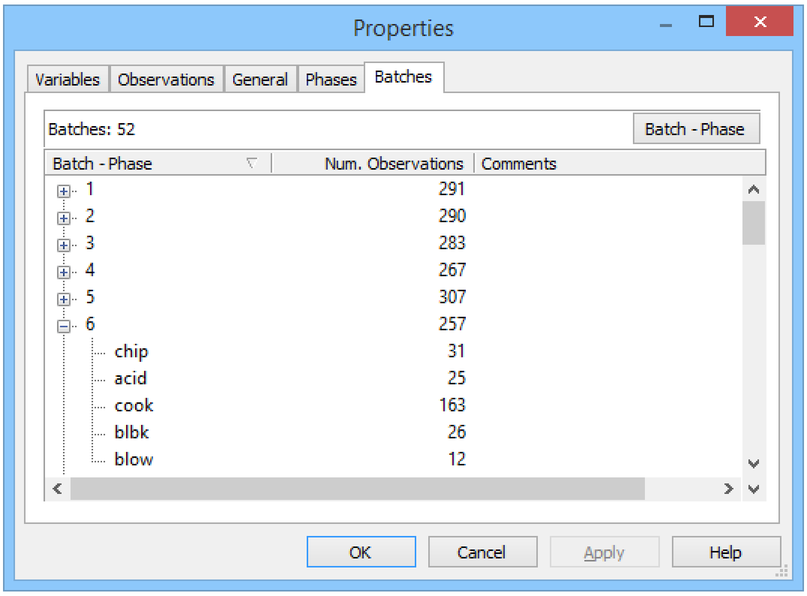


Phases: 5

Phase - Variables	Obs / Batch	Comments
⊞ chip	2549 / 52	
⊞ acid	1695 / 52	
⊞ cook	8538 / 52	
⊞ blbk	1284 / 52	
⊟ blow	534 / 52	
Acid state1		
Acid state2		
Vent state1		
Vent state2		
Steam state1		
Steam state2		
Pressure1		

8.11.5 Batches

The **Batches** page displays all batches with the number of observations included in each batch.



Batches: 52

Batch - Phase	Num. Observations	Comments
⊞ 1	291	
⊞ 2	290	
⊞ 3	283	
⊞ 4	267	
⊞ 5	307	
⊟ 6	257	
chip	31	
acid	25	
cook	163	
blbk	26	
blow	12	

When there are phases, clicking the + sign displays the phases included in the respective batch.

Clicking the **Batch - phase** or **Phase - batch** buttons switches what is displayed between:

- Batches with the phases displayed when clicking the + sign when the mode is **Batch-phase**.
- Phases with the batches displayed when clicking the + sign when the mode is **Phase-batch**.

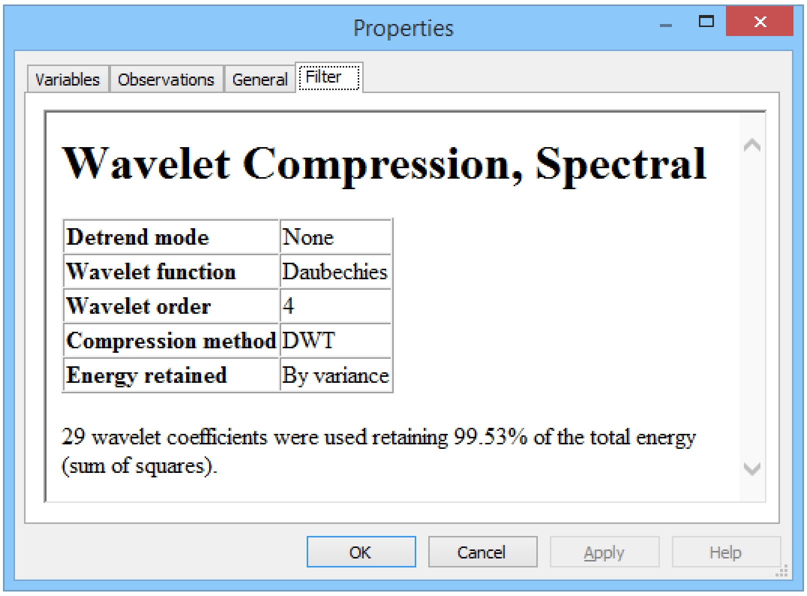
8.11.6 Filter summary

The **Filter** page holds details about the performed filtering in the selected preprocessed dataset. A preprocessed dataset is a dataset created by spectral filtering (**Data | Spectral filters**) or time series filtering (**Data | Time series filters**). The **Filter** page is available in the dataset **Properties** dialog.

To display the **Filter** page click:

- On the **Data** tab, in the **Summary** group, click **Dataset summary** and in the **Properties** dialog click the **Filter** tab.
- Right-click the filtered dataset spreadsheet and select **Properties**.

In the example here, the current dataset is the result of having filtered and decimated a time series dataset, and the **Filter** page displays the following:



Wavelet Compression, Spectral

Detrend mode	None
Wavelet function	Daubechies
Wavelet order	4
Compression method	DWT
Energy retained	By variance

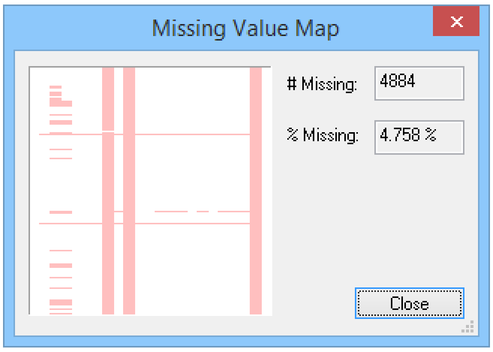
29 wavelet coefficients were used retaining 99.53% of the total energy (sum of squares).

8.12 Missing value map

To display an overview of a dataset with respect to missing values:

- On the **Data** tab, in the **Summary** group, click **Missing value map** and then the desired dataset in SIMCA.
- In SIMCA import, on the **View** tab in the **Missing values** group, click **Missing value map**.

Missing values are colored while data present are white.



Missing: 4884

% Missing: 4.758 %

8.13 Trimming overview

Trimming overview is available after trimming or Winsorizing the dataset.

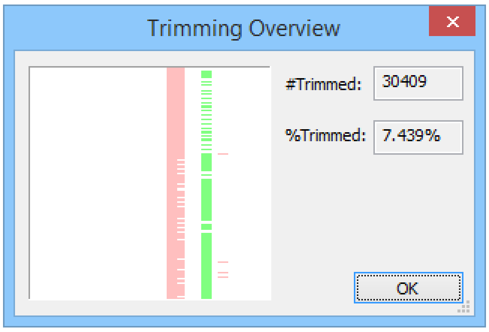
To get an overview of the trimming performed, open the **Trimming overview**.

The **Trimming overview** is available by:

- On the **Data** tab, in the **Summary** group, clicking **Trimming overview**.
- Right-clicking the dataset spreadsheet and selecting **Trimming Overview**.

The **Trimming overview** displays a summary of the trimmed or replaced values. Trimmed values replaced by missing appear in pink, Winsorized values appear in green.

Note: *The trimming-Winsorizing effects only the selected observations and variables.*



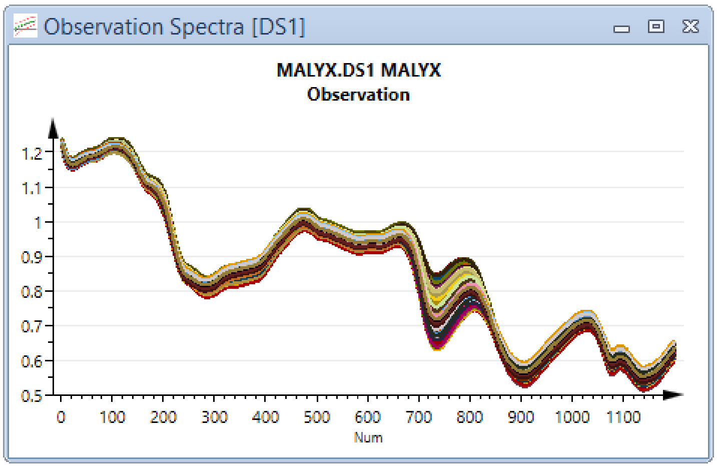
#Trimmed: 30409

%Trimmed: 7.439%

8.14 Spectra

With spectral data, it is particularly useful to display XObs of all observations in a line plot, the **Spectra** plot.

Open the **Spectra** plot on the **Data** tab, in the **Summary** group.



See also the Color subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs for details about coloring the line plot.

8.15 Hierarchical models

After fitting a model, the scores, residuals, and predicted y of that model can be used as variables in another model.

Models using scores, residuals, or predicted y from another model are named hierarchical top models. The model providing the score/residual/predicted y variables is named hierarchical base model.

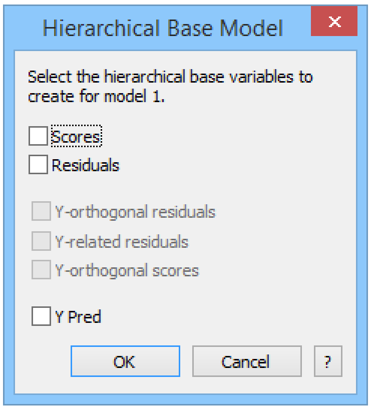
To create the hierarchical variables to use in another model, use one of the two methods:

- With the model marked in the **Project Window**, on the **Data** tab, in the **Base model** group click **Hierarchical base model** and select check boxes as desired.
- Right-click the model in the **Project Window**, click **Hierarchical base model** and select the check boxes as desired.

A new dataset named *$MxHierarchical* is created holding:

- The scores of all extracted components, when selecting **Scores**.
- The residuals of all the variables, when selecting the residual check boxes.
- The predictions for all y-variables when selecting **Y Pred**.

Models including the hierarchical dataset are marked T (hierarchical Top model), and the Base models are marked B in the **Project Window**.


Hierarchical Base Model

Select the hierarchical base variables to create for model 1.

□ Scores
□ Residuals

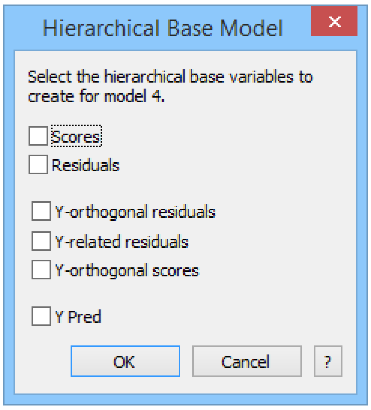
□ Y-orthogonal residuals
□ Y-related residuals
□ Y-orthogonal scores

□ Y Pred

8.15.1 Hierarchical models with OPLS or O2PLS

When the fitted model is an OPLS or O2PLS model, the following additional hierarchical terms can be added:

- **Y-orthogonal residuals** - the residuals after subtracting the predictive part of the model (X-TP'). Only available for OPLS and O2PLS models with at least one Y-Orthogonal component.
- **Y-related residuals** - the residuals after subtracting the Y-orthogonal part of the model (X-ToPo'). Only available for OPLS and O2PLS models with at least one Y-Orthogonal component.
- **Y-orthogonal scores** - the scores that are orthogonal to Y (To). Only available for OPLS and O2PLS models with at least one Y-Orthogonal component.


Hierarchical Base Model

Select the hierarchical base variables to create for model 4.

□ Scores
□ Residuals

□ Y-orthogonal residuals
□ Y-related residuals
□ Y-orthogonal scores

□ Y Pred

8.15.2 Hierarchical models with blocks

After assigning variables to blocks (see Assigning variables to blocks subsection in the Workset section in Chapter 7 Home), the hierarchical model types **PCA-Hierarchical**, and if y-variables were specified, **PLS-Hierarchical**, **OPLS-Hierarchical** and **O2PLS-Hierarchical** are available.

Selecting one of the hierarchical model types results in:

- Fitting one model for each block positioned in a CM wrapper.
- Setting each model as hierarchical base model creating the hierarchical scores datasets.

8.15.3 Hierarchical base models reverts to non hierarchical

A hierarchical base model reverts to a regular **Non hierarchical** when:

- Adding components
- Changing the model title
- Clicking **Non hierarchical**

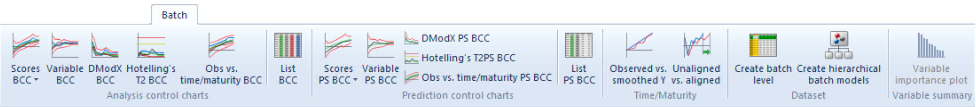
This results in that the B is removed and the hierarchical dataset is deleted. Consequently the hierarchical top models are deleted and the former base model has to be designated as a hierarchical base model again to recreate the hierarchical top models.

9 Batch

9.1 Introduction

The **Batch** tab holds the batch specific features and is unavailable for regular projects. The following features are available:

- Batch control charts (BCC) plots and lists, both for the model and for predictions. Available both for PLS and OPLS models.
- Batch plots illustrating smoothing and alignment.
- Creation of batch level and hierarchical batch datasets.
- Batch variable importance plot.



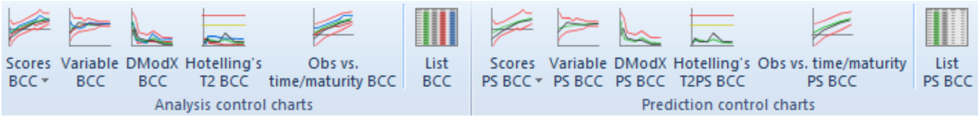
The batch evolution and batch level model types are described in the Batch modeling in SIMCA section, in Chapter 2, Introduction to multivariate data analysis.

9.2 Batch control charts

For batch evolution models, batch control charts are available on the **Batch** tab. The available batch control chart types are:

- **Scores**
- **Variable**
- **DModX**
- **Hotelling's T2**
- **Observed vs. time/maturity**
- **List**

All plots are available both in the **Analysis control charts** and the **Prediction control charts** groups, the buttons in the latter with the addition of *PS* in the button name.



Each plot type is described later in this section.

The batch control charts by default display the first batch in the workset. For batch projects with phases the active phase (class) is used. When the BEM is marked when clicking a BCC all phases are displayed.

Note: For any batch control chart with a batch outside the displayed control limits, you can display the Out of control summary plot by clicking **Out of control summary** in the **Create** group on the **Tools** tab. For more, see the Out of control summary plot (OOC) subsection in Chapter 14, Plot and list contextual tabs.

9.2.1 Batch control chart background

When batches have different length, alignment of the batch variables, scores, DModX, etc., is done by cutting or continuing with the last value so that all batches have the same length as the median batch length. This subsection describes the batch control chart calculations using, as example, the scores.

Note: With batches that vary in length more than 20% to 30%, you should use a maturity variable as Y.

The scores of the active model(s) are chopped up, aligned and reorganized so that the scores of one batch form one row vector (t1 followed by t2, followed by t3, etc.) in a matrix S_T. This matrix has N rows (one per batch) and x J (AJ) columns from the A score vectors and the J "time points" per batch.

When batches have phases, the alignment is done by phases using their respective Maturity or Time variable.

Time Normalized is equivalent to a linear time warping.

From the matrix S_T, SIMCA calculates the averages and standard deviations (SD) of the scores, (average trace of normal batches and control intervals as the averages ± 2, and ± 3 SD).

The batch control charts for Variables, DModX, Hotelling's T2, and Obs vs. time/maturity are calculated in the same manner.

9.2.2 Batch control chart plot and list customization

Batch control charts can be customized using the **Properties** and **Format Plot** dialogs. This section describes the **Properties** dialog for batch control charts. For more about Format Plot, see the Chapter 14, Plot and list contextual tabs.

Open the **Properties** dialog by clicking the plot and clicking **Properties** in the mini-toolbar

In the **Properties** dialog for the BCCs the following tabs are available:

- Select batch and phase
- Limits and averages
- Component
- Select variable for the **Variable BCC**.
- Color with only one phase selected.

The **Select batch and phase** tab is available for the **Batch control chart list** while the other tabs are not.

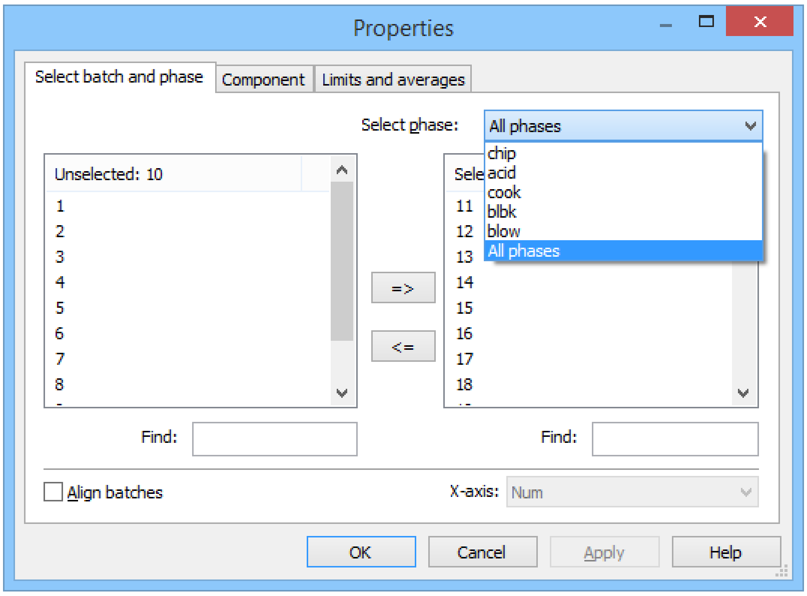
Each tab is described in the subsections that follow.

9.2.2.1 Selecting batch and phase

On the **Select batch and phase** page:

- In the **Select phase** box select one phase or **All phases**.
- In the **Unselected** list, select the batches to display and click the **=>** button.
- In the **Selected** list, mark available batches to no longer display and click the **<=** button.
- Select or clear the **Align batches** check box (by default both workset and predictionset batches are displayed unaligned) to display the batches aligned or unaligned. After clearing, select what to display on the **X-Axis**: **YVar**, **YVarDS**, or **Num**. Or for the batch control charts created from the **Prediction control charts** group: **YVarPS**, **YVarDSPS**, or **Num**. **YVar** and **YVarPS** are the time/maturity variable treated as in the workset; **YVarDS** and **YVarDSPS** are the time/maturity variable in original units (as in the respective datasets).

Note: Batch control charts displaying **All phases** use **Num** on the x-axis.



Select phase: All phases

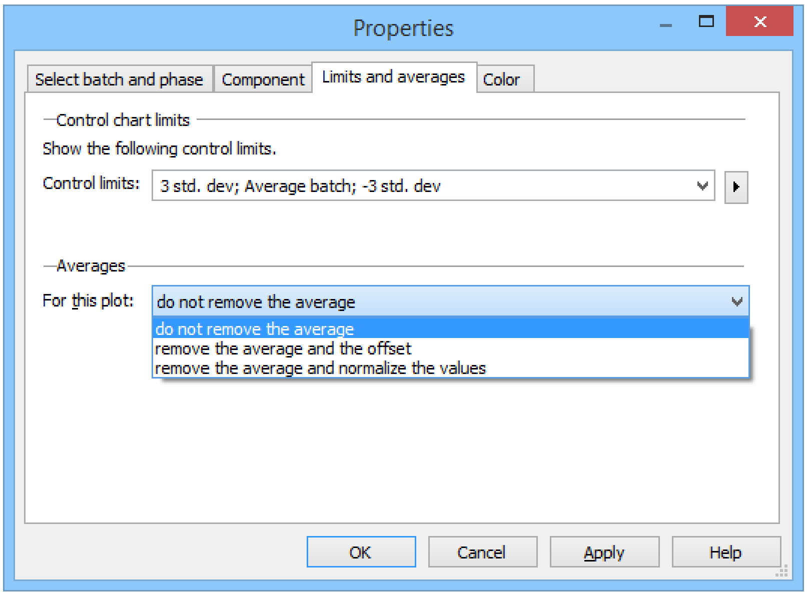
□ Align batches

X-axis: Num

9.2.2.2 Limits and averages

On the **Limits and averages** page:

- In the **Control limits** box, select which limits to display. Default is to display **Average batch** and when appropriate **+3 std. dev.** and **-3 std. dev**. Available limits are by default -3, -2, -1, Average Batch, 1, 2, 3 standard deviations.
- To display the standard deviation over all batches and phases, select the **Display steady state limits using the overall standard deviation** check box. This option is available for the **Variable BCCs** displaying one phase, and enables monitoring of steady state variables.
- In the **For this plot** box in the **Averages** section, select
  a. **do not remove the average** – to display the limits and values on the original scale.
  b. **remove the average** – to remove the average from limits and batches leading to a centered plot with y=0 as average batch.
  c. **remove the average and normalize the values** – to remove the average and normalize limits and batches leading to a plot with y=0 as average batch and horizontal limits.



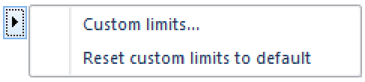
Show the following control limits.

Control limits: 3 std. dev; Average batch; -3 std. dev

For this plot: do not remove the average

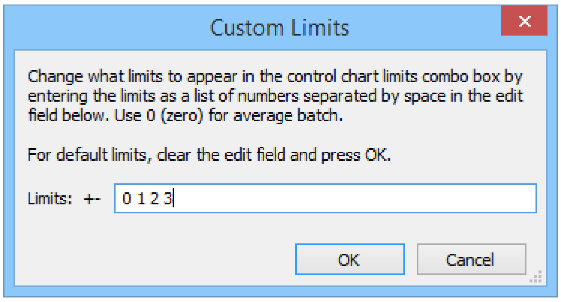
Adding limits

To add control limits, click the arrow next to the **Control limits** box and click **Custom limits**.



In the **Custom Limits** dialog, enter the limits to display in **Control limits**, with <space> parting the limits.

Note: The new entered limits replace the old. This means that typing '1.5' in **Limits** results in that –1.5 and +1.5 std. dev. will be the only available limits.



Change what limits to appear in the control chart limits combo box by entering the limits as a list of numbers separated by space in the edit field below. Use 0 (zero) for average batch.

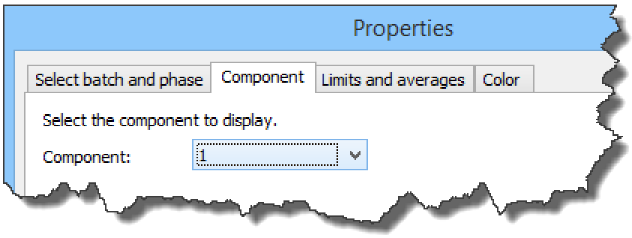
For default limits, clear the edit field and press OK.

Limits: +- 0 1 2 3

To restore the default limits, click the arrow next to the **Control limits** box and click **Reset custom limits to default**.

9.2.2.3 Component

On the **Component** page, select for which component to display the batch control chart. The **Component** page is not available for the **Variable BCC**.

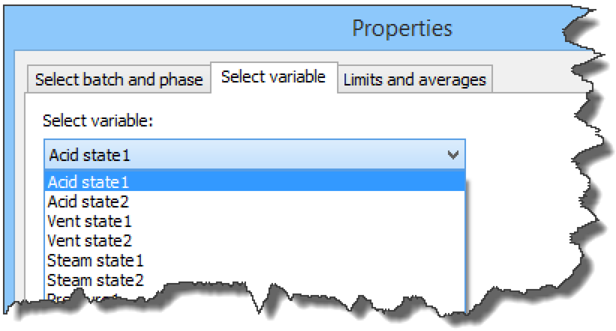


Select the component to display.

Component: 1

9.2.2.4 Select variable

On the **Select variable** page, select which variable to display in the **Variable BCC**.



Select variable: Acid state1

9.2.3 Excluding batches

An entire batch can be excluded from the batch evolution model by selecting the batch in a plot using the **Batch marking mode**.

To exclude a batch from the model:

1. Open a plot displaying batches, such as a batch control chart.
2. On the **Tools** tab, in the **Plot tools** group, click **Select** | **Batch marking mode**.
3. In the plot click the batch.

4. On the **Marked items** tab, in the **Modify model** group, click **Exclude**.

5. New unfitted models are created.

For exclusion of batches in batch level models, see the Excluding marked items section in the Marked Items tab section in Chapter 14, Plot and list contextual tabs.

For details on the tools, see the Select plot items - Marking tool section in the Marked Items tab section in Chapter 14, Plot and list contextual tabs.

See also the Including and excluding batches subsection in the Batch page section in Chapter 7, Home.

9.2.4 Score batch control chart

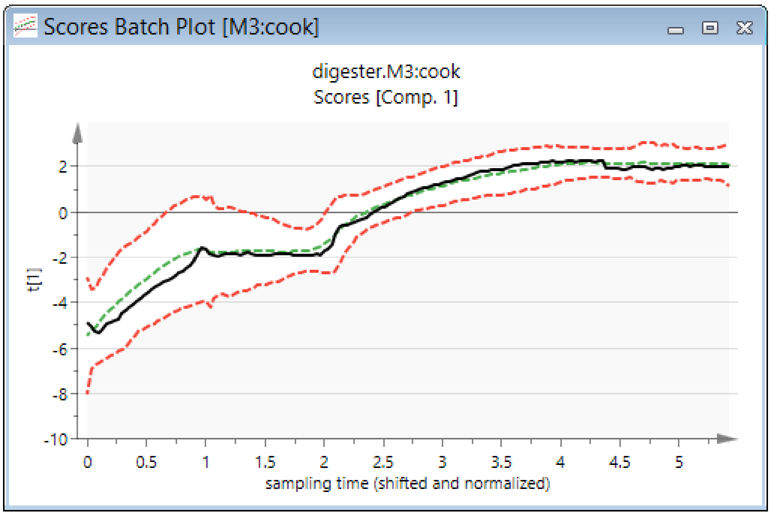
Open the **Scores BCC** by clicking it in the **Analysis control chart** group on the **Batch** tab. This plot displays the workset batches. For OPLS models **Scores BCC | Orth scores** is available displaying the orthogonal part for the model.

The advantage with OPLS is that it concentrates all predictive information in one control chart. This gives narrower control limits and facilitates early fault detection of problematic batches. In addition, the orthogonal components may display clues to variations not related to Y.

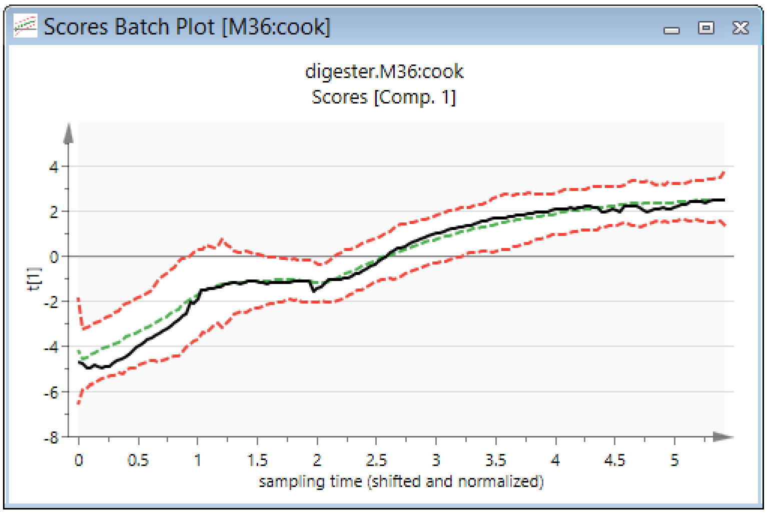
To see predictions, click **Scores PS BCC** in the **Prediction control chart** group.

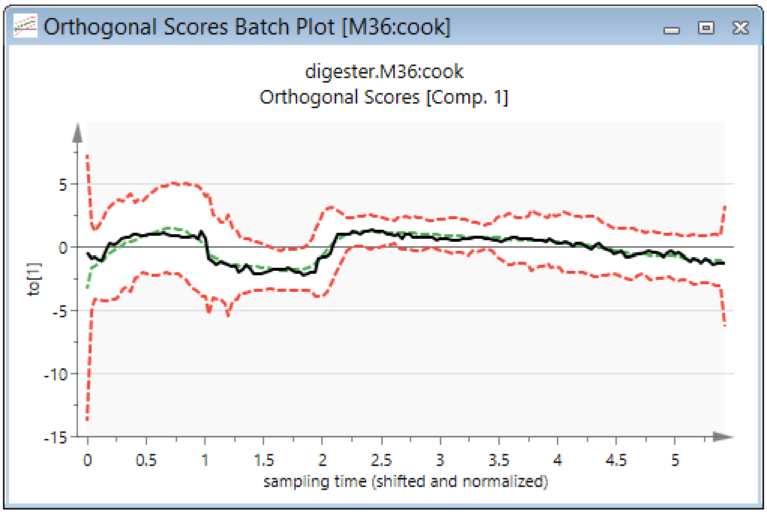
The limits that are displayed by default are the Average batch and -3 and +3 std. dev.

PLS:



OPLS:



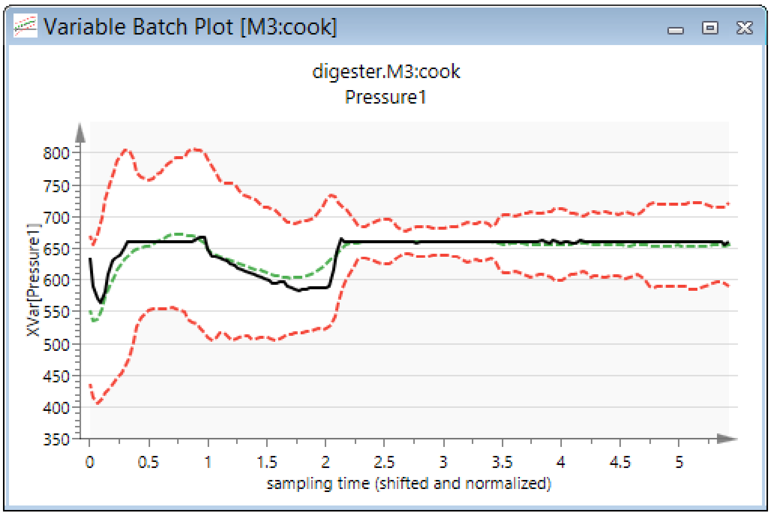

Orthogonal Scores Batch Plot [M36:cook]
digester.M36:cook
Orthogonal Scores [Comp. 1]
to[1]
5
0
-5
-10
-15
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
sampling time (shifted and normalized)

9.2.5 Variable batch control chart

Open the **Variable BCC** by clicking it in the **Analysis control chart** group on the **Batch** tab. This plot displays the workset batches.

To see predictions, click **DModX PS BCC** in the **Prediction control chart** group.

The limits that are displayed by default are the Average batch and -3 and +3 standard deviations.



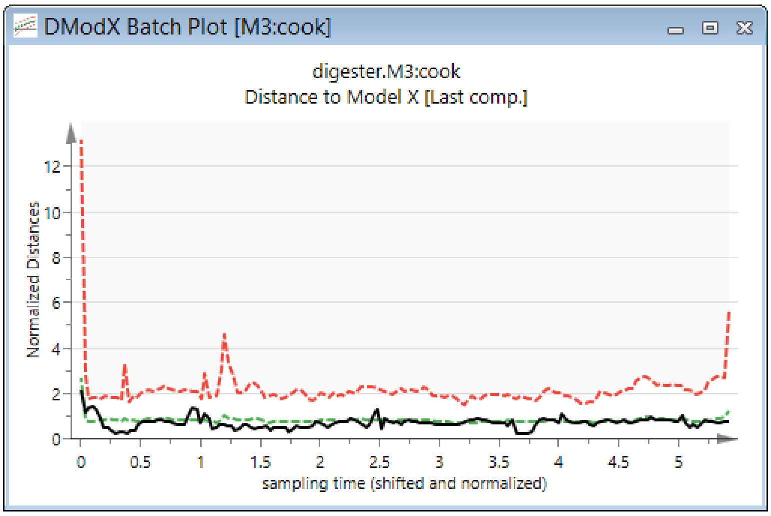
By selecting the **Display steady state limits using the overall standard deviation** check box, in the **Properties** dialog, **Limits and averages** tab, you can select to have the limits computed from the standard deviation of the variable as computed or specified in the workset.

9.2.6 DModX batch control chart

Open the **DModX BCC** by clicking it in the **Analysis control chart** group on the **Batch** tab. This plot displays the workset batches.

To see predictions, click **DModX PS BCC** in the **Prediction control chart** group.

The limits that are displayed by default are the Average batch and +3 std. dev.

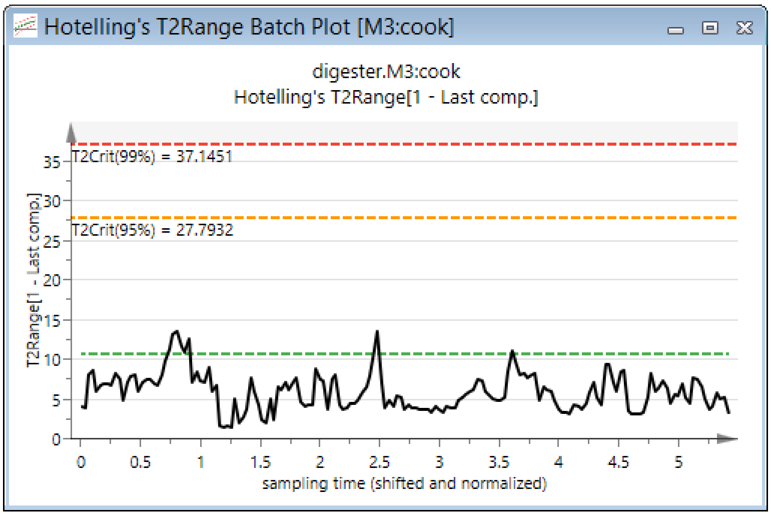

DModX Batch Plot [M3:cook]
digester.M3:cook
Distance to Model X [Last comp.]
Normalized Distances
0
2
4
6
8
10
12
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5
sampling time (shifted and normalized)

9.2.7 Hotelling’s T2Range batch control chart

Open the **Hotelling’s T2 BCC** by clicking it in the **Analysis control chart** group on the **Batch** tab. This plot displays the workset batches.

To see predictions, click **Hotelling's T2PS BCC** in the **Prediction control chart** group.

The limits that are displayed by default are the Average batch and T2Crit(95%) and T2Crit(99%).

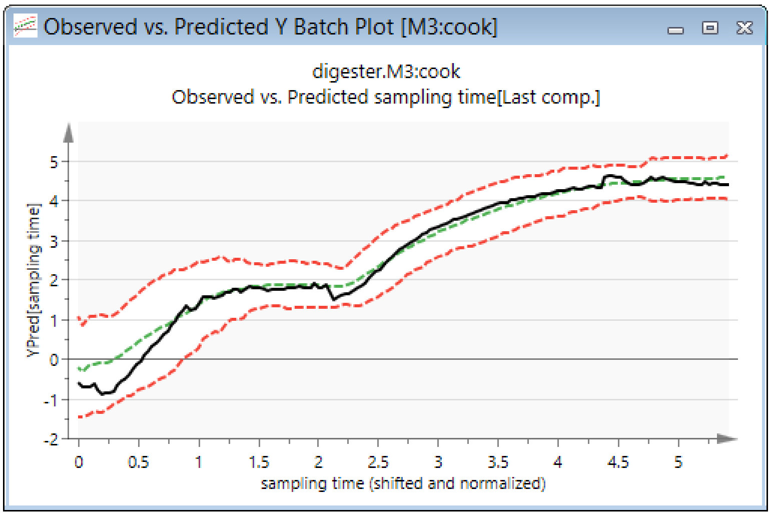


9.2.8 Observed vs. time/maturity batch control chart

Open the Observed vs. Predicted Y Batch Plot by clicking **Obs vs. time/maturity BCC** in the **Analysis control chart** group on the **Batch** tab. This plot displays the workset batches.

To see predictions, click **Obs vs. time/maturity PS BCC** in the **Prediction control chart** group.

The limits that are displayed by default are the Average batch and -3 and +3 std. dev.

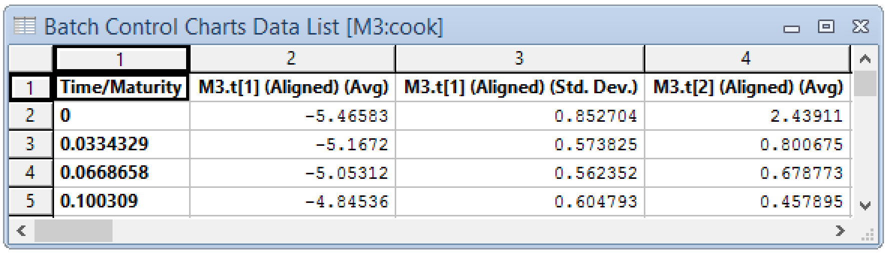


9.2.9 Batch control charts list

The **List BCC** displays a number of vectors for the active model or phase.

Open the **BCC List** by clicking it in the **Analysis control chart** group on the **Batch** tab. This plot displays the workset batches.

To see predictions, click **List PS BCC** in the **Prediction control chart** group.


Batch Control Charts Data List [M3:cook]

	1	2	3	4
1	Time/Maturity	M3.t[1] (Aligned) (Avg)	M3.t[1] (Aligned) (Std. Dev.)	M3.t[2] (Aligned) (Avg)
2	0	-5.46583	0.852704	2.43911
3	0.0334329	-5.1672	0.573825	0.800675
4	0.0668658	-5.05312	0.562352	0.678773
5	0.100309	-4.84536	0.604793	0.457895

Default is to display the list for unaligned batches. All t, YPred, and DModX vectors are then displayed unaligned while the averages and standard deviations are displayed aligned.

Note: The t, YPred, and DModX vectors referring to the specific batches are displayed alongside the YVarDS vector to the far right in the list.

To display the list for aligned batches, open Properties, and select the **Align batches** check box.

All vectors available from the **BCC List** are listed in the table.

General name	Description	Example
Mx.t['comp'] (Aligned) (Avg)	The average over all batches of the aligned score vectors, for each component.	M3.t[1] (Aligned) (Avg)
Mx.t['comp'] (Aligned) (Std. Dev.)	The standard deviation over all batches of the aligned score vectors, for each component.	M3.t[1] (Aligned) (Std. Dev.)
Mx.t['comp'] (Aligned): 'batch'	The aligned score vector for the listed batch, for each component. **Note**: This vector is only available when the **Align batches** check box is selected.	M3.t[1] (Aligned): 1
Mx.YPred['last comp']('y')(Aligned) (Avg)	The average over all batches of the aligned predicted y vectors, for the last component.	M3.YPred[2](timeb)(Aligned) (Avg)
Mx.YPred['last comp']('y')(Aligned) (Std. Dev.)	The standard deviation over all batches of the aligned predicted y vectors, for the last component.	M3.YPred[2](timeb)(Aligned) (Std. Dev.)
Mx.YPred['last comp']('y')(Aligned): 'batch'	The aligned predicted y vector for the listed batch and last component.	M3.YPred[2](timeb)(Aligned): 1

General name	Description	Example
	Note: This vector is only available when the **Align batches** check box is selected.	
Mx.DModX['last comp'] (Aligned) (Avg)	The average over all batches of the aligned DModX vectors, for the last component.	M3.DModX[2] (Aligned) (Avg)
Mx.DModX['last comp'] (Aligned) (Std. Dev.)	The standard deviation over all batches of the aligned DModX vectors, for the last component.	M3.DModX[2] (Aligned) (Std. Dev.)
Mx.DModX['last comp'] (Aligned): 'batch'	The aligned DModX vector, for the listed batch and last component. **Note**: This vector is only available when the **Align batches** check box is selected.	M3.DModX[2] (Aligned): 1
Mx.YVarDS('y'): 'batch'	The original y-vector for the listed batch. **Note**: This vector is only available when the **Align batches** check box has been cleared.	M3.YVarDS(timeb): 1
Mx.t['comp']: 'batch'	The unaligned score vector for the listed batch, for each component. **Note**: This vector is only available when the **Align batches** check box has been cleared.	M3.t[1]: 1
Mx.YPred['last comp'] ('y'): 'batch'	The unaligned predicted y vector for the listed batch and last component. **Note**: This vector is only available when the **Align batches** check box has been cleared.	M3.YPred[2] (timeb): 1
Mx.DModX['last comp']: 'batch'	The unaligned DModX vector for the listed batch and last component. **Note**: This vector is only available when the **Align batches** check box has been cleared.	M3.DModX[2]: 1

The to (orthogonal scores) vectors for OPLS are unavailable here but available in Plot/List | List.

9.3 Batch control charts for new batches

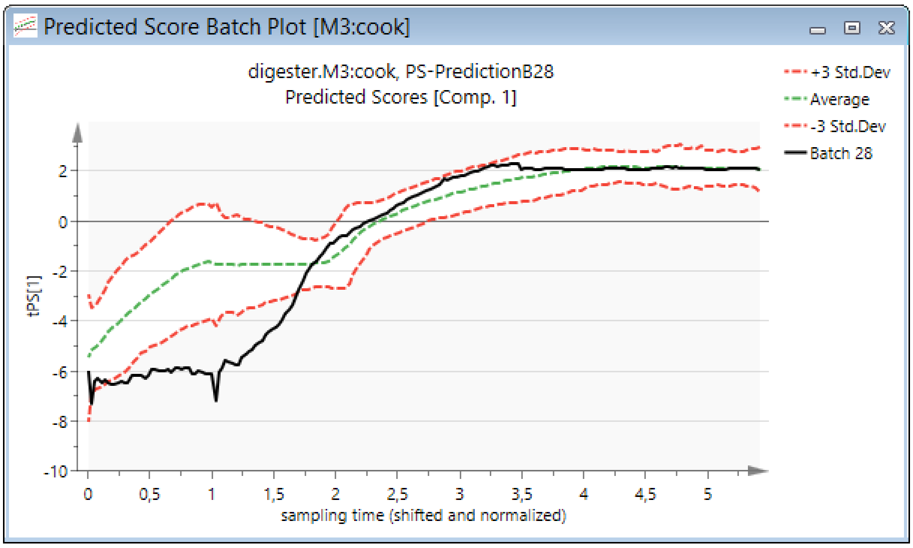
To monitor the evolution of new batches, use the buttons in the **Prediction control chart** group on the **Batch** tab, after specifying the predictionset in the **Specify predictionset** group on the **Predict** tab.

The data from each new batch are inserted into the batch evolution model, giving predicted values of the scores, TPS. In addition, predicted Y and DModX values are computed. These results can now be plotted in the appropriate control charts, with limits derived from the workset model.

The batch control charts indicate whether the batch is starting and running normally or not. If the values are outside the normal ranges, contribution plots based on the x-values or the residuals indicate which variables together are related to the deviations.

The new batches are by default displayed unaligned in the predicted batch control charts.

Use the **Properties** group, in the **Tools** tab, to select a different phase, different batches, etc.



For details about creating contribution plots for entire batches, see the second table in the Drill down contribution plots available subsection in the Marked items tab section in Chapter 14, Plot and list contextual tabs.

For details about the **Properties** dialog, see the Batch control chart plot and list customization subsection previously in this chapter.

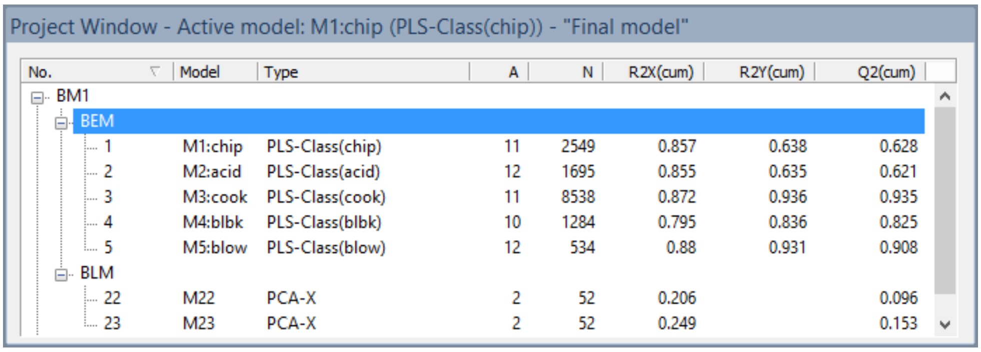
For details about the limits, see the Calculating limits to build control charts subsection in Chapter 2, Introduction to multivariate data analysis.

For info about the out of control summary plot, see the Out of control summary plot (OOC) subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs.

9.4 Create BLM

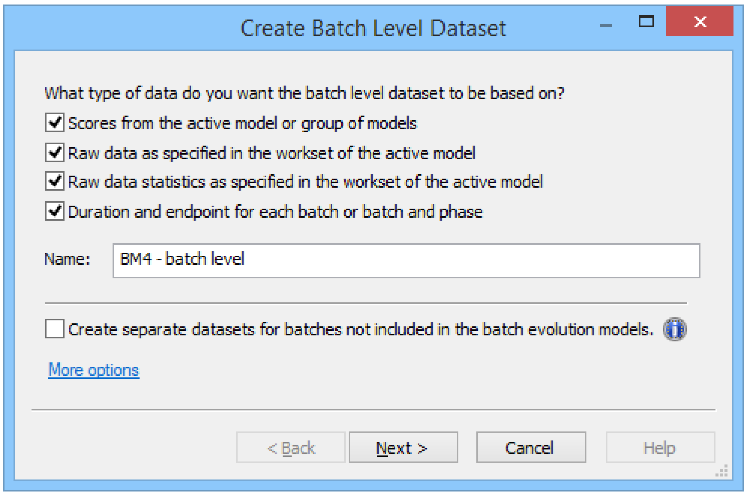
To be able to create a batch level model, BLM, you first have to create a batch level dataset, BL DS. The BL DS then resides in the same project as the batch evolution dataset.

Batch level models, BLM, created using the BL DS, are positioned in the same BM as the BEM the BL DS was created from.


Project Window - Active model: M1:chip (PLS-Class(chip)) - "Final model"

No.	Model	Type	A	N	R2X(cum)	R2Y(cum)	Q2(cum)
BM1							
BEM							
1	M1:chip	PLS-Class(chip)	11	2549	0.857	0.638	0.628
2	M2:acid	PLS-Class(acid)	12	1695	0.855	0.635	0.621
3	M3:cook	PLS-Class(cook)	11	8538	0.872	0.936	0.935
4	M4:blbk	PLS-Class(blbk)	10	1284	0.795	0.836	0.825
5	M5:blow	PLS-Class(blow)	12	534	0.88	0.931	0.908
BLM							
22	M22	PCA-X	2	52	0.206		0.096
23	M23	PCA-X	2	52	0.249		0.153

Create the batch level dataset by clicking **Create batch level** in the **Dataset** group on the **Batch** tab. The **Create Batch Level Dataset** wizard opens.



Create Batch Level Dataset

What type of data do you want the batch level dataset to be based on?

☑ Scores from the active model or group of models

☑ Raw data as specified in the workset of the active model

☑ Raw data statistics as specified in the workset of the active model

☑ Duration and endpoint for each batch or batch and phase

Name: BM4 - batch level

☐ Create separate datasets for batches not included in the batch evolution models.

Note: The **Scores from the active model or group of models** check box is unavailable for OPLS as creation of batch level datasets using orthogonal scores is not supported.

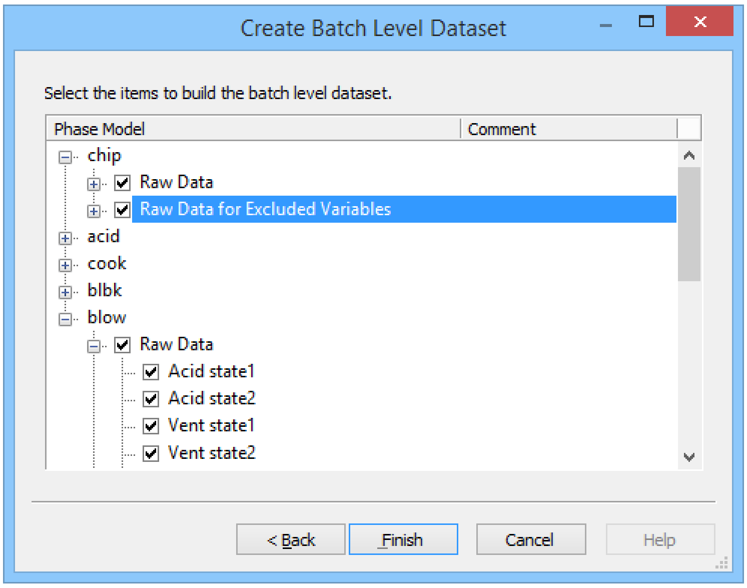
9.4.1 Selecting what to base the batch level dataset on

On the first page of the **Create Batch Level Dataset** wizard, you must select what to base the batch level dataset, BL DS, on. The BL DS can be created using the options described in the table. Note that all check boxes can be selected and multiple BL DS are then created simultaneously.

	Options	Action	Result after Next/Finish
1.	Create BL DS from scores. Available for PLS only.	Select the Scores from the active model or group of models check box.	A dataset containing scores is created after **Finish**. The variables are aligned using the time/maturity variable.
2.	Create BL DS from original variables.	Select the Raw data as specified in the workset of the active model check box.	A page for selecting variables for each phase. See **Selecting BEM variables for BL DS** section. **Finish** creates the dataset. The variables are aligned using the time/maturity variable.
3.	Create BL DS from statistics of the original variables.	Select the Raw data statistics as specified in the workset of the active model check box.	A page for selecting which statistics to include in the new dataset. **Finish** creates the dataset. For details about these variables, see the Raw Data Statistics Types dialog topic.
4.	Create a BL DS containing duration and endpoint.	Leave the Create duration and endpoint in a separate dataset check box selected.	A BL DS is created holding the duration and endpoint variables for all phases in the current BEM. Duration is calculated as the number of points in the batch for that phase. Endpoint is calculated as the time passed since the start of the batch, or maturity value at last point.
5	Create separate datasets for batches not included in the batch evolution models	Select the Create separate datasets for batches not included in the batch evolution modelscheck box.	One batch level dataset for each of the check boxes selected (Scores..., Raw data..., Raw data statistics..., Duration...) is created holding all batches available in the project but not included in the BEM. When selecting the check box after batch level datasets have already been created, the complementary datasets are created for all dataset types either already created or selected at this point.
6.	More options	Click **More options** to access advanced options.	The Options dialog opens with the Project options page active allowing you to change the batch level options as desired. The new options are applied to the newly created models as applicable.

9.4.2 Selecting BEM variables for BL DS dialog

When clicking **Raw data as specified in the workset of the active model**, to construct the BL DS with different variable selection depending on the phase, clicking **Next** opens a dialog box enabling custom settings for each phase. Projects without phases are treated as having one phase.



Create Batch Level Dataset

Select the items to build the batch level dataset.

Phase Model	Comment
⊟ chip	
⊞ ☑ Raw Data	
⊞ ☑ Raw Data for Excluded Variables	
⊞ acid	
⊞ cook	
⊞ blbk	
⊟ blow	
⊟ ☑ Raw Data	
☑ Acid state1	
☑ Acid state2	
☑ Vent state1	
☑ Vent state2	

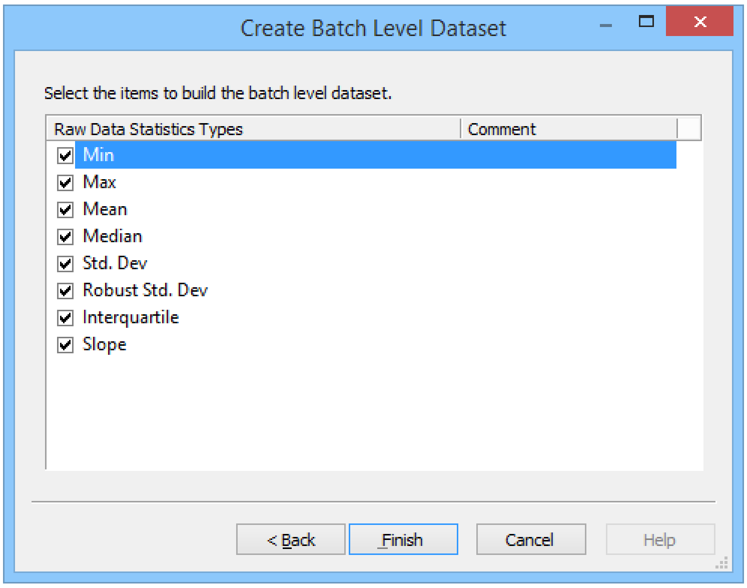
The original variables in the model and those excluded are available for selection for each phase.

Variable	Description	Comment
Raw Data	Original variables.	Click the + to select a subset of the original variables in the phase.
Raw Data for Excluded Variables	Original variables not included.	Click the + to select a subset of the original variables not included in the phase.

Select/clear the desired check boxes and click **Next/Finish**.

9.4.3 Raw Data Statistics Types dialog

When selecting **Raw data statistics as specified in the workset of the active model**, clicking **Next** opens a dialog box for selecting which statistical variables to create in the new BL DS.



Create Batch Level Dataset

Select the items to build the batch level dataset.

Raw Data Statistics Types	Comment
☑ Min	
☑ Max	
☑ Mean	
☑ Median	
☑ Std. Dev	
☑ Robust Std. Dev	
☑ Interquartile	
☑ Slope	

The statistical variables, listed in the table, are calculated for each variable in each phase.

Name in Raw Data Statistics page	Name in BL DS spreadsheet	Description
Min	MIN	Minimum value.
Max	MAX	Maximum value.
Mean	AVG	Average value.
Median	MEDIAN	Median value.
Std. Dev.	SD	Standard deviation.
Robust Std. Dev.	RSD	RSD = IQR/1.075
Interquartile	IQR	IQR = IQR[1] - IQR[3]. That is, the third interquartile subtracted from the first interquartile.
Slope	SLOPE	Slope of the variable.

Select the desired check boxes and click **Finish**.

9.4.4 Batch and phase condition datasets

Batch condition variables are variables pertaining to the whole batch used in BLM. Phase condition variables are variables pertaining to the whole phase and phase iteration conditions are variables pertaining to the whole phase iteration. Condition variables may be starting conditions or final (result) conditions.

Condition variables can be included in a batch level model after the **Create a batch level model** check box has been selected in the **Workset** dialog and the condition dataset has been selected. All selected datasets are automatically merged in the calculations after being selected in the **Workset** dialog.

A condition variable can be a continuous variable or discrete (qualitative).

If batch, phase, and phase iteration condition variables were imported in the BE DS, they are available in separate batch level DS (conditions dataset) created at import. For how to specify batch and phase conditions during import of the BE DS, see the Specifying data properties subsection in Chapter 6, SIMCA import.

For how to import batch conditions separately, see the Importing batch and phase conditions subsection in the Chapter 6, SIMCA import.

9.4.5 Batch level datasets and missing values

When creating batch level datasets, BL DS, from original variables, and there are ***missing values***, SIMCA interpolates all missing values. Missing values can still be present first or last, as no extrapolation is done.

When batches are ***missing phases***, this is usually due to the fact that these phases/steps are not needed for those particular batches. In SIMCA there are two options:

- Replacing these phases/steps with missing when creating the BL DS. This is the default in SIMCA. Note that this may cause bias in the results.
- Replacing the missing phases/steps by the average values of these phases/steps in the workset (batches that yielded good results). This is the way SIMCA treated missing phases pre 13 and by some viewed as the best way to ensure that these phases will not bias unfavorably the predicted quality.

9.5 Sources of variation plot

In batch level models it is useful to display the contribution and loading plots (or any other plot displaying variables) as line plots over time rather than column plots at every time point. Therefore the **Sources of variation plot** is the default loading and contribution plot for all BLM with one or more score or raw variables. The Sources of variation plot contains the exact same data as a loading or contribution plot would show. Instead of having the variable number on the x-axis, the maturity of the batch is used. This gives a better view of how the process variables relate to each other at different stages in the process.

For projects with phases, this plot is displayed showing all phases.

9.5.1 BLM with batch conditions

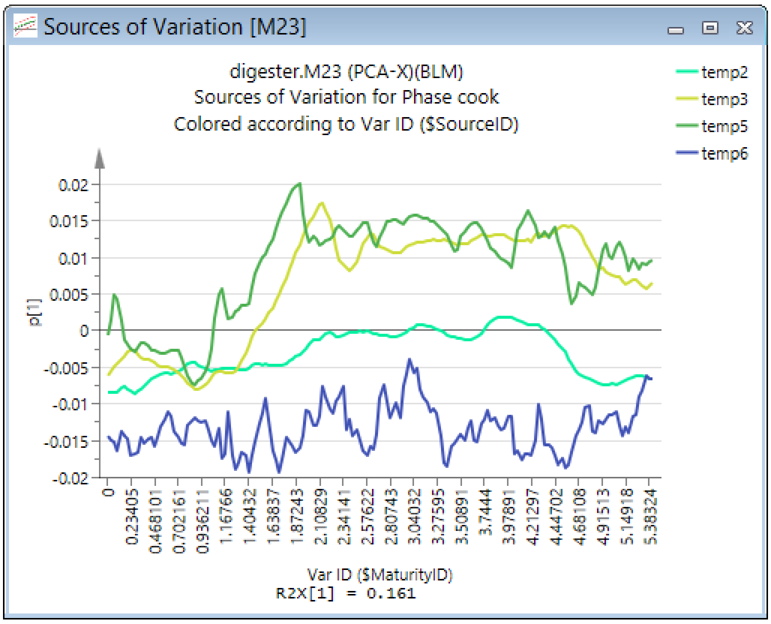
Variables without maturity, i.e. batch conditions, cannot be shown in Sources of variation plots. When the BLM contains batch conditions it can be useful to view the plot as a regular column plot too.

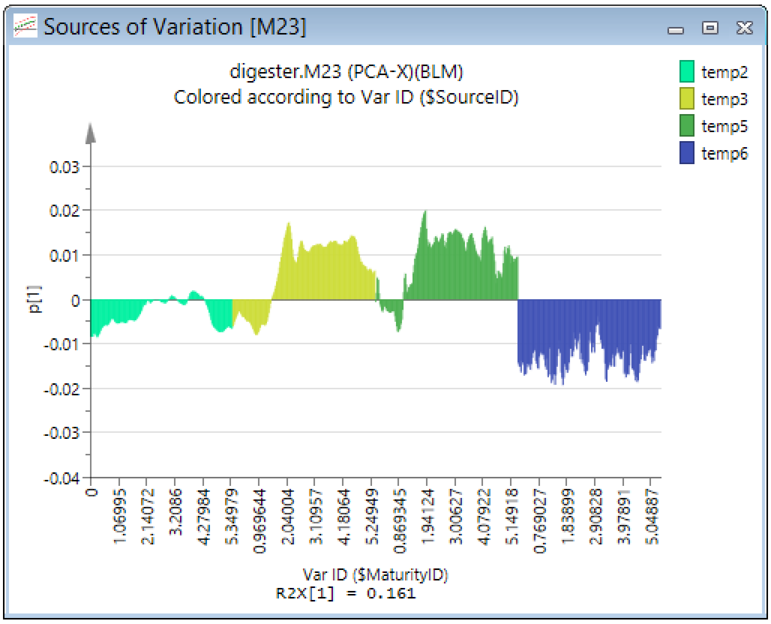
To switch the Sources of variation plot to a column plot, on the **Tools** tab, click **Change type** | **Column**. A normal loading plot can always be created from the **Loading** plot gallery, in the **Diagnostics & interpretation** group on the **Home** tab, by selecting one of the standard options.

Contribution plots in column form may be selected on the **Marked items** tab, in the **Drill down** group, by clicking **Column** in the comparison plot gallery.

9.5.2 BLM loading and contribution plots example

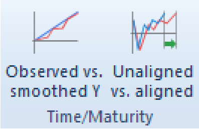
How to change between a Sources of variation plot and a column plot is described in the table. This example uses a loading plot, but is applicable for contribution plots as well.

Step	Illustration/description
1. On the **Home** tab, click **Loadings**.	 For a PCA loading sources of variation plot, the main systematic variation over time in the data for the selected variables is displayed. For a PLS/OPLS/O2PLS loading sources of variation plot, the variable loading over time, i.e. the variation over time that is related to the Y-variable is displayed. In a contribution sources of variation plot, how the variables over time differ between the selected batch and the average batch is displayed.

Step	Illustration/description
2. To transform to the column plot, on the **Tools** tab, click **Change type | Column**.	 Sources of Variation [M23] digester.M23 (PCA-X)(BLM) Colored according to Var ID ($SourceID) temp2 temp3 temp5 temp6 p[1] 0.03 0.02 0.01 0 -0.01 -0.02 -0.03 -0.04 0 1.06995 2.14072 3.2086 4.27984 5.34979 0.969644 2.04004 3.10957 4.18064 5.24949 0.869345 1.94124 3.00627 4.07922 5.14918 0.769027 1.83899 2.90828 3.97891 5.04887 Var ID ($MaturityID) R2X[1] = 0.161
3. To transform to the Sources of variation plot (from the column plot), on the **Tools** tab, in the **Create** group, click **Sources of variation**.	
4. To switch phases or displayed variables in the contribution plot open **Properties** and: • click the desired phase in the **Select phase** box. • add to the **Selected** list the variables to display.	

9.6 Time/maturity group plots

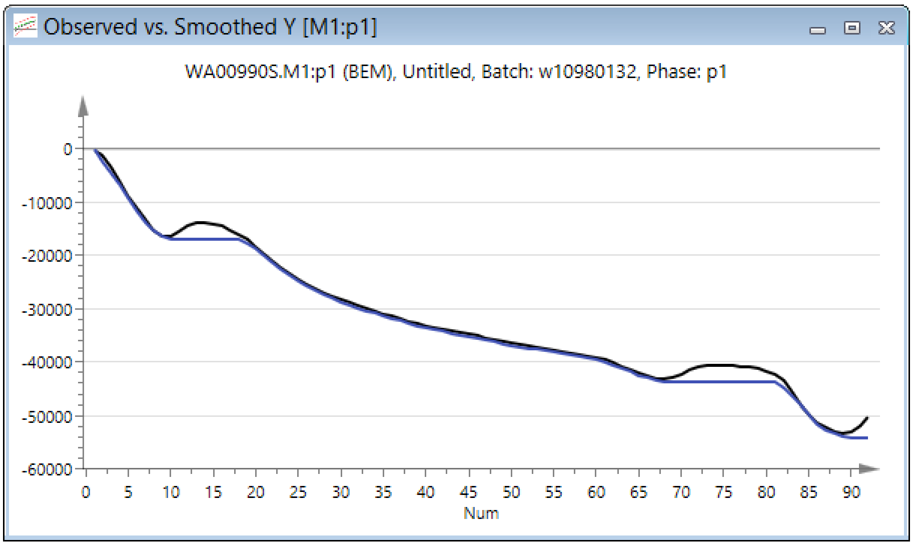
The two plots **Observed vs. smoothed Y** and **Unaligned vs. aligned** are found in the **Time/maturity** group on the **Batch** tab.



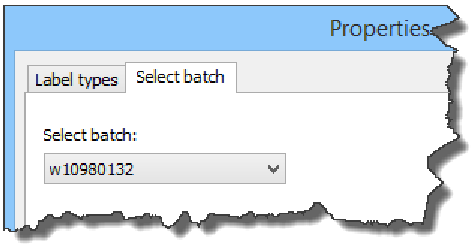
9.6.1 Observed vs. smoothed Y plot

The **Observed vs. Smoothed Y** plot displays the original maturity variable alongside the maturity variable as configured in the workset. This plot is displayed for each phase and is very illustrative when the maturity variable has been smoothed.

To open the **Observed vs. Smoothed Y** plot, click it in the **Time/maturity** group on the **Batch** tab.



Use **Properties** to select a different batch.



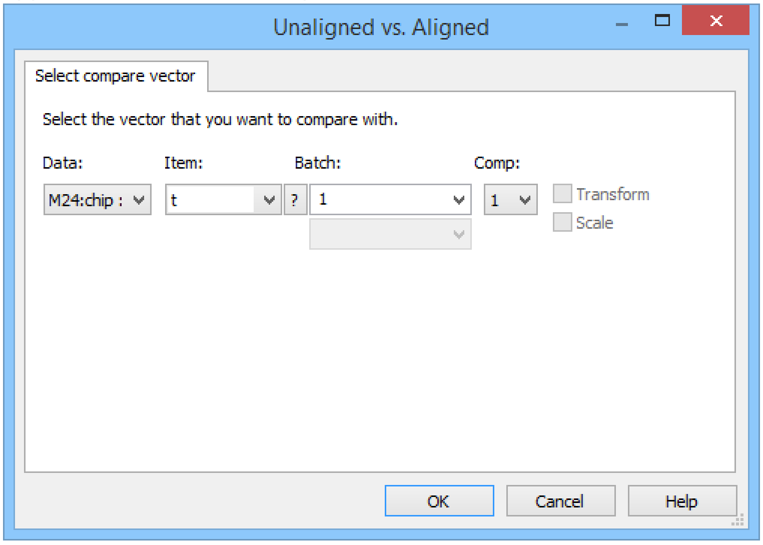
Select batch:

w10980132

9.6.2 Unaligned vs. aligned plot

To visualize the alignment of batches, i.e., how much a batch was stretched or shrunk to the median length of the workset batches:

1. On the **Batch** tab, in the **Time/maturity** group click **Unaligned vs. aligned Plot**.
2. In the dialog select the model in the **Data** box, vector in the **Item** box, and batch in the **Batch** box, and when applicable variable and component. Click **OK**.



Select the vector that you want to compare with.

Data: M24:chip :

Item: t

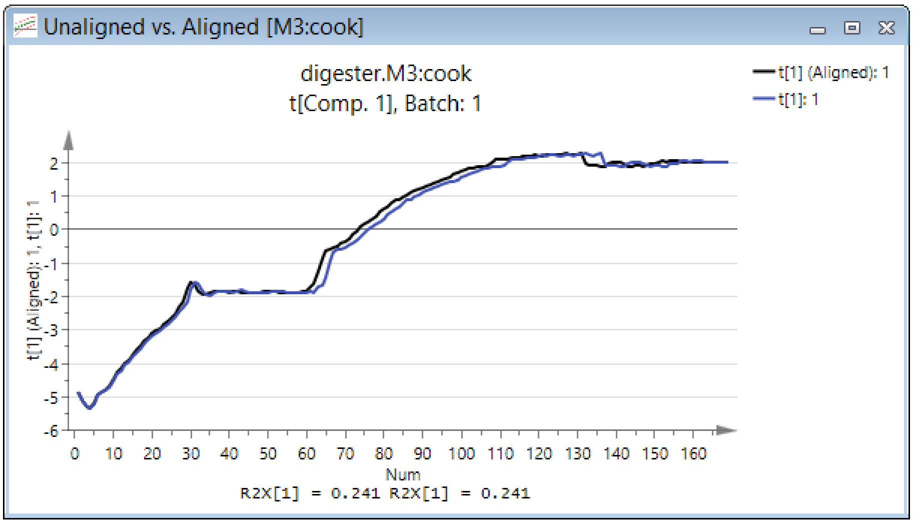
Batch: 1

Comp: 1

□ Transform

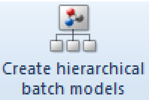
□ Scale

The resulting plot displays how well the aligned line follows the unaligned line.



9.7 Creating hierarchical models for batch level datasets

When there are batch level datasets (BL DS) present, hierarchical batch models can automatically be created by clicking **Create hierarchical batch models** in the **Dataset** group on the **Batch** tab.



The types of hierarchical base models possible are:

- One model for each phase and component – available when the variables in the BL DS are scores and the BEM has phases.
- One model for each component – available when the variables in the BL DS are scores but the BEM has no phases.
- One model for each phase in the BEM – available when the BEM has phases.
- Sequential models covering a part of completion of the batches – available when the BEM does not have phases.

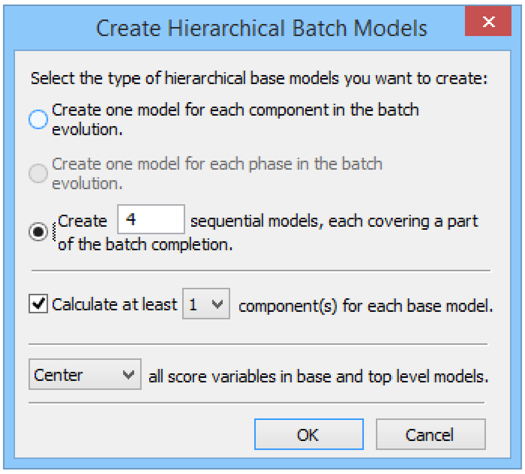
When there are more than one BL DS, a dialog allowing you to select which datasets to use is opened.

Note: You can only select datasets created from the same BEM.

9.7.1 Create Hierarchical Batch Models dialog

The **Create Hierarchical Batch Models** dialog has two interfaces, one where the BEM that the BL DS was created from has 2 or more phases and one where the BEM has one or no phases.

The interface with one or no phases:



Create Hierarchical Batch Models

Select the type of hierarchical base models you want to create:

○ Create one model for each component in the batch evolution.

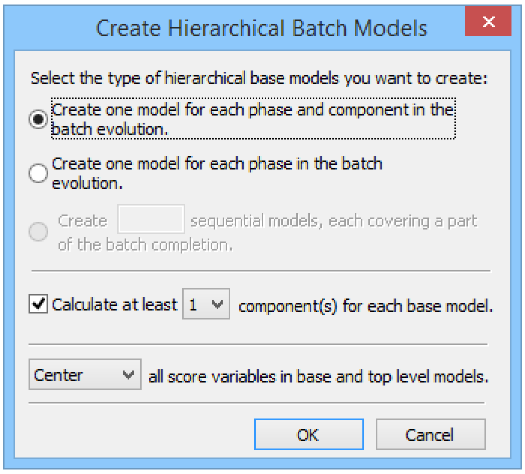
○ Create one model for each phase in the batch evolution.

● Create 4 sequential models, each covering a part of the batch completion.

☑ Calculate at least 1 component(s) for each base model.

Center all score variables in base and top level models.

The interface with two or more phases:



Create Hierarchical Batch Models

Select the type of hierarchical base models you want to create:

● Create one model for each phase and component in the batch evolution.

○ Create one model for each phase in the batch evolution.

○ Create ▭ sequential models, each covering a part of the batch completion.

☑ Calculate at least 1 component(s) for each base model.

Center all score variables in base and top level models.

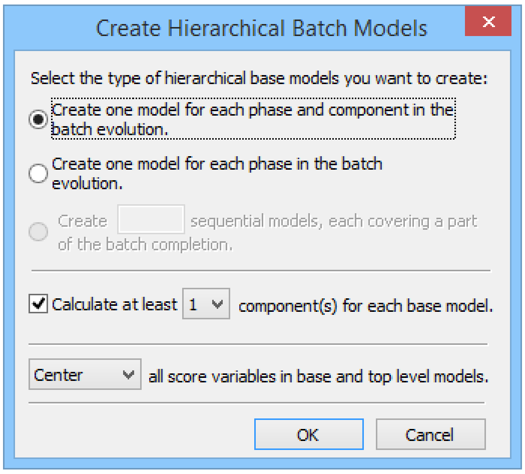
When creating the hierarchical batch models, the following options are always available:

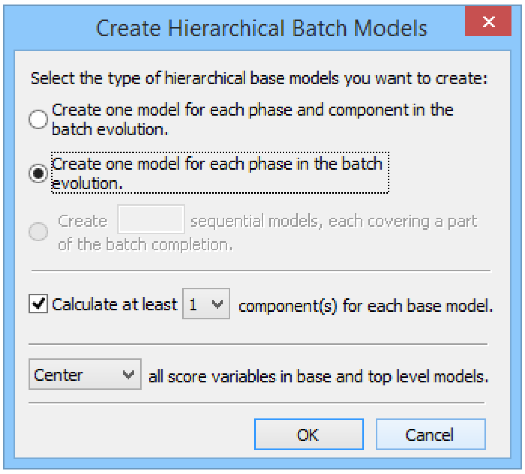
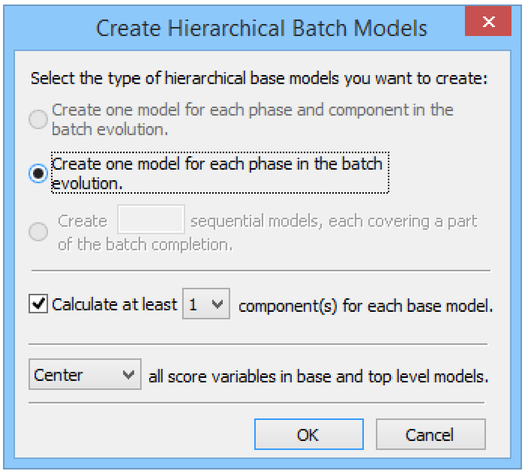
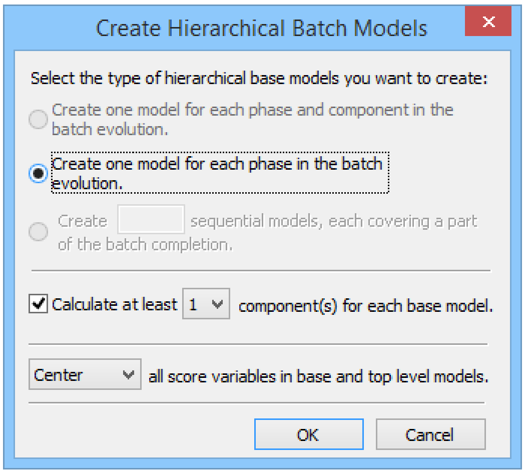
- **Calculate at least x component(s) for each base model**. This option forces extraction of x components when possible.
- **Center/UV scale all score variables in base and top level models**. The default is **Center**. Selecting **UV scale** scales all score variables in the base model, if there are score variables, to unit variance, leaving all other variables **Center** scaled. Also all top level model score variables are scaled to unit variance when **UV scale** is selected.

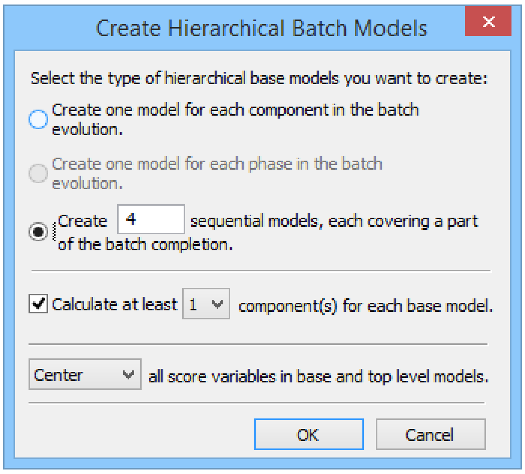
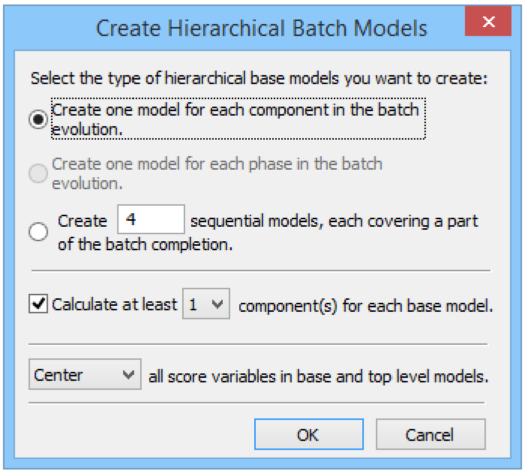
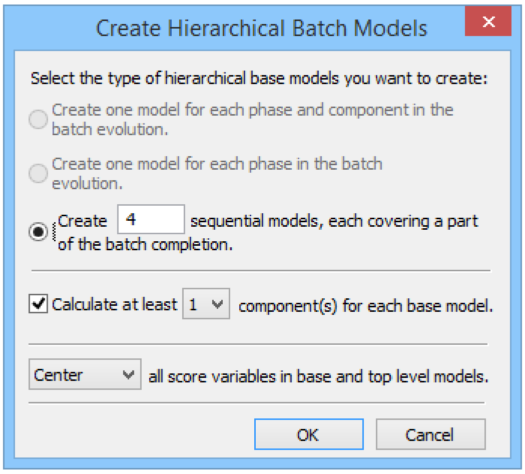
Note: The selection of Center or UV scale only affects the default scaling of the score variables. All other variables are default scaled to unit variance.

9.7.2 Create hierarchical batch models results

The resulting models from a few examples of using **Create hierarchical batch models** are described in the table:

Characteristics	Dialog settings	Description of resulting models
1. 5 phases in the BEM, each with two components. BL DS from scores.	 Create Hierarchical Batch Models Select the type of hierarchical base models you want to create: ● Create one model for each phase and component in the batch evolution. ○ Create one model for each phase in the batch evolution. ○ Create ▭ sequential models, each covering a part of the batch completion. ☑ Calculate at least 1 component(s) for each base model. Center all score variables in base and top level models. 	10 autofitted (but at least one component) base models – one for each phase and component – with all variables scaled Ctr. The variables included in each base model are the score variables related to each phase and component. One hierarchical top model holding the hierarchical score variables scaled Ctr.

Characteristics	Dialog settings	Description of resulting models
2. 5 phases in the BEM, each with two components. BL DS from scores.	 Create Hierarchical Batch Models Select the type of hierarchical base models you want to create: ○ Create one model for each phase and component in the batch evolution. ● Create one model for each phase in the batch evolution. ○ Create sequential models, each covering a part of the batch completion. ☑ Calculate at least 1 component(s) for each base model. Center all score variables in base and top level models. 	5 autofitted (but at least two components) base models – one for each phase – with all variables scaled UV. The variables included in each base model are the score variables. One hierarchical top model holding the hierarchical score variables all scaled UV.
3. 5 phases in the BEM, each with two components. BL DS from raw (original) data.	 Create Hierarchical Batch Models Select the type of hierarchical base models you want to create: ○ Create one model for each phase and component in the batch evolution. ● Create one model for each phase in the batch evolution. ○ Create sequential models, each covering a part of the batch completion. ☑ Calculate at least 1 component(s) for each base model. Center all score variables in base and top level models. 	5 autofitted base models – one for each phase – with all variables scaled UV. The variables included in each base model are the original variables. One hierarchical top model holding the hierarchical score variables scaled Ctr.
4. 5 phases in BEM, each with two components. BL DS from raw data statistics.	 Create Hierarchical Batch Models Select the type of hierarchical base models you want to create: ○ Create one model for each phase and component in the batch evolution. ● Create one model for each phase in the batch evolution. ○ Create sequential models, each covering a part of the batch completion. ☑ Calculate at least 1 component(s) for each base model. Center all score variables in base and top level models. 	5 autofitted base models – one for each phase – with all variables scaled UV. The variables included in each base model are the statistics variables. One hierarchical top model holding the hierarchical score variables scaled Ctr.

Characteristics	Dialog settings	Description of resulting models
5. No phases in the BEM, two components. BL DS from scores.	 Create Hierarchical Batch Models Select the type of hierarchical base models you want to create: ○ Create one model for each component in the batch evolution. ○ Create one model for each phase in the batch evolution. ● Create 4 sequential models, each covering a part of the batch completion. ☑ Calculate at least 1 component(s) for each base model. Center all score variables in base and top level models. OK Cancel	4 autofitted (but at least one component) models – each covering 25% of the batch completion according to the maturity. The first model covers 0-25%, the second 25%-50% etc. The base model variables are scaled UV. One hierarchical top model holding the hierarchical scores scaled UV.
6. No phases in the BEM, two components. BL DS from scores.	 Create Hierarchical Batch Models Select the type of hierarchical base models you want to create: ● Create one model for each component in the batch evolution. ○ Create one model for each phase in the batch evolution. ○ Create 4 sequential models, each covering a part of the batch completion. ☑ Calculate at least 1 component(s) for each base model. Center all score variables in base and top level models. OK Cancel	2 autofitted base models – one for each component. The variables included in each base model are the score variables. All score variables in the base and top models are Ctr scaled.
7. No phases in the BEM, two components. BL DS from raw (original) data.	 Create Hierarchical Batch Models Select the type of hierarchical base models you want to create: ○ Create one model for each phase and component in the batch evolution. ○ Create one model for each phase in the batch evolution. ● Create 4 sequential models, each covering a part of the batch completion. ☑ Calculate at least 1 component(s) for each base model. Center all score variables in base and top level models. OK Cancel	4 autofitted (but at least one component) models – each covering 25% of the batch completion according to the maturity. The first model covers 0-25%, the second 25%-50% etc. All variables in the base model are UV scaled. One hierarchical top model holding the hierarchical score variables scaled Ctr.
8. No phases in the BEM, two components. BL DS from only raw data statistics variables.	No hierarchical batch models can be created since there are: 1. No score variables. 2. No phases. 3. No components related to the batch level variables 4. No maturity variable to create sequential models.	

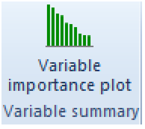
9.7.3 Hierarchical top level model

All the hierarchical base models are fitted while the hierarchical top level model is created using the scores of the base models. This last model is unfitted for editing of the model by for instance including other variables, such as quality variables as Y.

Note: Changing the order of the included datasets resets the default workset resulting in that centering, if default done by SIMCA, must be redone manually.

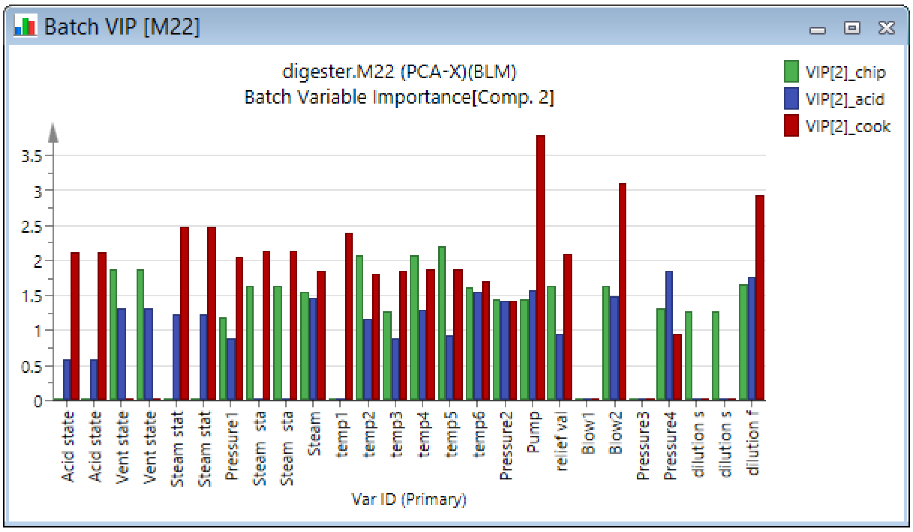
9.8 Batch Variable importance plot

The **Variable Importance Plot** (also named **Batch VIP**), available for batch level models created from a scores dataset, displays the overall importance of the variable over the whole evolution on the final quality of the batch. With phases, the plot displays the importance of a variable by phase. With a PLS model, the **Batch VIP** displays one plot for each y-variable with a column per selected phase.



To open the plot:

1. On the **Batch** tab, in the **Variable summary** group, click **Variable importance plot**.
2. In the **Batch Variable Importance** dialog, select the phases for which to display the Batch VIP. With no phases, the Batch VIP is displayed for the BEM used to create the batch level dataset the model was built on.
3. Click **OK**.



Note: The Variable importance plot, Batch VIP, is only available when scores in the scores BL DS are selected as X in the BLM.

10Analyze

10.1 Introduction

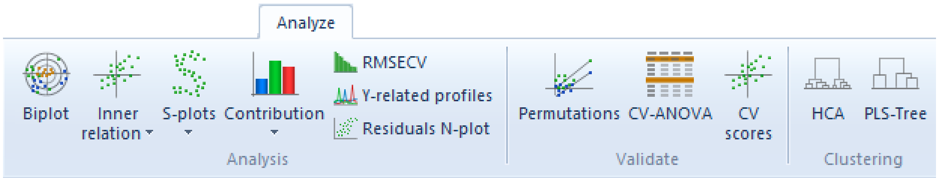
This chapter describes all commands on the **Analyze** tab.

The **Analyze** tab displays the analysis features not common enough to end up on the **Home** tab.

Content

The following commands are available on the **Analyze** tab:

1. Biplot to display the scores and loadings in the same plot.
2. Inner relation to illustrate the goodness of fit.
3. S-plots to display the S-plot, S-line or SUS Plot.
4. Contribution plots to display the influence on each variable when comparing a point or group of points with the center, another point, or a group of points.
5. RMSECV to indicate predictive power.
6. Y-related profiles to display the pure profiles of the underlying spectrum for OPLS and O2PLS models.
7. Residuals N-plot to display the residuals on a normal probability scale.
8. Permutations to display a measure of the overfit.
9. CV-ANOVA to display the cross validated ANOVA table.
10. CV scores to display a cross validated complement to the regular score plot.
11. HCA for cluster analysis.
12. PLS-Tree for cluster analysis highlighting subgroup formations in latent variables.



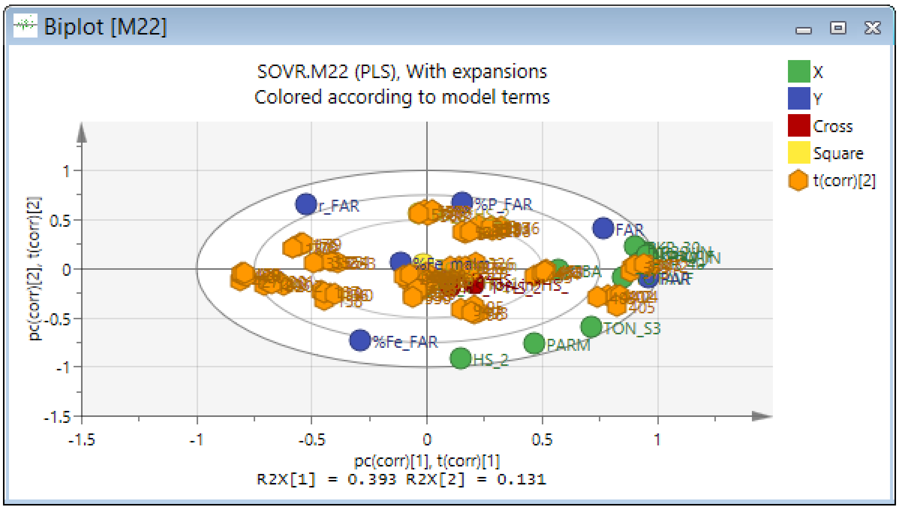
10.2 Biplot

The loading vectors p, c and pc and the score vector t can be displayed **Correlation scaled** leading to the vectors p(corr), c(corr), pc(corr) and t(corr). Additionally poso and pq for OPLS and O2PLS can be displayed correlation scaled, poso(corr) and pq(corr). The selected correlation scaled loading vector can be displayed together with the correlation scaled score vector in a **Biplot** where all points end up inside the correlation circle of radius 1.

Open the plot by clicking **Biplot** in the **Analysis** group on the **Analyze** tab. The **Biplot** is available for all fit methods.

Note: The weights w and w*, cannot be displayed as correlations, as the u vectors are not orthogonal.

In the **Biplot** here pc(corr) and t(corr) are displayed for the first and second components.



The default coloring for the loading vector is by **Terms** and is found in the **Color** tab in the **Properties** dialog. For coloring of the score vector an additional tab **Score color** is available. For details about coloring see the Coloring from Properties subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs.

In the **Properties** dialog, in addition to the **Label types** tab referring to the labels on the loading vectors, there is a **Score labels** tab which refers to the labels on the scores. The default is to not display labels on the observations.

10.2.1 Colors in the Biplot

In the **Biplot**, the different points are by default colored by **Terms** coloring x-variables, y-variables, cross, square, cubic, lags and observations in different colors.

The color scheme is the same as for the regular loadings scatter plot.

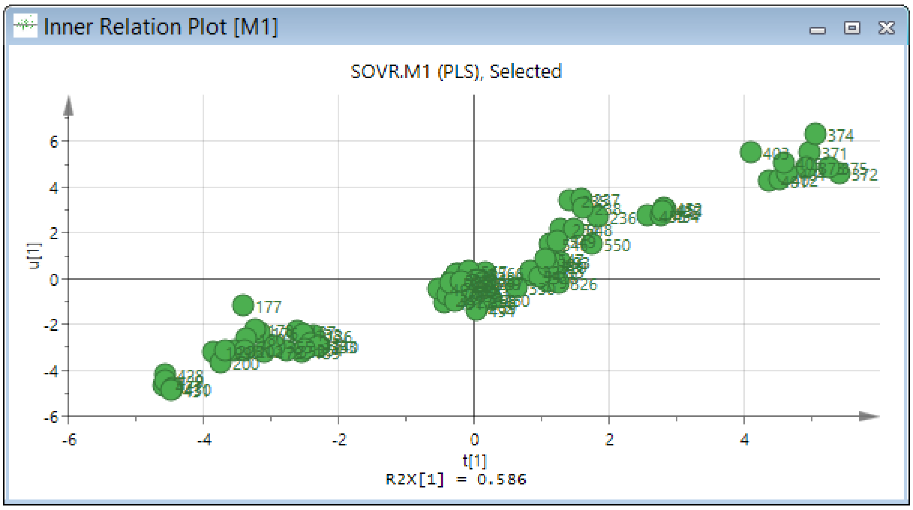
The colors and symbols can be changed in the **Format Plot** dialog, **Styles** node.

10.3 Inner relation plot

For a PLS model the Y space can be explored by plotting u1 vs. u2 and interpreting it in the same way as the t1 vs. t2 plot.

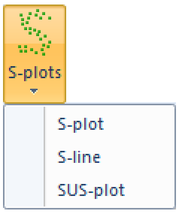
When plotting a t vector vs. a u vector for the same component, the goodness of the fit is illustrated.

Open the plot by clicking **Inner relation** in the **Analysis** group on the **Analyze** tab.



10.4 S-plots

S-plots menu holds the three plots: **S-plot**, **S-line** and **SUS-plot**.

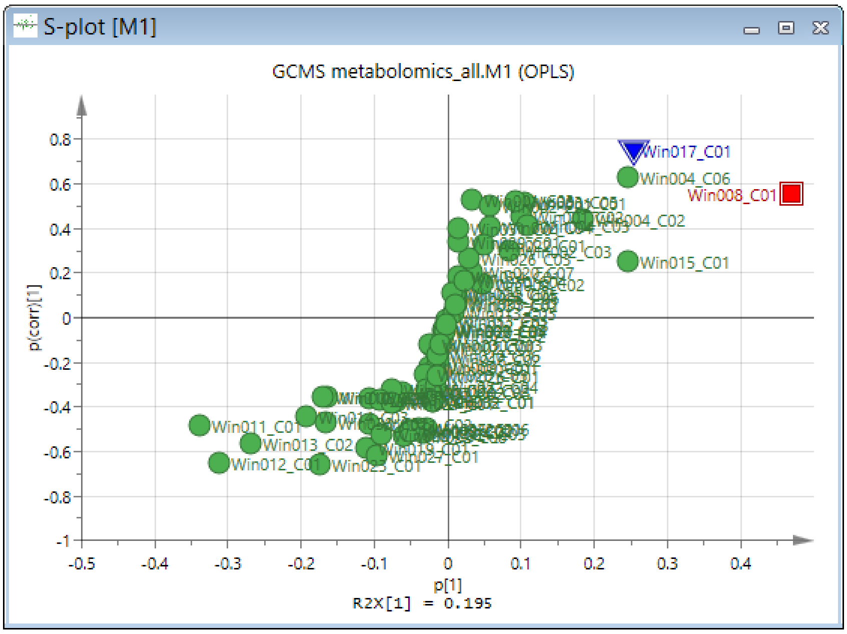


The S-plots provide visualization of the OPLS/OPLS-DA predictive component loading to facilitate model interpretation. The plots are only available for OPLS models with one y-variable and OPLS-DA models with two classes.

10.4.1 S-plot

The **S-plot**™ is used to visualize both the covariance and the correlation structure between the X-variables and the predictive score t[1]. Thus, the S-plot is a scatter plot of the p[1] vs p(corr)[1] vectors of the predictive component [Wiklund, et al., Analytical Chemistry, 2008]. With Pareto and Ctr scaling this plot often takes the shape of the letter 'S'. X-variables situated far out on the wings of the S combine high model influence with high reliability and are of relevance in the search for e.g. biomarkers that are up- or downregulated.

In the example below, the triangle has a high p(corr) which means a very high reliability while the square has a high model influence partly due to its high variance in the dataset.

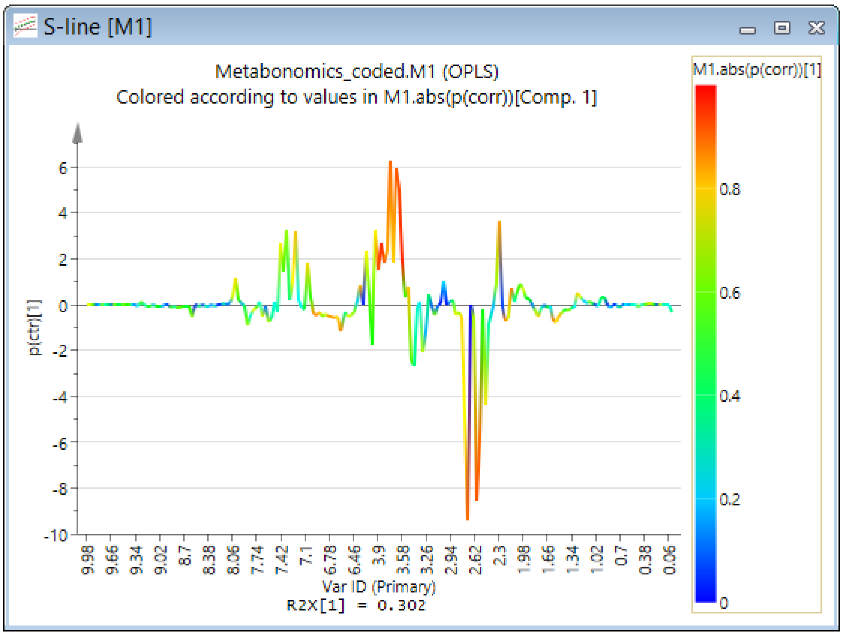


10.4.2 S-line plot

The **S-line** plot is tailor-made for NMR spectroscopy data. It visualizes the p(ctr)[1] loading colored according to the absolute value of the correlation loading, p(corr)[1]. Thus, the S-line plot is conceptually similar to the STOCSY™ plot pioneered by the Nicholson group at Imperial College, London, UK [Cloarec, et al., Analytical Chemistry, 2005]. However, it should be noted that the coloring principle is slightly different between the two plots.

The plot below displays the predictive loading in a form resembling the original spectra, colored according to p(corr). The top end of the color scale visualizes the NMR shifts that influence the separation of the groups.

Figure. The S-line for an OPLS-DA model.

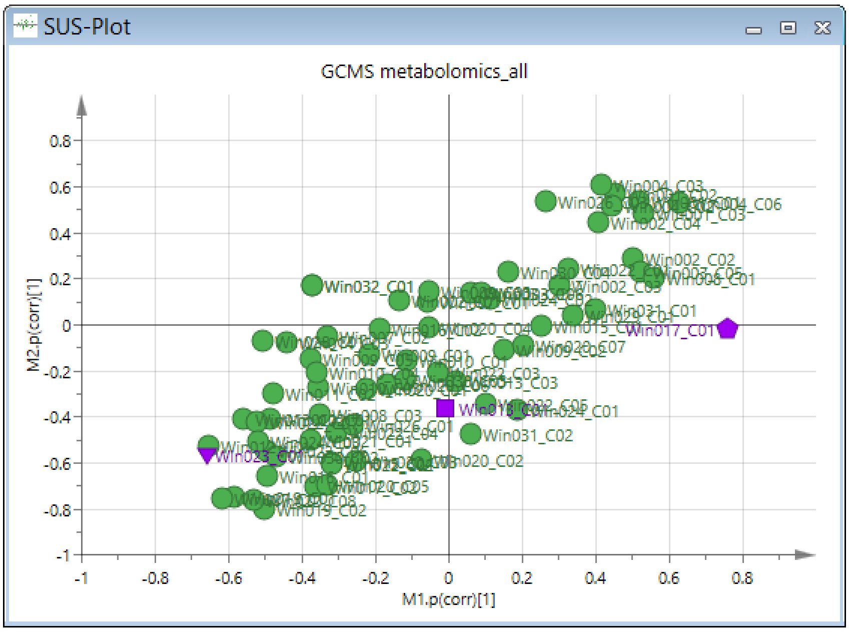


10.4.3 SUS-plot

The **SUS-Plot** is a scatter plot of the p(corr)[1] vector from two separate OPLS models [Wiklund, et al., 2008]. If two OPLS models have similar profiles (they capture similar relationships between the X-variables and the single Y-variable) the X-variables will line up along the diagonal running from the lower left corner to the upper right corner. Such variables represent the Shared structure among the two compared OPLS models. Conversely, X-variables that are not located along this thought diagonal, e.g. in the upper left corner, represent structures that are Unique to either of the two models compared.

SUS is an acronym for Shared and Unique Structures.

In the plot below, in the lower left corner, the variable with plot mark triangle is a *Shared* variable. It has a negative correlation of the same size in both models meaning that it is down regulated, i.e. lower in the genetically modified samples compared with the control in both models. The square (at 6 o'clock) is a Unique variable for M2 as the p(corr) for M1 is 0. The opposite is true for the pentagon variable which is *Unique* for M1 and has a p(corr) close to 0 for M2.

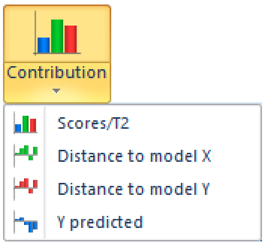


10.5 Contribution plots

Contribution plots are used to understand why an observation differs from the others in an X score (t), in DModX, in DModY, in Hotelling's T2Range, or in the observed vs. predicted Y plot.

The contribution plot displays the differences, in scaled units, for all the terms in the model, between the outlying observation and the normal (or average) observation, multiplied by the absolute value of the normalized weight.

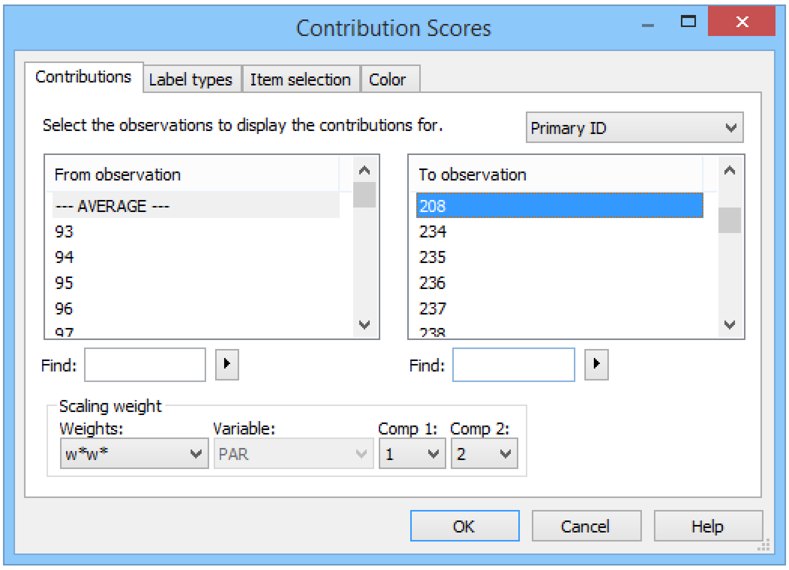
Contribution plots for the model can be displayed from plots or by clicking **Contribution**, in the **Analysis** group, on the **Analyze** tab.



For batch level models, it is often useful to display the variation of a variable from a selected phase in a contribution plot, as a line plot over time, rather than a column plot at every time point. Therefore the **Sources of Variation Plot** is by default displayed when creating the contribution plot from a plot when the BLM was created from scores or original data. For more, see the Sources of variation plot subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs.

10.5.1 Scores/T2 contribution plot

To create the score contribution plot using the ribbon, on the **Analyze** tab, in the **Analysis** group, click **Contribution | Scores/T2**. The **Contribution Scores** dialog opens:



Select the observations to display the contributions for. Primary ID

From observation	To observation
--- AVERAGE ---	208
93	234
94	235
95	236
96	237
97	238

Find:

Find:

Scaling weight

Weights: w*w*

Variable: PAR

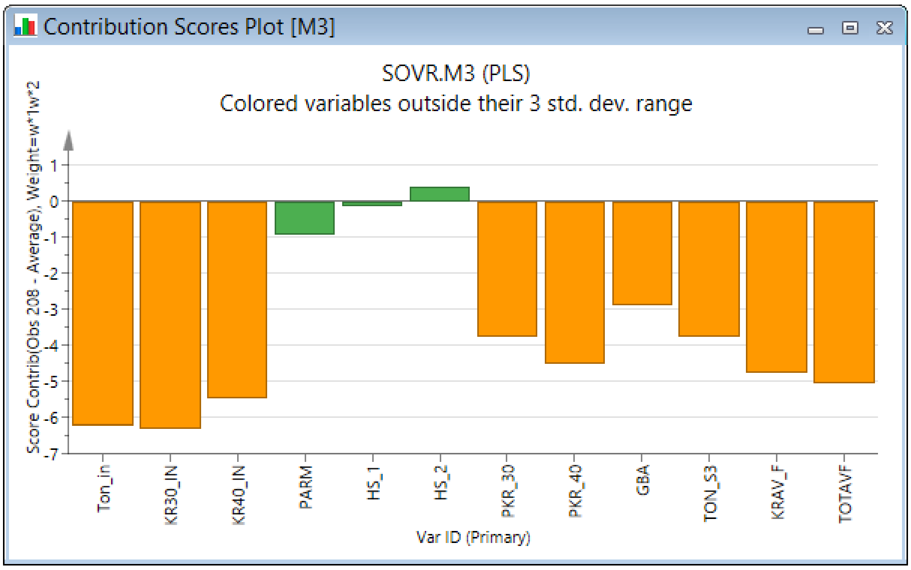
Comp 1: 1

Comp 2: 2

In the dialog:

1. Select the ID to display in the box positioned top right.
2. Select the observation ID of a normal observation, a group of observations, or **AVERAGE** in the **From observation** list. When selecting **AVERAGE**, this corresponds to a hypothetical observation with all its elements equal to the variable means.
3. Select the observation ID of the suspect observation or group of suspect observations in the **To observation** list.
4. Select the weight parameter in the **Weights** box. If the point is outside in only one dimension, select a single weight.
5. Select the dimension of the scores of the outlying observation in the **Comp 1** box and, if applicable, in the **Comp 2** box.

For details about the **Find** feature, see the Find feature in workset dialog subsection in the Workset section in Chapter 7, Home.


Contribution Scores Plot [M3]
SOVR.M3 (PLS)
Colored variables outside their 3 std. dev. range
Score Contrib(Obs 208 - Average), Weight=w*1w*2
1
0
-1
-2
-3
-4
-5
-6
-7
Ton_in
KR30_IN
KR40_IN
PARM
HS_1
HS_2
PKR_30
PKR_40
GBA
TON_S3
KRAV_F
TOTAVF
Var ID (Primary)

10.5.1.1 Weights available for Scores/T2 contribution

The following weights listed in the table are available in the **Weights** box.

Note: The absolute values for the weight vector are used.

Weight	Description
Raw	No weights are used. Displays the subtraction of the values in one observation minus the other in original units.
Normalized	No weights are used, but displayed in the units of the workset.
p	Using the selected dimension (of the outlying observation), the p loadings for that dimension are used as weights.
pp	Using the two selected dimensions (of the outlying observation), the corresponding linear combinations of the p vectors are used as weights.
PRange	Using all selected dimensions, the corresponding p vectors are used as weights, for OPLS including po vectors. Use this option for Hotelling's T2Range.
po	Using the selected dimension (of the outlying observation), the po loadings for that dimension are used as weights.
ppo	Using the selected dimension (of the outlying observation), the p and po loadings for that dimension are used as weights.
popo	Using the selected dimension (of the outlying observation), the po loadings for that dimension are used as weights.
w*	Using the selected dimension (of the outlying observation), the w* vector of that dimension is used as weights.
w*w*	Using the two selected dimensions (of the outlying observation), the corresponding linear combinations of the w* vectors are used as weights.
CoeffCS	The weights are the absolute values of the PLS scaled and centered regression coefficients, for the selected y-variable, after the selected dimension.
VIP	The weights are the VIP values after the selected component.
W*Range	Using all selected dimensions, the corresponding w* vectors are used as weights. Select this option for Hotelling's T2Range.
RX	The weights are the square root of the fraction of the Sum of Squares (SS) of every term explained by the model, after the selected dimension listed as R2VX(cum). PCA only.

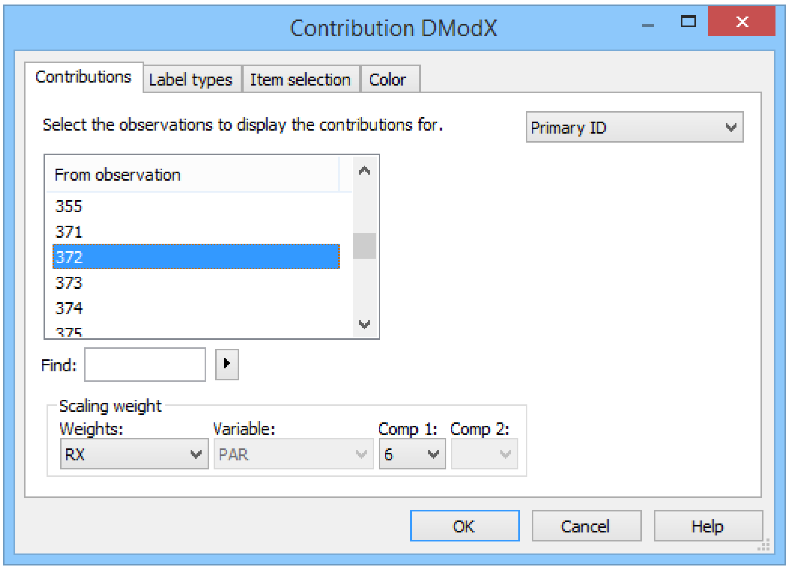
10.5.1.2 Hotelling's T2Range outlier

When an observation is an outlier in a Hotelling's T2Range plot, use **Contribution Scores**, select **AVERAGE** in the **From observation** list and the suspect observation in the **To observation** list. Select the weights **PRange** for a PC model and **W*Range** for a PLS model. Select the range of the Hotelling's T2Range plot and click **OK**.

Note: Group contribution is not available from the Hotelling's T2Range plot.

10.5.2 Distance to model X contribution plot

To create the DModX contribution plot using the ribbon, on the **Analyze** tab, in the **Analysis** group, click **Contribution | Distance to model X**. The **Contribution DModX** dialog opens:



Contribution DModX

Select the observations to display the contributions for.

Primary ID

From observation: 355, 371, 372 (selected), 373, 374, 375

Find:

Scaling weight

Weights: RX

Variable: PAR

Comp 1: 6

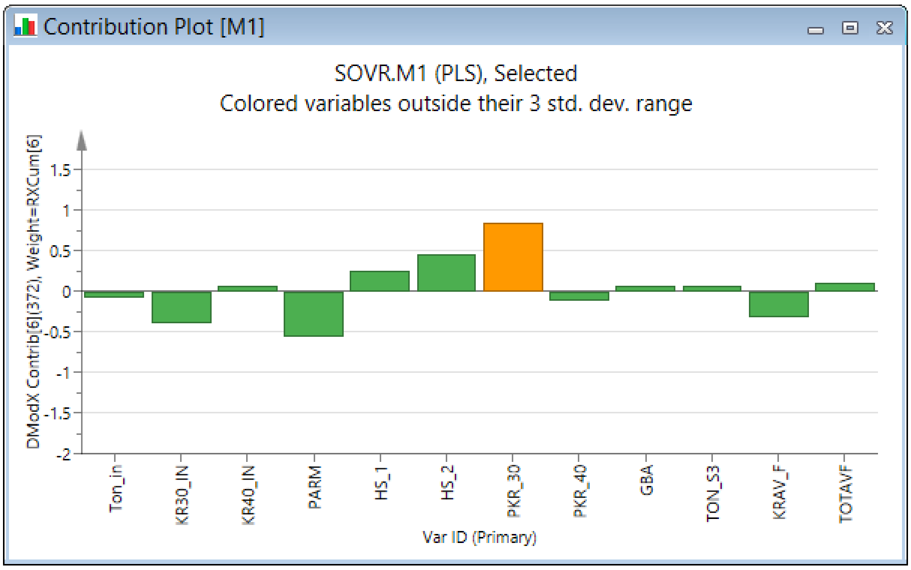
Comp 2:

In the dialog:

1. Select the ID to display in the box positioned top right.
2. Select the observation ID of the observation(s) with a large DModX in the list.
3. Select the weight parameter in the **Weights** box.
4. With weight **RX**, select the number of components to use. Default is to use all components of the active model.

For details about the Find feature, see the Find feature in workset dialog subsection in Chapter 7, Home.

The **Contribution** plot displays the scaled residuals of every term in the model, for that observation multiplied by the absolute value of the weight parameter.



10.5.2.1 Weights available for DModX contribution

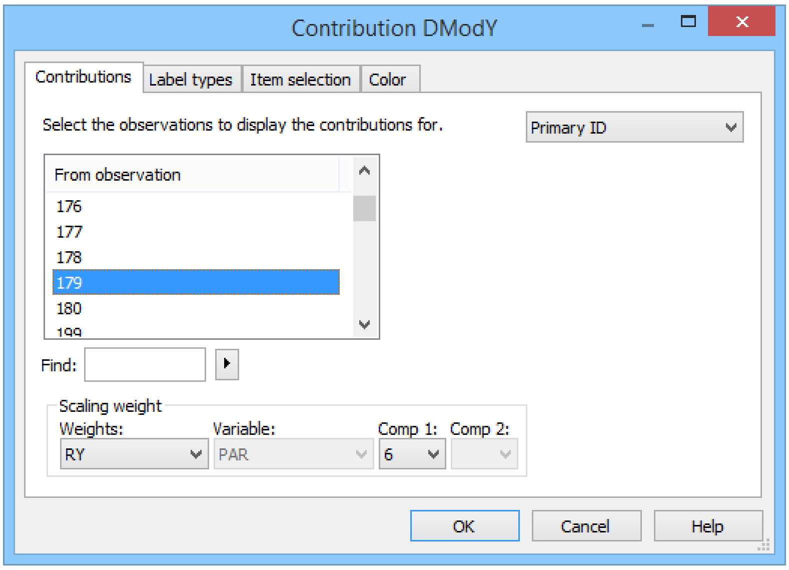
The following weights listed in the table are available in the **Weights** box.

Note: The absolute values for the weight vector are used.

Weight	Description
Normalized	No weights are used, but displayed in the units of the workset.
RX	The weights are the square root of the fraction of the Sum of Squares (SS) of every term explained by the model, after the selected dimension listed as R2VX(cum). This is the default.
CoeffCS	The weights are the absolute values of the PLS scaled and centered regression coefficients, for the selected y-variable, after the selected dimension.
VIP	The weights are the VIP values after the selected component.

10.5.3 Distance to model Y contribution plot

Create the DModY contribution plot using the ribbon, on the **Analyze** tab, in the **Analysis** group, click **Contribution | Distance to model Y**. The **Contribution DModY** dialog opens:



Contribution DModY

Contributions | Label types | Item selection | Color

Select the observations to display the contributions for.

Primary ID

From observation
176
177
178
179
180
199

Find:

Scaling weight
Weights: RY
Variable: PAR
Comp 1: 6
Comp 2:

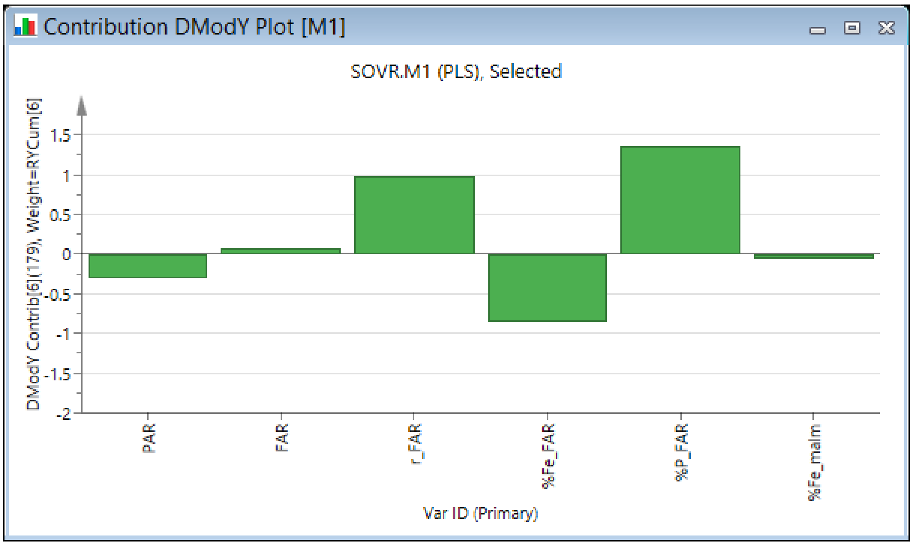
In the dialog:

1. Select the ID to display in the box positioned top right.

2. Select the observation ID of the observation(s) with a large DModY in the list.
3. Select the weight parameter in the **Weights** box.
4. With weight **RY**, select the number of components to use. Default is to use all components of the active model.

For details about the Find feature, see the Find feature in workset dialog subsection in Chapter 7, Home.

The contribution plot displays the Y scaled residuals for that observation multiplied by the absolute value of the weight parameter.



This plot is unavailable for PCA.

10.5.3.1 Weights available for DModY contribution

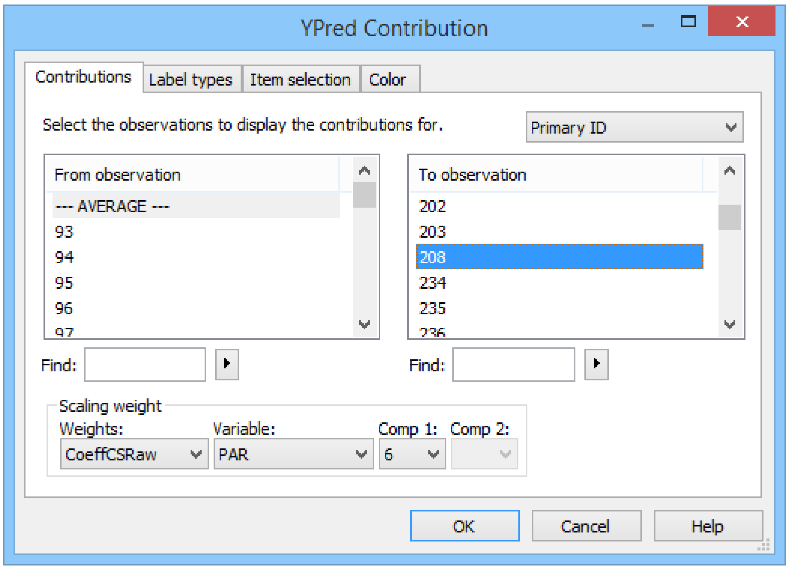
The following weights listed in the table are available in the **Weights** box.

Note: The absolute values for the weight vector are used.

Weight	Description
Normalized	No weights are used, but displayed in the units of the workset.
RY	The weights are the square roots of the fraction of the Sum of Squares (SS) of every Y explained by the model, after the selected dimension listed as R2VY(cum). This is the default

10.5.4 Y predicted contribution plot

Create the YPred contribution plot using the ribbon, on the **Analyze** tab, in the **Analysis** group, click **Contribution | Y predicted**. The **YPred Contribution** dialog opens:



YPred Contribution

Select the observations to display the contributions for. Primary ID

From observation: --- AVERAGE ---, 93, 94, 95, 96, 97

To observation: 202, 203, 208 (selected), 234, 235, 236

Find:

Find:

Scaling weight

Weights: CoeffCSRaw

Variable: PAR

Comp 1: 6

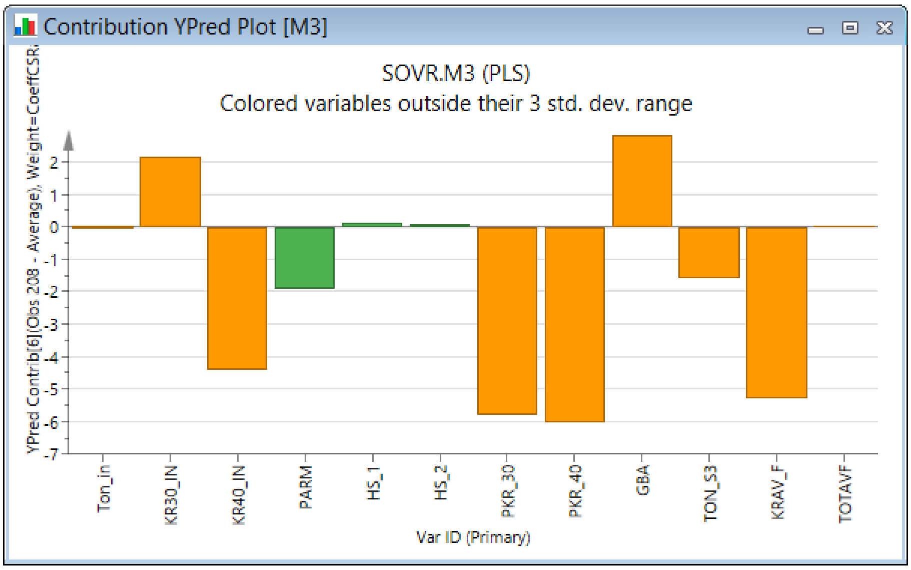
Comp 2:

In the dialog:

1. Select the ID to display in the box positioned top right.
2. Select the observation ID of a normal observation, group of observations, or **AVERAGE** in the **From Observation** list. When selecting **AVERAGE**, this corresponds to a hypothetical observation with all its elements equal to the variable means.
3. Select the observation ID of the suspect observation or group of observations in the **To Observation** list.
4. Select the weight parameter in the **Weights** box. There is one weight: **CoeffCSRaw**.
5. Select the y-variable the observation is an outlier for in the **Variable** box and the number of components to use in the **Comp 1** box.

For details about the Find feature, see the Find feature in workset dialog subsection in Chapter 7, Home.

The **Contribution** plot displays the differences, in scaled units, for all the terms in the model, between the deviating observation and the normal (or average) observation, multiplied by the normalized regression coefficient (Centered and Scaled) i.e., divided by the length of the coefficient vector (i.e. square root of sum of squares of the coefficients for all the terms in the model.)



In the contribution plot, the variables are colored orange if the original variable is outside the + 3 standard deviation limits for the investigated observations. To color outside 3 standard deviations is the default and changeable in Properties.

This plot is unavailable for PCA models.

10.5.4.1 Weights available for YPred contribution

The following weights listed in the table are available in the **Weights** box.

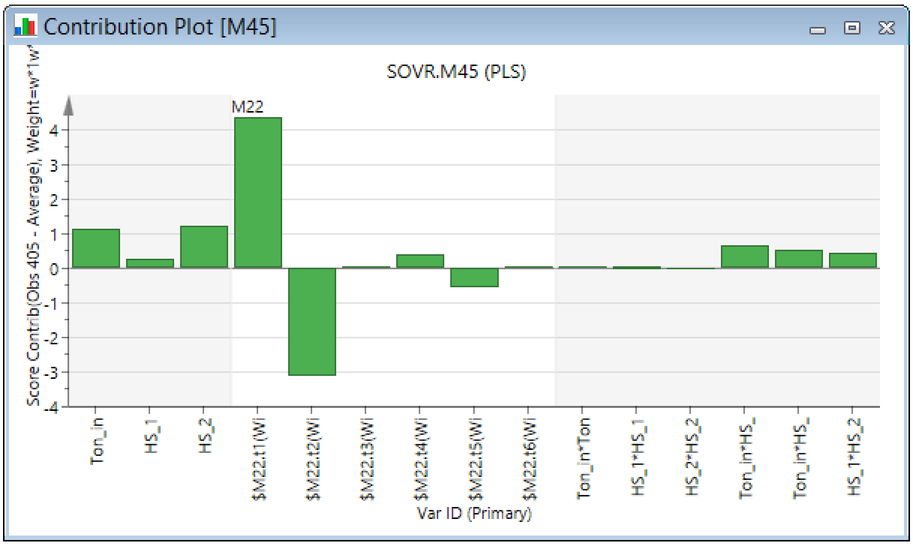
Note: The YPred contribution plot can only be created from menu. When creating contribution plots from observed vs. predicted plots the displayed plot is a Score contribution.

Weight	Description
CoeffCSRaw	The weights are the values of the scaled and centered regression coefficients, for the selected Y variable, after the selected dimension.

10.5.5 Contribution plot for hierarchical top level models

In hierarchical top models, the contribution plot refers to the top level variables, usually scores of base models. The background is shaded to separate variables from the different models.

For hierarchical top level models the **Contribution** plot displays the top level contributions. Double-click a variable to display the individual underlying variable contributions.



Hint: To line plot the hierarchical variable, mark it and click **Variable trend plot** on the **Marked items** tab.

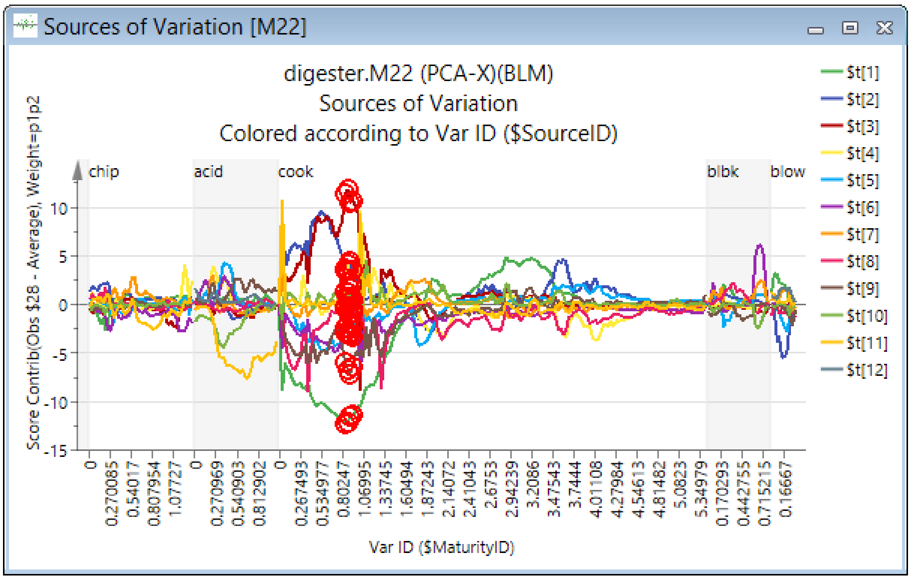
10.5.6 Combined contribution plot for batch level model

The combined contribution plot displays how the process variables contribute to an observed deviation of a batch or group of batches. The contribution value is an aggregate index across all selected time points or maturity values.

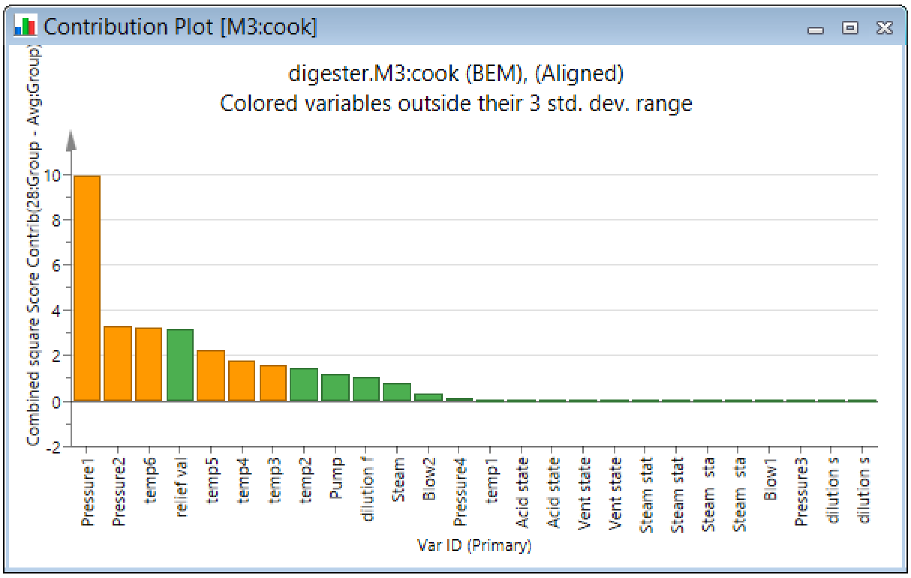
The combined contribution plot can only be created for batch level models created from *score variables*, by following the steps described:

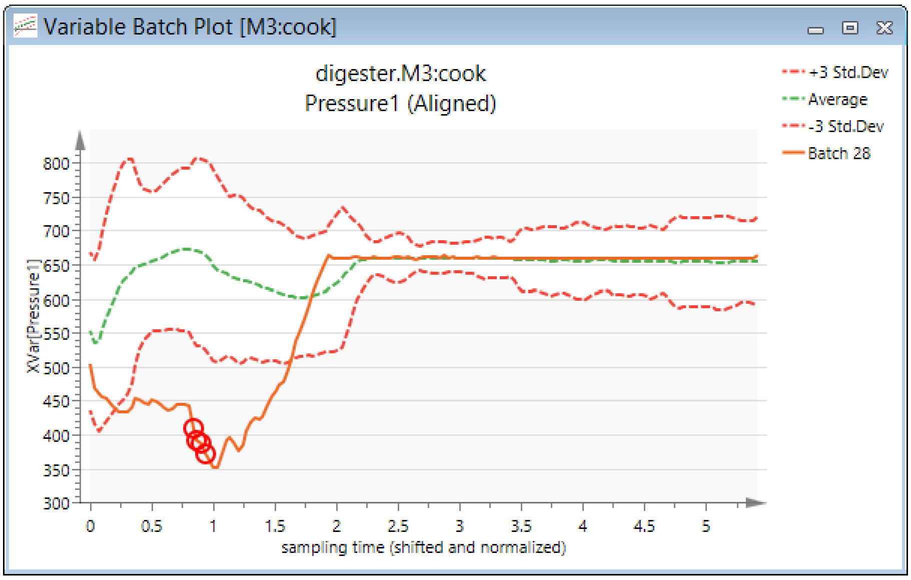
1. Open the contribution plot of interest.
2. Mark several score variables corresponding to the time period or maturity region of interest.
3. On the **Marked items** tab, in the **Drill down** group, click **Combined contribution**.

The Combined contribution plot is a sorted batch evolution contribution plot displaying original variables.



In the contribution plot, the variables are colored orange if the original variable is outside the + 3 standard deviation limits for the investigated observations. To color outside 3 standard deviations is the default and changeable in Properties.





10.5.7 Contribution plot from plot

Contribution plots can be created from plots displaying observations, that is, scores, Hotelling's T2Range, DModX, DModY, and Observed vs. Predicted plots.

To display a contribution plot not using the menus, use one of the following methods:

- Select the observations and click the relevant comparison plot in **Drill down** group on the **Marked items** tab.
- Double-click the point or column.
- Select the observations, right-click the selection, and click **Create | Contribution plot**.

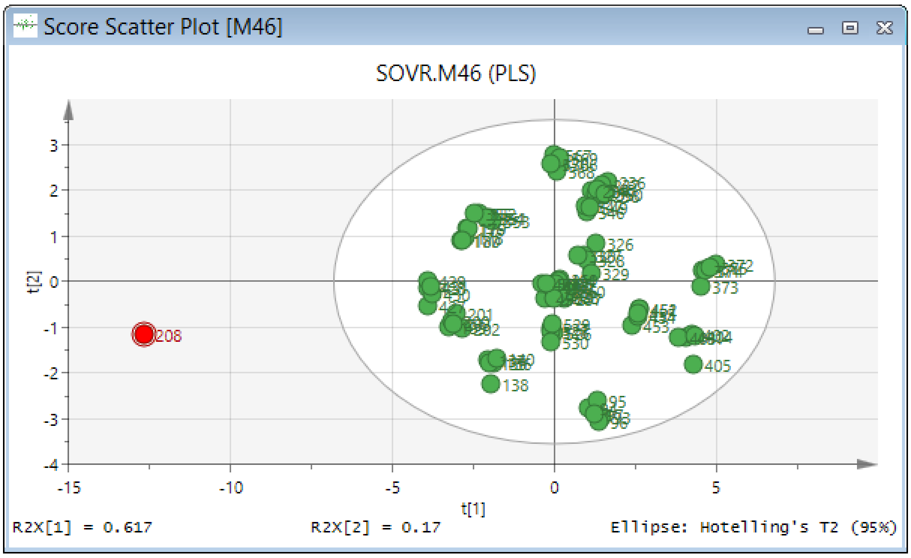
Note: Group contribution is not available from the Hotelling's T2Range plot.

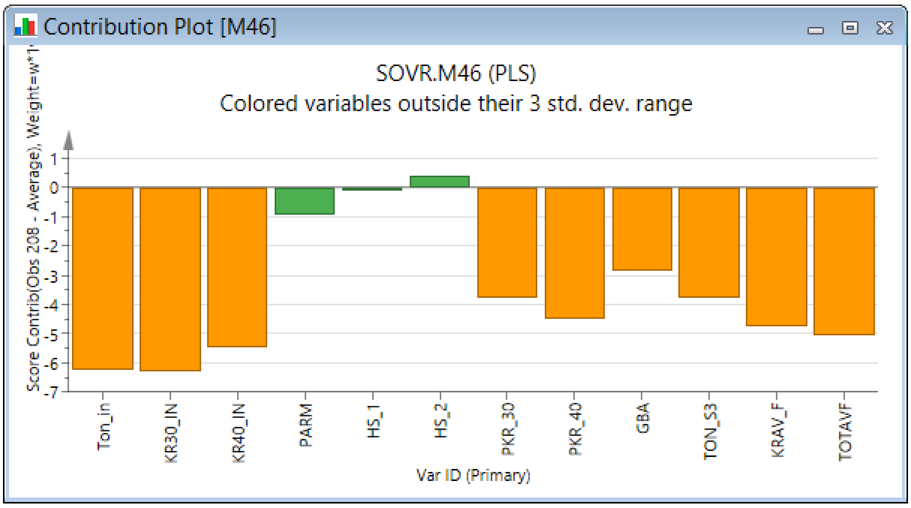
For more about the **Drill down** plots, see the Drill down group section in the Marked items tab section in Chapter 14, Plot and list contextual tabs.

10.5.7.1.1 Example of contribution plot directly from plot

In the example here, observation 208 was double-clicked in the score plot resulting in that the contribution plot comparing observation 208 to the average was displayed.

In the contribution plot, the variables are colored orange if the original variable is outside the ± 3 standard deviation limits for the investigated observations. To color outside 3 standard deviations is the default and changeable in Properties.

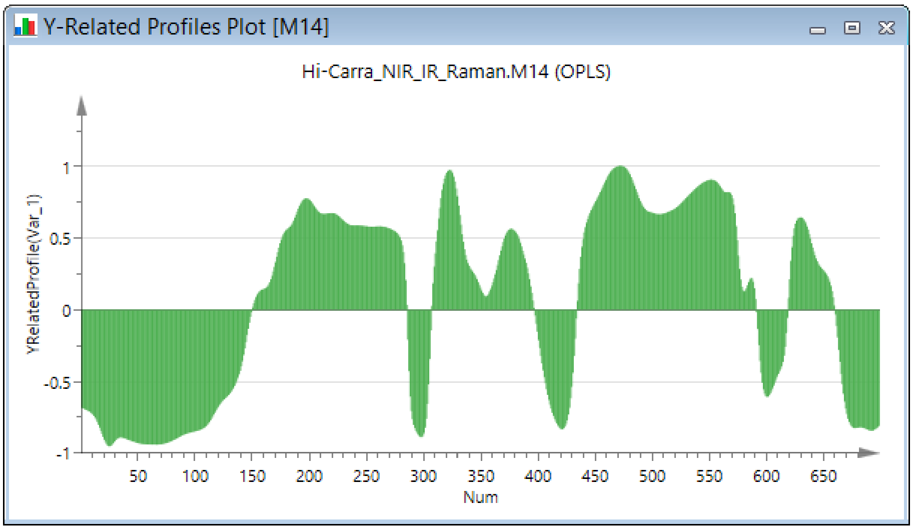




10.6 Coefficient Y-related profiles plot

When the fitted model is OPLS or O2PLS, the **Y-related profiles** plot can be displayed. The **Y-related profiles** are the coefficients rotated so that they display the pure profiles of the underlying constituents in X.

This plot is only available when the number of significant predictive components is equal to the number of y-variables.



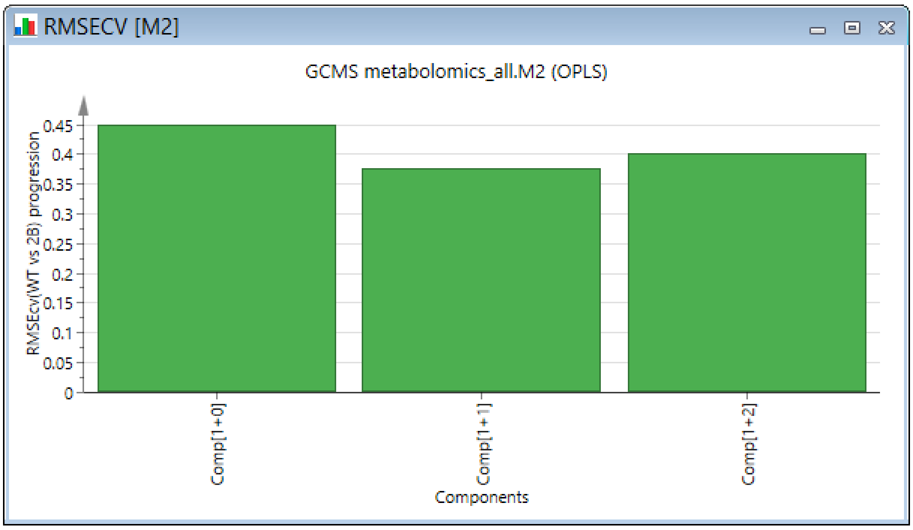
Y-related profiles is available in the **Analysis** group on the **Analyze** tab.

For more, see the OPLS/O2PLS - Orthogonal PLS modeling section in the Statistical appendix.

10.7 RMSECV plot

RMSECV can be regarded as an intermediary to RMSEE and RMSEP, as it applies to the workset (as does RMSEE) but indicates predictive power (as does RMSEP). The RMSEE, RMSEP and RMSECV values are listed at the bottom of plots wherever these parameters are applicable.

In the plot, we can see that the 3rd component results in a higher RMSECV-value, which is why the autofit will retain only two components.



The **RMSECV** plot is available on the **Analyze** tab, in the **Analysis** group.

For more about RMSEcv, see the **RMSEE, RMSEP and RMSECV** subsection in the Statistical appendix.

10.8 Residual normal probability plot

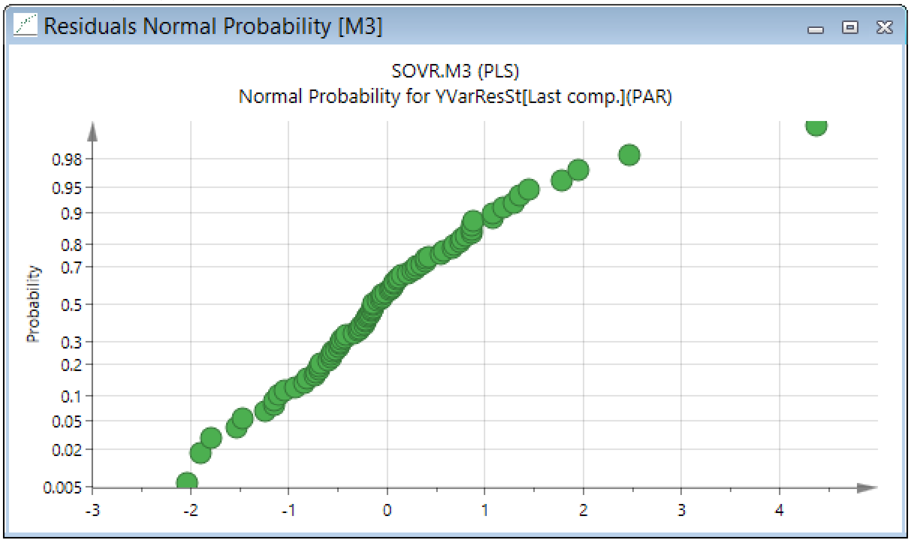
The residuals are the difference between fitted and observed values and exist both for the X block (residual matrix named E) and the Y block (residual matrix named F).

In the **Residuals N-plot**, available in the **Analysis** group on the **Analyze** tab, the residuals for the Y block are displayed. Consequently the plot is unavailable for PCA models.

For transformed responses, all values are, by default, in the original (back transformed) units. To display them in transformed units, select the **Transform predictions** check box in the Predictions page in **Model Options**. Alternatively, to apply the change to future models only select **Transform predictions** *Yes* in Project options.

The residuals displayed in the residuals normal probability plot can be expressed as:

- Raw residuals – The Y-residuals in original units.
- Standardized residuals – The standardized residuals are the scaled Y-residuals divided by the residual standard deviation (RSD). This is the SIMCA default.



The Y-residuals are plotted on a cumulative normal probability scale. This plot makes it easy to detect the following:

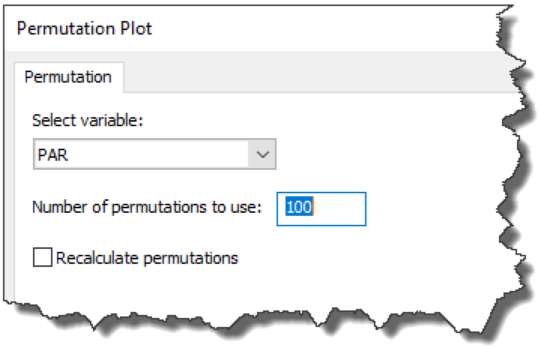
- Normality of the residuals – If the residuals are normally distributed the points on the probability plot follow close to a straight line.
- Outliers – One or more points are below and to the right of the normal line, or above and to the left of the normal line, usually greater than +4 or – 4 standard deviations.

To switch to another y-variable use the **Y-variable** box in the **Properties** group on the **Tools** tab, or use the Properties dialog.

10.9 Permutation plot

Use the **Permutation** plot to check the validity and the degree of overfit for the PLS, OPLS or O2PLS model.

Open the **Permutation Plot** dialog by clicking **Permutations** in the **Validate** group on the **Analyze** tab.


Permutation Plot

Select variable: PAR

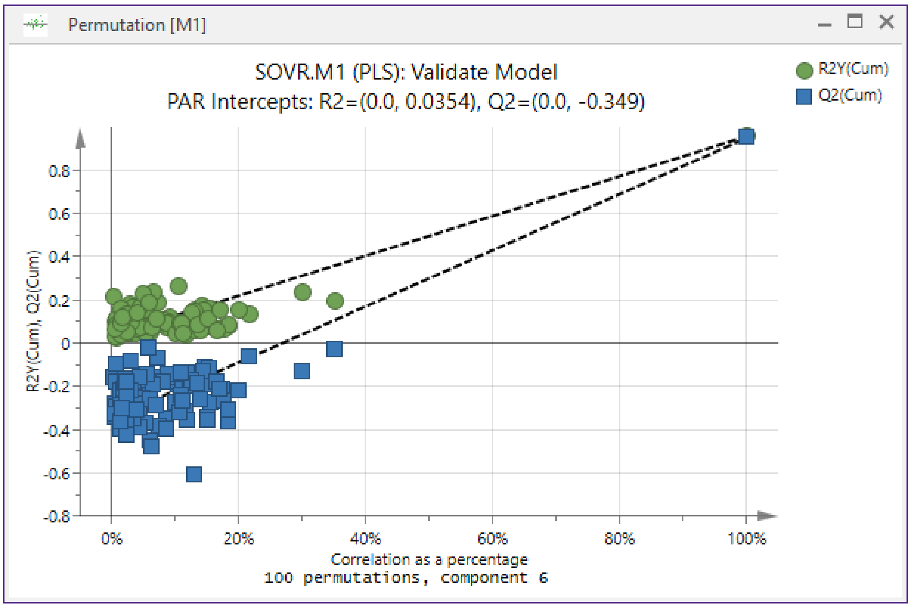
Number of permutations to use: 100

☐ Recalculate permutations

In the dialog:

1. Select the y-variable to make the calculations for in the **Select variable** box.
2. Enter the number of permutations in the **Number of permutations to use** field. Default is 20.

3. Select the **Recalculate permutations** check box in the case where the calculations have been done but you want to recalculate.



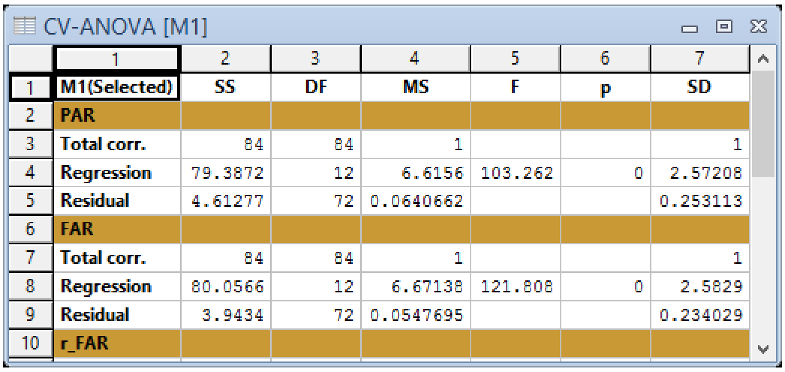
When clicking **OK** in the dialog, the order of the y-variable is randomly permuted the specified number of times, and separate models are fitted to all the permuted y-variables, extracting as many components as was done with the original Y matrix.

The **Permutation** plot then displays the correlation coefficient between the original y-variable and the permuted y-variable on the x-axis versus the cumulative R^2 and Q^2 on the Y-axis, and draws the regression line. The intercept is a measure of the overfit.

10.10 CV-ANOVA

The CV-ANOVA is a diagnostic tool for assessing the reliability of PLS, OPLS, and O2PLS models.

For more see the CV-ANOVA section in the Statistical appendix.



	1	2	3	4	5	6	7
1	M1(Selected)	SS	DF	MS	F	p	SD
2	PAR						
3	Total corr.	84	84	1			1
4	Regression	79.3872	12	6.6156	103.262	0	2.57208
5	Residual	4.61277	72	0.0640662			0.253113
6	FAR						
7	Total corr.	84	84	1			1
8	Regression	80.0566	12	6.67138	121.808	0	2.5829
9	Residual	3.9434	72	0.0547695			0.234029
10	r_FAR						

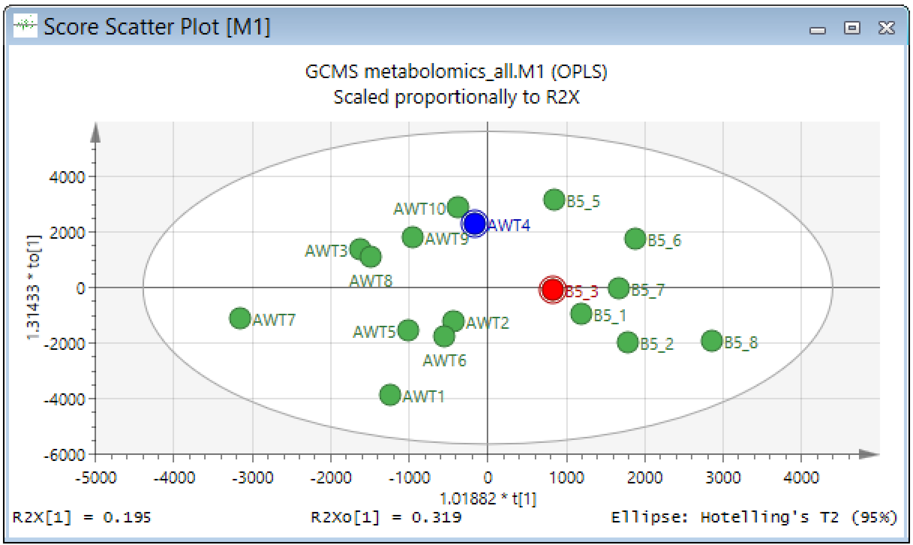
10.11 CV scores plot

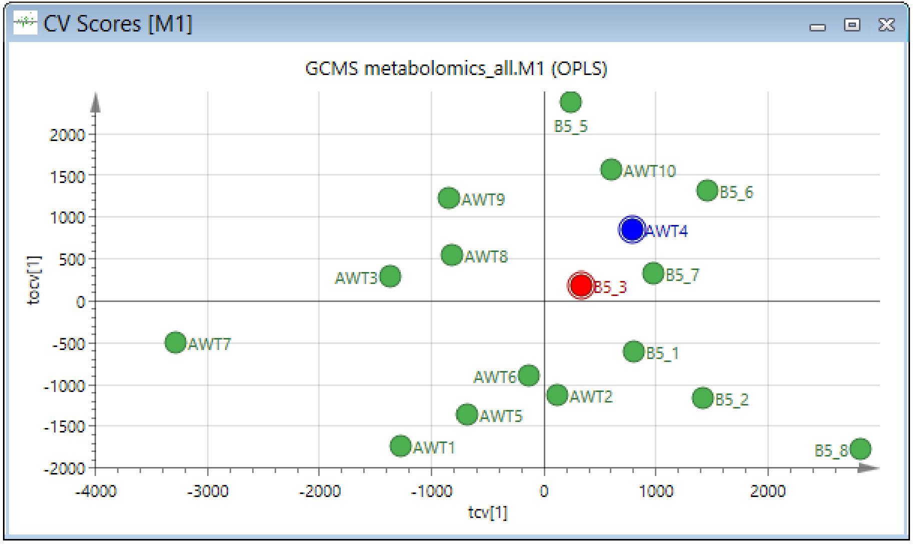
The scatter plot of the cross-validated score vectors is analogous to the scatter plot of regular score vectors, but indicates how sensitive a model is to the exclusion of an observation of the workset.

Open the **CV Scores** plot to display the cross-validated complement to the regular scores plot. Investigate the stability of single points as well as groups by displaying the two plots side by side.

Small changes between the regular score plot and the corresponding cross-validated score plot, indicates a model that is stable towards the inclusion or exclusion of the observations of the workset.

In the example below, we start with the regular score plot and mark samples in each group close to 0, that is, close to being assigned to the wrong class. In the **CV Scores** plot we see that the B5_1 sample is still on the correct side of the 0-line while the AWT samples end up on the wrong side. If and when we have samples that cross over to the other side, this indicates that their class assignment is uncertain.

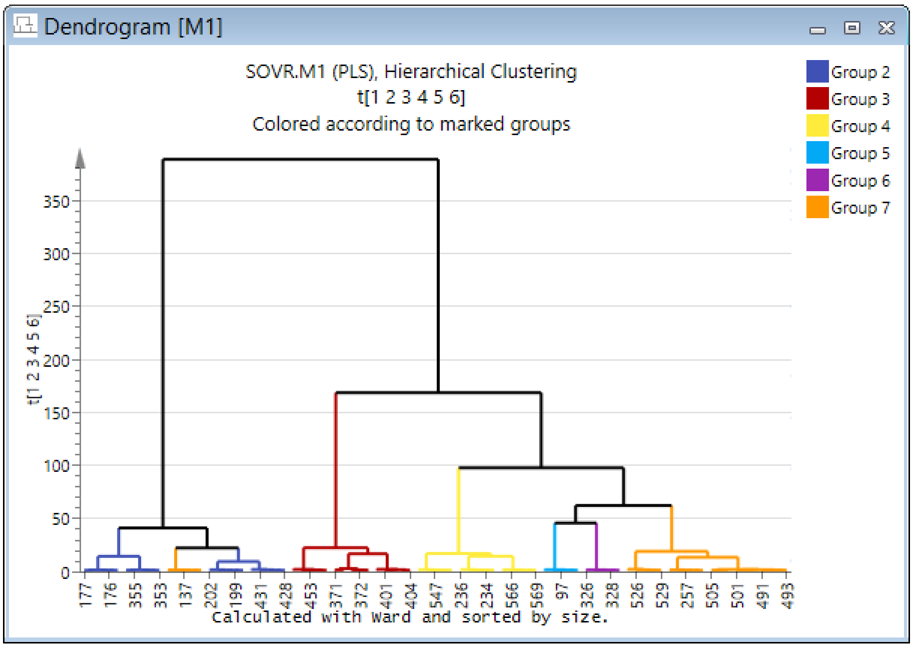




10.12 HCA

The **HCA** dendrogram, available in the **Clustering** group on the **Analyze** tab, is a tree diagram used for showing the clusters generated by hierarchical cluster analysis of the data.

For more about hierarchical cluster analysis, see the Cluster Analysis (CA), dendrograms, Hierarchical CA (HCA), PLS section in the Statistical appendix.



The heights of the clusters are proportional to the distance between the clusters. That is, when the vertical lines are tall the clusters are far apart, and when they are short the clusters are close together.

See also the PLS-Tree section later in this chapter.

10.12.1 Clustering of observations (matrix rows)

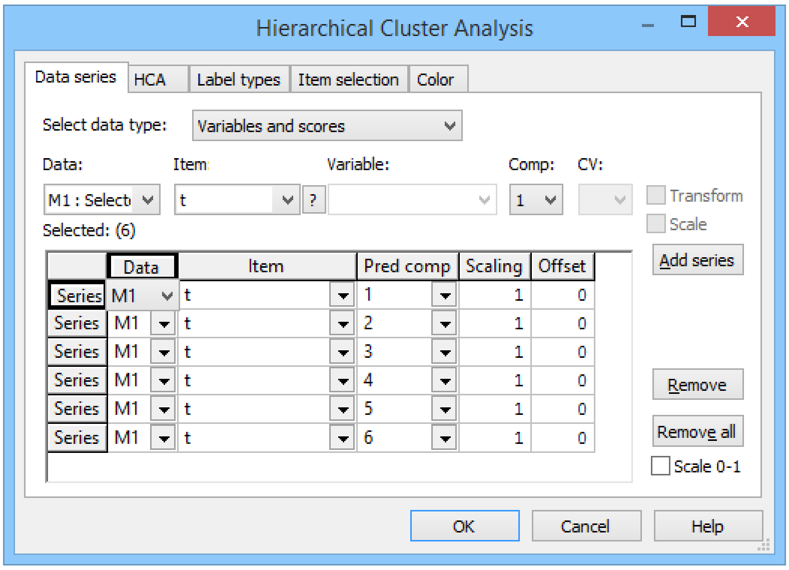
For the clustering of observations, the HCA can be applied to either a score matrix T (recommended) or a data matrix X.

HCA can be started as follows:

- Click **HCA**, in the **Clustering** group on the **Analyze** tab, and select the desired data series, i.e., the basis for the clustering (specific loadings or specific observations).
- With a score scatter plot (2D or 3D) open, on the **Tools** tab, click **Change type** | **Other plot types** and click **Dendrogram**. This cluster analysis is calculated using the vectors displayed in the plot.
- With a score scatter plot (2D or 3D) open, mark points, right-click and click **Create | Plot**, **Dendrogram**. This cluster analysis is calculated using the vectors displayed in the plot but only the selected items.

When clicking **HCA** the **Hierarchical Cluster Analysis** dialog opens.

With, for example, a PCA model with 6 components, the default clustering basis consists of the 6 scores, by default added in the **Selected** list. In the case where the active model was not fitted, the original x-variables are by default available in the **Selected** list.



Hierarchical Cluster Analysis

Select data type: Variables and scores

Data: M1 : Selecte | Item: t | Variable: | Comp: 1 | CV:

□ Transform
□ Scale

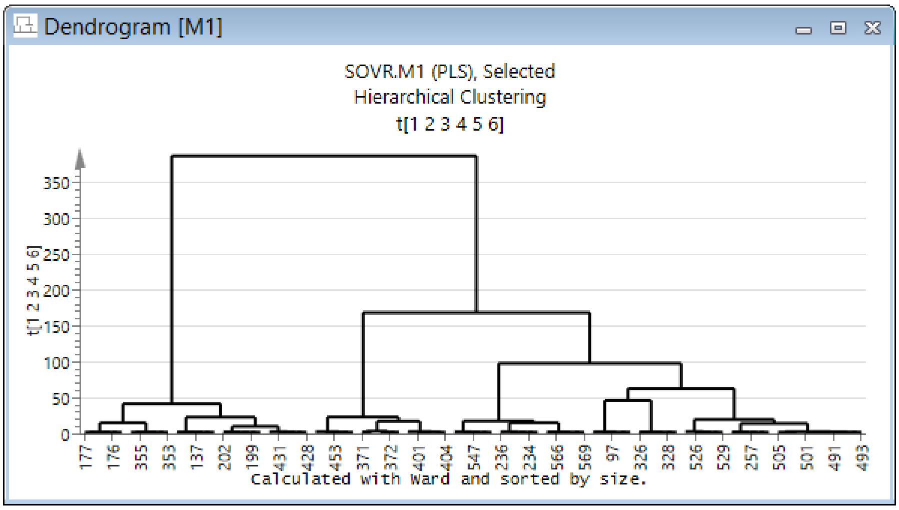
Selected: (6)

	Data	Item	Pred comp	Scaling	Offset
Series	M1	t	1	1	0
Series	M1	t	2	1	0
Series	M1	t	3	1	0
Series	M1	t	4	1	0
Series	M1	t	5	1	0
Series	M1	t	6	1	0

□ Scale 0-1

When clicking **OK** the cluster analysis starts. HCA uses the default similarity criterion (**Ward**) and sorting principle (**Size**), both changeable in the **HCA** tab in the **Properties** dialog. For more, see the HCA options subsection later in this chapter.

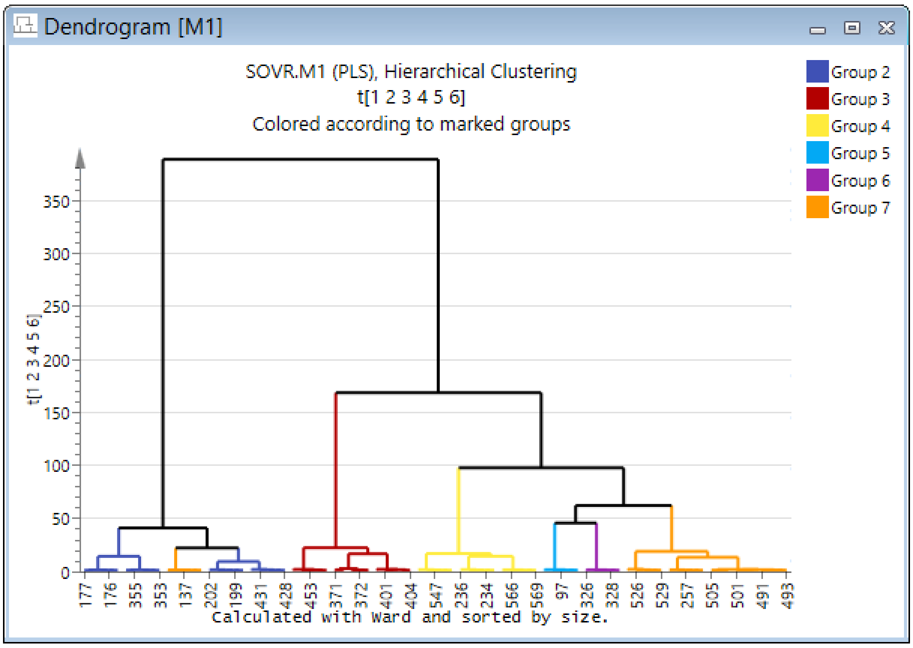
When the calculations are finished, the resulting dendrogram is displayed.



If not by default selected, clicking the **Select plot items** marking tool, and clicking **Group dendrogram clusters** displays a horizontal line with which the resolution of the dendrogram is specified, and thereby the number of clusters.

After selecting the position of the horizontal line and clicking once, the dendrogram and all open scores and similar plots are colored according to the groupings. For more about the marking tool, see the Group dendrogram clusters marking tool subsection later in this chapter.

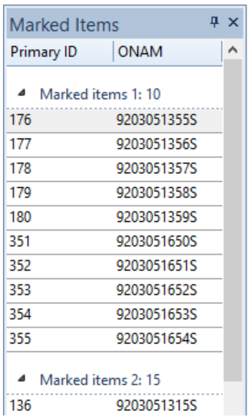
After marking, classes can be created according to this marking. For more, see the Creating class models from plot marking subsection later in this chapter.



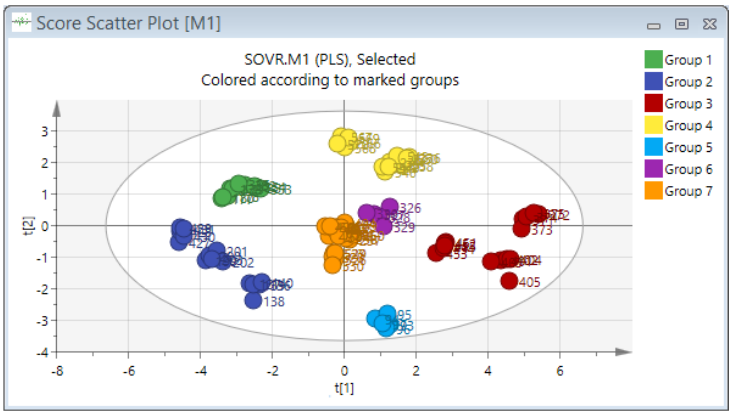
The groups found by the HCA and colored in the dendrogram are colored accordingly in all open plots displaying observations, and are also listed in the **Marked Item** pane, opened by selecting the **Marked items** check box on the **View** tab.

The marked items list can be copied and pasted to e.g., Excel or Word, either group-wise or the whole list. See also the Clustering of variables (matrix columns) subsection next.

With the colored dendrogram or the colored score plot active, clicking **Class | Create class models** in the **Modify model** group on the **Marked items** tab, initiates one model per class so that data can be further analyzed. For more, see the Creating class models from plot marking subsection in Chapter 14, Plot and list contextual tabs.


Marked Items

Primary ID	ONAM
Marked items 1: 10	
176	9203051355S
177	9203051356S
178	9203051357S
179	9203051358S
180	9203051359S
351	9203051650S
352	9203051651S
353	9203051652S
354	9203051653S
355	9203051654S
Marked items 2: 15	
136	9203051315S



10.12.2 Clustering of variables (matrix columns)

For the clustering of variables, the HCA is applied to a loading matrix P (recommended) or a data matrix in this domain. The clustering of variables is similar to clustering of observations. Details about coloring, marking etc., are not described here, see the Clustering of observations (matrix rows) subsection earlier in this chapter. See also the PLS-Tree section later in this chapter.

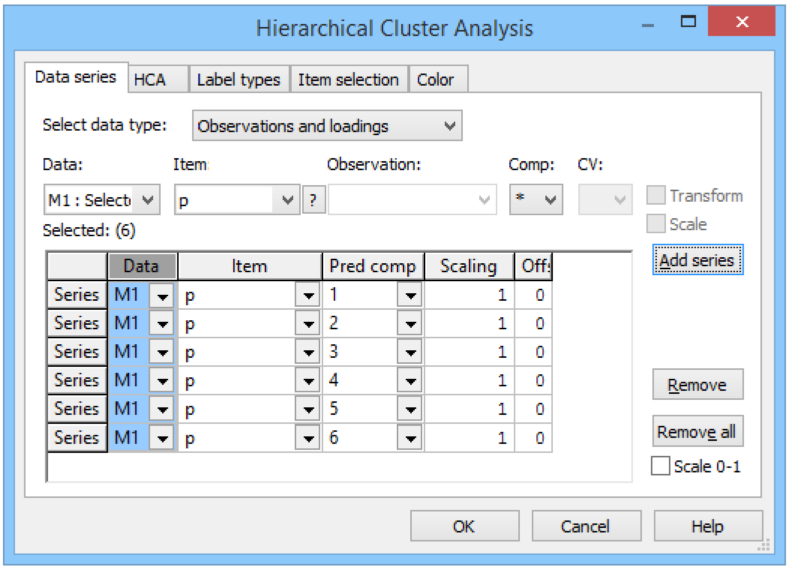
HCA can be started as follows:

- Click **HCA**, in the **Clustering** group on the **Analyze** tab, and select the desired data series, i.e., the basis for the clustering (specific loadings or specific observations).
- With a score scatter plot (2D or 3D) open, on the **Tools** tab, click **Change type** | **Other plot types** and click **Dendrogram**. This cluster analysis is calculated using the vectors displayed in the plot.

- With a score scatter plot (2D or 3D) open, mark points, right-click and click **Create | Plot**, **Dendrogram**. This cluster analysis is calculated using the vectors displayed in the plot but only the selected items.

When clicking **HCA** the **Hierarchical Cluster Analysis** dialog opens.

To investigate clustering in variables, in the **Select data type** box select **Observations and loadings** and add the series.



Select data type: Observations and loadings

Data: M1 : Selecti

Item p ?

Observation:

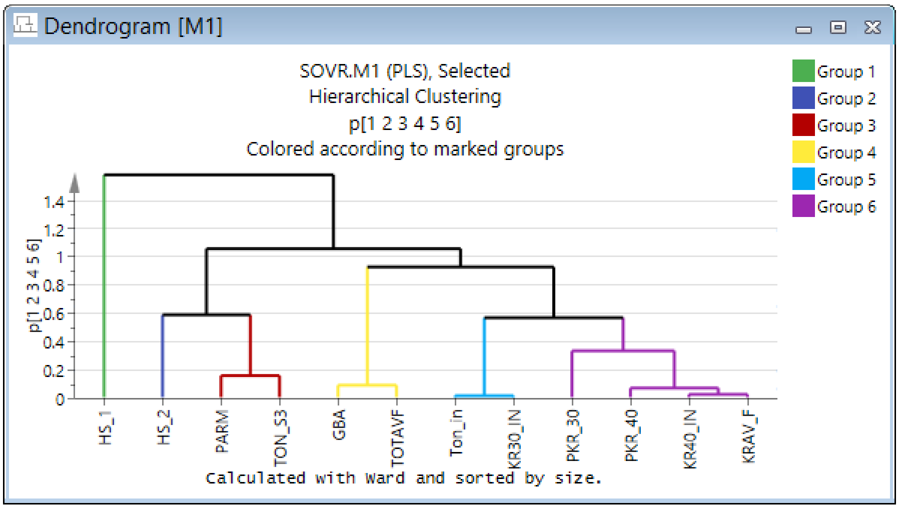
Comp: *

CV:

Selected: (6)

	Data	Item	Pred comp	Scaling	Off
Series	M1	p	1	1	0
Series	M1	p	2	1	0
Series	M1	p	3	1	0
Series	M1	p	4	1	0
Series	M1	p	5	1	0
Series	M1	p	6	1	0

Since a PLS with 6 components was the active model, the clustering basis consists of the 6 loadings. Clicking **OK** starts the cluster analysis and results in a dendrogram.



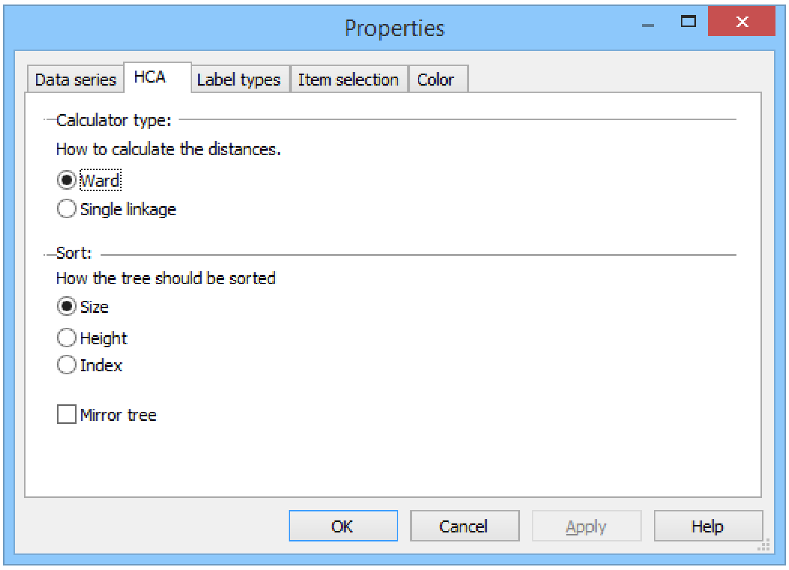
The groups found by the HCA and colored in the dendrogram are colored accordingly in all open plots displaying variables, and are also listed in the **Marked Item** pane, opened by selecting the **Marked items** check box on the **View** tab.

10.12.3 HCA options

In the **Calculator type** section the two methods to calculate the distances between clusters are available. **Ward** is by default selected. Select **Single linkage** by clicking it. For more about these methods, see the Cluster Analysis (CA), dendrograms, Hierarchical CA (HCA) section in the Statistical appendix.

In the **Sort** section, the sorting methods **Size**, **Height**, and **Index** are listed. For more about the **Sort** section, see the Clustering algorithm parameters subsection later in this chapter.

To flip the dendrogram, select the **Mirror tree** check box.



Calculator type:

How to calculate the distances.

● Ward

○ Single linkage

Sort:

How the tree should be sorted

● Size

○ Height

○ Index

□ Mirror tree

See also the PLS-Tree section later in this chapter.

10.12.4 Group dendrogram clusters marking tool

The **Group dendrogram clusters** marker tool displays a slider (line) running horizontally across the plot enabling the marking of clusters. This slider is moved up and down by the mouse.

Adjusting it to a vertical position corresponds to the selection of as many groups as the number of vertical line intersections. This means that by moving the slider up and clicking the plot, the data are divided in fewer clusters and by moving it down and clicking the plot, the data are divided in more clusters.

The current clusters are color coded.

When the **Group dendrogram clusters** is not the selected marker tool, clicking the dendrogram plot selects all observations or variables in the clicked branch.

10.12.5 Creating a PLS-DA or OPLS-DA model from plot marking

To create a PLS-DA or OPLS-DA model from a dendrogram plot (HCA):

1. Mark in the dendrogram plot so that the desired groups are displayed in different colors.
2. On the **Marked items** tab, in the **Modify model** group, click **Class | Create PLS-DA model** or **Create OPLS-DA model**.

Class | Create PLS-DA model and **Create OPLS-DA model** are available when two (or more groups) are marked in a plot displaying observations.

10.12.6 Creating class models from plot marking

To create classes from a dendrogram plot (HCA):

1. Mark in the dendrogram plot so that the desired groups are displayed in different colors.
2. On the **Marked items** tab, in the **Modify model** group, click **Class | Create class models**.

Class | Create class models is available when two (or more) groups are marked in any plot displaying observations.

10.13 PLS-Tree

The PLS-Tree is a hierarchical clustering tool designed to highlight sub-group formation in latent variable space. The PLS-Tree is useful for detecting subtle clustering occurring in higher dimensional data spaces.

To read about the background to PLS-Trees and cluster analysis, see the Cluster Analysis (CA), dendrograms, Hierarchical CA (HCA), PLS-Trees section in the Statistical appendix and the HCA section earlier in this chapter.

10.13.1 Initializing a PLS-Tree

Before running a PLS-Tree estimation, the user must specify the data in terms of a workset:

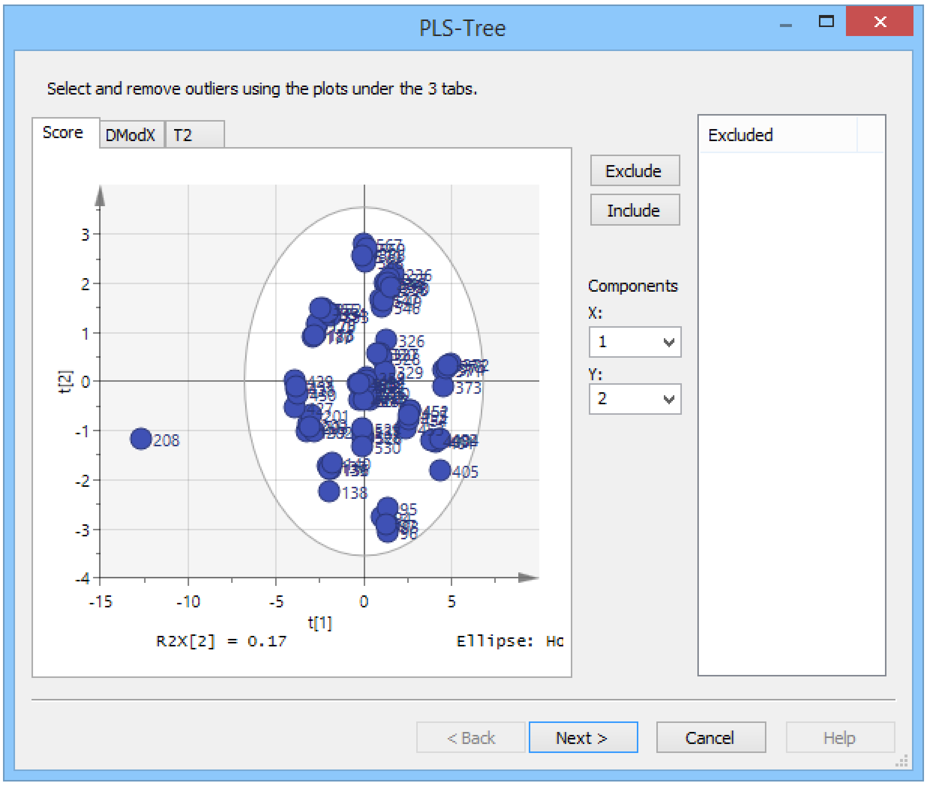
- X and Y,
- observations,
- transformation,
- scaling and centering,
- etc.

Note: There must be at least one Y-variable and at least one X-variable since the models comprising the PLS-Tree are PLS models.

10.13.2 PLS-Tree wizard - removing outliers

With a PLS model active (mark it in the project window), start the PLS-Tree by clicking **PLS-Tree** in the **Clustering** group on the **Analyze** tab. Note that the PLS model can be unfitted or previously fitted.

A wizard is started with its first page shown here. This first page allows the user to exclude obvious outliers based on scores, DModX, and Hotelling's T2.



PLS-Tree

Select and remove outliers using the plots under the 3 tabs.

Components

X: 1

Y: 2

10.13.3 Clustering algorithm parameters

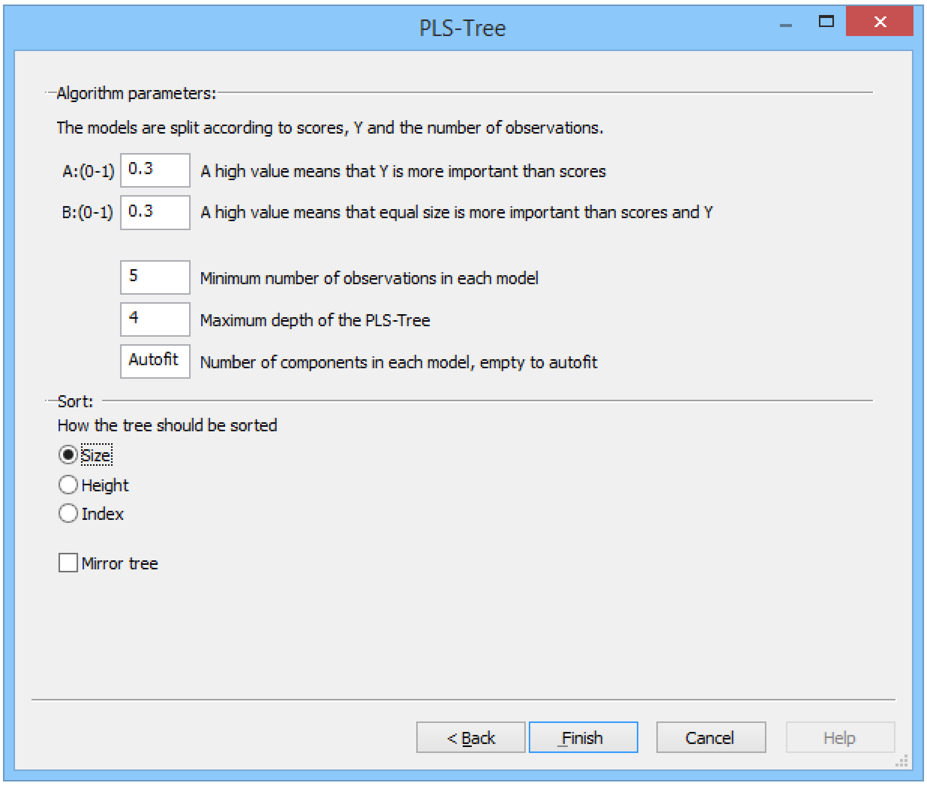
After clicking **Next**, the **Algorithm Parameters** page appears, where the PLS-Tree parameters are specified. The default values are chosen to be reasonable in situations when knowledge about the given problem is scarce.

The performance of the PLS-Tree can be influenced by means of two adjustable algorithm parameters. These parameters are called A and B and run between 0 and 1 and regulate how the PLS models are split.

A sets the balance between the score t1 and the Y. The closer the value for A is to zero, the more weight is attributed to the score t1.

B takes into account the group size of the resulting clusters. The closer the value for B is to zero, the less important it becomes to have equal group sizes in the dendrogram.

This means that a division along t1 is sought that minimizes the within group variation and hence maximizes the between group differences in t1 and Y.



Algorithm parameters:

The models are split according to scores, Y and the number of observations.

A:(0-1) 0.3 A high value means that Y is more important than scores

B:(0-1) 0.3 A high value means that equal size is more important than scores and Y

5 Minimum number of observations in each model

4 Maximum depth of the PLS-Tree

Autofit Number of components in each model, empty to autofit

Sort:

How the tree should be sorted

● Size

○ Height

○ Index

□ Mirror tree

Other parameters that can be adjusted are:

- **Minimum number of observations in each model** - by default 5. This number has to be > 4.
- **Maximum depth of the PLS-Tree** - by default 4.
- **Number of components in each model** - by default Autofit.

For large datasets the Autofit option takes a long time, and a ‘1’ for single component models is recommended. Also, for large datasets the minimum size and the maximum depth can be increased from 5 and 4 to, say, 10 and 7, respectively.

In the **Sort** section the sorting of the resulting dendrogram can be changed.

- **Size** - positions the clusters with the most observations to the right.
- **Height** - positions the clusters with highest bar to the right.
- **Index** - positions the clusters with the lowest index number to the left.

To flip the **Dendrogram**, select the **Mirror tree** check box.

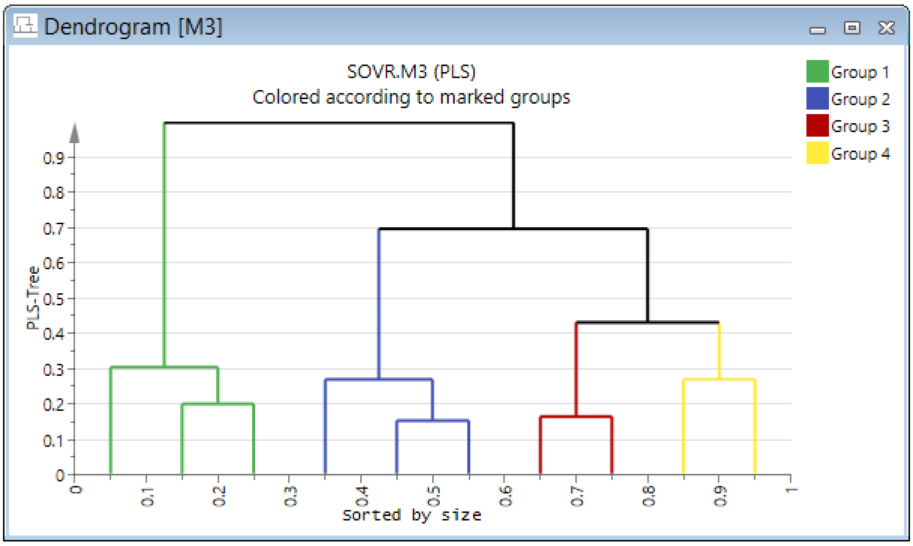
10.13.4 PLS-Tree resulting dendrogram

Clicking **Finish** in the last page of the PLS-Tree wizard starts the PLS-Tree calculations.

After a while, a tree (dendrogram), an uncolored score plot, and the PLS-Tree model window displaying all PLS-Tree models, are opened.

The **Group dendrogram clusters** marker tool is automatically active when a dendrogram is the active plot. Adjusting it to a vertical position corresponds to the selection of as many groups as the number of vertical line intersections. In this example 5 groups were selected.

Note: The heights of the clusters are by default proportional to the number of observations in the clusters.



After selecting the position of the horizontal line and clicking once, the dendrogram and all open scores and similar plots are colored according to the colored groups. For more about the marking tool, see the Group dendrogram clusters marking tool subsection later in this chapter.

After marking, classes can be created according to this marking. For more, see the Creating class models from plot marking subsection later in this chapter.

The **Marked Items** pane, opened by selecting the **Marked items** check box in the **View** tab, displays the members of the colored groups.

For the interpretation of the individual models, mark them as active (one at a time) and investigate in the usual way.

To reopen the dendrogram, mark the top model of the PLS-Tree in the Project window and click **PLS-Tree** on the **Analyze** tab. The PLS-Tree model window and dendrogram both open.

10.13.5 Group dendrogram clusters marking tool

The **Group dendrogram clusters** marker tool displays a slider (line) running horizontally across the plot enabling the marking of clusters. This slider is moved up and down by the mouse.

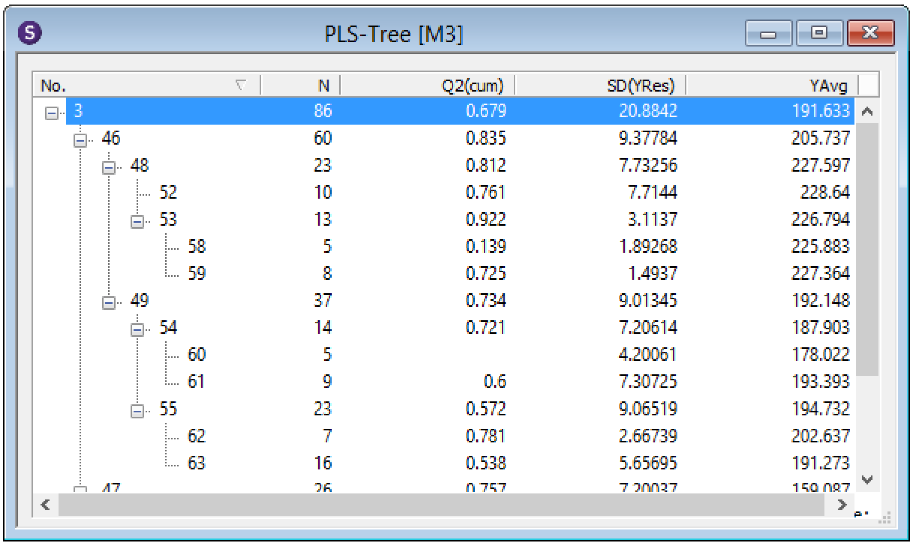
Adjusting it to a vertical position corresponds to the selection of as many groups as the number of vertical line intersections. This means that by moving the slider up and clicking the plot, the data are divided in fewer clusters and by moving it down and clicking the plot, the data are divided in more clusters.

The current clusters are color coded.

When the **Group dendrogram clusters** is not the selected marker tool, clicking the dendrogram plot selects all observations or variables in the clicked branch.

10.13.6 PLS-Tree model window and partial models

Any model can be further modified and investigated by making the model active either in the project window or – recommended – the PLS Tree model window.



No.	N	Q2(cum)	SD(YRes)	YAvg
3	86	0.679	20.8842	191.633
46	60	0.835	9.37784	205.737
48	23	0.812	7.73256	227.597
52	10	0.761	7.7144	228.64
53	13	0.922	3.1137	226.794
58	5	0.139	1.89268	225.883
59	8	0.725	1.4937	227.364
49	37	0.734	9.01345	192.148
54	14	0.721	7.20614	187.903
60	5		4.20061	178.022
61	9	0.6	7.30725	193.393
55	23	0.572	9.06519	194.732
62	7	0.781	2.66739	202.637
63	16	0.538	5.65695	191.273
47	26	0.757	7.20037	159.087

As always, we recommend a score plot, loading plot, and DModX plot for each interesting model, augmented by coefficients and VIP.

Finally, any partial PLS model in a tree can be the starting point for a new tree. Hence, a prudent strategy for a large dataset would be to first develop a tree with depth of, say, 3, then selecting the one or two most promising/interesting models as starting points for additional levels (sub-models) of just those branches, etc. In this way the user keeps some control of the number of models and branches, and hence avoids the incomprehensible mess resulting from letting any clustering loose on a large dataset with unrestricted depth of the tree.

11 Predict

11.1 Introduction

This chapter describes all commands on the **Predict** tab.

Use the **Predict** tab to:

1. Specify a prediction dataset.
2. Classify observations with respect to a model and display the result in plots and lists.
3. Predict results for new observations with respect to a model and display the result in plots and lists.

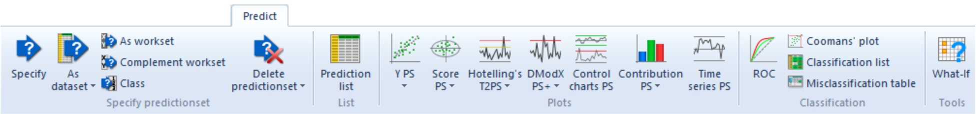
Note: All vectors with the suffix PS are predicted vectors.

All predictions are made using the active model and current predictionset. When a predictionset has not been specified, SIMCA uses the first dataset as predictionset.

Content

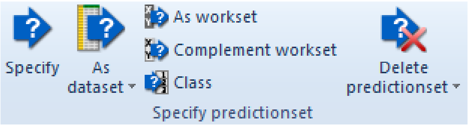
The commands and groups available on the **Predict** tab are listed here.

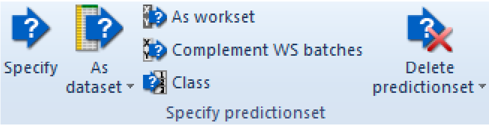
- **Specify predictionset** group: **Specify**, **As dataset**, **As workset**, **Complement workset** (**Complement WS batches** for batch projects), **Class**, **Delete predictionset**.
- **List** group: **Prediction list**.
- **Plots** group: **Y PS**, **Score PS**, **Hotelling's T2PS**, **DModX PS**, **Control charts PS**, **Contribution PS**, **Time series PS**.
- **Classification** group: **ROC**, **Coomans' plot**, **Classification list**, **Misclassification table**.
- **Tools** group: **What-If**.



11.2 Specify predictionset

In the **Specify predictionset** group the following buttons are available: **Specify**, **As dataset**, **As workset**, **Complement workset** or **Complement WS batches**, **Class**, and **Delete predictionset**.



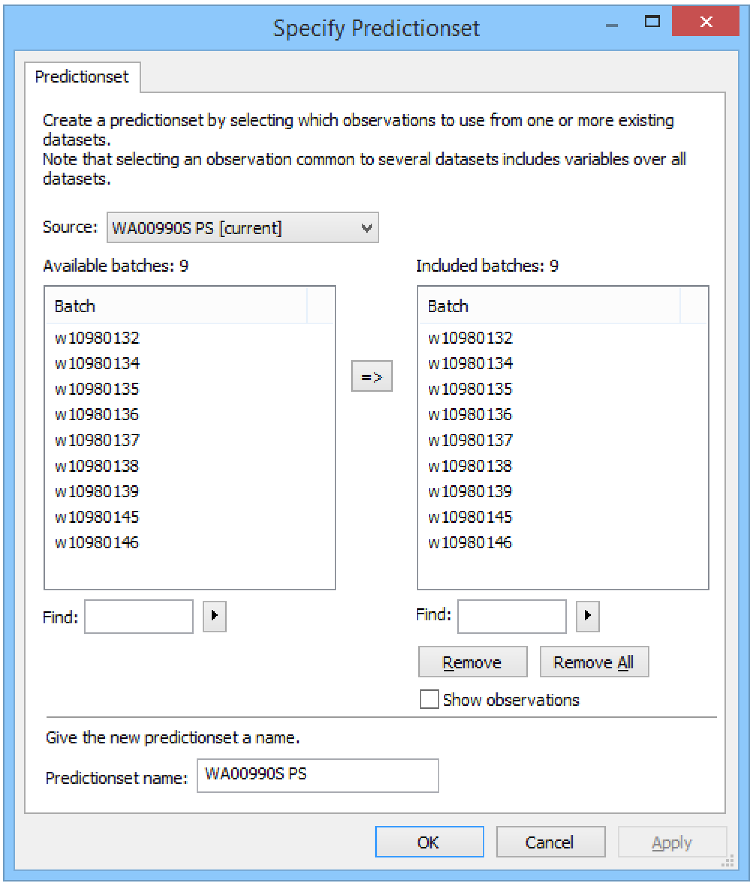


Note: With a lagged variables model, the predictionset must have the same sampling interval as the workset used to develop the model. The first Maximum lag number of observations is incomplete and should therefore be discarded.

11.2.1 Specify Predictionset dialog

To build a predictionset, by combining observations/batches from different datasets or removing observations/batches from the predictionset, click **Specify**.

The **Specify Predictionset** dialog displays the currently selected predictionset.



Specify Predictionset

Predictionset

Create a predictionset by selecting which observations to use from one or more existing datasets.
Note that selecting an observation common to several datasets includes variables over all datasets.

Source: WA00990S PS [current]

Available batches: 9

Batch
w10980132
w10980134
w10980135
w10980136
w10980137
w10980138
w10980139
w10980145
w10980146

Included batches: 9

Batch
w10980132
w10980134
w10980135
w10980136
w10980137
w10980138
w10980139
w10980145
w10980146

□ Show observations

Give the new predictionset a name.

Predictionset name: WA00990S PS

The table lists the functionality of the page and how to use it.

Functionality	Description
Source list box	Select from which source the observations in the **Available observations/batches** list should originate. The available sources are: • Workset section – Workset the observations/batches in the active model. – Classes/phases when available. • Datasets section – all currently available datasets. • Predictionsets section – the currently available predictionsets with the current predictionset default selected. To combine observations from different datasets, click the **Source** box, click the desired dataset, and add the observations. Repeat selecting another dataset in the **Source** box.
Predictionset name field	Enter the name for the new predictionset in the **Predictionset name** field. **Note**: Entering/leaving a name of an already existing predictionset overwrites that predictionset without warning.
Available observations/batches list	In the **Available observations/batches** list, all observations/batches in the currently selected dataset in the **Source** box are displayed. The number of observations/batches, in the selected dataset, is listed. To specify the predictionset, select the observations/batches and click the => to find them in the **Included observations/batches list**.
Find feature	The **Find** feature works as in other dialogs. For details, see the relevant parts of the Find feature subsection, in the Workset section in Chapter 7, Home.
Included observations/batches list	In the **Included observations/batches** list, the observations/batches of the current predictionset are displayed. If no predictionset was selected, the observations/batches in the first dataset are displayed.

Functionality	Description
Show observations check box	In a batch project, the batches are by default displayed. To display the underlying observations, select the **Show observations** check box.
Remove-buttons	After selecting observations in the **Included observations/batches list**, clicking **Remove** removes them from the predictionset specification. Clicking **Remove all** removes all, independent of selection.

11.2.2 As dataset

To select an entire dataset as predictionset, click **As dataset** and click the dataset name. The **Prediction list** spreadsheet opens displaying the selected dataset with predictions using the active model.

Clicking **As dataset** displays a menu with two headers:

- **Dataset** where all datasets are listed.
- **Predictionset** where all specified predictionsets are listed. If you have not specified any predictionsets only the default predictionset is listed here, which is the first imported dataset.

In the predictionset the primary observation IDs/batch IDs are saved. This means that if you have two datasets with the same primary observation IDs/batch IDs but different variables, predictionsets created from these datasets define the same predictionset.

Note: The predictionset uses all variables for each included observation/batch whichever dataset the observation or batch was selected from.

11.2.3 As workset

To select the observations/batches included in the active model as predictionset, click **As workset**. The **Prediction list** spreadsheet opens displaying the observations/batches of the selected model with predictions using the active model.

11.2.4 Complement workset

To select the observations in the selected datasets *not* included in the workset of the active model as predictionset, click **Complement workset**. The **Prediction list** spreadsheet opens displaying the observations with predictions using the active model.

For batch evolution models, the command is named **Complement WS batches**.

For instance, if you have excluded batches from the workset, you can specify them as a predictionset by clicking **Complement workset**.

11.2.5 Class

To select the observations included in a class as predictionset, click **Class**, and click the class name. The **Prediction list** spreadsheet opens displaying the observations of the selected class with predictions using the active model.

This command is available for class and phase models.

11.2.6 Delete predictionset

All predictionsets, but the current one, can be deleted.

Predictionsets hold references to the selected observations or batches. Deleting a predictionset thus only removes the references and does not affect the datasets.

11.2.7 Batch predictionset

For batch projects, only batch evolution datasets, BE DS, are available to select as predictionsets, even if the active model is a BLM.

When specifying a BE DS as predictionset and the active model is a batch level model, BLM, the predictionset is automatically rearranged to a batch level predictionset behind the scenes.

For batch evolution models, when the active model is a phase model, the **Prediction list** displays only the batches belonging to that phase.

The predictionset for the BLM is limited to the batches and observations included in the BEM the BLM was created from. This means that to specify batches excluded in the BEM as predictionset, you have to mark the BEM and on the **Predict** tab, in the **Specify predictionset** group, click **Complement WS batches**. Then mark the BLM and open the plots on the **Predict** tab.

Note: The **Specify Predictionset** dialog by default displays batches. To view the observations in the batches, and exclude observations, select the **Show observations** check box.

11.2.8 Predictionset for filtered datasets

For models built on filtered data, only original datasets are available to select as predictionsets.

When specifying a dataset as predictionset and the active model was built from filtered data, the predictionset is automatically filtered in the same way.

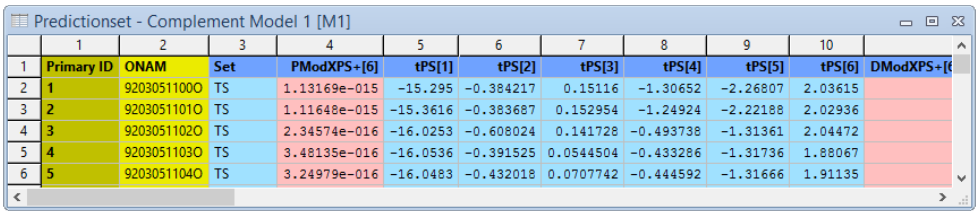
11.2.9 Missing values in the predictionset

The threshold of missing values is by default 50%. When the number of missing values in an observation or a variable exceeds the specified threshold, SIMCA displays a warning message. The threshold default can be changed in **File | Options** | Project options.

11.3 Prediction list

To open the Predictionset, click **Prediction list** in the **List** group on the **Predict** tab.

In this list the model membership probability (PModXPS+) and distances to the model (DModXPS, DModXPS+) values are colored red when the observation has a probability (PModXPS+) value smaller than the limit (default 0.05).



Predictionset - Complement Model 1 [M1]

	1	2	3	4	5	6	7	8	9	10	
1	Primary ID	ONAM	Set	PModXPS+[6]	tPS[1]	tPS[2]	tPS[3]	tPS[4]	tPS[5]	tPS[6]	DModXPS+[(
2	1	92030511000	TS	1.13169e-015	-15.295	-0.384217	0.15116	-1.30652	-2.26807	2.03615	
3	2	92030511010	TS	1.11648e-015	-15.3616	-0.383687	0.152954	-1.24924	-2.22188	2.02936	
4	3	92030511020	TS	2.34574e-016	-16.0253	-0.608024	0.141728	-0.493738	-1.31361	2.04472	
5	4	92030511030	TS	3.48135e-016	-16.0536	-0.391525	0.0544504	-0.433286	-1.31736	1.88067	
6	5	92030511040	TS	3.24979e-016	-16.0483	-0.432018	0.0707742	-0.444592	-1.31666	1.91135	

The columns displaying Primary ID, Secondary IDs, Y variables, and X variables are always displayed in the **Prediction list**, along with the default result columns. To select to display other columns, right-click the spreadsheet, and then click **Properties**.

11.3.1 Properties in Prediction list

In the **Properties** dialog, select the prediction results to display by selecting the corresponding check boxes.

Results for all fit methods

1. **Model membership probability – PModXPS+**
   Displayed for the last component and lists the probability that the observation belongs to the model. With a 95% confidence level, observations with a probability of membership less than 5% (i.e. less than 0.05) are considered to be outliers and not belonging to the model. The PModXPS+, DModXPS, and DModXPS+ values are colored red when the observation is outside the critical limit.

2. **Distance to model (DModXPS)**
   By default SIMCA displays the normalized distance to the model, i.e., standard deviation of the residuals divided by the pooled RSD of the model. To change, open **Project Options** or **Model Options**. The PModXPS+, DModXPS, and DModXPS+ values are colored red when the observation is outside the critical limit.

3. **Distance to model + (DModXPS+)**
   Combination of distance to the model (DModXPS) and the distance of its score to the normal score range of the model (when its predicted score is outside the model score range). The PModXPS+, DModXPS, and DModXPS+ values are colored red when the observation is outside the critical limit.

4. **t predictionset (tPS)**
   The predicted scores, tPS, for all components.

5. **Workset / Testset membership (Set)**
   A column labeling the observation as WS, the observation was part of the workset, or TS, the observation was not used to fit the model and belongs to the test set (predictionset).

6. **Confidence interval of tPS (± C.I. tPS[1])**

7. **X predicted (XVarPredPS)**
   A reconstructed variable as the appropriate part of TP' from the predictionset.

Results for PLS/OPLS/O2PLS models only

The results in the columns shown for PLS/OPLS/O2PLS are always back transformed to original units independent of whether the **Transform predictions** and **Scale predictions** check boxes are selected in **Model Options**.

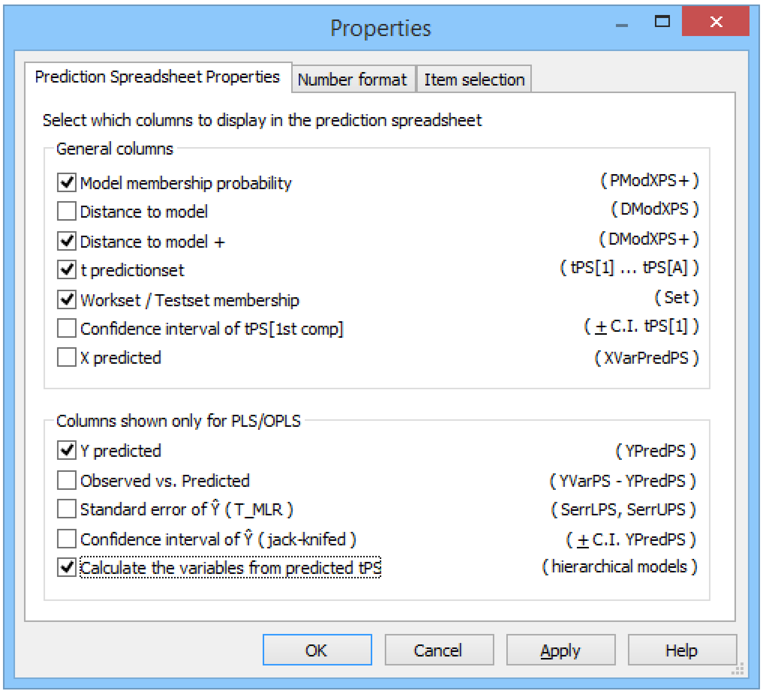
1. **Y predicted (YPredPS)**
   Displays the predicted response value for all responses using the last component.

2. **Observed – Predicted (YVarPS – YPredPS)**
   Displays the differences between the y-variable in the predictionset and the predicted y-variable for all responses. **YPredPS** using the last component.

3. **Standard error of Y (SerrLPS, SerrUPS)**
   Displays the standard errors for the predicted Y values. The standard errors are displayed for all responses using the last component. For details about the computation, see the Statistical appendix**.**

4. **Confidence interval of Y (± C.I. YPredPS)**
   Confidence interval computed from all the cross validation rounds and jack-knifing. These confidence intervals can only be computed for predictionset observations, i.e., observations not used to fit the model.

5. **Calculate the variables from predicted tPS**
   For hierarchical models the predicted Y derived from the predicted scores.



Select which columns to display in the prediction spreadsheet

General columns

☑ Model membership probability (PModXPS+)
☐ Distance to model (DModXPS)
☑ Distance to model + (DModXPS+)
☑ t predictionset (tPS[1] ... tPS[A])
☑ Workset / Testset membership (Set)
☐ Confidence interval of tPS[1st comp] (± C.I. tPS[1])
☐ X predicted (XVarPredPS)

Columns shown only for PLS/OPLS

☑ Y predicted (YPredPS)
☐ Observed vs. Predicted (YVarPS - YPredPS)
☐ Standard error of Ŷ (T_MLR) (SerrLPS, SerrUPS)
☐ Confidence interval of Ŷ (jack-knifed) (± C.I. YPredPS)
☑ Calculate the variables from predicted tPS (hierarchical models)

11.4 Y PS plots

The plots and lists displaying predicted responses are found on the **Predict** tab, in the **Plots** group, by clicking **Y PS**. The available plots and lists are: **Scatter**, **Line**, **Column**, and **List**.

With transformed Y variables, the observed and predicted y-variables are, by default, back transformed to original units. To display the plot or list in transformed units, select the **Transform predictions** check box in **Model Options** and recreate the plot.

Note: The Y PS plots and lists are only available for PLS, OPLS, and O2PLS models and their class models.

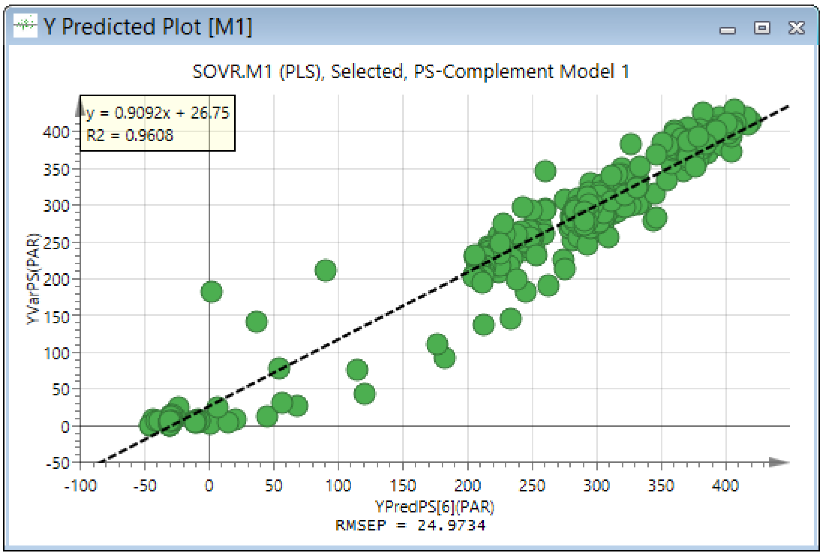
11.4.1 RMSEP

At the bottom of the plots, RMSEP (Root Mean Square Error of Prediction) is displayed. This is the standard deviation of the predicted residuals (errors). It is computed as the square root of (Σ(obs-pred)²/N).

11.4.2 Y PS scatter plot

To display observed vs. predicted y as a scatter plot, click **Y PS | Scatter**.

An example of the plot follows:

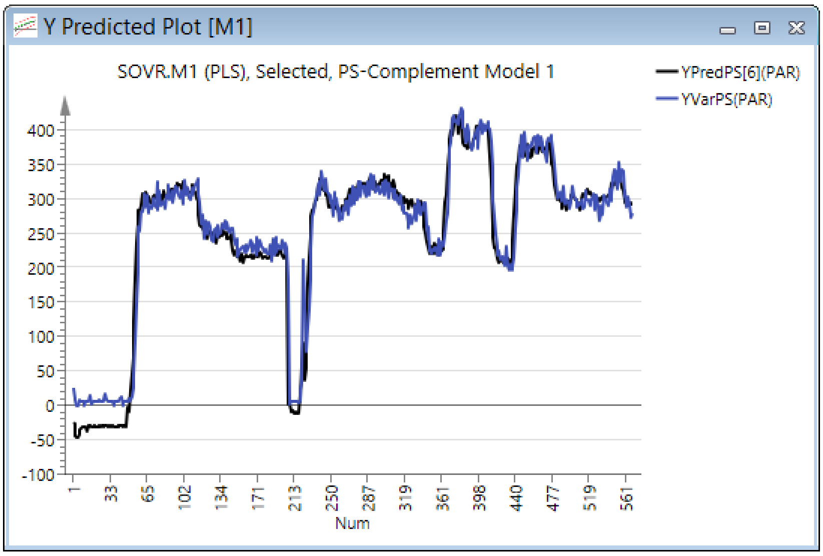


RMSEP = 24.9734

11.4.3 Y PS line plot

To display the predictionset variable **YVarPS** and the predicted variable **YPredPS** versus Num, click **Y PS | Line**.

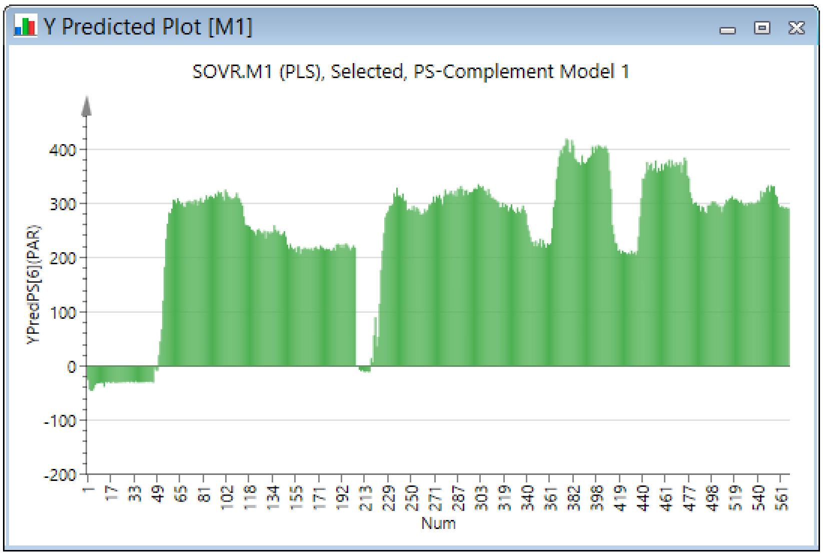
An example of the plot follows:



11.4.4 Y PS column plot

To display Y Predicted as a column plot with confidence intervals, click **Y PS | Column**.

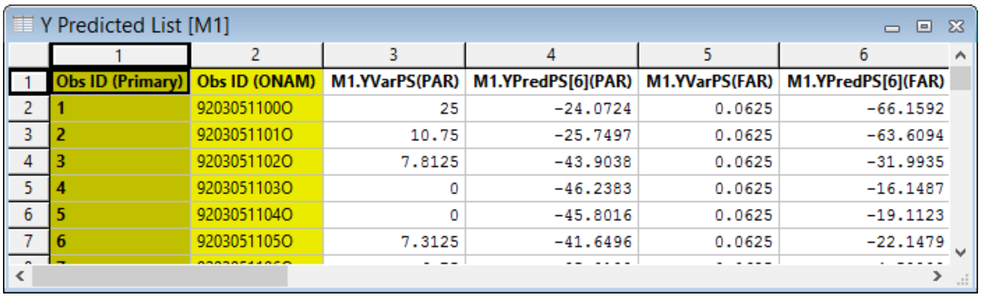
The plot is displayed with jack-knife uncertainty bars. These limits can be modified in the **Properties** dialog. For more, see the Limits subsection in Chapter 14, Plot and list contextual tabs.



11.4.5 Y PS list

The **Y Predicted List** displays for each y-variable:

Vector	Description
YVarPS	Measured or observed Y if present.
YPredPS	Predicted Y.


Y Predicted List [M1]

	1	2	3	4	5	6
1	Obs ID (Primary)	Obs ID (ONAM)	M1.YVarPS(PAR)	M1.YPredPS[6](PAR)	M1.YVarPS(FAR)	M1.YPredPS[6](FAR)
2	1	9203051100O	25	-24.0724	0.0625	-66.1592
3	2	9203051101O	10.75	-25.7497	0.0625	-63.6094
4	3	9203051102O	7.8125	-43.9038	0.0625	-31.9935
5	4	9203051103O	0	-46.2383	0.0625	-16.1487
6	5	9203051104O	0	-45.8016	0.0625	-19.1123
7	6	9203051105O	7.3125	-41.6496	0.0625	-22.1479

Note: For discriminant models the **Y Predicted List** is identical to the Classification List.

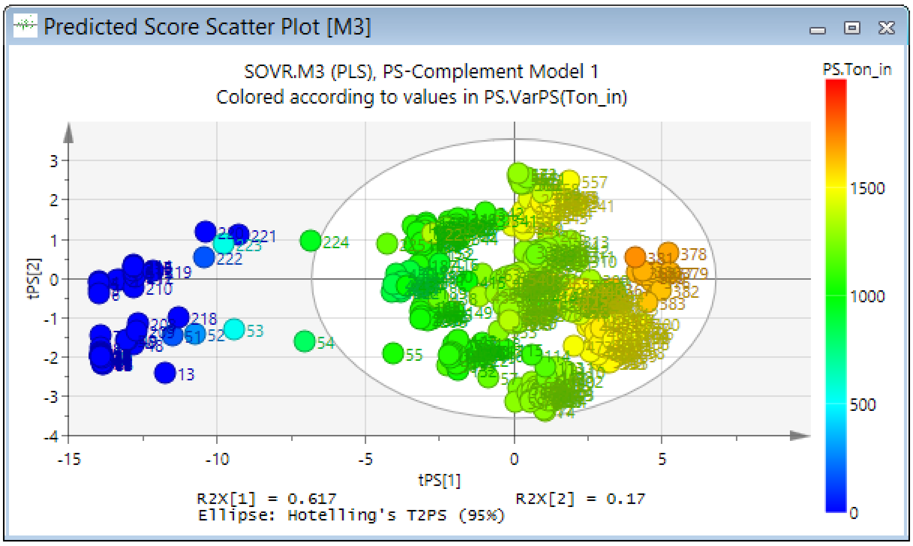
11.5 Score PS plots

There are four types of predicted score plots available by clicking **Score PS**: **Scatter**, **Line**, **Column**, and **3D**.

These plots and dialogs are very similar to those of the score plots found on the **Home** tab. For details about the dialog, see the Scores section in Chapter 7, Home. An example of each plot type follows here.

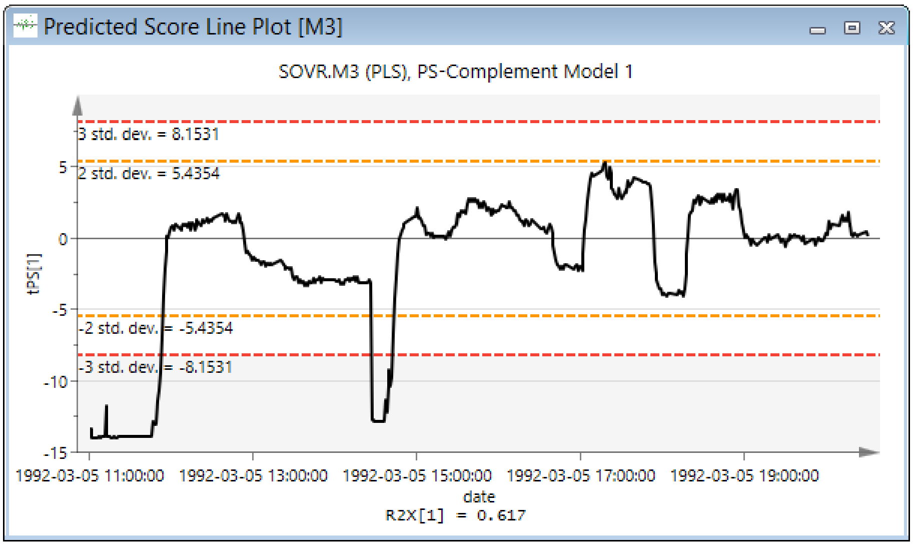
11.5.1 Predicted score scatter plot

To open the scatter plot displaying predicted scores, tPS, click **Score PS | Scatter**.


Predicted Score Scatter Plot [M3]
SOVR.M3 (PLS), PS-Complement Model 1
Colored according to values in PS.VarPS(Ton_in)
PS.Ton_in
1500
1000
500
0
tPS[2]
tPS[1]
-15
-10
-5
0
5
3
2
1
0
-1
-2
-3
-4
R2X[1] = 0.617
R2X[2] = 0.17
Ellipse: Hotelling's T2PS (95%)

11.5.2 Predicted score line plot

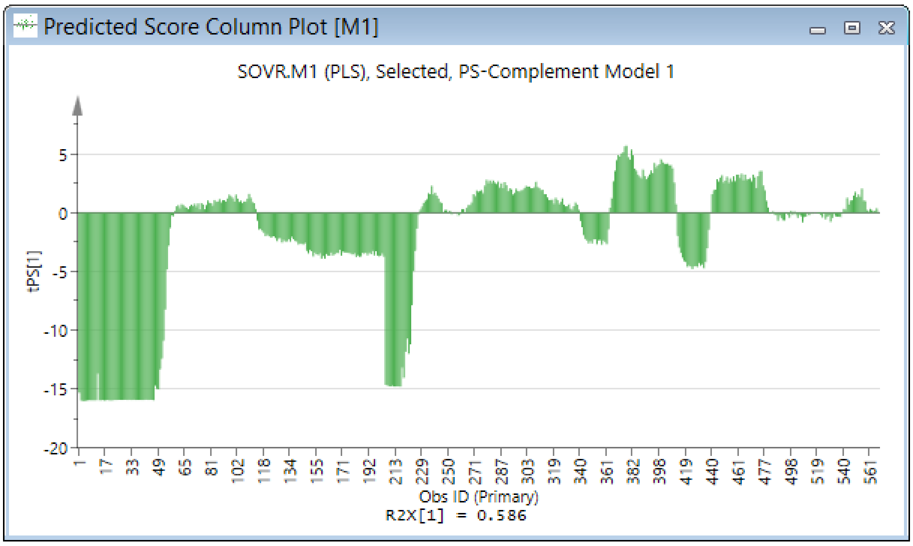
To open the line plot displaying predicted scores, tPS, click **Score PS | Line**.



11.5.3 Predicted score column plot

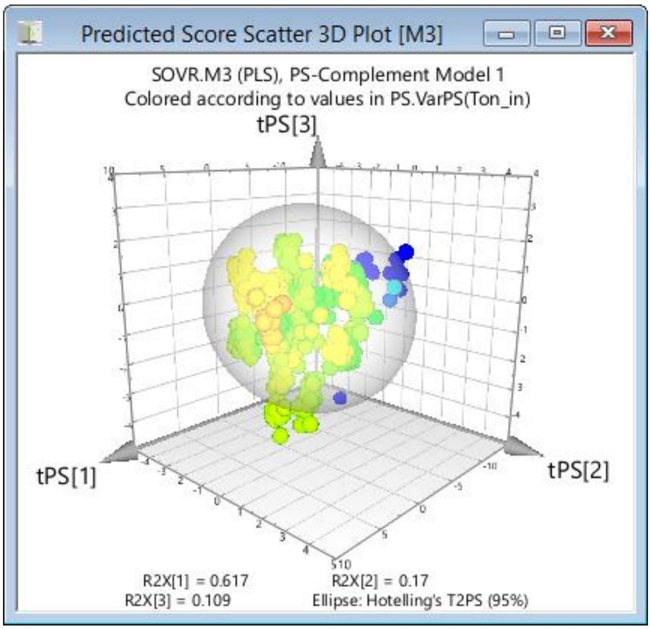
To open the column plot displaying predicted scores, tPS, click **Score PS | Column**.

The plot is displayed with jack-knife uncertainty bars. These limits can be modified in the **Properties** dialog. For more, see the Limits subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs.



11.5.4 Predicted score 3D plot

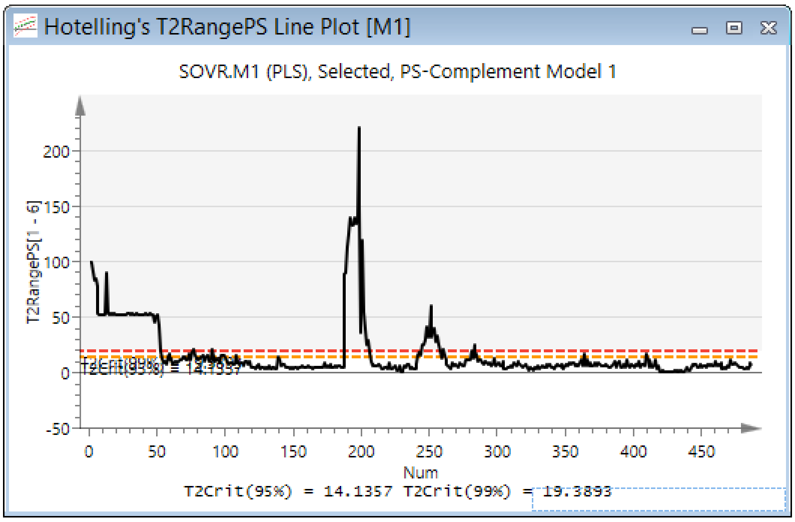
To open the 3D scatter plot displaying predicted scores, tPS, click **Score PS | 3D**.


Predicted Score Scatter 3D Plot [M3]
SOVR.M3 (PLS), PS-Complement Model 1
Colored according to values in PS.VarPS(Ton_in)
tPS[3]
tPS[1]
tPS[2]
R2X[1] = 0.617
R2X[3] = 0.109
R2X[2] = 0.17
Ellipse: Hotelling's T2PS (95%)

For how to mark, zoom, rotate, move the plot in its window, color and size the 3D plot, see the 3D Score Scatter Plot section in Chapter 7, Home.

11.6 Hotelling’s T2Range plot

Predicted Hotelling's T2Range can be displayed in two plot types available by clicking **Hotelling's T2PS | Line** and **Column**.



The Hotelling's T²Range plot displays the distance from the origin in the model plane (score space) for each selected observation. The plot shows the T² calculated for the range of selected components, e.g., 1 to 7, or 3 to 6.

Default is to display from the first to the last component. For OPLS and O2PLS the range is locked to from first predictive to last orthogonal in X component.

To change the range of components, right-click the plot and select **Properties**, tab **Component**.

Values larger than the 95% limit are suspect, and values larger than the 99% limit can be considered serious outliers.

See also the Hotelling's T2Range section in Chapter 7, Home.

For more, see the Limits topic in the Shortcut menu chapter.

11.7 DModX PS+

Distance to model is an estimate of how far from the model plane, in the X or Y space, the observation is positioned.

The distance to the model can be displayed in absolute and normalized units. By default the distance to model plots are displayed in normalized units after the last component.

Use **Model Options** or **Project Options**, to change units of the DMod plot.

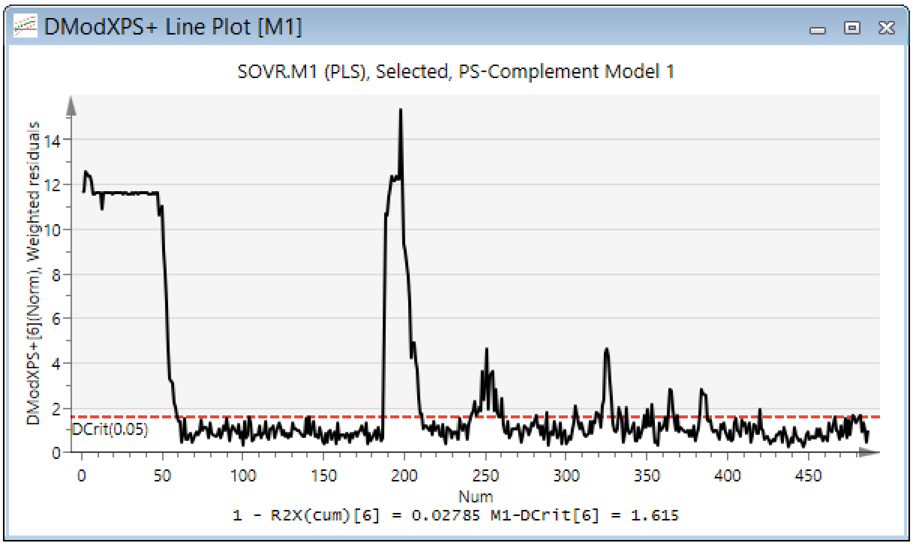
For details about the calculations of DModXPS, DModXPS+, DModYPS and DCrit, see the Distance to the model section in the Statistical appendix.

11.7.1 DModX PS+ - Distance to the model X-block

To display the DModX for the predictionset, click **DModX PS+** and under the **DModX** header click **Line** or **Column**.

The plot by default displays DModXPS+ after the selected component with limit at significance level 0.05.

To switch to the regular DModXPS, open the **Properties** dialog, click the **DMod** tab, and click **Regular**.

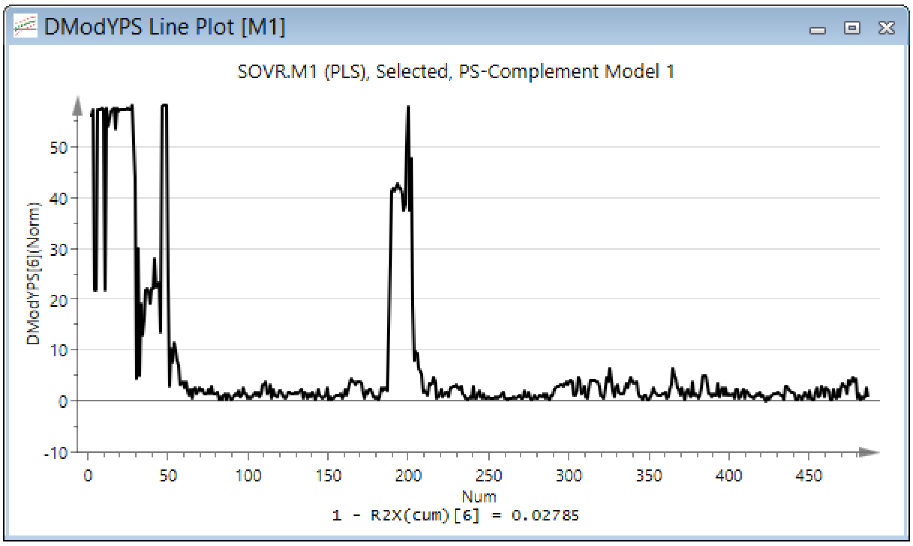


DModXPS+, displayed in this plot, is a combination of the regular DModXPS and the distance to normal score range. For details, see the Distance to the model of new observations in the predictionset subsection in the Statistical appendix.

11.7.2 DModY PS - Distance to the model Y-Block

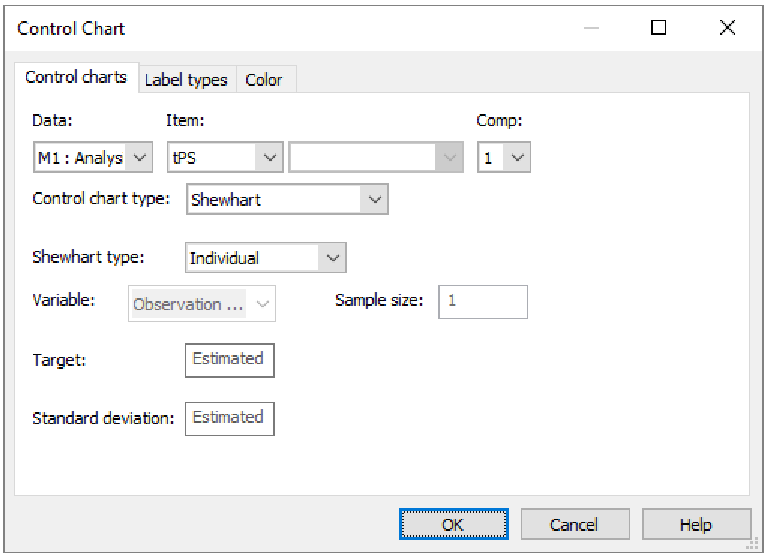
To display the DModY for the predictionset, click **DModX PS+**, and under the **DModY** header click **Line** or **Column**.

The plot displays DModYPS after the selected component.



11.8 Control charts PS

With a fitted model, the predicted scores, x and y-variables and their residuals can be displayed in control charts available by clicking **Control charts PS**.



To display a control chart:

1. Select:
   a. The data source in the **Data** box.
   b. The vector to display in the **Item** box. **tPS**, **XVarPS**, **XVarResPS**, **YVarPS**, and **YVarResPS** are available.
   c. Variable and/or component in the **Variable** or **Comp** boxes when appropriate.
2. In the **Type of control chart** box, select **Shewhart**, **EWMA**, **CUSUM**, or **EWMA/Shewhart**.
3. Depending on the selected control chart, select the properties as desired. Note that you can select to group on observation groups or any monotonically increasing variable or time variable.
4. Clicking **OK** opens the control chart with limits computed from the workset.

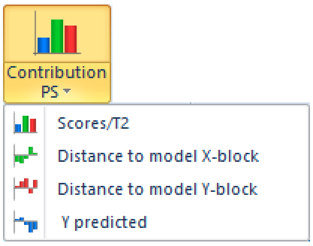
For details, see the Control charts section in Chapter 12, Plot/List.

11.9 Contribution PS

Contribution plots are used to understand why an observation differs from the others in an X score (t), in DModX, in DModY, in Hotelling's T2Range, or in the observed vs. predicted Y plot.

The contribution plot displays the differences, in scaled units, for all the terms in the model, between the outlying observation and the normal (or average) observation, multiplied by the (absolute) value of the normalized weight.

Contribution plots for the predictionset can be displayed from plots or by clicking **Contributions PS**.

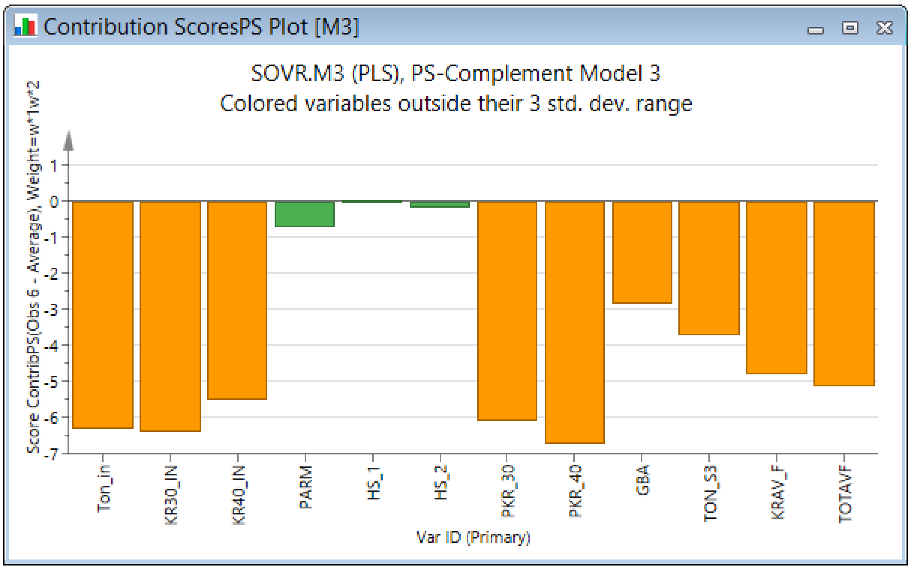


For BLM with one or more variables created from scores or original variables in the BEM, it is useful to display the variation of a variable from a selected phase in a contribution plot, as a line plot over time, rather than a column plot at every time point. For this purpose the **Sources of Variation Plot** is by default displayed when creating the contribution plot from a plot. For more, see the Sources of variation plot subsection in Chapter 9, Batch.

11.9.1 Scores/T2

To create the score contribution plot for the predictionset using the buttons, click **Contribution PS | Scores/T2**.

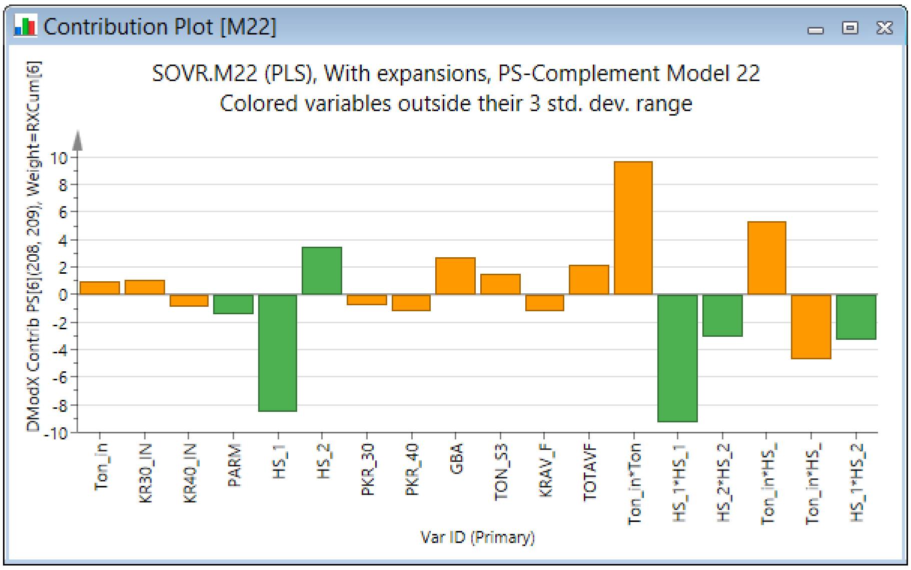
The **Contribution Scores** dialog that opens is identical to the one opened by clicking **Contribution | Scores/T2** in the **Analysis** group on the **Analyze** tab. For more about this dialog and the available weights, see the Scores/T2 contribution plot section in Chapter 10, Analyze.


Contribution ScoresPS Plot [M3]
SOVR.M3 (PLS), PS-Complement Model 3
Colored variables outside their 3 std. dev. range
Score ContribPS(Obs 6 - Average), Weight=w*1w*2
1
0
-1
-2
-3
-4
-5
-6
-7
Ton_in
KR30_IN
KR40_IN
PARM
HS_1
HS_2
PKR_30
PKR_40
GBA
TON_S3
KRAV_F
TOTAVF
Var ID (Primary)

11.9.2 Distance to model X contribution plot

To create the DModX contribution plot for the predictionset using the menus, click **Contribution PS | Distance to model X**.

The **Contribution DModX** dialog that opens is identical to the one opened by clicking **Contribution | Distance to model X** in the **Analysis** group on the **Analyze** tab. For more about this dialog and the available weights, see the Distance to model X contribution plot section in Chapter 10, Analyze.

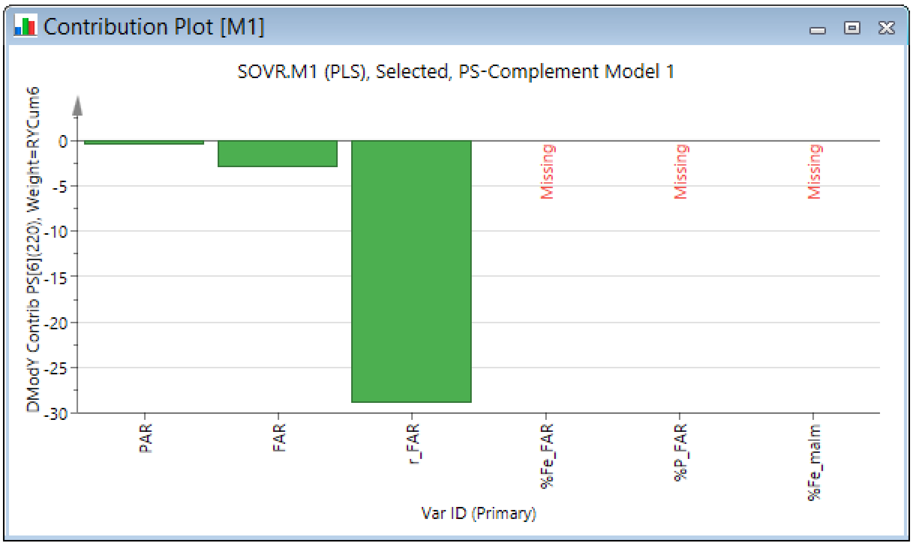


In the contribution plot, the variables are colored orange if the original variable is outside the + 3 standard deviation limits for the investigated observations. To color outside 3 standard deviations is the default and changeable in Properties.

11.9.3 Distance to model Y contribution plot

With a PLS model, create the DModY contribution plot for the predictionset using the menus by clicking **Contribution PS | Distance to model Y**.

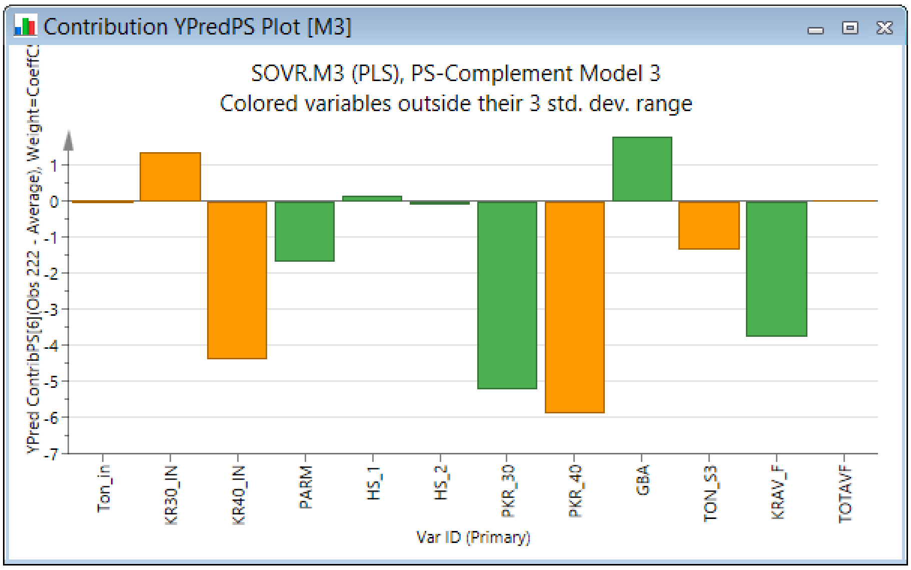
The **Contribution DModY** dialog that opens is identical to the one opened by clicking **Contribution | Distance to model Y** in the **Analysis** group on the **Analyze** tab. For more about this dialog and the available weights, see the Distance to model Y contribution plot section in Chapter 10, Analyze.



11.9.4 Y predicted contribution plot

With a PLS model, create the YPred contribution plot using the menus by clicking **Contribution PS | Y predicted**.

The **YPred Contribution** dialog that opens is identical to the one opened by clicking **Contribution | Y predicted** in the **Analysis** group on the **Analyze** tab. For more about this dialog and the available weights, see the Y Predicted contribution plot section in Chapter 10, Analyze.



11.9.5 Contribution plot from plot

Contribution plots can be created from plots displaying observations, that is, scores, Hotelling's T2Range, DModX, DModY, and Observed vs. Predicted plots.

To display a contribution plot not using the menus, use one of the following methods:

- Select the observations and click the relevant comparison plot in **Drill down** group on the **Marked items** tab.
- Double-click the point or column.
- Select the observations, right-click the selection, and click **Create | Contribution plot**.

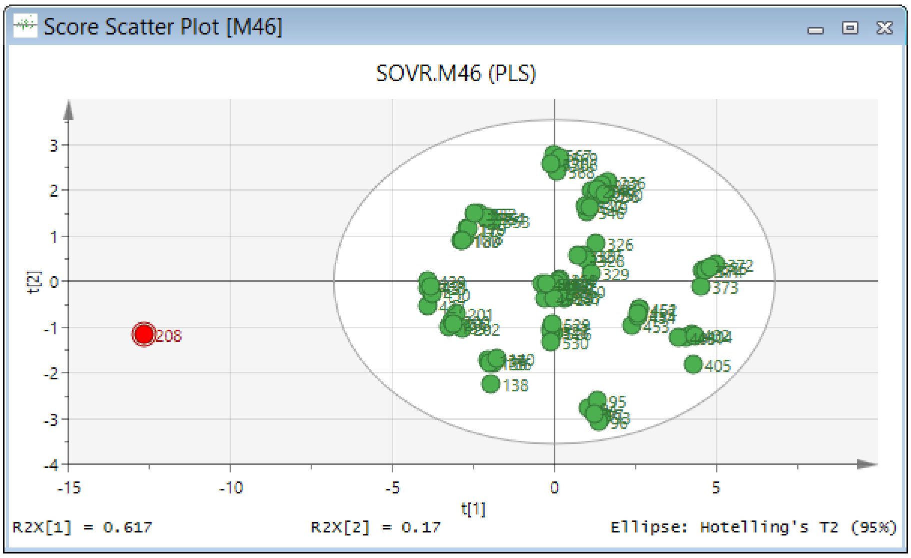
Note: Group contribution is not available from the Hotelling's T2Range plot.

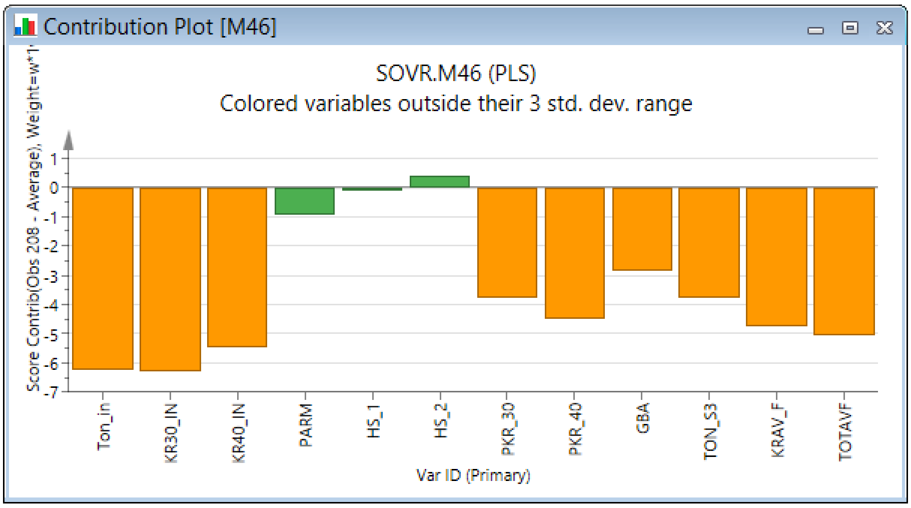
For more about the **Drill down** plots, see the Drill down group section in the Marked items tab section in Chapter 14, Plot and list contextual tabs.

11.9.5.1.1 Example of contribution plot directly from plot

In the example here, observation 208 was double-clicked in the score plot resulting in that the contribution plot comparing observation 208 to the average was displayed.

In the contribution plot, the variables are colored orange if the original variable is outside the ± 3 standard deviation limits for the investigated observations. To color outside 3 standard deviations is the default and changeable in Properties.





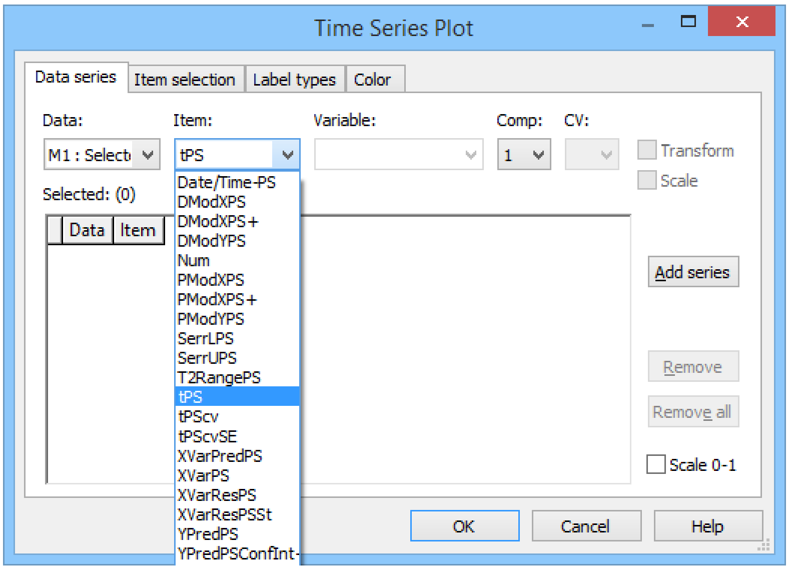
11.10 Time series PS

The **Time series PS** plots, display selected prediction vectors as series on the Y-axis and **Num** on the X-axis. The differences versus using the **Plot/List | Line** is that **Num**, or **Date/Time** when available, is always plotted on the X-axis and the vectors available in the **Item** box are the prediction vectors only.

To open a time series plot, click **Time series PS** in the **Plots** group on the **Predict** tab (or **Time series** in the **Control charts** group on the **Plot/List** tab).

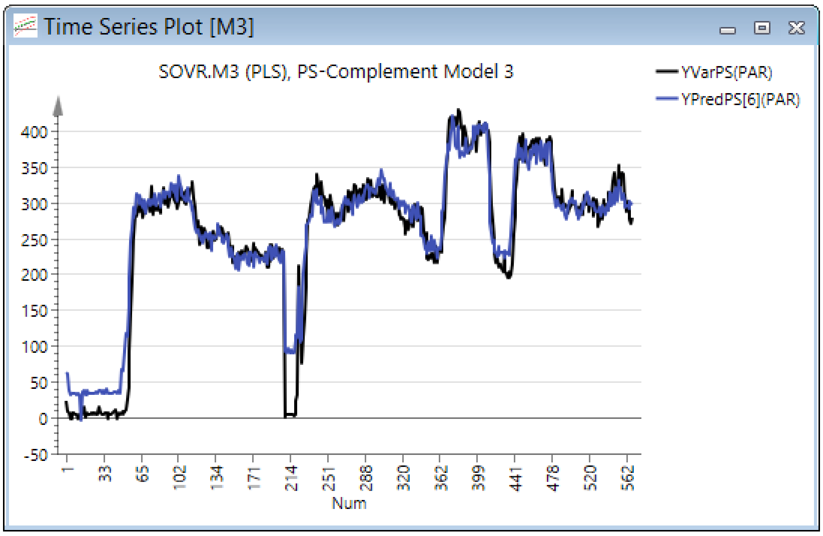
In the **Time Series Plot** dialog, select the vectors to plot in the **Item** box and click the **Add series**-button.

To display all vectors scaled to range 0 – 1, select the **Scale 0-1** check box.



11.10.1 Time series plot example

The plot here displays the observed y-variable in the predictionset, YVarPS, and the predicted y-variable, YPredPS.



11.11 ROC - Receiver operating characteristic

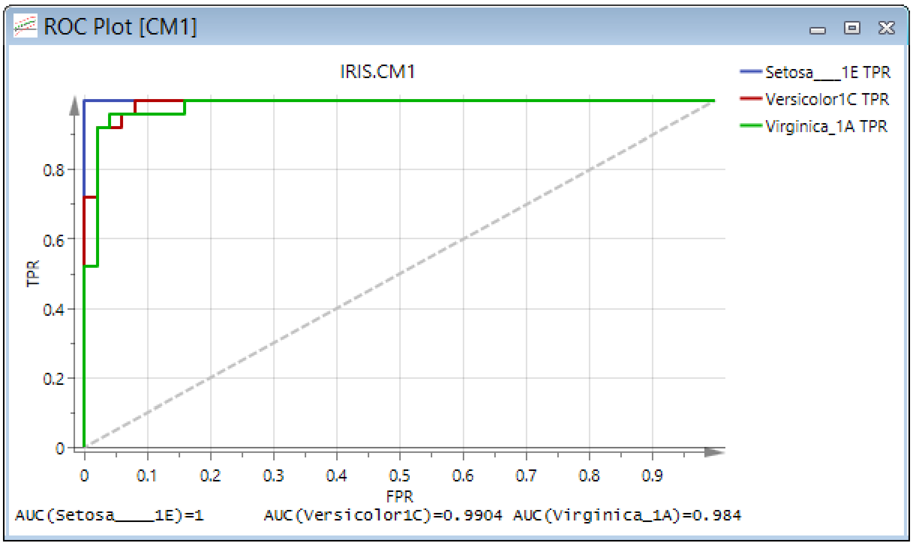
The **ROC** plot is available on the **Predict** tab for class and discriminant analysis models.

The ROC plot is a tool for visualizing and summarizing the performance of classification and discrimination models. This tool supplements the existing tools Coomans' plot, classification list and misclassification table, in the sense that it provides a quantitative measure of the performance of the model.

The ROC plot displays the true positive classification rate (TPR) of a classifier model plotted against the corresponding false positive classification rate (FPR) at various threshold settings of the criterion parameter (PModXPS for class models and YPredPS for DA models).

As a quantitative measure of the classification success the area under the (ROC) curve (AUC) is computed and visualized in the footer of the plot. This parameter ranges between 0.5 (bad classification) and 1.0 (perfect classification).

See the ROC background section in the Statistical appendix for more.



AUC(Setosa____1E)=1 AUC(Versicolor1C)=0.9904 AUC(Virginica_1A)=0.984

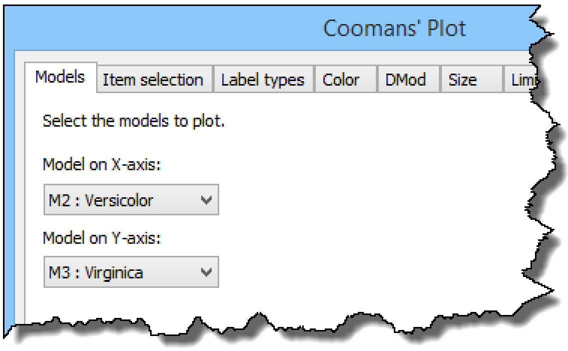
11.12 Coomans' plot

Use Coomans' plot to classify new observations with respect to two selected models.

For each observation in the predictionset, the distance to each of the selected models is computed and plotted along with the selected models' critical distances.

To display **Coomans' Plot**:

1. Specify the predictionset.
2. On the **Predict** tab, in the **Classification** group, click **Coomans' plot**.
3. In the **Coomans' Plot** dialog, select the two models to plot the DModXPS+ for.
4. Optionally click the **Color** tab and select to color by classes.
5. Click **OK**.



Select the models to plot.

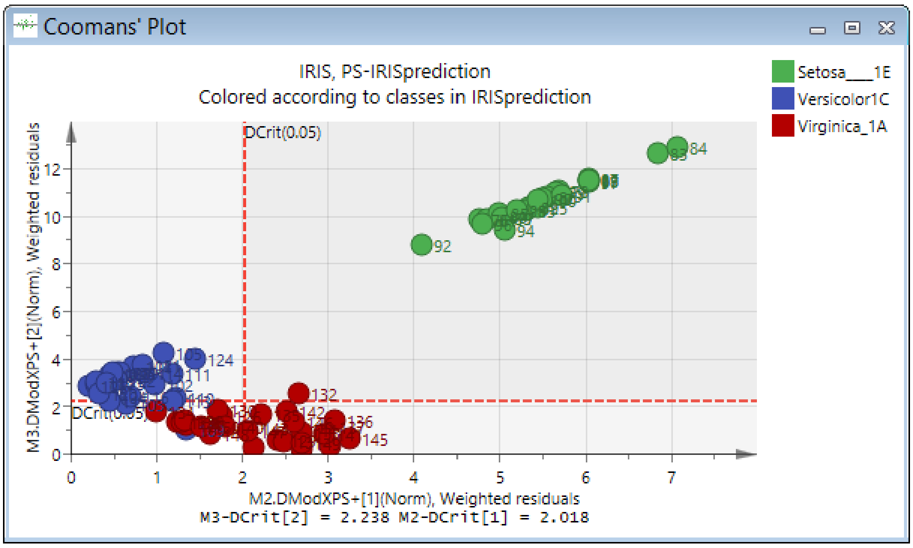
Model on X-axis:

M2 : Versicolor

Model on Y-axis:

M3 : Virginica

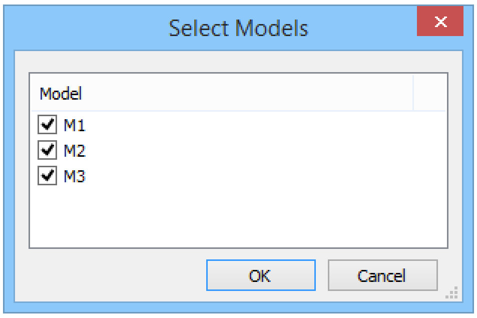
In the Limits page you can select to hide the critical lines. In the **DMod** page you can select to display **Regular** DModX. The other tabs are general and described in detail in the Properties dialog section in Chapter 14, Plot and list contextual tabs.



11.13 Classification list for class models

With class models you can automatically classify a predictionset with respect to all the class models by:

1. clicking **Classification list** in the **Classification** group on the **Predict** tab,
2. selecting the desired models, and clicking **OK**.



The **Classification List** displays the observations of the predictionset as rows, and the class models probability of membership, PModXPS+, as columns. The model title in the second row identifies the class.

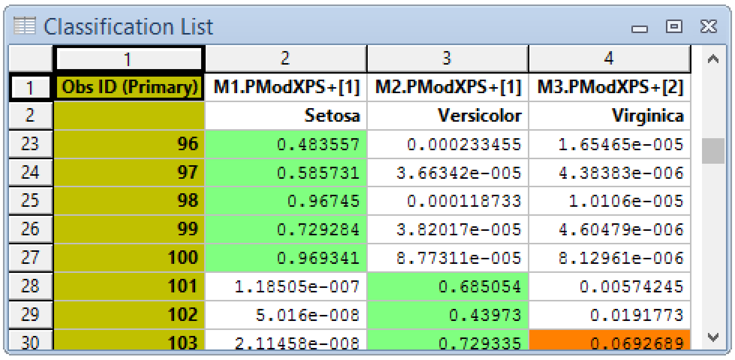
Note: By default the primary observation ID is displayed. To display all observation IDs, on the **Tools** tab, in the **Properties** group, click Labels. For more see the Label Types for lists subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs.

11.13.1 Coloring in the Classification List

The values displayed in the **Classification List** are probabilities.

The observations are colored such that probabilities:

- > 0.10 are green (inside 90% confidence of the normal probability curve).
- between 0.10 and 0.05 are orange (inside 95% confidence).
- < 0.05 are white and the observation is deemed to be outside the class (outside 95% confidence).



Classification List

	1	2	3	4
1	Obs ID (Primary)	M1.PModXPS+[1]	M2.PModXPS+[1]	M3.PModXPS+[2]
2		Setosa	Versicolor	Virginica
23	96	0.483557	0.000233455	1.65465e-005
24	97	0.585731	3.66342e-005	4.38383e-006
25	98	0.96745	0.000118733	1.0106e-005
26	99	0.729284	3.82017e-005	4.60479e-006
27	100	0.969341	8.77311e-005	8.12961e-006
28	101	1.18505e-007	0.685054	0.00574245
29	102	5.016e-008	0.43973	0.0191773
30	103	2.11458e-008	0.729335	0.0692689

11.14 Classification list for Discriminant Analysis models

The **Classification List** for discriminant analysis models provides the predicted Y value for the dummy variables (0 or 1) used to direct the projection.

The **Classification List** displays the observations of the predictionset as rows, and the original dummy variable in YVarPS and predicted dummy variable in YPredPS, as columns.

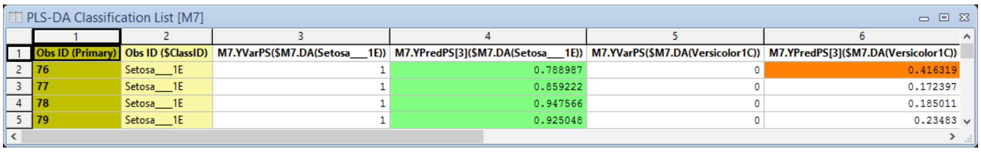
Note: By default all observation IDs are displayed. To display different IDs, on the **Tools** tab, in the **Properties** group, click Labels. For more see the Label Types for lists subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs.

11.14.1 Coloring in the Classification List

The values displayed in the **Classification List** for discriminant analysis models are the predictionset original values and predicted values.

The observations are colored such that predicted values:

- < 0.35 are white (do not belong to the class).
- between 0.35 and 0.65 are orange (borderline).
- above 0.65 are green (belong to the class).



PLS-DA Classification List [M7]

	1	2	3	4	5	6
1	Obs ID (Primary)	Obs ID ($ClassID)	M7.YVarPS($M7.DA(Setosa___1E))	M7.YPredPS[3]($M7.DA(Setosa___1E))	M7.YVarPS($M7.DA(Versicolor1C))	M7.YPredPS[3]($M7.DA(Versicolor1C))
2	76	Setosa___1E	1	0.788987	0	0.416319
3	77	Setosa___1E	1	0.859222	0	0.172397
4	78	Setosa___1E	1	0.947566	0	0.185011
5	79	Setosa___1E	1	0.925048	0	0.23483

Membership of a class depends upon matching the value of the dummy variable, so a value close to one indicates membership of the workset class. In practice 0.5 is often used as a practical threshold in order to classify an observation as belonging to one class or another.

11.15 Misclassification table

The **Misclassification table** is available for all class models and discriminant analysis models.

The **Misclassification table** shows the proportion of correctly classified observations in the predictionset.

If the class information is not available in the dataset that the predictionset was created from, the class information has to be defined. This is achieved by:

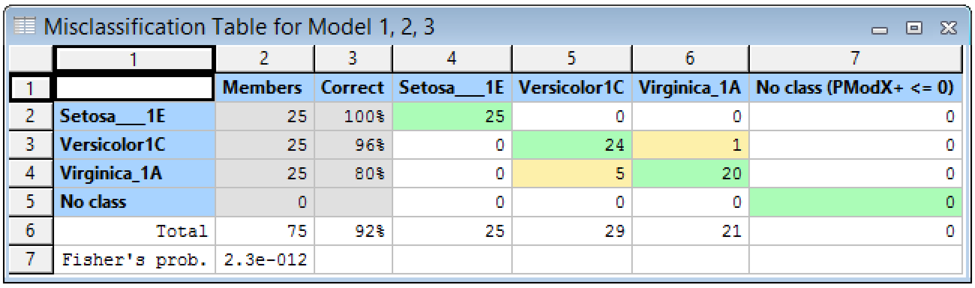
- Using the dataset **Properties** dialog, **Observations** page. See the Observations page subsection in Dataset summary section Chapter 8, Data.
- Specifying a **Class ID** while importing the file. See Class ID specification subsection in the Home tab section in Chapter 6, SIMCA import.

11.15.1 Misclassification table for class models

The **Misclassification table** is available for all class models.

With specified classes, the **Misclassification Table** summarizes how well the selected models classify the observations into the known classes. By default the **Assign each observation only to the nearest class** option is used (see the Properties dialog subsection described in the Misclassification table Properties subsection later in this chapter).

Note: In order to classify observations they all need appropriate class assignment, that is, they need to be assigned to the relevant classes. If the dataset used as prediction set lacks class assignment, there will be no estimates of correct classifications in this table. Setting classes can be done in Dataset Properties, Observations page.



Misclassification Table for Model 1, 2, 3

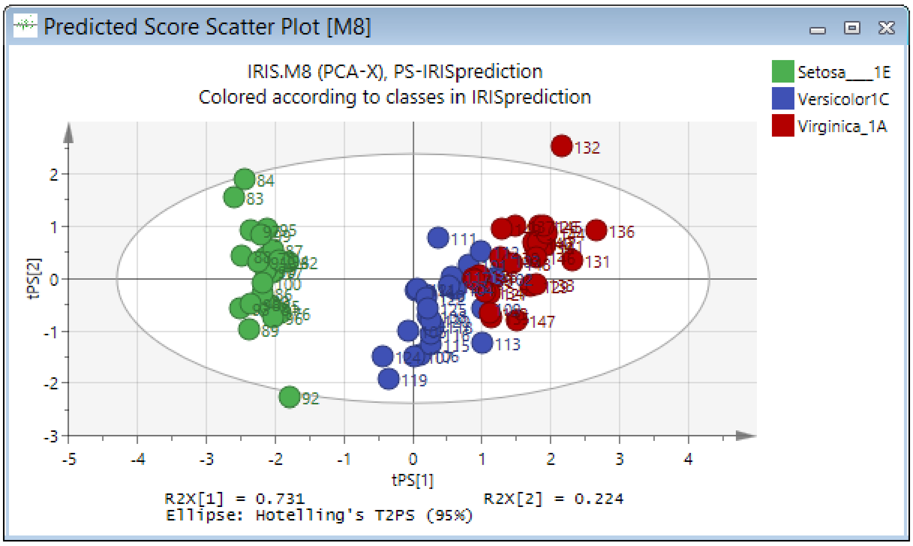
	1	2	3	4	5	6	7
1		Members	Correct	Setosa___1E	Versicolor1C	Virginica_1A	No class (PModX+ <= 0)
2	Setosa___1E	25	100%	25	0	0	0
3	Versicolor1C	25	96%	0	24	1	0
4	Virginica_1A	25	80%	0	5	20	0
5	No class	0		0	0	0	0
6	Total	75	92%	25	29	21	0
7	Fisher's prob.	2.3e-012					

The **Misclassification Table** is organized as follows:

Column	Content
First column	The class names, No class, Total, and Fishers probability. The **Total** row displays: the total number of observations in the predictionset, the average percentage correctly classified, and the number of observations classified to each class. Fisher's probability is the probability of the table occurring by chance and is satisfied when p < 0.05 for 95% confidence. For more, see the Fisher's exact test subsection in the Statistical appendix. Fisher's probability is displayed when **Assign each observation only to the nearest class** is the selected option in **Properties**.
Members	The number of observations assigned to each class in the selected predictionset. At the bottom of the list Fisher's probability value is listed.
Correct	The percentage correctly classified for each class and at the bottom the average percentage.
Individual classes	The number of observations classified as belonging to the class on that row. The correct classifications are colored green while the incorrect are colored yellow.
No class (PModX+<='limit')	The observations that are not classified to any one of the available classes.
Combined classes	The observations that overlap between classes. When **Assign all observations to classes above the limit** is selected, all combinations of classes are displayed with number of overlapping observations.

Note: All entries on the diagonal are observations that have been correctly classified.

In the above table, we can see that all the observations but 6 observations were correctly classified, one belonging to **Ver** was classified as **Vir**, and 5 belonging to **Vir** were classified as **Ver**. The reason for this is the closeness of the two classes, illustrated in the score plot here.

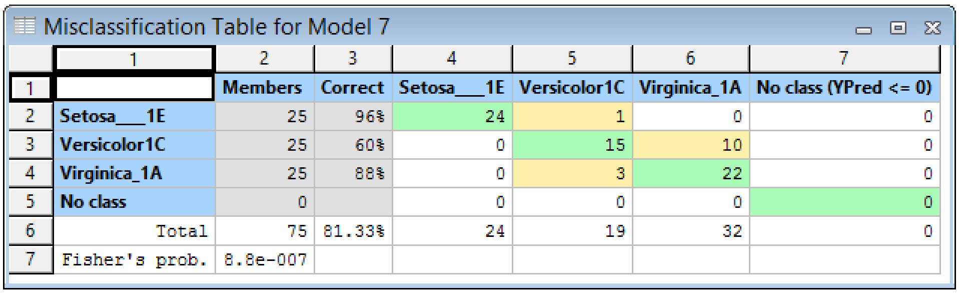


11.15.2 Misclassification table for Discriminant Analysis models

The **Misclassification table** is available for all discriminant analysis models.

By default the observations are assigned to the nearest class only, using no threshold.

To see the options available, see the Misclassification table Properties subsection later in this section.


Misclassification Table for Model 7

	1	2	3	4	5	6	7
1		Members	Correct	Setosa___1E	Versicolor1C	Virginica_1A	No class (YPred <= 0)
2	Setosa___1E	25	96%	24	1	0	0
3	Versicolor1C	25	60%	0	15	10	0
4	Virginica_1A	25	88%	0	3	22	0
5	No class	0		0	0	0	0
6	Total	75	81.33%	24	19	32	0
7	Fisher's prob.	8.8e-007					

For a description of the content of the table, see the Misclassification table for class models subsection earlier in this section.

11.15.3 Misclassification table Properties

The Misclassification table **Properties** dialog contains options to change the way of classifying the observations.

Use the **Properties** dialog to:

- Select models in the **Model(s)** box.
- Select how to classify the observations and probability level according to the method below.

11.15.3.1 Method for assigning observations

Select whether to assign each observation:

1. Only to the nearest class, with an optional PModX cut-off by clicking **Assign each observation only to the nearest class**.
2. To all classes if they exceed the probability limit listed by clicking **Assign observations to all classes above the limit**. When there are overlapping classes, or classes close to each other, this may result in that observations are assigned to several classes.

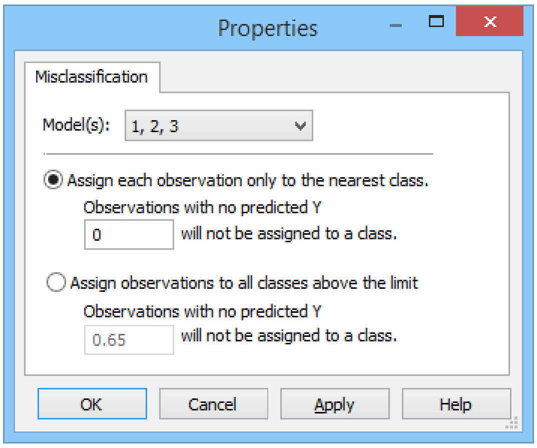
In the **Do not assign observations with PModX less than or equal to** 'limit' **will not be assigned to a class** field, optionally enter the probability limit to use.

A possible reason for entering a probability limit is in cases of unequally sized groups where the discriminating threshold may not be in the center of the projection.

The default values in this field are:

- '0' for **Assign each observation only to the nearest class** always.
- '0.1' for **Assign observations to all classes above the limit**, when the models are class models
- '0.65' for **Assign observations to all classes above the limit**, when the model is a DA-model. Another common value is '0.5'.

Note: The fields remember the last entered value.



Model(s): 1, 2, 3

● Assign each observation only to the nearest class.
Observations with no predicted Y
0 will not be assigned to a class.

○ Assign observations to all classes above the limit
Observations with no predicted Y
0.65 will not be assigned to a class.

11.16 What-If

The **What-If** feature is a simulation based on the active model, which for batches with phases means the selected phase. Marking a BEM is the same as marking the first phase as far as the What-If is concerned. This means that for a plot displaying all phases, and introducing changes in What-If, the changes apply only to the first phase.

The **What-If** allows you to graphically increase or decrease the values of selected variables and observe the effects in prediction plots. Technically, the predictionset expands to the double, adjusting for the introduced changes in the second half of the predictionset. This second part of the predictionset is named the What-If dataset and can be opened separately from the What-If pane.

Note: For batch projects with phases, changes in variables are made to one phase at a time.

11.16.1 Work process using What-If for regular models

An overview of the work process when working with regular projects follows:

1. Select a predictionset in the **Specify predictionset** group on the **Predict** tab.
2. In the Project Window, mark the desired model. With classes, marking a CM is the same as marking the first class model.
3. Open the **What-If** pane from the **View** or **Predict** tabs.
4. Select the desired What-If mode.
5. In **Select variables** select the variables you want to simulate a change in.
6. Introduce changes in the variables and investigate the effect in the prediction plots.

When you introduce the first change in a variable the default prediction plots open, Scores PS and DModXPS if no prediction plots are open. The original predictionset items are displayed in one color and the What-If predictions in another.

11.16.2 Work process using What-If for batch evolution models

An overview of the work process when working with batch evolution models follows:

1. Select a predictionset in the **Specify predictionset** group on the **Predict** tab.

2. In the Project Window, mark the desired phase model. Marking the BEM is the same as marking the first phase.
3. Open the **What-If** pane on the **View** or **Predict** tabs.
4. Select the desired What-If mode.
5. In **Select variables** select the variables you want to simulate a change in.
6. Introduce changes in the variables and investigate the effect in the prediction plots.
7. If you want to apply another offset at a later maturity;
    1. Click the plus-sign to add another row.
    2. Specify the start maturity either by selecting one in the list or by typing in the field.
    3. Specify and apply your new offset, applicable from that maturity until the end or the next specified maturity range.

When you introduce the first change in a variable the default prediction plots open, Scores PS BCC and DModXPS PS BCC if no prediction plots are open. The original predictionset items are displayed in one color and the What-If predictions in another.

11.16.3 Work process using What-If for batch level models

The work process when using the What-If with batch level models is the same as for regular models, see the Work process using What-If for regular projects subsection earlier in this section. This means that changes are specified and applied to the original variables.

When there are batch condition variables in the model these are found last in the variable list.

Note: Batch condition variables are only available in the variable list when available in the predictionset.

For details on specifying a predictionset for batch models, see the Batch predictionset section in Chapter 11, Predict.

11.16.4 What-If pane

The **Select variables** combo box lists all variables available in the workset of the current model. However, for batch level models the displayed variables are those of the batch evolution models the batch level models were created from, with the addition of batch condition variables when such variables are available in the predictionset.

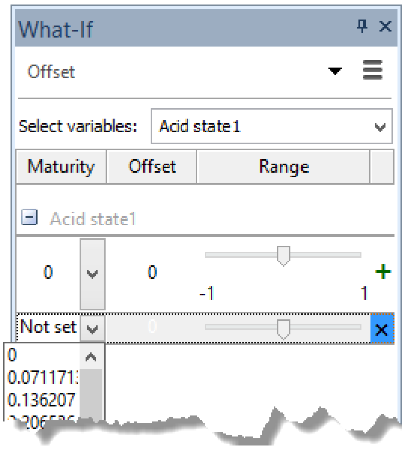
The available modes for the What-If are described in the What-If mode subsection next.

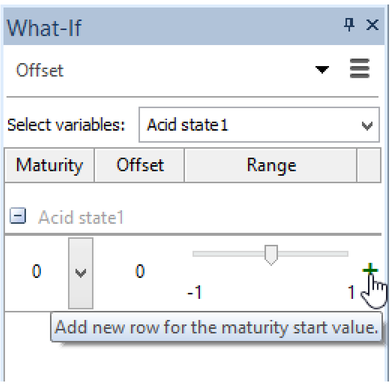
The commands available on the **Options** menu are described in the What-If Options menu subsection later in this section.

11.16.4.1 Variable sliders and columns

The columns available for the selected variables are:

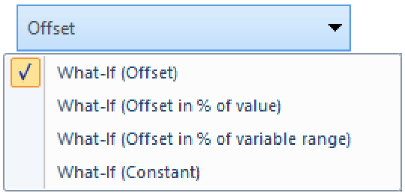
- **Maturity** - Only for batch evolution models. Allows you to specify from which maturity the specified variable adjustment should apply. The adjustment then applies until the end or the next specified maturity. Note that you can select one of the available maturities or type a maturity here.
- **Offset** - The value added to the What-If dataset. Available for the Offset modes. Note that you can type a value here.
- **Setpoint** - The constant value in the What-If dataset. Available for the Constant mode. Note that you can type a value here.
- **Variable range** - The slider with *Minimum slider value*, the current setting for the slider and the *Maximum slider value.* The minimum and maximum slider values can be changed by typing in the value fields beneath the slider endpoints.
- New row plus-sign - Only for batch evolution models. When clicked, another row is added for that variable, allowing you to introduce a new offset/setpoint starting from another maturity.





11.16.4.2 What-If mode

There are four What-If modes.


Offset
✓ What-If (Offset)
What-If (Offset in % of value)
What-If (Offset in % of variable range)
What-If (Constant)

11.16.4.2.1 Offset

With **Offset** selected, changing a variable adds that value to all items in the expanded part of the predictionset, the What-If dataset. The slider range is by default that of the variable in the workset, centered at the median of the variable range in the predictionset.

11.16.4.2.2 Offset in percent of value

With **Offset in % of value** selected, the added offset is expressed in percent of the original variable value. For example, specifying 10% results in that for that variable each value will be the original value times 1.1.

11.16.4.2.3 Offset in percent of range

With **Offset in % of range** selected, the added offset is expressed in percent of the workset variable range. For example, specifying 10% for a variable with the range 55 results in that for that variable each value is increased with 5.5.

11.16.4.2.4 Constant

With **Constant** selected, the selected setpoint is the value used for that variable in the What-If dataset.

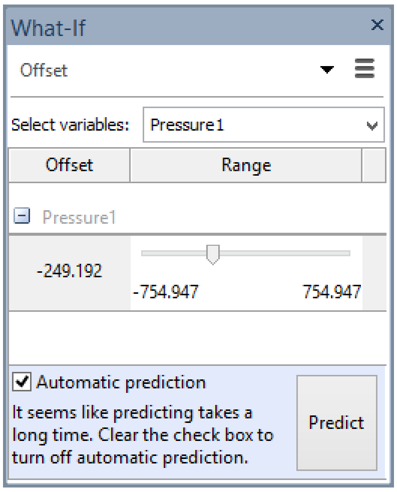
The slider range is by default the range of the variable in the workset.

11.16.4.3 What-If Options menu

In the **Options** menu you can:

- **Create default plots** - opens the Score PS and DModXPS plots for regular and batch level models, Score PS BCC and DModX PS BCC for batch models.
- **Reset sliders** - moves all sliders to their default positions and resets the What-If dataset to the default.
- **View What-If dataset** - opens the current What-If dataset.
- **Save as dataset -** saves the current What-If dataset to the entered dataset name.
- **Automatic prediction** is by default selected, which means that after each change in the What-If, the predictionset and the open prediction plots are updated. Disabling **Automatic prediction** by clicking it enables the **Predict** button at the bottom of the What-If pane, so that you can manually predict when done with the variable adjustments.

Note: SIMCA displays a message at the bottom of the What-If pane suggesting to turn **Automatic prediction** off when the predictions take more than 2 seconds.



What-If

Offset

Select variables: Pressure1

Offset	Range
Pressure1	
-249.192	-754.947 754.947

☑ Automatic prediction

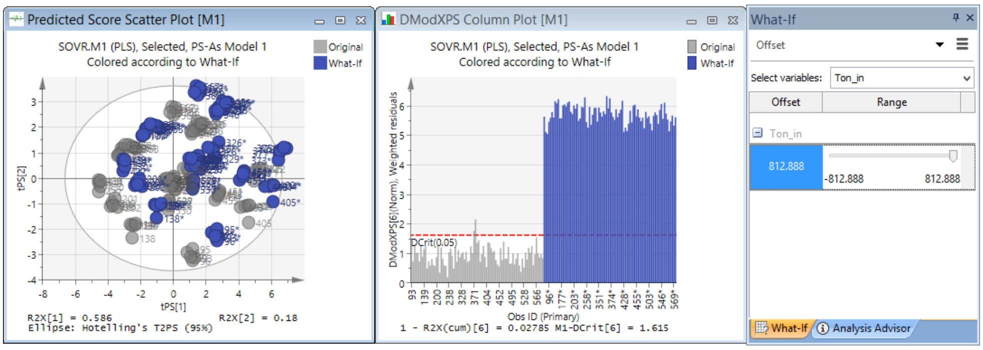
It seems like predicting takes a long time. Clear the check box to turn off automatic prediction.

Predict

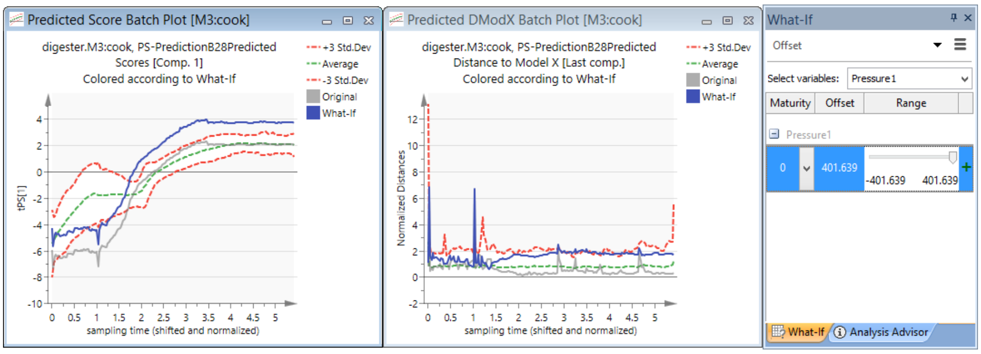
11.16.5 What-If results

The What-If predictions are by default displayed in blue while the original variables are gray. With column plots, the first set of columns refers to the original observations and the second set to the modified observations.

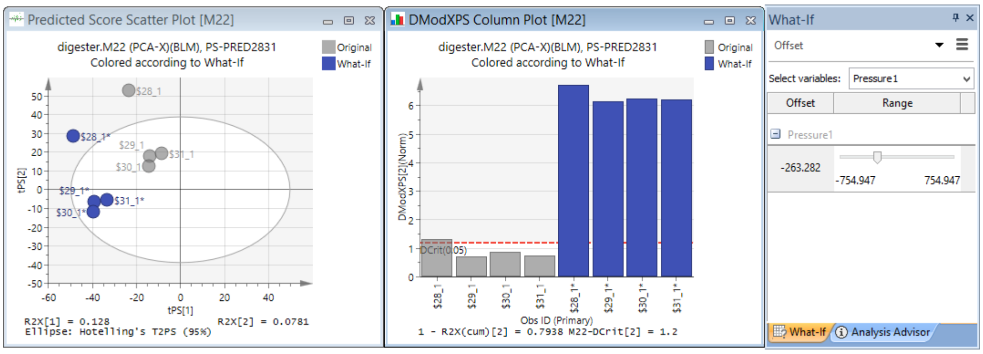
Regular


Predicted Score Scatter Plot [M1]
SOVR.M1 (PLS), Selected, PS-As Model 1
Colored according to What-If
Original
What-If
tPS[2]
tPS[1]
R2X[1] = 0.586
R2X[2] = 0.18
Ellipse: Hotelling's T2PS (95%)
DModXPS Column Plot [M1]
SOVR.M1 (PLS), Selected, PS-As Model 1
Colored according to What-If
Original
What-If
DModXPS[6](Norm), Weighted residuals
DCrit(0.05)
Obs ID (Primary)
1 - R2X(cum)[6] = 0.02785 M1-DCrit[6] = 1.615
What-If
Offset
Select variables: Ton_in
Offset
Range
Ton_in
812.888
-812.888
812.888
What-If
Analysis Advisor

Batch evolution model, BEM


Predicted Score Batch Plot [M3:cook]
digester.M3:cook, PS-PredictionB28Predicted
Scores [Comp. 1]
Colored according to What-If
+3 Std.Dev
Average
-3 Std.Dev
Original
What-If
tPS[1]
sampling time (shifted and normalized)
Predicted DModX Batch Plot [M3:cook]
digester.M3:cook, PS-PredictionB28Predicted
Distance to Model X [Last comp.]
Colored according to What-If
Normalized Distances
What-If
Offset
Select variables: Pressure1
Maturity
Offset
Range
Pressure1
0
401.639
-401.639
401.639
What-If
Analysis Advisor

Batch level model, BLM


Predicted Score Scatter Plot [M22]
digester.M22 (PCA-X)(BLM), PS-PRED2831
Colored according to What-If
Original
What-If
$28_1
$28_1*
$29_1
$31_1
$30_1
$29_1*
$31_1*
$30_1*
tPS[2]
tPS[1]
R2X[1] = 0.128
R2X[2] = 0.0781
Ellipse: Hotelling's T2PS (95%)
DModXPS Column Plot [M22]
digester.M22 (PCA-X)(BLM), PS-PRED2831
Colored according to What-If
DModXPS[2](Norm)
DCrit(0.05)
Obs ID (Primary)
1 - R2X(cum)[2] = 0.7938 M22-DCrit[2] = 1.2
What-If
Offset
Select variables: Pressure1
Offset
Range
Pressure1
-263.282
-754.947
754.947
What-If
Analysis Advisor

Note: When the predictionset includes observations also in the model (workset), the DModXPS will be slightly smaller for the items not in the model. See the Absolute distance to the model of an observation in the workset subsection in the Statistical appendix.

12Plot/List

12.1 Introduction

This chapter describes the **Plot/List** tab features.

The **Plot/List** tab allows plotting and listing input data such as observations and variable values, computed elements such as scaling weights, variable variances, etc., as well as results such as loadings, scores, predictions, etc., of all the fitted models.

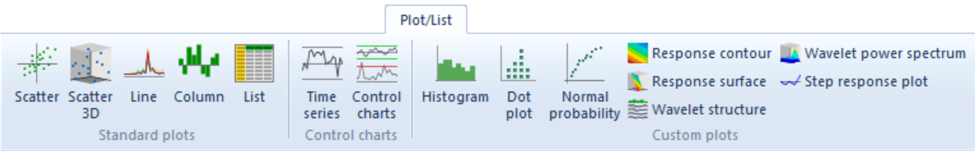
The plot types available on the **Plot/List** tab are:

- The **Standard plots** and list: **Scatter**, **Scatter 3D**, **Line**, **Column**, and **List**.
- The **Control charts: Time series** and **Control charts**.
- The **Custom plots: Histogram**, Dot plot, **Normal probability**, **Response contour**, **Response surface**, **Wavelet structure**, **Wavelet power spectrum** and **Step response plot**.

The plot types in the **Standard plots** group are not described in this user guide, but the dialog interface is described in this chapter.

Content

This chapter describes the following plots: Control charts, Response contour, Response surface, Wavelet structure, Wavelet power spectrum, and the Step response plot.



12.2 Name conventions

Some vectors have letters appended to them at the end of the item (vector) name. These indicate the source of the data, e.g. intermediate model results from cross validation rounds, statistics computed from all the cross validation rounds, or other information about the presented vector.

***Note**: Vectors containing Y are available for PLS, OPLS, and O2PLS models but unavailable for PCA models.*

See the table for the added endings and their description.

Ending	Description
DS	Any DataSet. Variables or observations in datasets are always the original raw variables with no role definition, or treatment. To access them, select the appropriate dataset in the **Data** box in the **Plot/List** dialog.
PS	The current PredictionSet. There is only one current predictionset at any time. Variables or observations in predictionsets are always the original raw variables with no role definition, or treatment. All items with the two letters PS are available when selecting a model in the **Data** box. All items without the two source letters are part of the selected model i.e., they pertain to variables or observations in the workset associated with the model. To plot or list variables from the predictionset directly, select the predictionset as data source in the **Data** box.
cv	Intermediate results such as scores, loadings, PLS weights, predicted values, etc., computed from a selected cross validation round.
cvSE	Jack-knife standard error computed for model results from all the cross validation rounds.
St	The vector is in standardized units, i.e. divided by its standard deviation.
(trans)	The vector is in transformed units according to the workset specification.

Ending	Description
(as WS)	The vector is displayed in the same units as the workset, WS. This means that a variable scaled to unit variance in the workset is displayed in scaled and centered units, while a transformed variable is displayed in the transformed metric, scaled and centered.
Cum	The vector is cumulative over all components up to the listed one. **Note**: There are a number of vectors that are cumulative without displaying this ending.
OOCSum	The vector is an Out Of Control summary vector.

12.3 Plot/List general dialog

The following commands on the **Plot/List** tab open a general dialog with a selection of the pages listed below: **Scatter**, **Scatter 3D**, **Line**, **Column**, **List**, **Time series**, **Control chart**, **Histogram**, **Dot plot**, and **Normal probability**.

A selection of the following pages is available in the different **Plot/List** dialogs: **Data series**, **Label types**, **Item selection**, **Color**, **Transformation**, **Size**, **Limits**, and **Number format**.

The Data series and Transformation pages are unique to the **Standard plot** group items (Scatter, Scatter 3D, Line, Column, List) and are described in the subsections that follow.

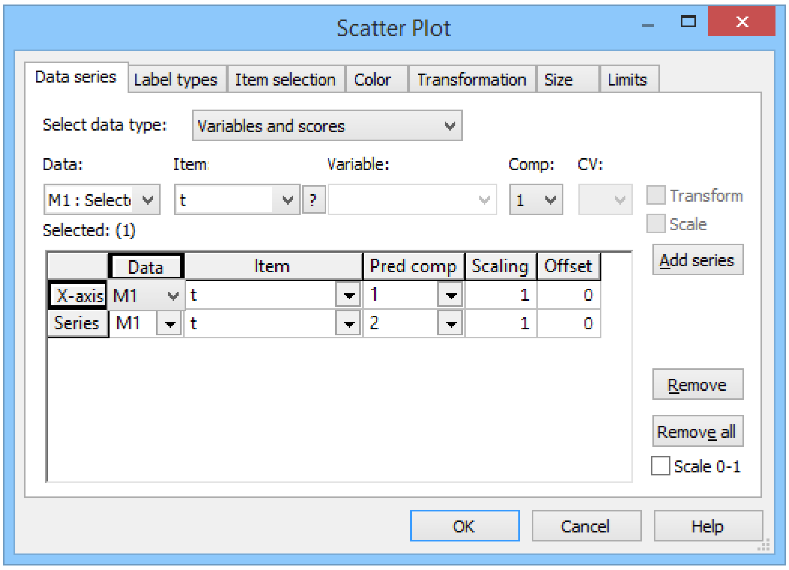
For more about the other pages, see the Properties dialog subsection in Tools tab section in Chapter 14, Plot and list contextual tabs.

12.3.1 Data series page

In the **Data series** page the vectors (series) to be displayed in the selected plot or list can be selected. To make the vector available in the **Item** box, the appropriate data type and data source have to be selected. Some vectors require selecting a variable, component(s), or CV group and some can be displayed in transformed and scaled units.

The list of currently added series is displayed in the **Selected** list. To remove series from the list, select them and click the **Remove** button, or click the **Remove all** button.

By selecting the **Scale 0-1** check box all series are scaled so that the maximum value is 1 and minimum is 0.



Select data type: Variables and scores

Data: M1 : Select　Item: t　Variable:　Comp: 1　CV:

□ Transform
□ Scale

Selected: (1)

	Data	Item	Pred comp	Scaling	Offset
X-axis	M1	t	1	1	0
Series	M1	t	2	1	0

□ Scale 0-1

Note: When the dataset contains numerical IDs, they can be selected and plotted on any axis.

12.3.1.1 Select data type

Before selecting the data series for plotting, the appropriate data type has to be selected from the **Select data type** box.

The available data types are:

- **Variables and scores** – vectors with one element per observation.
- **Observations and loadings** – vectors with one element per variable.

- Function of component, **F(Component)** – vectors that apply per component.
- Function of Lags, **F(Lags)** – vectors specific to a lagged model, such as pLag.
- **Aligned vectors** – aligned vectors available in batch control charts for batch evolution models.
- **Batch vectors** – Out Of Control (OOC) variables for the aligned vectors for batch evolution models.

12.3.1.2 Data source

By default the active model is the selected data source. For computed elements such as scaled variable values, variable variances, model results, or intermediate results from cross validation, the data source can only be a fitted model, not a dataset.

The data sources available in the **Data** box are:

1. **DS1** – dataset first imported.
2. **DS2**, **DS3** etc. – other datasets.
3. **PS** – current predictionset.
4. **M1**, **M2** etc. – fitted models.

To access items specific to another data source than the default, select the data source in the **Data** box.

For instance, for datasets preprocessed using Orthogonal Signal Correction (OSC), the OSC scores and loadings are available after selecting the OSCed dataset in the **Data** box.

12.3.1.3 Item

In the **Plot/List** tab dialogs, all items from the selected data type and source are available in the **Item** box.

Some vectors require selecting:

- Variable from the **Variable** box.
- Dimension from the **Component** box for some model results.
- Cross validation round from the **CV** box for intermediate results from cross validation.

Some items, such as DModX, are available for component 0, which correspond to scaled and centered data as specified in the workset (WS).

For Hotelling's **T2Range** specifying the starting and ending components is required.

Note: Vectors containing Y are available for PLS, OPLS, and O2PLS models but unavailable for PCA models.

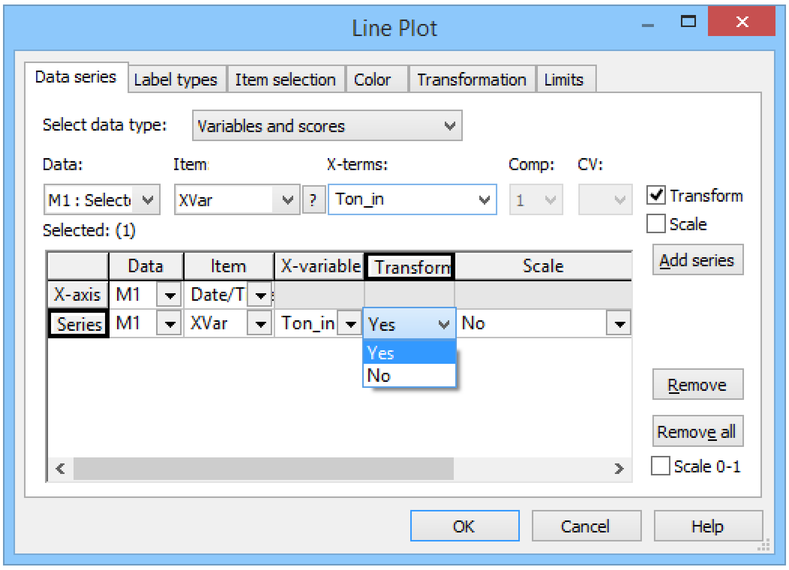
For a description of all vectors available for the **Plot/List** tab plot types, see the Vectors available in SIMCA section in the Statistical appendix.

12.3.1.4 Scale and Transform

When there are transformed variables in the model, many vectors can be displayed in the transformed metric. These same vectors can always be displayed scaled as the workset. Examples of such vectors are XVar and XVarRes.

- Select the **Transform** check box, before clicking **Add series**, to display the vector in the transformed metric. Or after adding the vector, in the **Selected** list, select **Yes** in the **Transform** column on the row of the vector.
- Select the **Scale** check box before clicking **Add series**, to display the vector in the metric of the workset. Or after adding the vector, in the **Selected** list, select **Yes** in the **Scale** column on the row of the vector.

For example, with **Scale** selected, a variable scaled to unit variance in the workset is displayed in scaled and centered units. If the variable was transformed, it is displayed in the transformed metric, scaled and centered. Hence, when selecting the **Scale** check box, the **Transform** check box is automatically selected.



Select data type: Variables and scores

Data: M1 : Selecti | Item: XVar | X-terms: Ton_in | Comp: 1 | CV:

☑ Transform

□ Scale

Selected: (1)

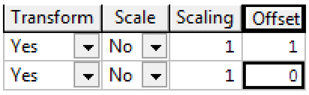
	Data	Item	X-variable	Transform	Scale
X-axis	M1	Date/T			
Series	M1	XVar	Ton_in	Yes	No

□ Scale 0-1

Note: *When both the* ***Scale*** *and* ***Transform*** *boxes are cleared, the added vector is displayed in original (back-transformed) units.*

12.3.1.5 Scaling and Offset

Specifying a **Scaling** value or **Offset** value is useful with **Line** and **Time series plots** when the selected vectors need to be visually separated.



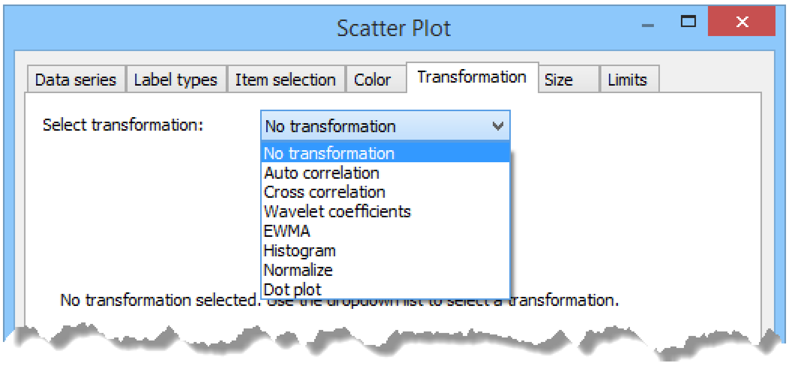
Transform	Scale	Scaling	Offset
Yes	No	1	1
Yes	No	1	0

After adding the series, enter values in the **Scaling** and/or **Offset** columns in the **Selected** list.

12.3.2 Transformation

On the **Transformation** page the following data transformations are available:

- Auto correlation
- Cross correlation
- Power spectrum
- Wavelet coefficients
- EWMA
- Histogram
- Normalize
- R2X
- Dot plot



Select transformation: No transformation

No transformation selected. Use the dropdown list to select a transformation.

12.3.2.1 Auto or cross correlation of variables or observations

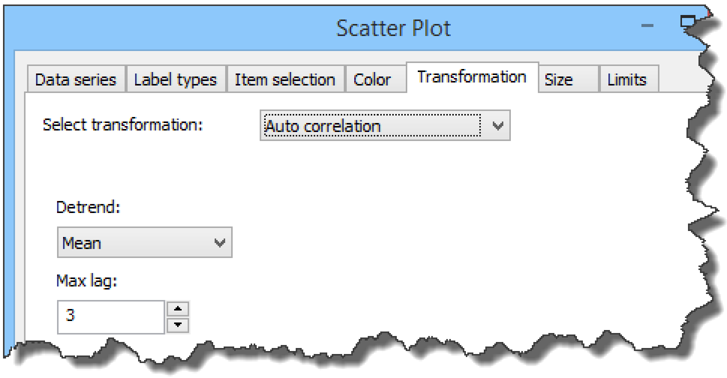
The auto and cross correlation are measures of dependence of adjacent observations and characterizes a time series or observation profile, in the time domain.

For technical details, see the Auto and cross correlation of variables or observations section in the Preprocessing appendix.

12.3.2.1.1 Applying Auto correlation

To apply auto correlation to a variable or observation;

1. On the **Plot/List** tab, click **Scatter**, **Line**, **Column** or **List**.
2. Select the desired vector on the **Data series** page.
3. Click the **Transformation** tab.
4. Select **Auto correlation** in the **Select transformation** box.
5. In the **Detrend** box the default is **Mean**. Select
   a. **Linear** to remove the best linear fit, or
   b. **None** to do nothing, or
   c. leave **Mean** to remove the mean.
6. To change maximum lagging, type a new value in the **Max lag** field. The auto correlation is default max lag L=30 or N/4, whichever is smaller, and can be displayed up to L=N.



Select transformation: Auto correlation

Detrend: Mean

Max lag: 3

12.3.2.1.2 Applying cross correlation

To apply cross correlation to a variable or observation:

1. On the **Plot/List** tab, click **Scatter**, **Line**, **Column** or **List**.
2. Select the desired vector on the **Data series** page.
3. Click the **Transformation** tab.
4. Select **Cross correlation** in the **Select transformation** box.

5. **Select the common vector to use cross correlation with** by selecting data source in the **Data** box, vector in the **Item** box, and if applicable, variable in the **Variable** box, component in the **Comp** box, and cross validation group in the **CV** box.

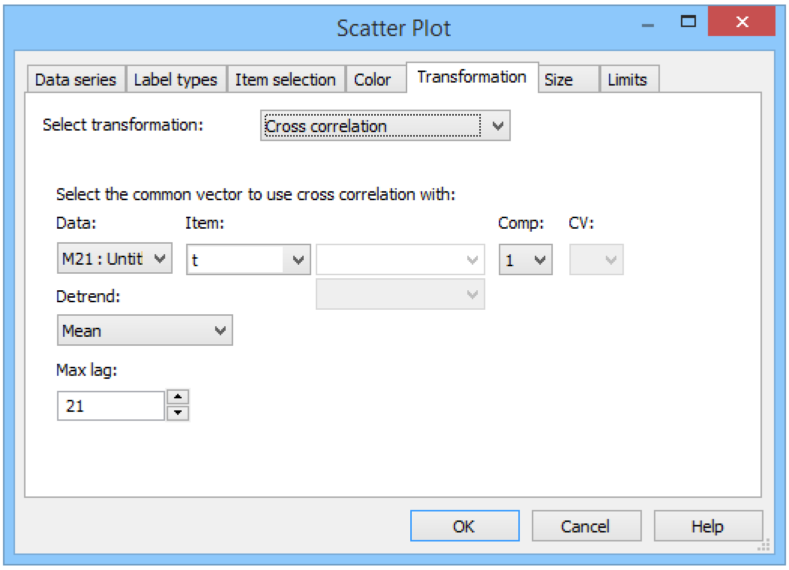
6. In the **Detrend** box the default is **Mean**. Select

   a. **Linear** to remove the best linear fit, or

   b. **None** to do nothing, or

   c. leave **Mean** to remove the mean.

7. To change maximum lagging, type a new value in the **Max lag** field. The auto correlation is default max lag L=30 or N/4, whichever is smaller, and can be displayed up to L=N. The plot displays the cross correlation for –L to +L.



Select transformation: Cross correlation

Select the common vector to use cross correlation with:

Data: M21 : Untit

Item: t

Comp: 1

CV:

Detrend: Mean

Max lag: 21

12.3.2.1.3 Spectral filtered wavelet data

With a dataset that has been wavelet transformed and compressed variable wise (using **Spectral filters** on the **Data** tab), the auto/cross correlation observation wise refers to the reconstructed observations, when the **Reconstruct wavelets** check box is selected.

To display the auto/cross correlation in the wavelet domain clear the **Reconstruct wavelets** check box found in **Project Options** dialog opened by clicking **File | Options | Project options**.

12.3.2.2 Power spectrum density of variables or observations

The power spectrum density (PSD) is the representation of the sequence x (t) in the frequency domain. The power spectrum is the square of the amplitude of the Fourier component at each frequency.

The frequency domain representation is particularly helpful to detect irregular cycles and pseudo periodic behavior, i.e. tendency towards cyclic movements centered on a particular frequency.

SIMCA uses the Welsch’s non-parametric method to estimate the PSD.

For more information see the Power spectrum density section in the Preprocessing appendix.

12.3.2.2.1 Spectral filtered wavelet data

With a dataset that has been wavelet transformed and compressed variable wise (using **Spectral filters** on the **Data** tab), the PSD observation wise refers to the reconstructed observations, when the **Reconstruct wavelets** check box is selected.

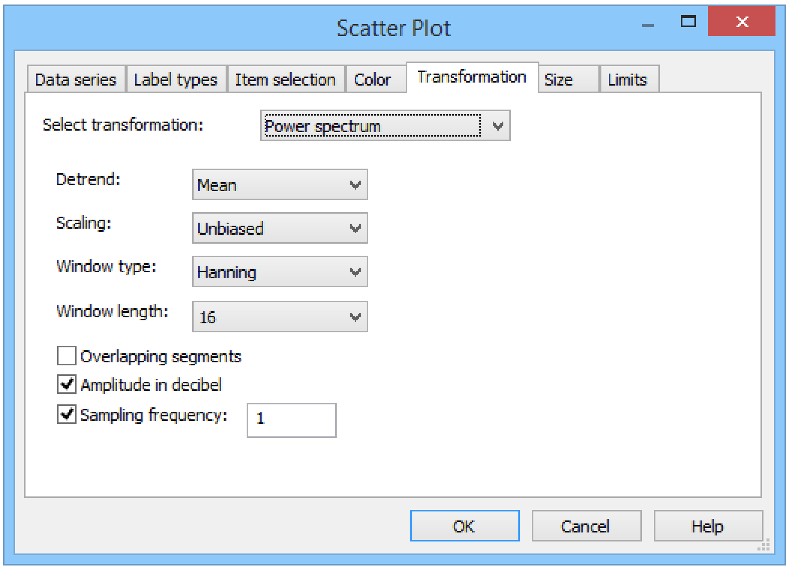
To display the PSD in the wavelet domain, clear the **Reconstruct wavelets** check box found in the **Project Options** dialog opened by clicking **File | Options | Project**.

12.3.2.2.2 Applying power spectrum

To apply the Power Spectrum to an observation or a variable, either use the Plot/List dialog described here, or use the **Quick info**:

1. Select the desired vector on the **Data series** page.
2. Click the **Transformation** tab.
3. Select **Power spectrum** in the **Select transformation** box.

Change the options as warranted and click **OK** to create the plot. For more about these options see the Power spectrum options tab subsection in the Quick info section in Chapter 13, View.



Select transformation: Power spectrum

Detrend: Mean

Scaling: Unbiased

Window type: Hanning

Window length: 16

□ Overlapping segments

☑ Amplitude in decibel

☑ Sampling frequency: 1

12.3.2.3 Wavelet coefficients

The wavelet transform of a signal X(t) is the representation of the signal in both the time and frequency domain. It is the scalar product between the signal x(t) and a mother wavelet function, stretched or compressed to create different scales (inverse of frequency), changing the window width.

Because of the repeated re-scaling, the variable or observation is decomposed into its details at every scale; these are the wavelet transform coefficients.

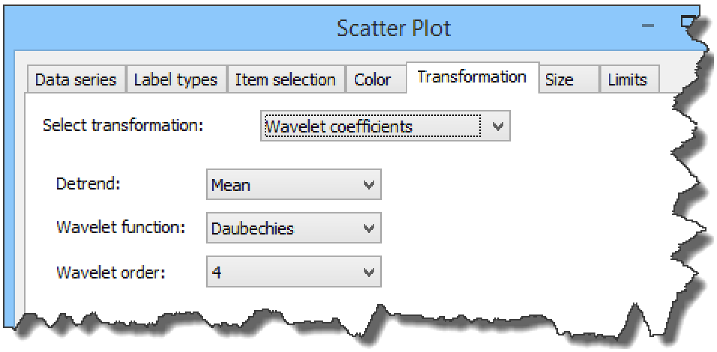
SIMCA uses the Discrete Wavelet transform, with orthogonal or biorthogonal wavelets and the fast Multi Resolution Analysis algorithm of S. Mallat.

Select the variables or observations you want to wavelet transform and the range of observations or variables to include.

12.3.2.3.1 Applying wavelet coefficients

To apply the wavelet coefficients to an observation or a variable, either use the **Plot/List** dialog described here, or **Spectral filters** in the **Filter** group on the **Data** tab:

1. Select the desired vector on the **Data series** page.
2. Click the **Transformation** tab.
3. Select **Wavelet coefficients** in the **Select transformation** box.
4. Change from the default detrending, wavelet function, and wavelet order if warranted. For more details about these options, see Wavelet transformations section in the Preprocessing appendix.



Scatter Plot

Select transformation: Wavelet coefficients

Detrend: Mean

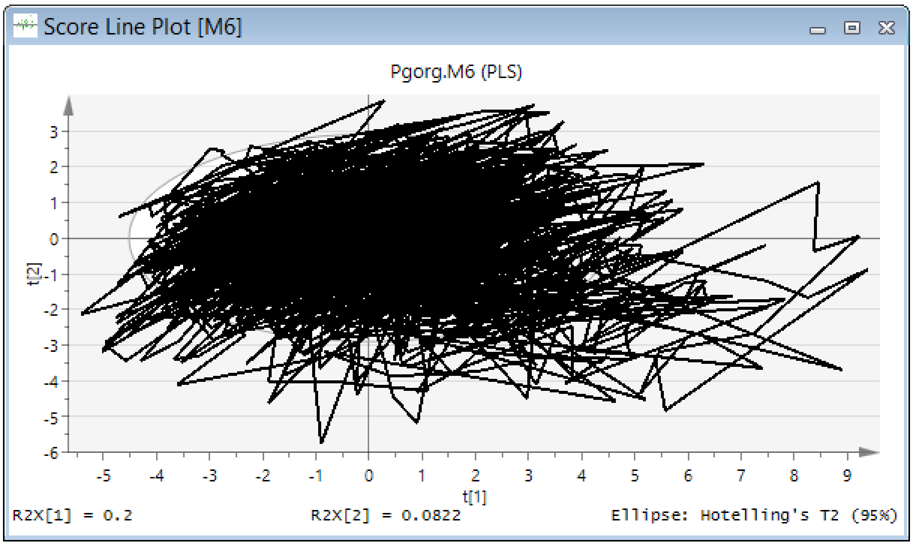
Wavelet function: Daubechies

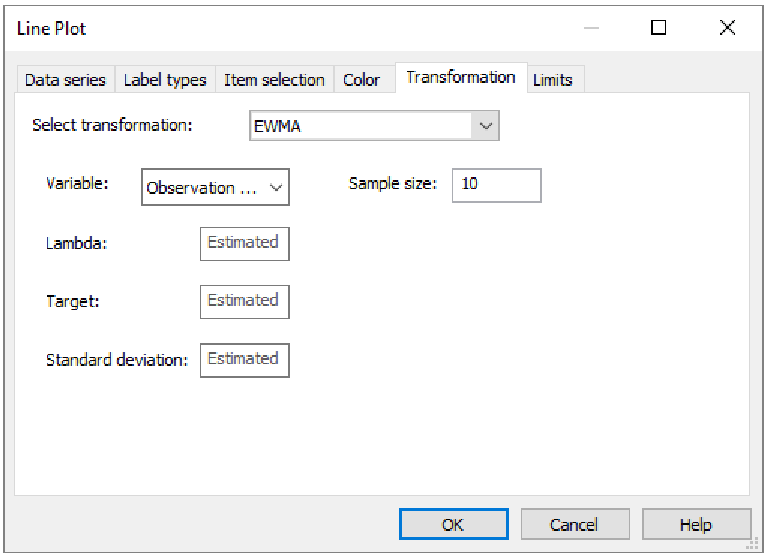
Wavelet order: 4

12.3.2.4 EWMA transformation

The EWMA transformation can be used to smooth scores or variables in plots.

As an example the following line score plot of t1 vs. t2 was transformed by EWMA and selecting subgroup 10.





Line Plot

Select transformation: EWMA

Variable: Observation ...

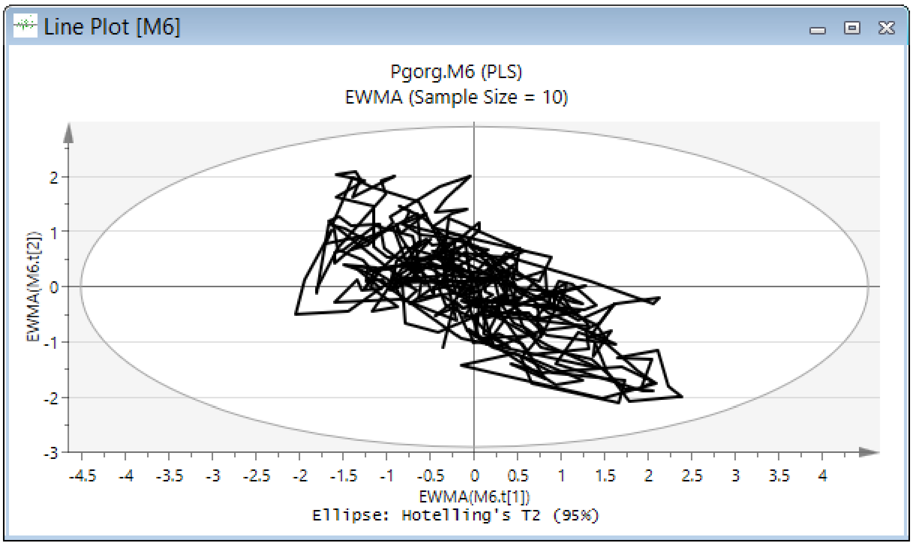
Sample size: 10

Lambda: Estimated

Target: Estimated

Standard deviation: Estimated

The EWMA transformed plot is easier to interpret.



12.3.2.4.1 Applying the EWMA transformation

To apply the EWMA to an observation or a variable:

1. Select the desired vector on the **Data series** page.
2. Click the **Transformation** tab.
3. Select **EWMA** in the **Select transformation** box.
4. In **Variable**, select **Observation group** or a variable under the Time range/Variable range headers.

a. With **Observation groups** selected, enter the desired sample size in the **Sample size** field (default 5).

b. With a monotonically increasing variable selected, enter the desired subgroup range in the units of the variable.

c. With a monotonically increasing time variable selected, enter the desired time range in the storing unit specified at import.

5. Select **User entered** in the **Target** box and enter a value in the field, or leave **Estimated**.
6. Select **User entered** in the **Standard dev.** box and enter a value in the field, or leave **Estimated**.
7. Click **OK**.

12.3.2.5 Histogram

To transform an observation or a variable to a histogram:

1. Select the desired vector on the **Data series** page.
2. Click the **Transformation** tab.
3. Select **Histogram** in the **Select transformation** box.
4. Click **OK**.

Note: Histogram is available in the Transformation page when only one series was added.

Histograms can also be created by clicking **Histogram** in the **Custom plots** group on the **Plot/List** tab.

12.3.2.6 Normalize in Transformation page

OPLS and O2PLS loading plots are by default normalized to unit length (**Normalize to unit length** check box is selected in **Properties**). When creating loading plots on **Plot/List** tab, the **Transformation** page must be used.

The **Normalize** transformation is only available for the vectors p, po, q, qo, so, and r when the model type is OPLS and O2PLS.

The normalization will make the sum of squared vector elements equal to 1. One advantage with this is that the loading line plots of spectral data are much easier to interpret. Normalize transformed loading plots should be used in conjunction with R2X transformed score plots.

12.3.2.7 R2X in Transformation page

OPLS and O2PLS score plots are by default scaled proportionally to R2X (**Scale proportionally to R2X** check box is selected in **Properties**). When creating score plots on **Plot/List** tab, the **Transformation** page must be used.

The **R2X** transformation is only available for the vectors t, to, u, uo, tPS and toPS when the model type is OPLS and O2PLS.

The R2X transformation will make distances in the score plot correspond with the explained variation (R2X). R2X transformed score plots should be used in conjunction with normalized loading plots.

12.3.2.8 Dot plot

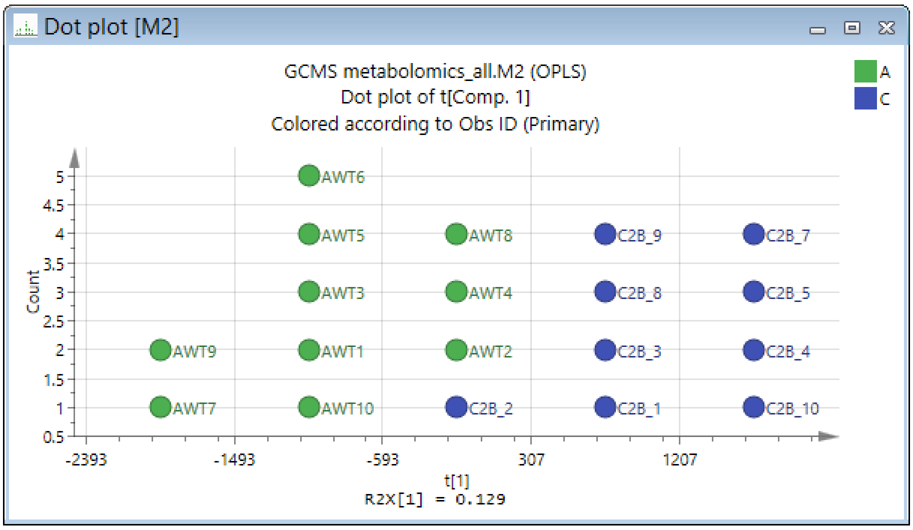
The dot plot is an alternative to the histogram and shows the distribution of a vector, but gives a better view of any separation present in the vector when colored according to the separating vector. You can color the dot plot as any scatter plot and also sort it by class. When sorting the dot plot by class, the sorting is done within each bin.

The dot plot can be created by clicking **Dot plot** in the **Custom plots** group on the **Plot/List** tab and as a **Transformation** in the general **Scatter** plot on the **Plot/List** tab; as the former is straight forward, the latter is described here.

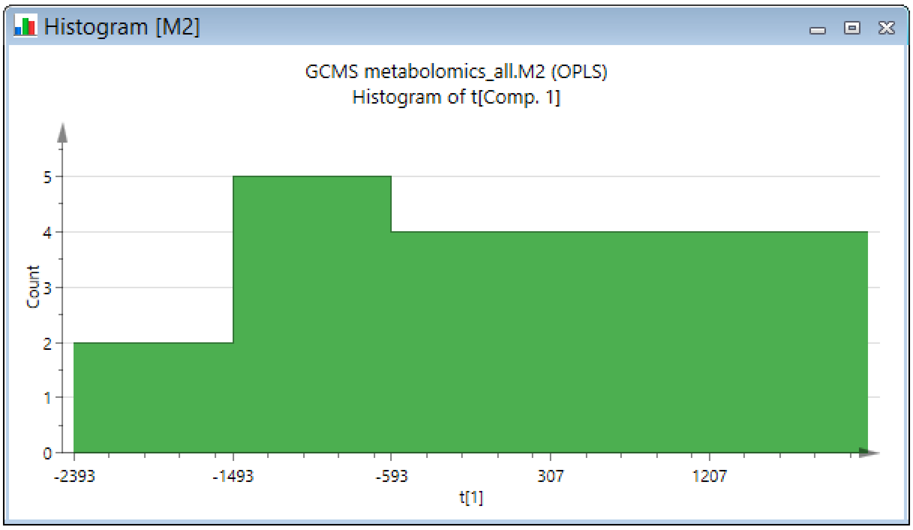
To transform a vector to a dot plot:

1. On the Plot/List tab, click **Scatter**.
2. On the **Data series** page, select Num on the x-axis and the desired vector (one) as series.
3. Click the **Transformation** tab.
4. Select **Dot plot** in the **Select transformation** box.
5. Click **OK**.

Note: **Dot plot** is available in the **Transformation** page when only one series was added and the X-axis is Num.



The corresponding histogram:



12.4 Control charts

Control charts are available on the **Predict** and **Plot/List** tabs.

The control charts from the **Predict** tab, will only display items from the predictionset. Opening the control chart from the **Plot/List** tab includes both the predictionset and workset vectors (items).

The **Control chart** group on the **Plot/List** tab holds both **Control chart** and **Time series** whilst this section only documents the **Control chart**. For more about the **Time series** plot, see the Time series PS section in Chapter 11, Predict.

12.4.1 What is a control chart?

The nature of process data is often noisy why individual observations are often grouped together in subgroups prior to visualization. Such averaging of data reveals trends more clearly. Sub groups can be based on a set number of observations or on a time range. Some control charts then display the variable range and/or standard deviation within each subgroup.

Control charts, also called statistical process control charts, constitute one of the major tools of “Total Quality Management”. They enable displaying the data measured on the process (or product) over time, and thereby detect process upsets, shifts, trends, etc., thus helping to improve the quality of the products.

However, processes generate collinear multivariate data. Therefore, monitoring and charting each variable as if it is independent from the others (univariate control charts) may be highly misleading, and may actually lead to the degradation of the product quality. *Multivariate* control charts use *all* the process variables simultaneously, and also extract the information contained in their correlation structure. This allows tracking of the process over time, identify process points and regions where the process is operating normally, as well as when the process starts to go out of control.

Because the scores (T and U) are linear combinations of the original variables, they are close to normally distributed as long as the process is stable. The scores are also much less noisy than the original variables since they have the characteristics of weighted averages. Hence, multivariate control charts are more reliable than univariate charts, and in addition much more informative.

12.4.1.1 Multivariate control charts

Multivariate control charts are model dependent, because the combination of all the variables to summaries are made *via* a multivariate model, here PCA, PLS, OPLS or O2PLS.

PC models

With a principal components (PC) model, the scores (T) are the best summary of all the process variables. Using the score values of one model dimension (t1, t2, etc.) as the control chart variable, yields a multivariate control chart based on all the process variables. The chart shows the position of the process along the direction of the specified model dimension. This chart can be used to track and follow the process as summarized by that dimension.

PLS models

With a PLS model, the X-scores (T) provide the best summary of the process variables that dominate the product qualities, and the Y-scores (U) provide the best summary of the product quality. Control charting the t-vectors or the u-vectors allows tracking the process using all the data.

OPLS and O2PLS models

For OPLS and O2PLS models, the X-scores (T) provide the best summary of the process variables that dominate the product qualities, and the Y-scores (U) provide the best summary of the product quality. Control charting the t-vectors or the u-vectors allows tracking the process using all the data.

In addition, the charting of To and Uo open up for analysis of the orthogonal information.

12.4.1.2 Univariate control charts

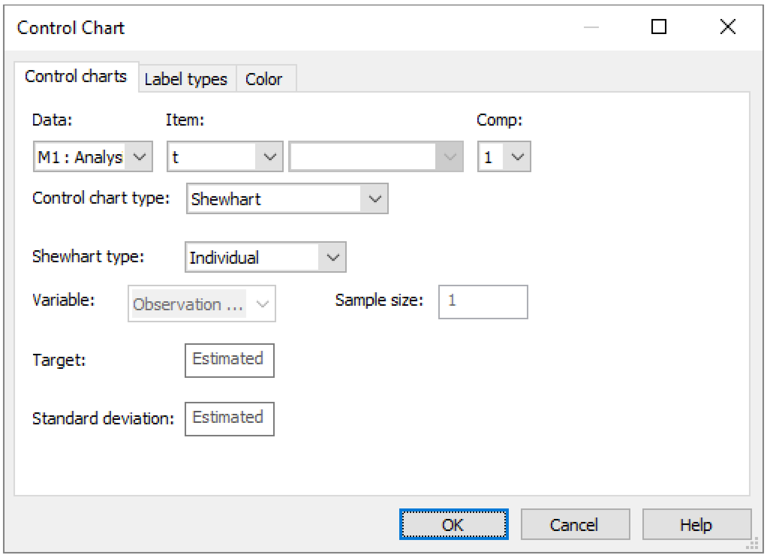
Univariate control charts are model independent, and can be plotted for a specified dataset.

To display a univariate control chart with some observations excluded: create an appropriate model. Control charting a variable from the model displays only the observations of that model's workset.

Note: *To look at special details of a variable, create control charts of an individual variable.*

12.4.2 Control Chart dialog

To open the **Control Chart** dialog, click **Control chart PS** in the **Plots** group on the **Predict** tab or **Control chart** in the **Control charts** group on the **Plot/List** tab.


Control Chart

Data: M1 : Analys

Item: t

Comp: 1

Control chart type: Shewhart

Shewhart type: Individual

Variable: Observation ...

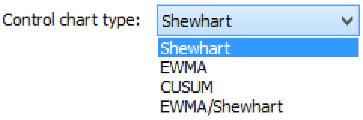
Sample size: 1

Target: Estimated

Standard deviation: Estimated

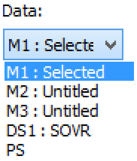
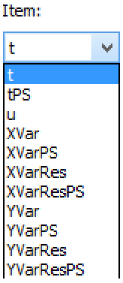
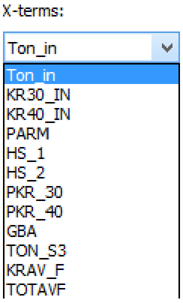
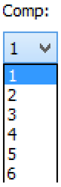
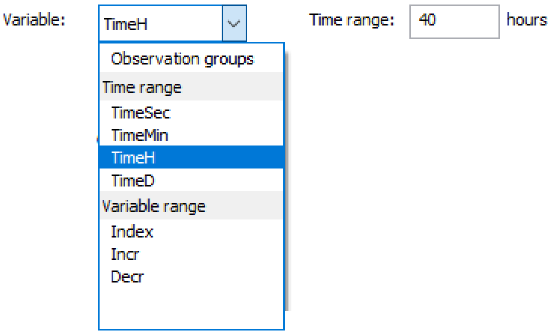
12.4.2.1 Types of control charts

There are four types of control charts available in the **Type of control chart** box: **Shewhart**, **EWMA**, **CUSUM**, and **EWMA/Shewhart**.


Control chart type: Shewhart

12.4.2.2 Selecting vector and x-axis options for control charts

To select the vector (item) to display in the control chart:

Step	Description	Action	Screen shot
1	In the **Data** box, the available data sources are listed. The data sources are the models (Mxx), datasets (DS1, DS2, etc.) and the current predictionset (PS).	Select the data source in the **Data** box.	 Data: M1 : Selecte M1 : Selected M2 : Untitled M3 : Untitled DS1 : SOVR PS
2	**In the Item box**, the available items are listed: **t**, **u**, **XVar**, **XVarRes**, **YVar** and **YVarRes**.	Select the vector in the **Item box**.	 Item: t t tPS u XVar XVarPS XVarRes XVarResPS YVar YVarPS YVarRes YVarResPS
3	For univariate control charts the variables are listed in the **Variable/X terms/Y terms box**. For the X terms the expanded terms are also listed.	Select the variable in the **Variable/X terms/Y terms box**.	 X-terms: Ton_in Ton_in KR30_IN KR40_IN PARM HS_1 HS_2 PKR_30 PKR_40 GBA TON_S3 KRAV_F TOTAVF
4	**In the Comp** box, the components for the selected vector are listed when the vector is a score or residual vector.	Select the **component** to display the vector for in the **Comp box**.	 Comp: 1
5	The Variable box, available for all control charts that can be displayed with subgroups specified. In the **Variable** box, observation groups, or any monotonically increasing variable or time variable are listed.	Select the Variable to use to specify the subgroups in the control chart. With **Observation groups**, the subgroups will be filled with as many samples as specified in **Sample size**, starting from the beginning of the data in the model.	 Variable: TimeH Time range: 40 hours Observation groups Time range TimeSec TimeMin TimeH TimeD Variable range Index Incr Decr

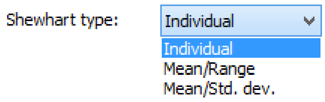
Step	Description	Action	Screen shot
		With a Time range variable, the range specifying the subgroup size is defined by the parsing at import. With Variable range, the range is specified in the units of the selected variable.	

***Note**: To display multivariate control charts of t or u, and for items from the predictionset, you must select a model in the **Data** box.*

12.4.2.3 Shewhart

Three types of Shewhart charts are available in SIMCA:

- **Individual** (default) – where the sample size is 1.
- **Mean/Range** – where the default sample size, when using observation groups, is 5 and can be changed as desired. Grouping can be applied using any monotonically increasing variable or time variable.
- **Mean/Std. dev.** – where the default sample size, when using observation groups, is 5 and can be changed as desired. Grouping can be applied using any monotonically increasing variable or time variable.


Shewhart type: Individual

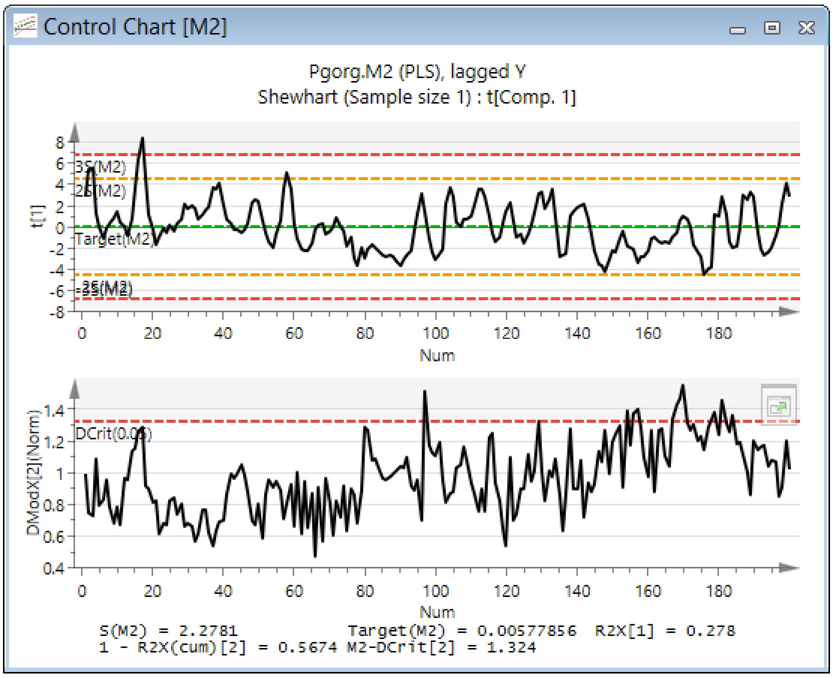
Individual

To create the **Shewhart** control chart without subgroups:

1. Click **Control chart**.
2. Select **Shewhart** in the **Type of control chart** box.
3. Leave **Individual** (the default) selected in the **Shewhart type** box, and then click **OK**.

The resulting plot displays the **Shewhart** control chart with values for each observation of the selected vector, with the 2 and 3 sigma limits displayed.

When plotting t or tPS, a plot of DModX or DModXPS is displayed beneath, with its critical distance. Observations outside the critical distance indicate process behavior different from the model.



Control Chart [M2]

Pgorg.M2 (PLS), lagged Y
Shewhart (Sample size 1) : t[Comp. 1]

```
S(M2) = 2.2781            Target(M2) = 0.00577856  R2X[1] = 0.278
1 - R2X(cum)[2] = 0.5674 M2-DCrit[2] = 1.324
```

The plot footer displays: **S(Mxx)**, **S(UE)** when defined, **Target(Mxx)** or **Target(UE)** when defined, **R2X[a]**, **1 – R2X(cum)[last component]** and **Mxx – DCrit[last component]**.

To view the nomenclature and calculations of target and standard deviation, see the Nomenclature and notation and Target and Standard deviation subsections in the Statistical appendix.

12.4.2.3.1 Mean/Range

When creating a Shewhart control chart of type Mean/Range, any monotonically increasing variable available can be used. When the plotted data originates from a model, any monotonically increasing variable in any of the included datasets, can be used to base the subgroups on, whether included or not.

To create the **Shewhart** control chart of type **Mean/Range**:

1. Click **Control chart**.
2. Select **Shewhart** in the **Type of control chart** box.
3. Select **Mean/Range** in the **Shewhart type** box.
4. In **Variable**, select **Observation group** or a variable under the Time range/Variable range headers. The value displayed in the plot is the average of the subgroup.

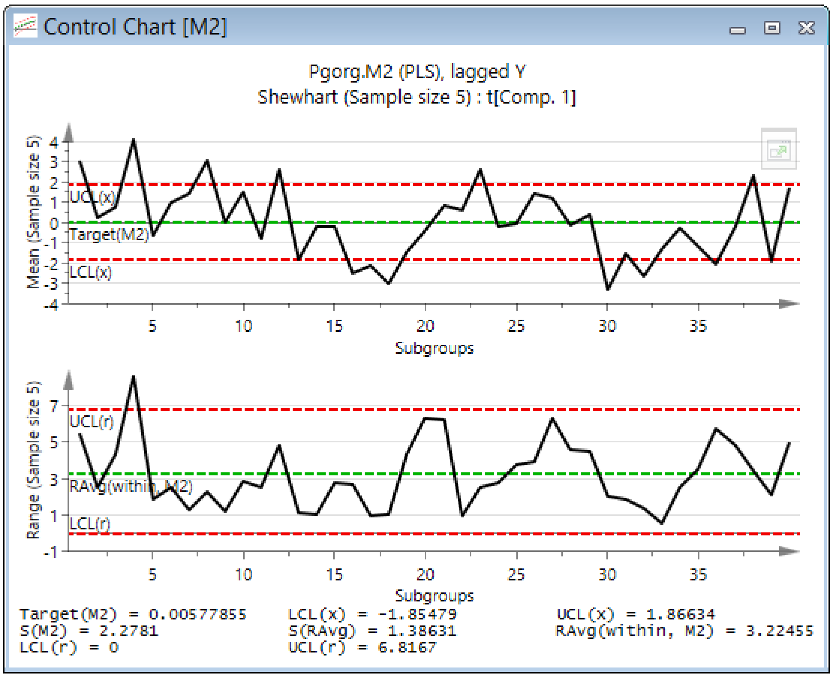
a. With **Observation groups** selected, enter the desired sample size in the **Sample size** field (default 5).

b. With a monotonically increasing variable selected, enter the desired subgroup range in the units of the variable.

c. With a monotonically increasing time variable selected, enter the desired time range in the storing unit specified at import.

5. Click **OK**.

The resulting plot displays the control charts for the selected vector, with the target and upper and lower limits displayed.



```
Target(M2) = 0.00577855    LCL(x) = -1.85479    UCL(x) = 1.86634
S(M2) = 2.2781             S(RAvg) = 1.38631    RAvg(within, M2) = 3.22455
LCL(r) = 0                 UCL(r) = 6.8167
```

The plot footer displays: **Target(Mxx)** or **Target(UE)** when defined, **LCL(x)**, **UCL(x)**, **S(Mxx)**, **S(RAvg)** or **S(UE)** when defined, **RAvg(within, Mxx** or **S(UE)** when defined), **LCL(r)** and **UCL(r)**.

To view the nomenclature and calculations of target and standard deviation, see the Nomenclature and notation and Target and Standard deviation subsections in the Statistical appendix.

Control limits and process range

Control limits and estimates of the process range in the **Shewhart Mean/Range** control chart are computed as follows:

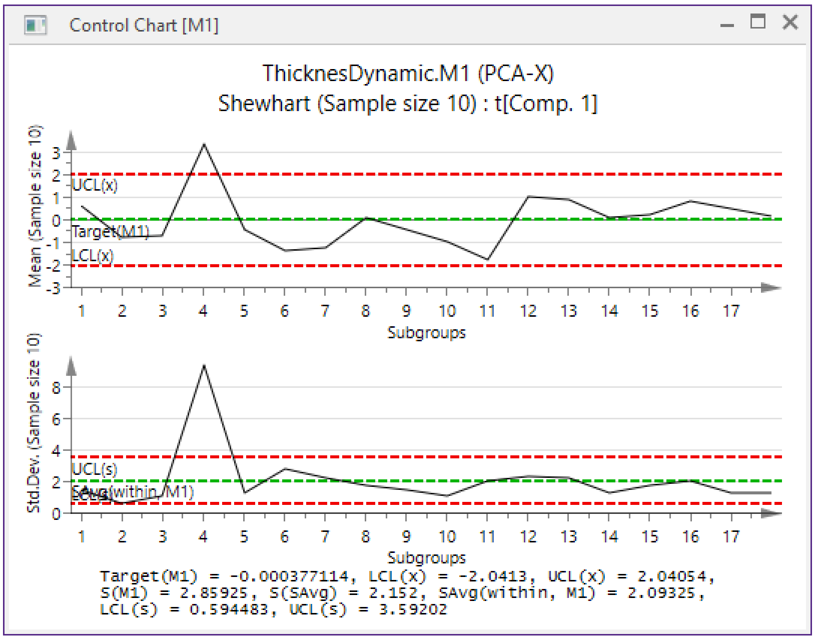
- S(RAvg) = RAvg /d2, estimate of process standard deviation.
- LCLx = Target - A2*RAvg
- UCLx = Target + A2*RAvg
- RAvg = Average range of subgroup (RAvg)
- LCLr = D3*RAvg
- UCLr = D4*RAvg
- D3, D4, A2, d2 are from McNeese. Reference McNeese, W.H., Klein, R.A., (1991) *Statistical methods for the process industries,* Quality and Reliability/28, chapter 16 table 1, p. 224.

12.4.2.3.2 Mean/Range using time range

When creating a Shewhart control chart of type Mean/Range., any monotonically increasing variable available can be used. The value displayed in the plot is the average of the subgroup.

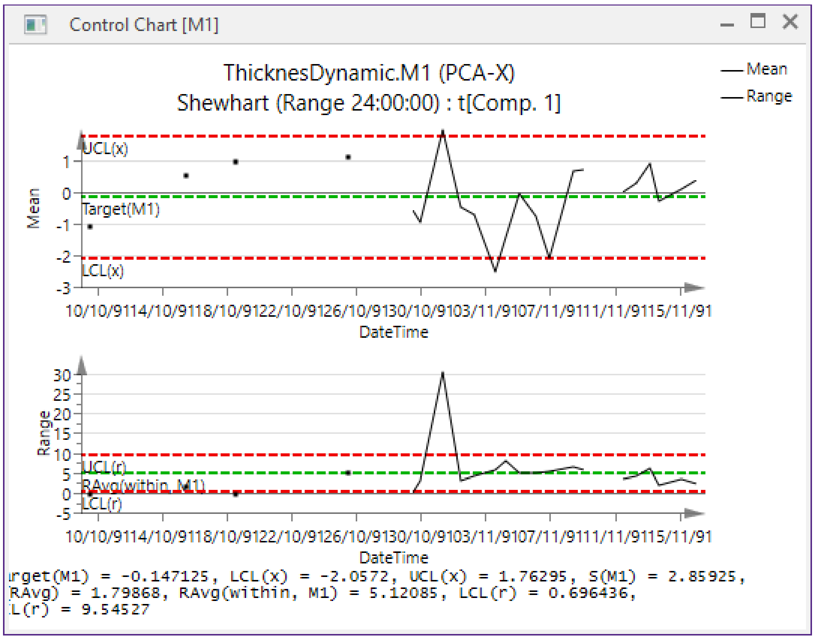
When the plotted data originates from a model, any monotonically increasing variable in any of the included datasets, can be used to base the subgroups on, whether included or not.

Applying groups based on time range is useful to review e.g. daily process changes since number of observations per day, hour etc may vary. For instance, in the first plot below the subgroups are defined as 10 per subgroup. Here we get no impression of how time matters.



```
Target(M1) = -0.000377114, LCL(x) = -2.0413, UCL(x) = 2.04054,
S(M1) = 2.85925, S(SAvg) = 2.152, SAvg(within, M1) = 2.09325,
LCL(s) = 0.594483, UCL(s) = 3.59202
```

In this second plot, where each subgroup is 1 day long, the time influence is clear. Note that the sub group size varies when variable range is used. The Range cannot be calculated for groups containing only 1 observation.



```
rget(M1) = -0.147125, LCL(x) = -2.0572, UCL(x) = 1.76295, S(M1) = 2.85925,
RAvg) = 1.79868, RAvg(within, M1) = 5.12085, LCL(r) = 0.696436,
L(r) = 9.54527
```

12.4.2.3.3 Mean/Standard deviation

When creating a Shewhart control chart of type Mean/Std. dev., any monotonically increasing variable available can be used. When the plotted data originates from a model, any monotonically increasing variable in any of the included datasets, can be used to base the subgroups on, whether included or not.

To create the **Shewhart** control chart of type Mean/standard deviation:

1. Click **Control chart**.
2. Select **Shewhart** in the **Type of control chart** box
3. Select **Mean/Std. dev.** in the **Shewhart type** box.

4. In **Variable**, select **Observation group** or a variable under the Time range/Variable range headers. The value displayed in the plot is the average of the subgroup.

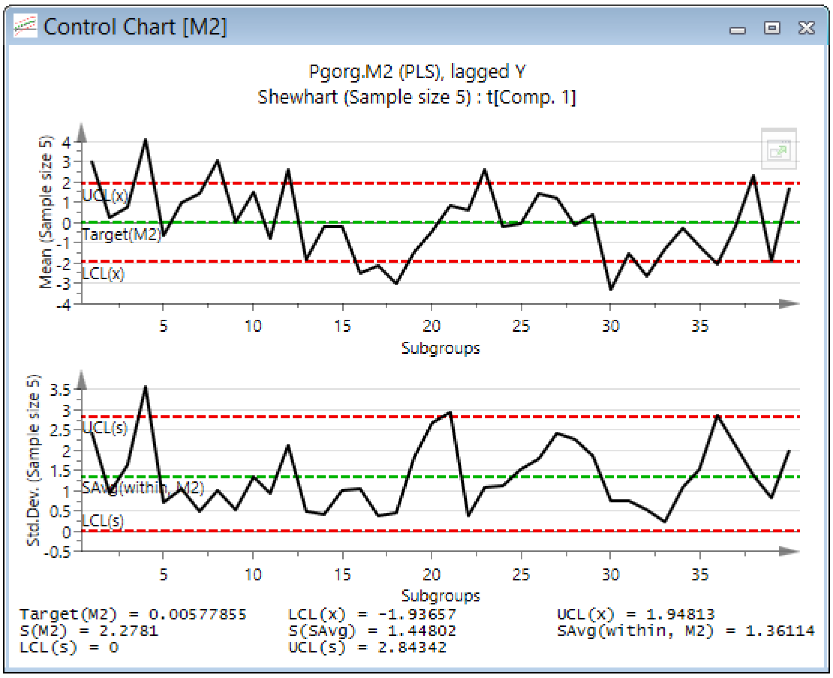
a. With **Observation groups** selected, enter the desired sample size in the **Sample size** field (default 5).

b. With a monotonically increasing variable selected, enter the desired subgroup range in the units of the variable.

c. With a monotonically increasing time variable selected, enter the desired time range in the storing unit specified at import.

5. Click **OK**..

The resulting plot displays the control charts for the selected vector, with the target and upper and lower limits displayed.



```
Target(M2) = 0.00577855    LCL(x) = -1.93657      UCL(x) = 1.94813
S(M2) = 2.2781             S(SAvg) = 1.44802      SAvg(within, M2) = 1.36114
LCL(s) = 0                 UCL(s) = 2.84342
```

The plot footer displays: **Target(Mxx)** or **Target(UE)** when defined, **LCL(x)**, **UCL(x)**, **S(Mxx)**, **S(SAvg)** or **S(UE)** when defined, **SAvg(within, S(Mxx))** or **SAvg(within, S(UE))** when defined, **LCL(s)** and **UCL(s)**.

To view the nomenclature and calculations of target and standard deviation, see the Nomenclature and notation and Target and Standard deviation subsections in the Statistical appendix.

Control limits and standard deviation

Control limits and estimates of the standard deviation are computed as follows:

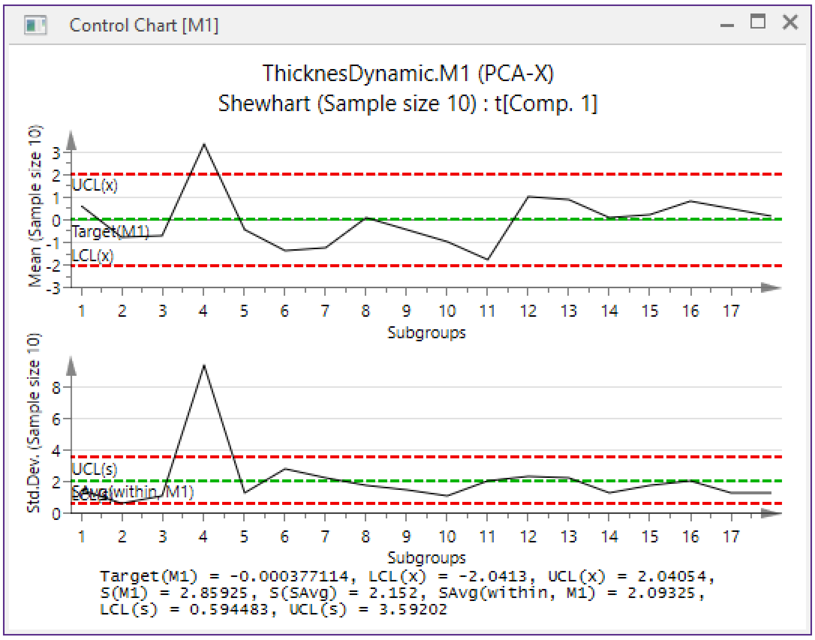
- S(SAvg) = SAvg/c4, estimate of the process standard deviation.
- LCLx = Target - A3*SAvg
- UCLx = Target + A3*SAvg
- LCLs = B3*SAvg
- UCLs = B4*SAvg
- SAvg(within, M1 or S(UE)) = average of the standard deviations of subgroups, or, when the standard deviation is user entered, c4 multiplied by S(UE).
- B3, B4, A3, c4 are from McNeese. Reference McNeese, W.H., Klein, R.A., (1991) *Statistical methods for the process industries,* Quality and Reliability/28, chapter 19 table 1, p. 272.

12.4.2.3.4 Mean/Std. dev. using time range

When creating a Shewhart control chart of type Mean/Std. dev., any monotonically increasing variable available can be used. The value displayed in the plot is the average of the subgroup.

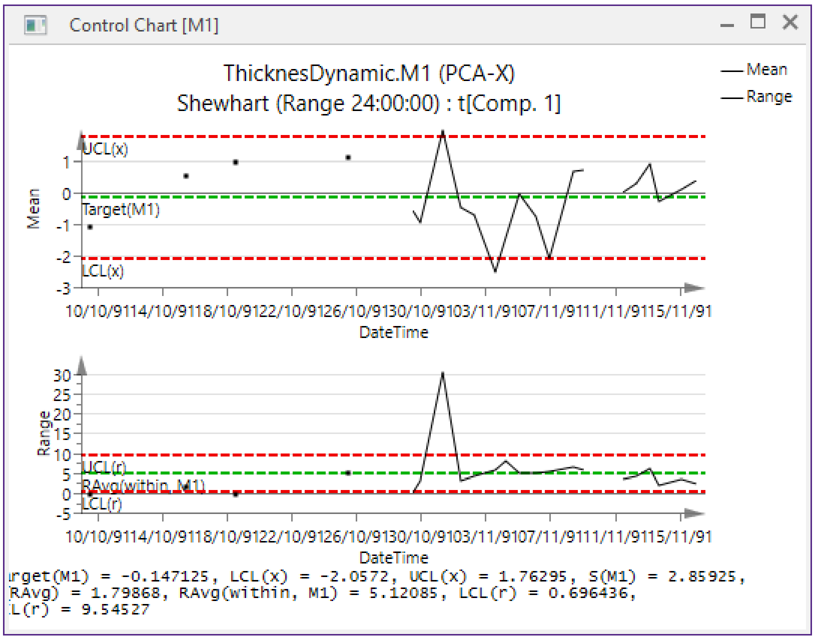
When the plotted data originates from a model, any monotonically increasing variable in any of the included datasets, can be used to base the subgroups on, whether included or not.

Applying groups based on time range is useful to review e.g. daily process changes since number of observations per day, hour etc may vary. For instance, in the first plot below the subgroups are defined as 10 per subgroup. Here we get no impression of how time matters.



```
Target(M1) = -0.000377114, LCL(x) = -2.0413, UCL(x) = 2.04054,
S(M1) = 2.85925, S(SAvg) = 2.152, SAvg(within, M1) = 2.09325,
LCL(s) = 0.594483, UCL(s) = 3.59202
```

In this second plot, where each subgroup is 1 day long, the time influence is clear. Note that the subgroup size varies when variable range is used. The standard deviation is calculated based on actual number of observations in each group and cannot be calculated for group sizes smaller than 3.

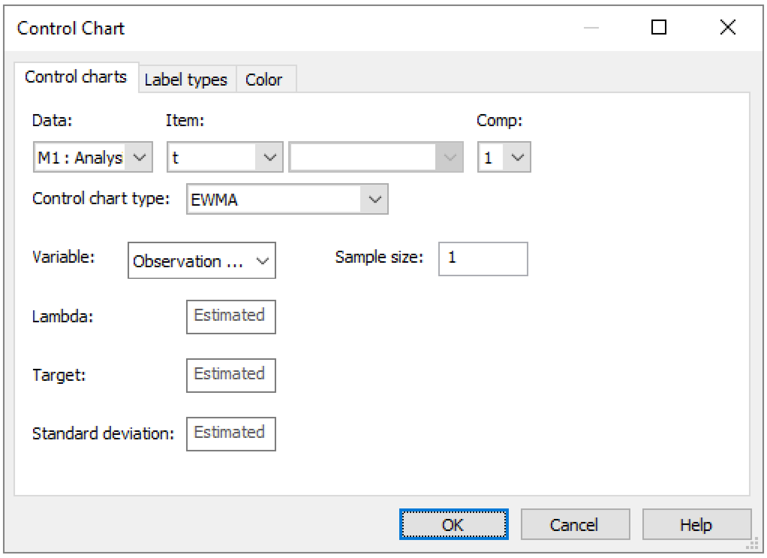


```
rget(M1) = -0.147125, LCL(x) = -2.0572, UCL(x) = 1.76295, S(M1) = 2.85925,
RAvg) = 1.79868, RAvg(within, M1) = 5.12085, LCL(r) = 0.696436,
L(r) = 9.54527
```

12.4.2.4 EWMA – Exponentially Weighted Moving Average

The EWMA, Exponentially Weighted Moving Average, control chart can be displayed both with sample size = 1 and sample size > 1.

Open the EWMA control chart by clicking **Control chart** on the **Plot/List** or **Predict** tabs, selecting **EWMA** in the **Type of control chart** box.



Control Chart

Data: M1 : Analys

Item: t

Comp: 1

Control chart type: EWMA

Variable: Observation ...

Sample size: 1

Lambda: Estimated

Target: Estimated

Standard deviation: Estimated

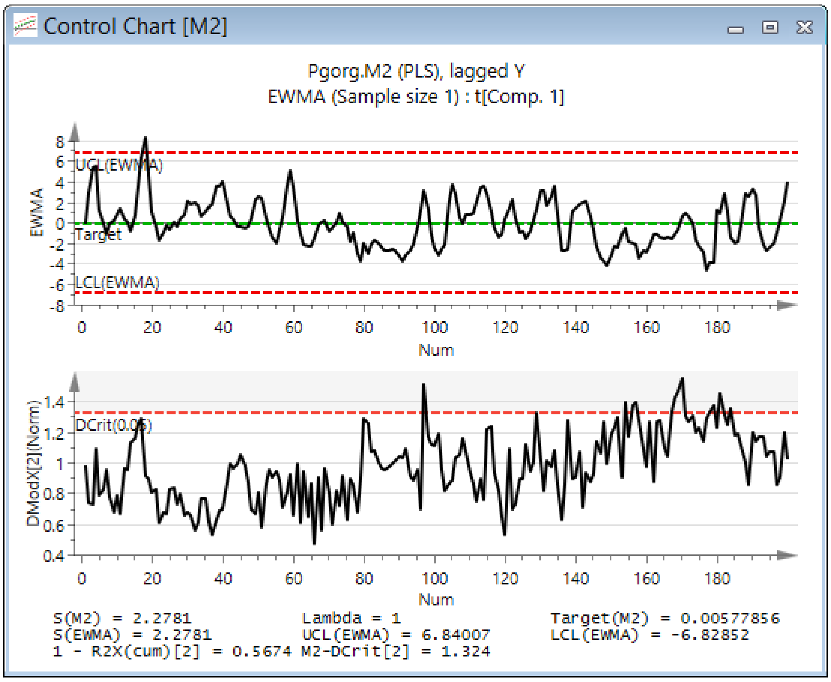
12.4.2.4.1 EWMA with sample size = 1

To create the **EWMA** control chart:

1. Click **Control chart**.
2. Select **EWMA** in the **Type of control chart** box.
3. Leave the default value = 1 in the **Sample size** field, and then click **OK**.

The resulting plot displays the selected vector, target and upper and lower limits in the EWMA control chart.

When plotting t or tPS, a plot of DModX or DModXPS is displayed beneath, with its critical distance. Observations outside the critical distance indicate process behavior different from the model.



```
S(M2) = 2.2781                Lambda = 1                Target(M2) = 0.00577856
S(EWMA) = 2.2781              UCL(EWMA) = 6.84007       LCL(EWMA) = -6.82852
1 - R2X(cum)[2] = 0.5674 M2-DCrit[2] = 1.324
```

The plot footer displays: S(Mxx), S(UE) when defined, **Lambda** (estimated or user defined), **Target(Mxx)** or **Target(UE)** when defined, **S(EWMA)**, **UCL(EWMA)**, **LCL(EWMA)**, **1 – R2X(cum)[last component]**and **Mxx – DCrit[last component]**.

To view the nomenclature and calculations of target and standard deviation, or calculations of limits, see the Nomenclature and notation, Target and Standard deviation, respective Control limits and standard deviation subsections in the Statistical appendix.

12.4.2.4.2 EWMA with subgroups

To create the EWMA control chart with subgroups:

1. Click **Control chart**.
2. Select **EWMA** in the **Type of control chart** box.
3. In **Variable**, select **Observation group** or a variable under the Time range/Variable range headers. The value displayed in the plot is the average of the subgroup.

a. With **Observation groups** selected, enter the desired sample size in the **Sample size** field (default 5).

b. With a monotonically increasing variable selected, enter the desired subgroup range in the units of the variable.

c. With a monotonically increasing time variable selected, enter the desired time range in the storing unit specified at import.

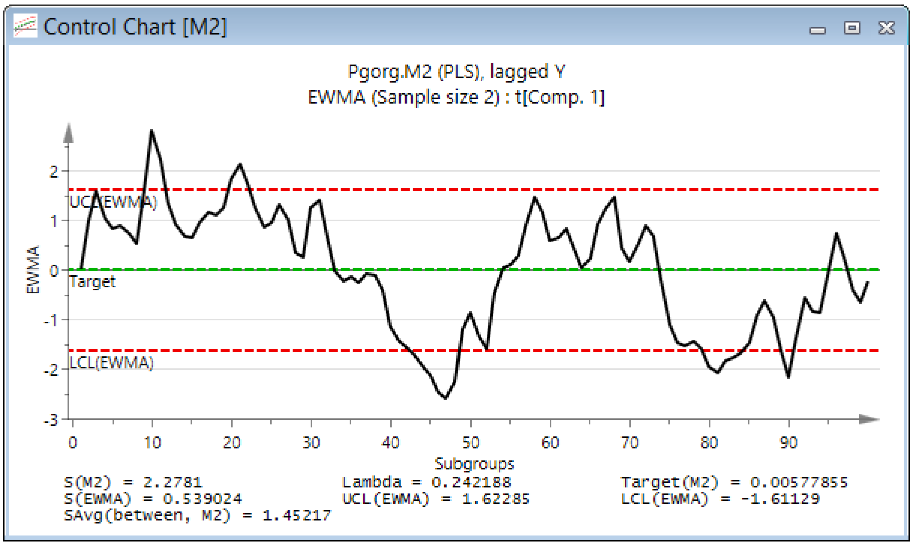
4. Click **OK**.

The resulting plot displays the selected vector, target and upper and lower limits in the EWMA control chart.

With sample size > 1 the EWMA is calculated as:

yhat$_{t+1}$ = yhat$_t$ + λ(Y$_t$ – yhat$_t$)

where t is time and yhat is predicted y.



Control Chart [M2]

Pgorg.M2 (PLS), lagged Y
EWMA (Sample size 2) : t[Comp. 1]

```
S(M2) = 2.2781                  Lambda = 0.242188          Target(M2) = 0.00577855
S(EWMA) = 0.539024              UCL(EWMA) = 1.62285        LCL(EWMA) = -1.61129
SAvg(between, M2) = 1.45217
```

The plot footer displays: **S(Mxx)**, **S(UE)** when defined, **Lambda** (estimated or user defined), **Target(Mxx)** or **Target(UE)** when defined, **S(EWMA)**, **UCL(EWMA)**, **LCL(EWMA)** and **SAvg(between, Mxx)** or **SAvg(between, S(UE)** if entered.

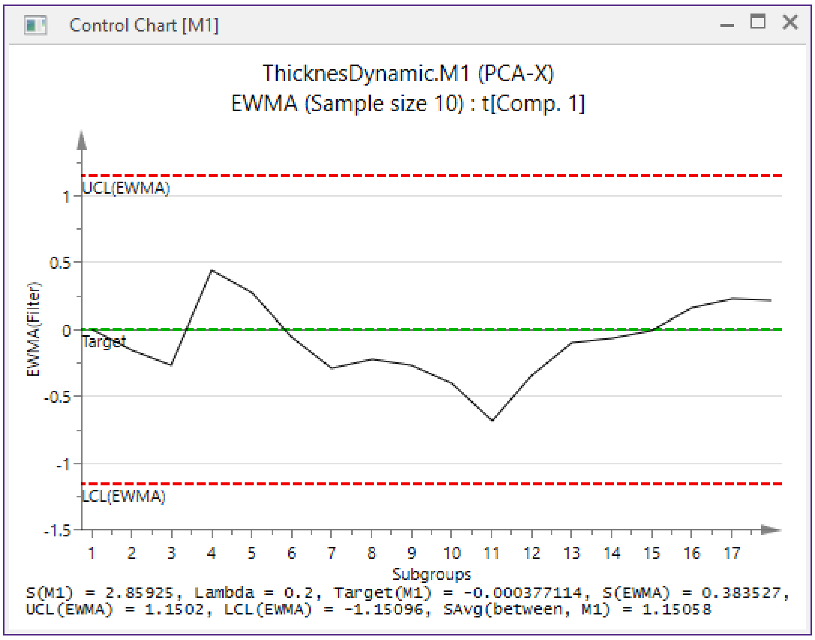
To view the nomenclature and calculations of target and standard deviation, or calculations of limits, see the Nomenclature and notation, Target and Standard deviation, respective Control limits and standard deviation subsections in the Statistical appendix.

12.4.2.4.3 EWMA with subgroups using time

When creating a EWMA control chart with subgroups, any monotonically increasing variable available can be used. The value displayed in the plot is the average of the subgroup.

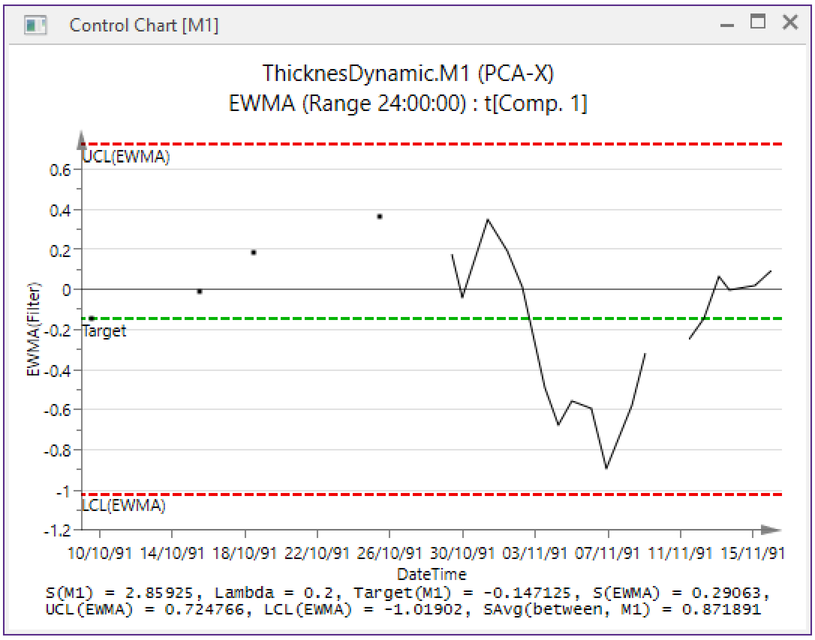
When the plotted data originates from a model, any monotonically increasing variable in any of the included datasets, can be used to base the subgroups on, whether included or not.

Applying groups based on time range is useful to review e.g. daily process changes since number of observations per day, hour etc may vary. For instance, in the first plot below the subgroups are defined as 10 per subgroup. Here we get no impression of how time matters.



```
S(M1) = 2.85925, Lambda = 0.2, Target(M1) = -0.000377114, S(EWMA) = 0.383527,
UCL(EWMA) = 1.1502, LCL(EWMA) = -1.15096, SAvg(between, M1) = 1.15058
```

In this second plot, where each subgroup is 1 day long, the time influence is clear. Note here also that the subgroup size varies when variable range is used.



```
S(M1) = 2.85925, Lambda = 0.2, Target(M1) = -0.147125, S(EWMA) = 0.29063,
UCL(EWMA) = 0.724766, LCL(EWMA) = -1.01902, SAvg(between, M1) = 0.871891
```

12.4.2.4.4 Control limits and standard deviation

Control limits and estimates of the standard deviation are computed as follows:

S(EWMA) = MSSD, Mean Square Successive Difference = SAvg * $(\lambda/(2-\lambda))^{1/2}$

The upper and lower control limits are computed as:

UCL(EWMA) = Target + 3 * S(EWMA)

LCL(EWMA) = Target – 3 * S(EWMA)

where λ is estimated (when not user entered) to minimize the error sum of squares.

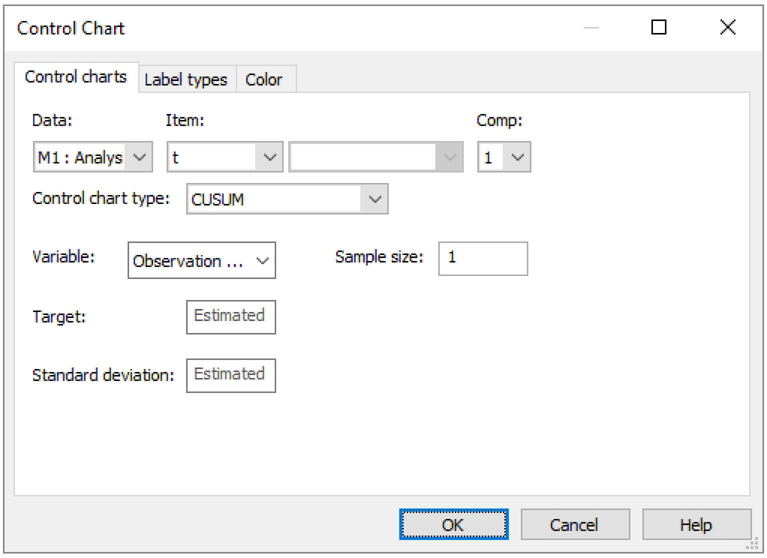
12.4.2.5 CUSUM

To create the CUSUM control chart:

1. Click **Control chart**.
2. Select **CUSUM** in the **Type of control chart** box.
3. (a) With **Observation groups** selected, enter the desired sample size in the **Sample size** field (default 5),
(b) With a monotonically increasing variable selected, enter the desired subgroup range in the units of the variable.
(c) With a monotonically increasing time variable selected, enter the desired time range in the storing unit specified at import.
4. Click **OK**.

The resulting plot displays the target, CUSUM lines and limits for the selected vector.

The CUSUM, CUmulative SUM, control chart can be displayed both with sample size = 1 and sample size > 1.



Data: M1 : Analys

Item: t

Comp: 1

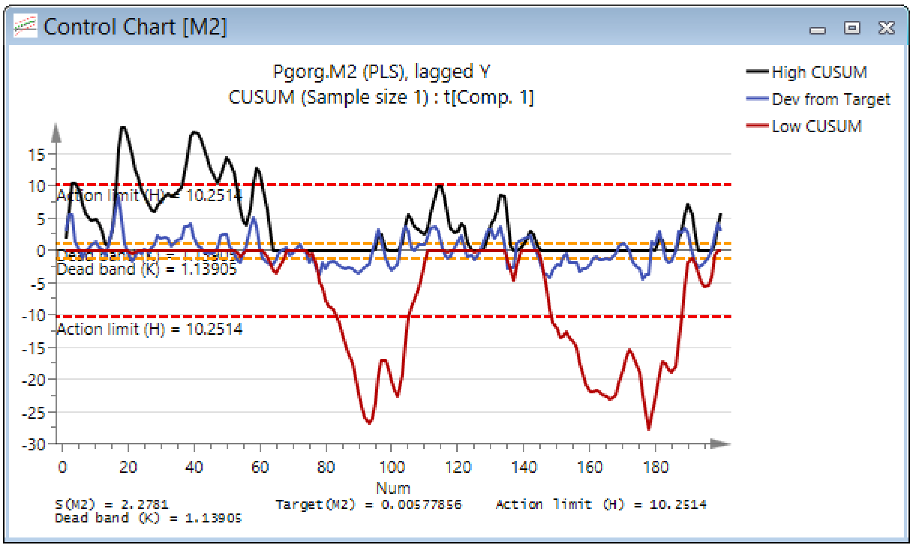
Control chart type: CUSUM

Variable: Observation ...

Sample size: 1

Target: Estimated

Standard deviation: Estimated



```
S(M2) = 2.2781                Target(M2) = 0.00577856        Action limit (H) = 10.2514
Dead band (K) = 1.13905
```

The plot footer displays: **S(Mxx)**, **Target(Mxx)** or **Target(UE)** when defined, **S(UE)** when defined, **Action limit (H)** and **Dead band (K)**.

To view the nomenclature, calculations of target and standard deviation, or calculations of limits, see the Nomenclature and notation and Target and Standard deviation subsections in the Statistical appendix, respective the Control limits section later.

12.4.2.5.1 CUSUM plot content

The series displayed in the plot are:

- **High CUSUM** = Cumulative sum on the high side difference used to detect a deviation from the target on the high side. High CUSUM is set to zero when negative.
- **Low CUSUM** = Cumulative sum on the low side difference used to detect a deviation from the target on the low side. Low CUSUM is set to zero when positive.
- **Dev from Target**, deviation from target **=** average of subgroup – target.

Reference McNeese, W.H., Klein, R.A., (1991) *Statistical methods for the process industries*, Quality and Reliability/28, chapter 21.

Note: The plot displays the Low CUSUM with reversed sign (- Low CUSUM) so that all values are displayed as negatives.

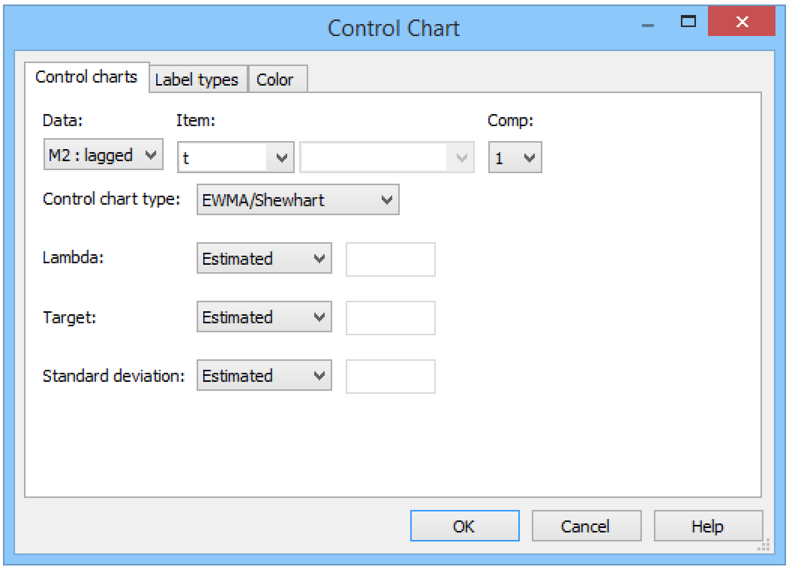
12.4.2.5.2 Control limits

The control limits are computed as follows:

- **Action limit (H)** = 4.5 standard deviation, using S(Mxx) when sample size = 1 and SAvg when sample size > 1.
- **Dead band (K)** (or allowable slack) = standard deviation/2, using S(Mxx) when sample size = 1 and SAvg when sample size > 1.

12.4.2.6 EWMA/Shewhart

Click **Control chart**, select **Shewhart/EWMA** in **Type of control chart**, and then click **OK** displays the Shewhart and EWMA lines, target and limits, all in the same plot.


Control Chart

Control charts | Label types | Color

Data: M2 : lagged

Item: t

Comp: 1

Control chart type: EWMA/Shewhart

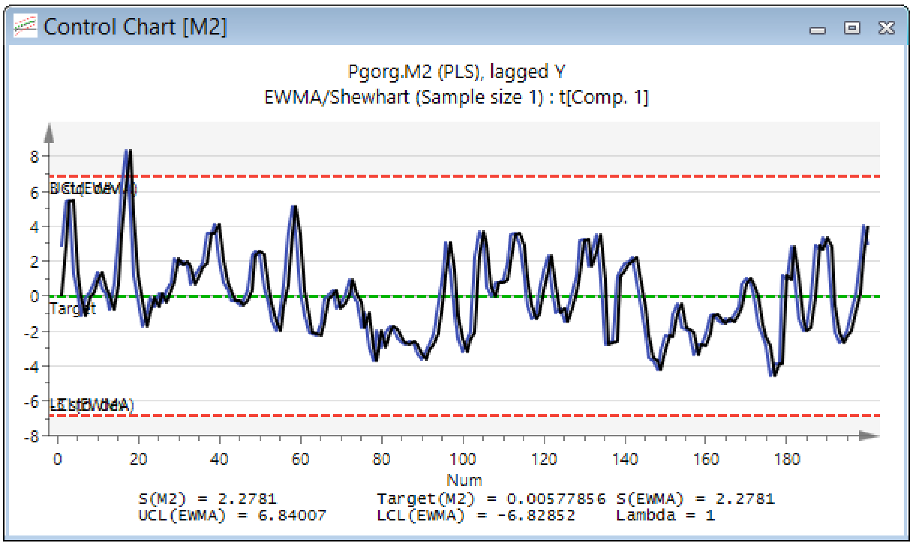
Lambda: Estimated

Target: Estimated

Standard deviation: Estimated

Note that the EWMA/Shewhart control chart is only available with sample size = 1. Consequently the Shewhart displayed is the **Individual**.

Lambda, **Target**, and **Standard deviation** can be **User entered** or **Estimated**. See the **Shewhart** and **EWMA** sections earlier for more.



```
S(M2) = 2.2781          Target(M2) = 0.00577856  S(EWMA) = 2.2781
UCL(EWMA) = 6.84007     LCL(EWMA) = -6.82852     Lambda = 1
```

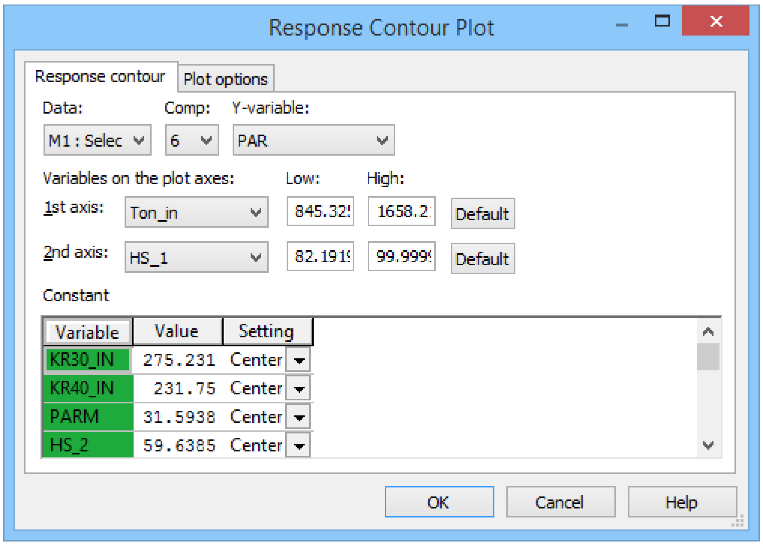
The plot footer displays: **S(Mxx)**, **S(UE)** when defined, **Target(Mxx)** or **Target(UE)** when defined, **S(EWMA)**, **UCL(EWMA)**, **LCL(EWMA)** and **Lambda** (estimated or user defined). See the Shewhart and EWMA sections earlier for more.

12.5 Response contour

The **Response contour** displays the response surface contour plot for the selected y-variable with the two selected x-variables on the axes, for a PLS model.

To create a **Response contour** plot:

1. On the **Plot/List** tab, in the **Custom plots** group, click **Response contour.**
2. Select the model in the **Data** box and the number of components to use in the **Comp** box.
3. Select the y-variable to display in the **Y-variable** box.
4. Select the x-variables to display on the x-axes in the 1^{st} **axis** and 2^{nd} **axis** boxes. The range of the selected variables is displayed using **Low** and **High** settings fields. These are the values used to limit the surface. Change them as warranted.
5. All x-variables not selected to be displayed on the axes, are held constant and listed in the **Constant variables** list, by default set at their average, **Center**. Change these settings as warranted by typing new values in the respective fields.
6. Click **OK** or click the **Plot options** tab (described next). After clicking **OK**, the values of the constant factors are displayed near the plot. Changing these values updates the plot instantly.



Data: M1 : Selec
Comp: 6
Y-variable: PAR

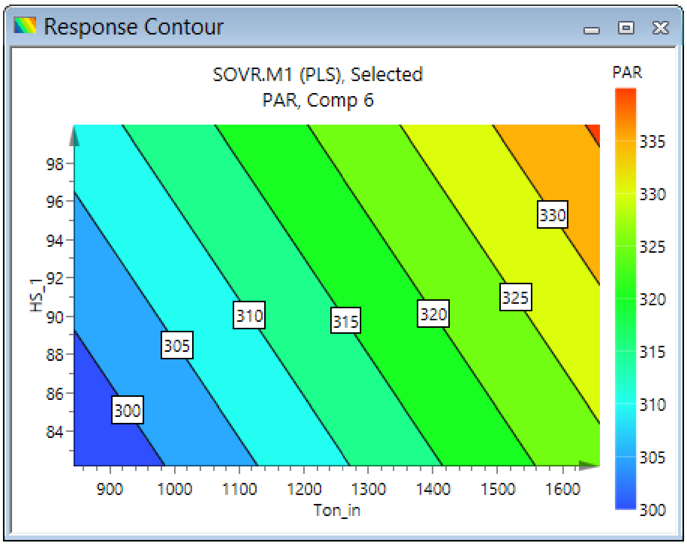
Variables on the plot axes: Low: High:

1st axis: Ton_in 845.32! 1658.2 Default

2nd axis: HS_1 82.191(99.999(Default

Constant

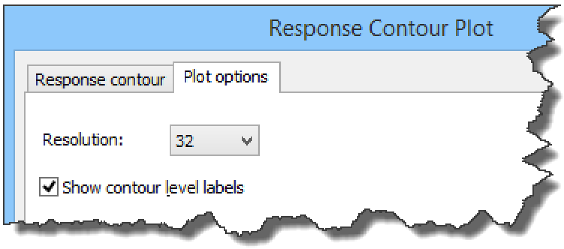
Variable	Value	Setting
KR30_IN	275.231	Center
KR40_IN	231.75	Center
PARM	31.5938	Center
HS_2	59.6385	Center



12.5.1 Response contour plot options

Clicking the **Plot options** tab enables changing the following options:

1. **Resolution** – 16, 32, 64, or 128. Resolution 32 is the default.
2. **Show contour level labels** - clear the check box to hide the labels in the plot.



Resolution: 32

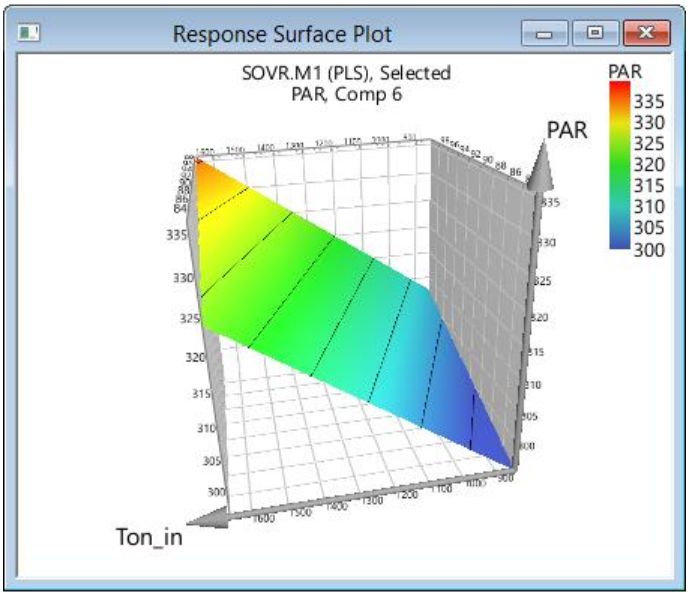
☑ Show contour level labels

See also the Contour subsection in the Tools tab section in Chapter 14, Plot and list contextual tabs.

12.6 Response surface plot

The **Response surface** plot displays the response surface contour plot in a 3D grid, for the selected y-variable with the two selected x-variables on the x and y-axes and the y-variable on the z-axis. The plot is only available for PLS, OPLS and O2PLS models.

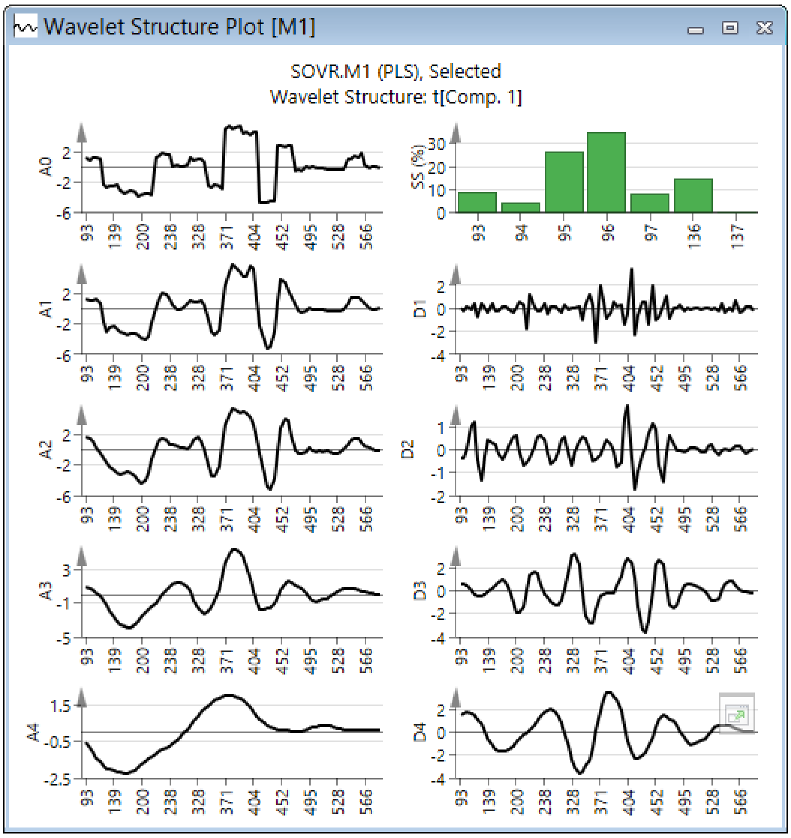
To create the **Response Surface Plot**, on the **Plot/List** tab, in the **Custom plots** group, click **Response surface**. The dialog that opens is the same as the one for the **Response contour**, see the Response contour section preceding this section.



12.7 Wavelet structure

In the Wavelet structure plot the selected vector is decomposed using DWT into its approximations and details at every scale. By default, the details and approximations for the first four lowest scales, scales 1 to 4 (the first 4 highest frequencies bands), are reconstructed and plotted using the same time axis. The original signal is A0. This is very useful in order to understand the structure of a signal.

Note: *In SIMCA the scales or levels are the inverse of the frequencies. Hence, scale 1 (D1) corresponds to the highest frequency band in the signal and the highest scale corresponds to the lowest frequency in the signal. The mean (DC component) is not included.*



The bar chart plot displays the percent of the total Sum of Squares of the signal (not including the DC component) contained in the details coefficients at every scale. Plots A1 to A4, and D1 to D4 are the reconstructed approximations and details coefficients at the scale 1 to 4. A0 is the original signal.

12.7.1 Displaying Wavelet structure plot

To display the **Wavelet Structure** plot:

1. Click **Wavelet structure**.
2. Select the vector to display.
3. Click the **Wavelet options** tab and select detrending, wavelet family, and wavelet order. For more, see the Wavelet Options subsection in Chapter 8, Data.
4. Click the **Wavelet details** tab and select the levels to display. For more, see the Wavelet compression/denoising By detail level subsection in Chapter 8, Data.
5. Click **OK**.

12.8 Wavelet power spectrum

The wavelet power spectrum plot is a 3-D plot displaying the scaled power density (the normalized squared wavelet coefficients) of the signal as a function of both time and frequency. Note that the frequencies are in logarithmic band passes (displayed on the plot as multiple of 2) up to the Nyquist frequency (the highest frequency in the signal). The smallest even scale (i.e. 2) on the plot represents the highest frequency band, that is frequencies in the signal from ½ the Nyquist up to the Nyquist frequency. The highest even scale in the plot is the single lowest frequency in the signal.

The DC component (average) when present is not included.

12.8.1 Displaying Wavelet power spectrum plot

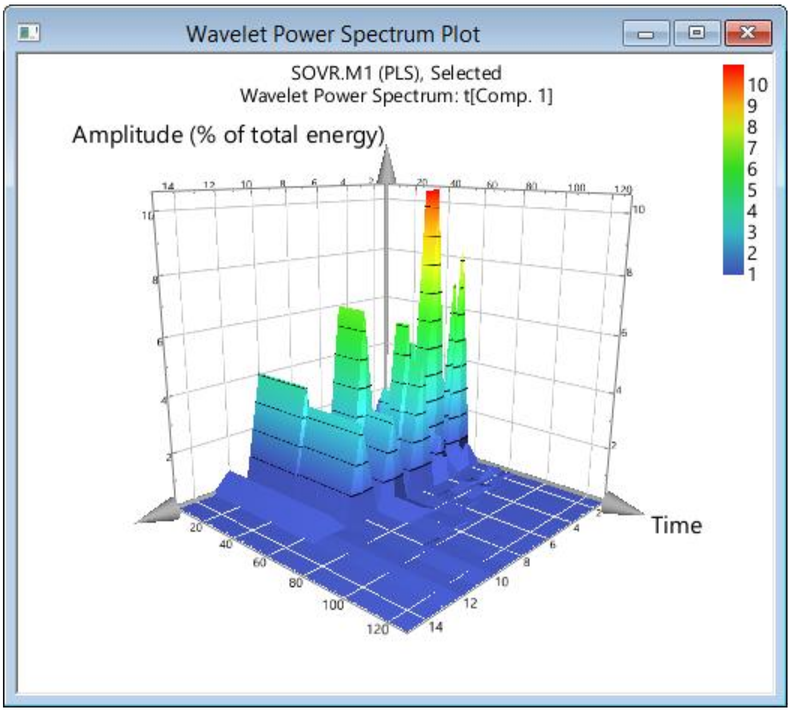
To display the **Wavelet power spectrum**:

1. Click **Wavelet power spectrum**.
2. Select the vector to display.
3. Click the **Wavelet options** tab and select detrending, wavelet family, and wavelet order. For more, see the Wavelet options subsection in Chapter 8, Data.
4. Click **OK**.

12.8.2 Wavelet power spectrum example

The following plots display a signal, which is 20-Hertz in the first half, and 100-Hertz in the second half. The sampling frequency of the signal is 1024- Hertz (i.e. 1024 points a second).

In the **Wavelet Power Spectrum Plot**, the 20-Hertz signal is displayed as continuous peaks across the first half of the time axis, on scale 10, i.e. frequency band between 16 and 32 Hertz. The 100-Hertz signal occurs across the second half of the time axis, with peaks centered on scale 6, i.e. frequency band between 64 and 128-Hertz.


Wavelet Power Spectrum Plot
SOVR.M1 (PLS), Selected
Wavelet Power Spectrum: t[Comp. 1]
Amplitude (% of total energy)
Time
10
9
8
7
6
5
4
3
2
1

4

12.9 Step response plot

The step response plot $\Sigma \nu_k$ is the sum or integral of the Impulse Response function v_k of the system. These are the response of the system at times t and k > 0 to a unit pulse input at time t = 0.

Hence

$Y_t = \Sigma \ \nu_k X_{t-k}$

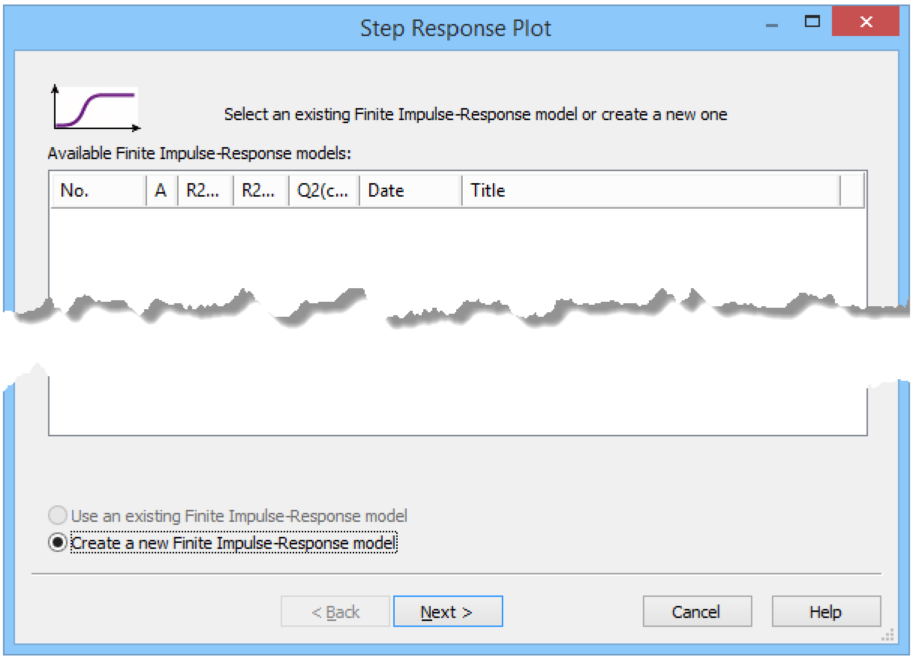
k=0 to ∞ is the deviation from steady state at time t.

12.9.1 Creating a finite impulse response model

When clicking **Step response plot**, a wizard opens with 2-6 pages depending on the selections in the wizard. The pages up to and including the page specifying the lag structure define the FIR model.

12.9.1.1 Selecting to create a new model

On the first page of the **Step Response Plot** wizard, select to create a new model by clicking **Create a new Finite Impulse Response model**. Then click **Next**.



Step Response Plot

Select an existing Finite Impulse-Response model or create a new one

Available Finite Impulse-Response models:

No.	A	R2...	R2...	Q2(c...	Date	Title

○ Use an existing Finite Impulse-Response model

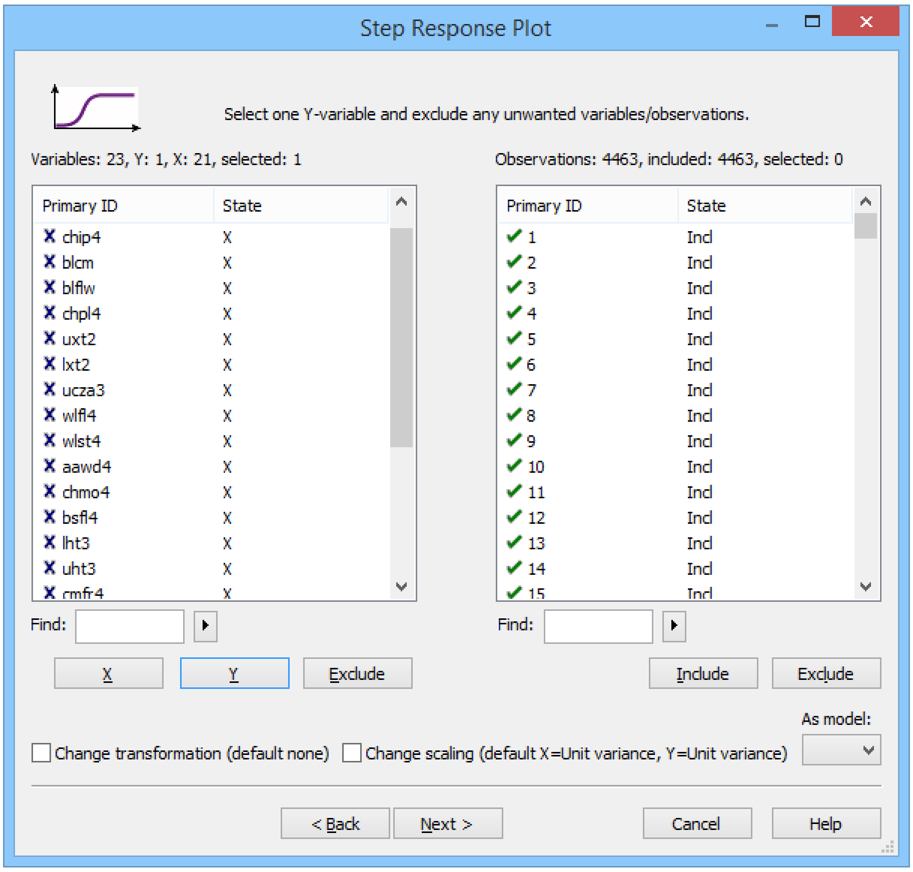
● Create a new Finite Impulse-Response model

12.9.1.2 Selecting y-variable and excluding variables or observations

On the 2nd page of the **Step Response Plot** wizard:

- Select the y-variable in the **Variables** list, and click the **Y**-button.
- Exclude undesired variables and observations by selecting them and clicking the respective **Exclude**-buttons.
- Optionally, select the **Change transformation** check box to transform variables. For more, see the Applying transformations subsection in the Workset section in Chapter 7, Home.
- Optionally select the **Change scaling** check box to change the scaling of variables. Then click **Next**, and customize the scaling using the **None**, **Pareto**, **Unit Variance**, and **Center**-buttons.

When done click **Next**.



Step Response Plot

Select one Y-variable and exclude any unwanted variables/observations.

Variables: 23, Y: 1, X: 21, selected: 1

Primary ID	State
chip4	X
blcm	X
blflw	X
chpl4	X
uxt2	X
lxt2	X
ucza3	X
wlfl4	X
wlst4	X
aawd4	X
chmo4	X
bsfl4	X
lht3	X
uht3	X
cmfr4	X

Observations: 4463, included: 4463, selected: 0

Primary ID	State
✓ 1	Incl
✓ 2	Incl
✓ 3	Incl
✓ 4	Incl
✓ 5	Incl
✓ 6	Incl
✓ 7	Incl
✓ 8	Incl
✓ 9	Incl
✓ 10	Incl
✓ 11	Incl
✓ 12	Incl
✓ 13	Incl
✓ 14	Incl
✓ 15	Incl

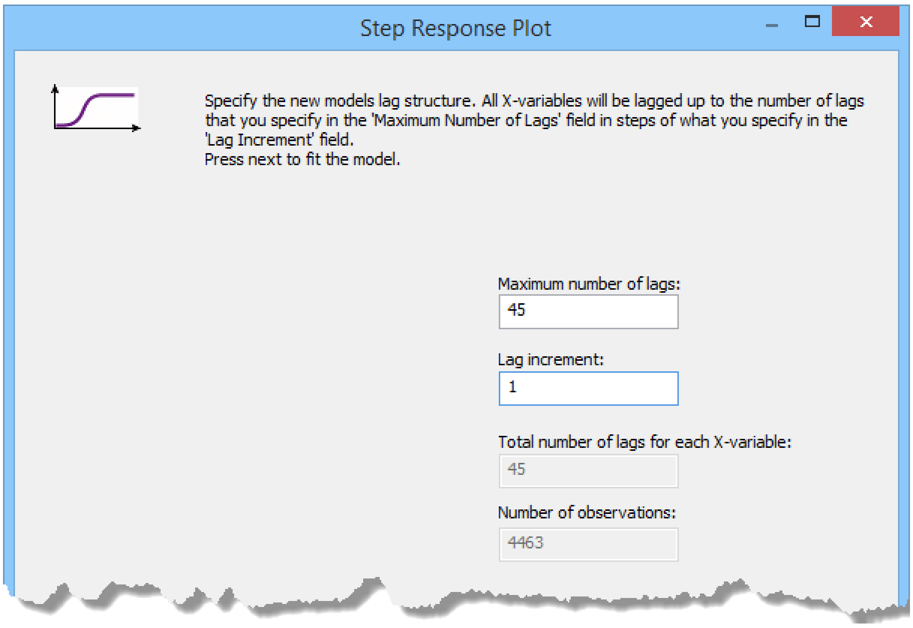
□ Change transformation (default none) □ Change scaling (default X=Unit variance, Y=Unit variance)

As model:

12.9.1.3 Specifying lag structure and fitting FIR model

To specify the new models lag structure:

1. The default **Maximum number of lags** is 45 or N-5 whichever is smaller. Specify a new maximum number of lags by typing a new value smaller than N-5.
2. The default **Lag increment** is 5 or **Maximum number of lags**/3 whichever is smaller. Specify a new lag increment by typing a new value smaller than **Maximum number of lags**/3.
3. Click **Next** and SIMCA fits an FIR model with the selected y-variable and all x-variables with their lags as selected.



Step Response Plot

Specify the new models lag structure. All X-variables will be lagged up to the number of lags that you specify in the 'Maximum Number of Lags' field in steps of what you specify in the 'Lag Increment' field.
Press next to fit the model.

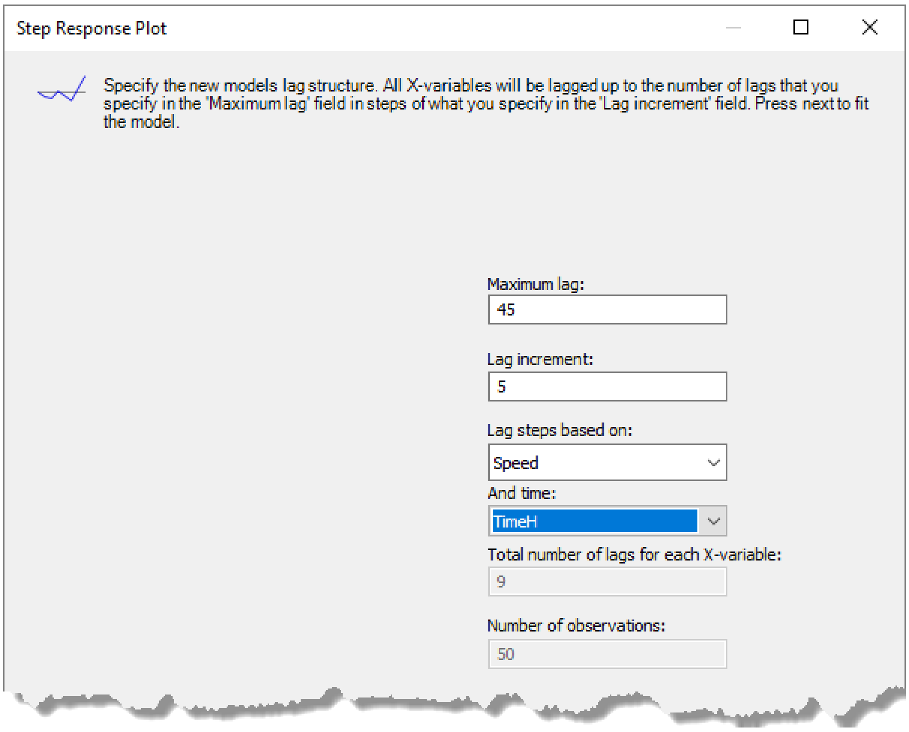
Maximum number of lags: 45

Lag increment: 1

Total number of lags for each X-variable: 45

Number of observations: 4463

We can also use monotonically increasing variables to specify lag structure here:



Step Response Plot

Specify the new models lag structure. All X-variables will be lagged up to the number of lags that you specify in the 'Maximum lag' field in steps of what you specify in the 'Lag increment' field. Press next to fit the model.

Maximum lag: 45

Lag increment: 5

Lag steps based on: Speed

And time: TimeH

Total number of lags for each X-variable: 9

Number of observations: 50

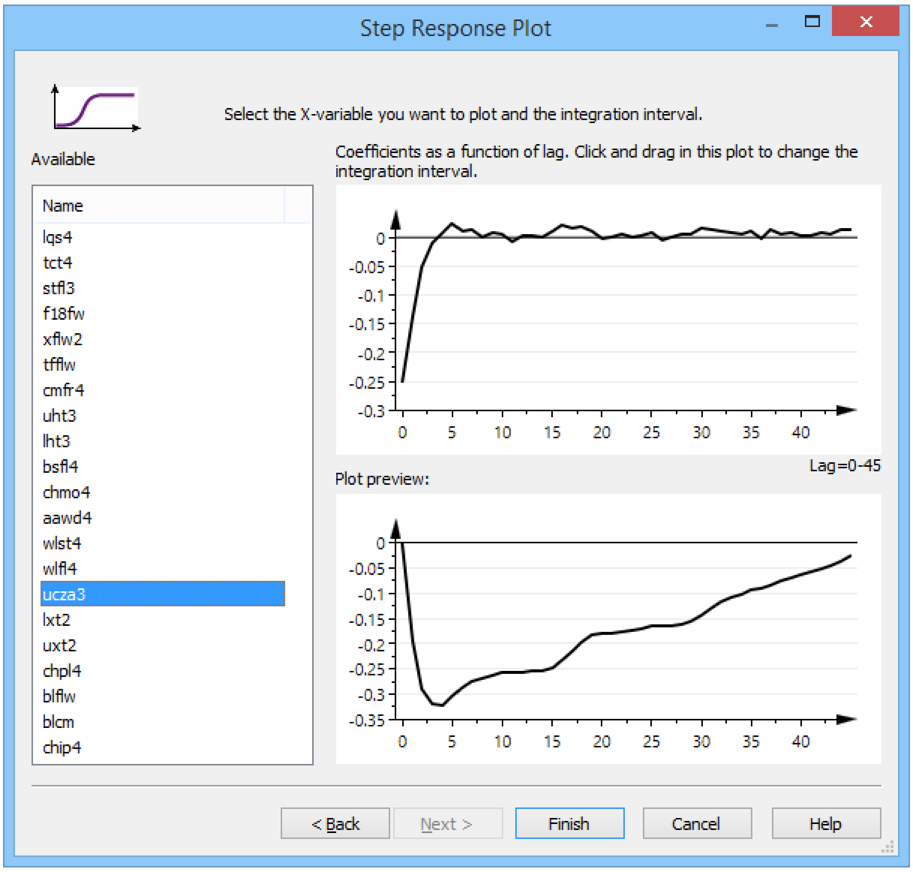
12.9.2 Displaying Step Response Plot

On the last page of the **Step Response Plot** wizard:

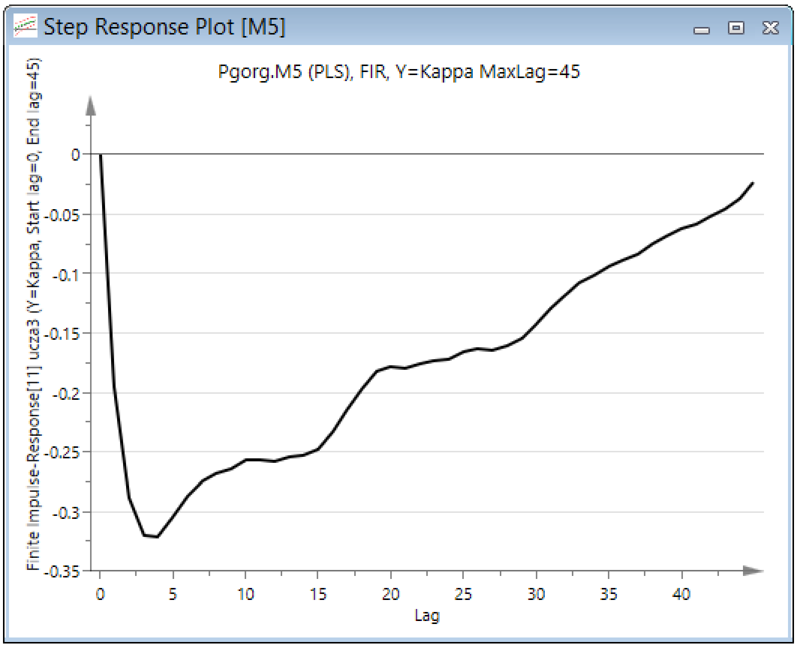
1. Select the x-variable to display in the **Available X-variables** list.
2. In the **Coefficients as a function of lag** plot, mark the integration interval to display in the step response plot. Leaving the plot as it is leads to displaying the entire integration.

Note that the **Plot preview** window displays the step response plot and is updated when switching x-variables and integration intervals.

When the FIR model is fitted the wizard displays the Impulse Response function of the selected x-variable.



Click **Finish** when done to display the final **Step Response Plot**. In this plot the integration always starts at 0.

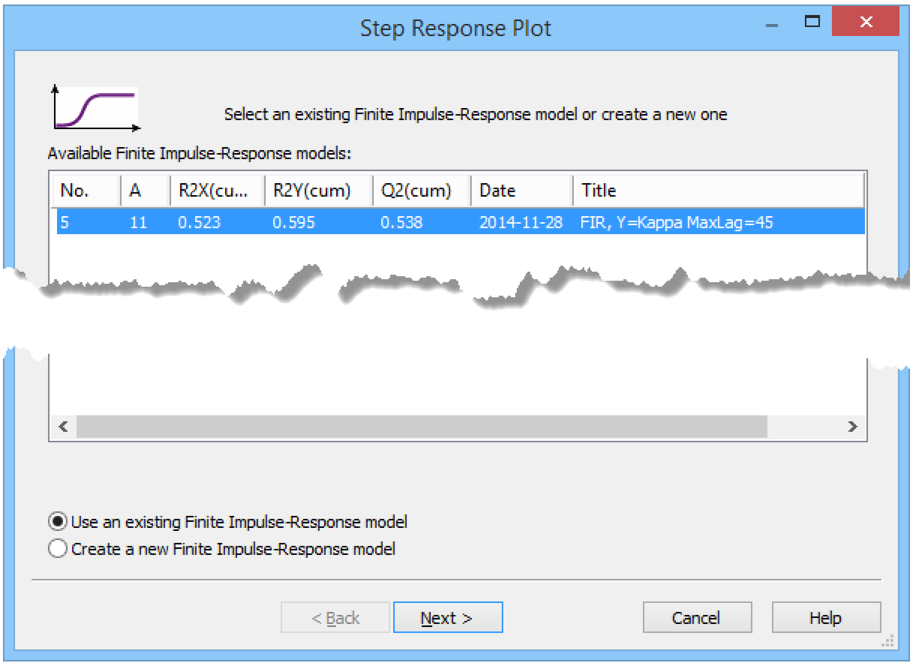


12.9.3 Using an existing finite impulse response model

To use an existing Finite Impulse-Response model to display another **Step Response Plot**:

1. Click **Step response plot**.
2. Click **Use an existing Finite Impulse Response model** and select one of the models listed in the **Available Finite Impulse-Response models** list.

3. Click **Next** to open the last page of the wizard. For more about this page, see the Displaying Step Response Plot subsection previously in this section.



Select an existing Finite Impulse-Response model or create a new one

Available Finite Impulse-Response models:

No.	A	R2X(cu...	R2Y(cum)	Q2(cum)	Date	Title
5	11	0.523	0.595	0.538	2014-11-28	FIR, Y=Kappa MaxLag=45

● Use an existing Finite Impulse-Response model

○ Create a new Finite Impulse-Response model

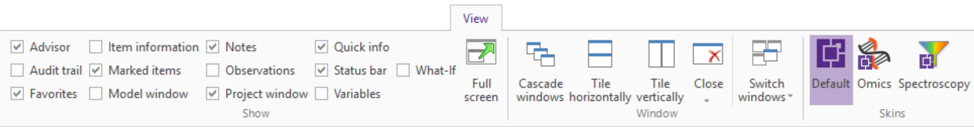
13View

13.1 Introduction

This chapter describes all commands on the **View** tab.

The following is available:

- The **Show** group including all panes, the **Model window** and the **Full screen** command.
- The **Window** group including **Cascade**, **Tile** and **Close** of windows.
- Optionally the **Skins** group if there are skins installed and enabled.



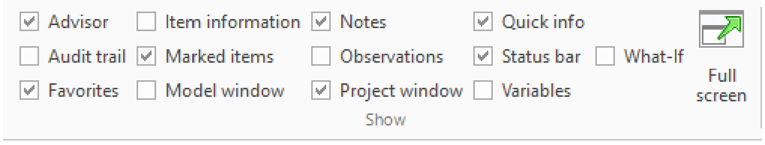
☑ Advisor □ Item information ☑ Notes ☑ Quick info

□ Audit trail ☑ Marked items □ Observations ☑ Status bar □ What-If

☑ Favorites □ Model window ☑ Project window □ Variables

13.2 Show

In the **Show** group on the **View** tab you can select to show or hide the following: **Advisor**, **Audit trail**, **Favorites**, **Item information**, **Marked items**, **Model window**, **Notes**, **Observations**, **Project window**, **Quick info**, **Status bar**, **Variables**, and the **What-If**. Clicking **Full screen** minimizes the ribbon as when Minimizing the ribbon.



☑ Advisor □ Item information ☑ Notes ☑ Quick info

□ Audit trail ☑ Marked items □ Observations ☑ Status bar □ What-If

☑ Favorites □ Model window ☑ Project window □ Variables

Selecting and clearing these check boxes opens and closes the respective pane, except for the **Model window** which is a regular window, and the **Status bar** which is always positioned at the bottom of SIMCA and displays the plot coordinates of the cursor or the first part of the current tooltip.

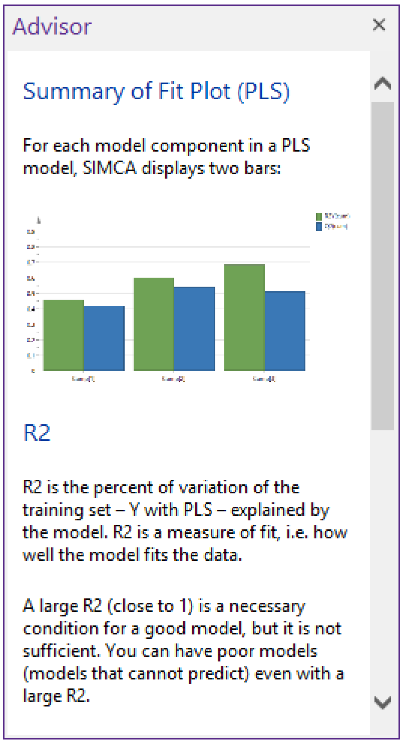
After selecting one of the panes, you can move and dock it as desired.

To auto hide the pane when not using it click the **Auto Hide** button 📌. The button changes to 📌 and the pane will slide away when not used and slide up on top of plots when clicked.

The features in the **Show** group are described in this section.

13.2.1 Advisor

The Advisor explains plots available on the **Home** tab. The **Advisor** pane by default opens on the right side of the screen and shows details about the open plot.



Advisor

Summary of Fit Plot (PLS)

For each model component in a PLS model, SIMCA displays two bars:

R2

R2 is the percent of variation of the training set – Y with PLS – explained by the model. R2 is a measure of fit, i.e. how well the model fits the data.

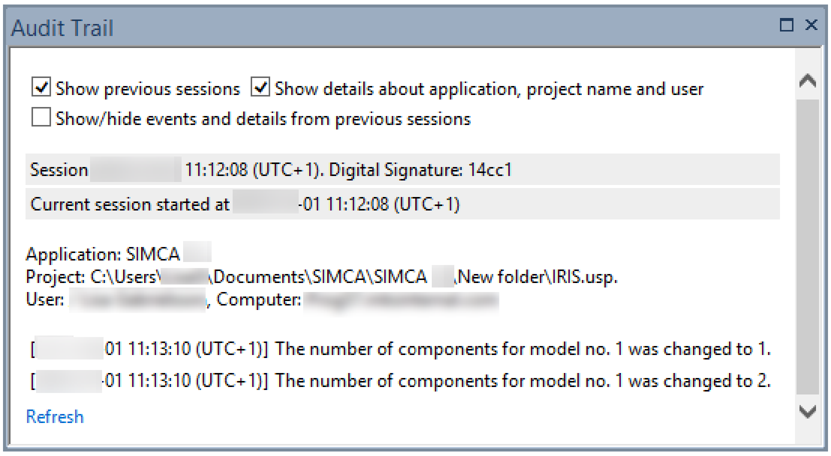
A large R2 (close to 1) is a necessary condition for a good model, but it is not sufficient. You can have poor models (models that cannot predict) even with a large R2.

13.2.2 Audit trail

The audit trail was implemented in SIMCA, in compliance with rules for keeping electronic records (21 CFR part 11).

When turned on, the **Audit Trail** pane logs all events in a session. A session starts with the creation or opening of a project and ends when the project is saved. When a project is reopened the current event logging is appended to the existing audit trail.

In addition to logging events, SIMCA logs information about the user and date and time of the events.



Audit Trail

☑ Show previous sessions ☑ Show details about application, project name and user
☐ Show/hide events and details from previous sessions

Session [redacted] 11:12:08 (UTC+1). Digital Signature: 14cc1

Current session started at [redacted]-01 11:12:08 (UTC+1)

Application: SIMCA [redacted]
Project: C:\Users\[redacted]\Documents\SIMCA\SIMCA [redacted]\New folder\IRIS.usp.
User: [redacted], Computer: [redacted]

[[redacted]01 11:13:10 (UTC+1)] The number of components for model no. 1 was changed to 1.

[[redacted]01 11:13:10 (UTC+1)] The number of components for model no. 1 was changed to 2.

13.2.2.1 Turning on logging to the audit trail

To turn on the logging to the audit trail:

- Before initilizing the creation of a new project, **File | Options** and in SIMCA options, select *Yes* in the **Enable the audit trail for new projects** box in the **Audit trail** section. The audit trail will then be turned on by default for all projects created thereafter.
- For projects already open in SIMCA, click **File | Options** and in Project options select *Yes* in the **Enable the audit trail** box in the **Audit trail** section. The audit trail will then log the events in this project that follow after it was turned on. This has no effect on projects created after.

The administrator can lock the audit trailed turned on. For administration of the audit trail, see the Administration of the audit trail subsection in the Project options section in Chapter 5, File.

The audit trail logs the actions listed in the Logged in the Audit Trail subsection next.

13.2.2.2 Logged in the audit trail

Note: Changes to a project introduced by scripts are **NOT** logged by the audit trail.

The following actions are logged by the audit trail:

Import and changes of the dataset during import/dataset creation:

- name and path of imported file(s).
- changes to the datasets done in SIMCA import, i.e. values changed, rows excluded etc.
- settings for creating batch level dataset.

Creation/changing of a workset:

- shows total number of X-variables.
- number of expansions.
- number of lags.
- number of Y-variables.
- number of observations.
- model type.
- number of excluded observations and variables.
- number of transformed variables.
- the datasets selected.

Changes of the model, such as:

- change in number of components.
- hierarchical model type.
- options.
- deletion of a model.

Creation/changes of datasets:

- logs the old and new values when changing values.
- logs the old and new value when changing observation or variable IDs.
- deletion of observations and variables.
- addition of observations and variables.
- sorting.
- splitting.
- merging.
- transposing.
- deletion of datasets.
- addition of variables using **Generate variables** on the **Data** tab.

- logs when there is a change in predictionset.

The data source name when the data comes from a database.

Save and Save as (including the name of the new project).

Registers when a digital signature in the audit trail is incorrect.

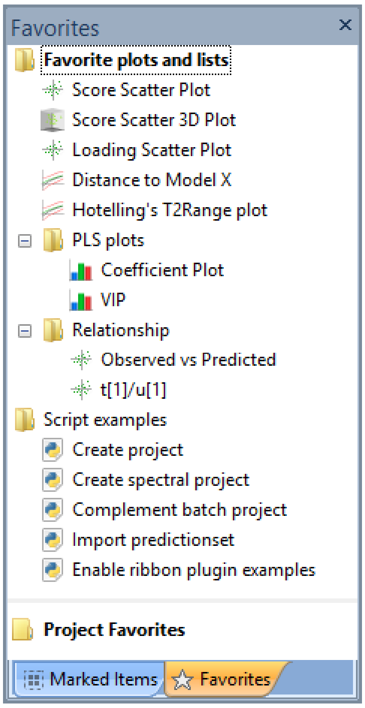
Clearing of the audit trail (File | Options | Project Options, Clear audit trail).

Turning on and off the audit trail.

Changes in the Audit trail extended user information.

13.2.3 Favorites

Open the **Favorites** pane by adding a plot or list to it, or by selecting the **Favorites** check box in the **Show** group on the **View** tab.

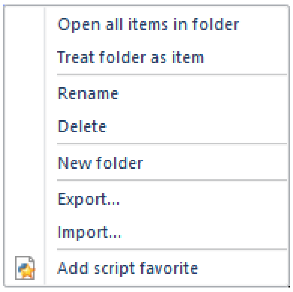


The **Favorites** pane by default contains a few plots and a folder with script examples. Clicking a plot opens the specified plot for the selected model in the current project. To move items or folders, grab and drag them.

13.2.3.1 Shortcut menu

The following commands are available from the **Favorites** shortcut menu:

- Open when a single item is marked.
- Open all items in folder when a folder is marked.
- Treat folder as item when a folder is marked. Toggles treating the folder as an item on or off.
- Rename folder or item.
- Delete folder or item.
- New folder.
- Export the **Favorites** configuration to file.
- Import the **Favorites** configuration from file.
- **Add script favorite** for quick access to your favorite scripts.



13.2.3.2 Organizing in folders in Favorites

Plots can be organized in folders in the **Favorites** pane. There are two global folders available by default, **Favorite plots and lists** and **Script examples**, and one local folder, **Project favorites**.

The default folders can be customized, and new global or local folders can be created.

Favorites positioned in **Project favorites** are saved with the current project and do not remain when another project is opened.

13.2.3.3 Script examples

In the *Script examples* folder a few example scripts are available. Clicking a script example displays an information-message describing what the script does and then runs that example provided your license allows running Python scripts.

You can add your own scripts to Favorites by clicking the **Add script favorite** on the **Developer** tab.

13.2.3.4 Opening plots, items, and executing folders in Favorites

Each item in the **Favorites** pane can be opened by double-clicking it or by marking, right-clicking, and clicking **Open**.

All items or commands in a folder can be opened, and the windows tiled, by marking the folder, right-clicking it and clicking:

- **Open all items in folder**.
- **Treat folder as item** and then double-clicking it.

13.2.3.5 Renaming in Favorites

Rename folders or items by:

- Right-clicking the item and selecting **Rename**.

Or

- Marking the item and pressing **F2**.

13.2.3.6 Deleting from Favorites

To delete a folder or an item, mark the item and:

- Right-click and select **Delete**.
- Press **DELETE** on your keyboard.

13.2.3.7 Creating folders in Favorites

It is convenient to group plots in folders, and automatically open all plots in the folder in sequence when often opening the same plots.

To create a folder:

1. Right-click in the **Favorites** pane.
2. Click **New folder**.
3. Type a name for the folder.

13.2.3.8 Exporting and importing Favorites configuration

The **Favorites** pane configuration can be saved as an .xml-file.

To save the current favorites configuration to file:

1. Right-click the **Favorites** pane.
2. Click **Export**.
3. Enter the name and location in the **Save As** dialog,
4. Click **Save**.

To import favorites from .xml-file:

1. Right-click the **Favorites** pane.
2. Click **Import**.
3. Browse for the file in the **Open** dialog.
4. Click **Open**.

Note: Importing a favorites file overwrites the current file.

13.2.3.9 Adding plots and lists to Favorites

To add a plot or list to **Favorites** use one of the following methods:

1. Right-click the plot or list, and then click **Add to favorites**.
2. With the plot or list active, press **CTRL+D**.
3. With the plot or list active, on the **View** tab, in the **Add** group, click **Add to favorites**.

13.2.4 Item information

The **Item Information** pane displays all the information about the items that are marked in a plot.

13.2.4.1.1 SMILES

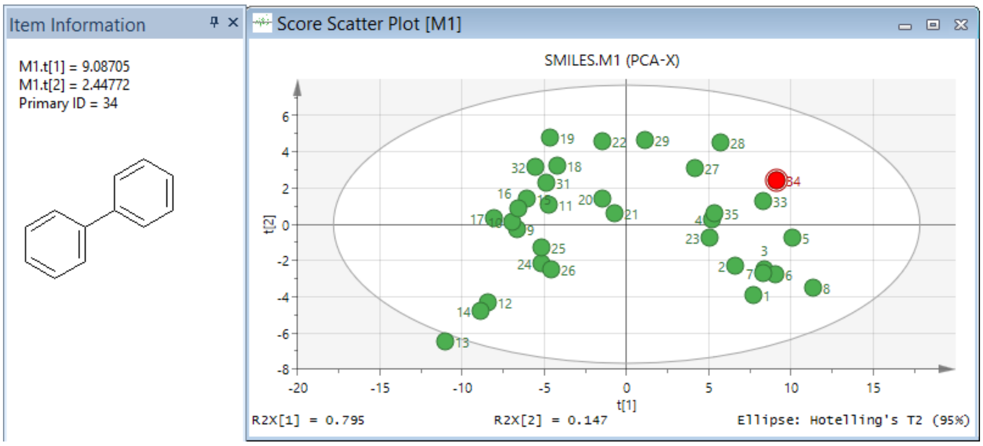
If you have SMILES code as a secondary Observation ID, and have the SMILES plug-in DLL, the Item Information pane displays the molecule.

When marking several observations holding down the CTRL-button, the Item Information pane only displays the chemical structure for the last marked observation.

To see the structure of several observations, all points need to be marked in one go. When the points are not adjacent:

1. Mark the points you want to see structure for.
2. Right-click, select **Create plot** or **Create list**.
3. Mark all the observations in one scope (not holding CTRL-button) and the chemical structure is displayed for all observations in Item Information.

For more information about SMILES, contact your Sartorius Stedim Data Analytics sales office.



M1.t[1] = 9.08705
M1.t[2] = 2.44772
Primary ID = 34

R2X[1] = 0.795 R2X[2] = 0.147 Ellipse: Hotelling's T2 (95%)

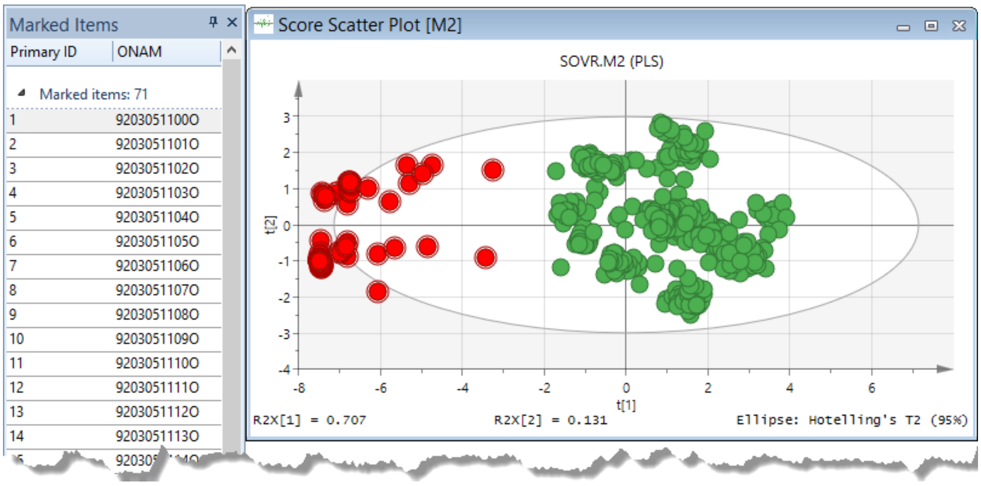
13.2.5 Marked items

The objective of the Marked Items pane is to display the items (observations or variables) that are marked in a plot. When there are many items in a plot, it is difficult to precisely know which items are marked.

The shortcut menu can be used to unmark observations or variables, exclude or include observations or variables, and organize observations in classes. The Exclude/Include and Set classes commands work exactly as on the Marked items contextual tab and creates a new unfitted model with the new specifications.

When items are unmarked in the Marked Items window the corresponding items are unmarked on the plot.

The Marked Items pane is also useful to display the observations used in a group contribution plot. When making a group contribution between two groups, the observations in the first group of observations are displayed under Previously marked items and the second group under Marked items.



Marked items: 71

Primary ID	ONAM
1	9203051100O
2	9203051101O
3	9203051102O
4	9203051103O
5	9203051104O
6	9203051105O
7	9203051106O
8	9203051107O
9	9203051108O
10	9203051109O
11	9203051110O
12	9203051111O
13	9203051112O
14	9203051113O

R2X[1] = 0.707 R2X[2] = 0.131 Ellipse: Hotelling's T2 (95%)

The Marked Items pane can be used for many purposes. For instance:

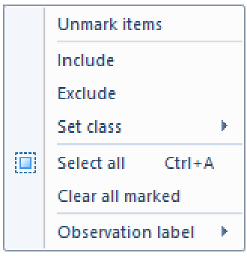
- To display the items, observations or variables, marked in a plot to visualize which items are actually marked. In plots with many items it can be difficult to see precisely which those items are.
- To visualize the marked points in the Marked Items pane when marking points to create a contribution plot.
- To unmark (deselect) points - Mark the points in the **Marked Items** pane, right-click the marking, and click **Unmark items**.

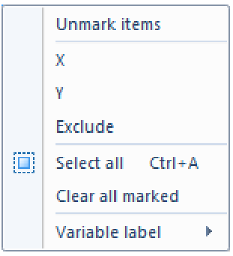
- To view the groups in the dendrogram plot, opened by clicking **HCA** in the **Clustering** group on the **Analyze** tab.

13.2.5.1 Marked Items pane features

There are a number of features available in the **Marked Items** pane shortcut menu.

With observations (left below) the shortcut menu holds the commands: **Unmark items**, **Include**, **Exclude**, **Set class**, **Select all**, **Clear all marked**, and **Observation label**.





With variables (right above) in **Marked Items**, the shortcut menu holds the commands: **Unmark items**, **X**, **Y**, **Exclude**, **Select all**, **Clear all marked**, and **Variable label**.

Clicking **Include**, **Exclude**, **Set class**, **X**, **Y**, or **Exclude** creates a new unfitted model unless there already is an unfitted model. If there already is an unfitted model the selected command is done for that model.

When a new unfitted model is created, that model is created as a copy (as **New as** in the **Workset** group) of the model used when marking the items displayed in the **Marked Items** pane.

Select	Result
Unmark items	Unmarks the marked items in the **Marked Items** pane both in the pane and in all open plots and lists.
Include	Creates a new model including only the marked items.
Exclude	Excludes the marked items.
Set class	Select **No class** or a class. Organizes in classes.
X	Sets the marked variables as X.
Y	Sets the marked variables as Y.
Select all	Marks all items in the **Marked Items** pane.
Clear all marked	Clears all marking in the pane and in all open plots and lists.
Observation label and Variable label	The **Marked Items** pane lists all identifiers. Select to remove labels under **Observation label** or **Variable label**.

13.2.5.2 Creating contribution plots using Marked Items pane and tab

The **Marked Items** pane is useful when creating contribution plots, and especially group contribution plots.

When creating a group contribution plot, the observations in the group marked first are displayed under **Previously marked items** and the group marked last under **Marked items**.

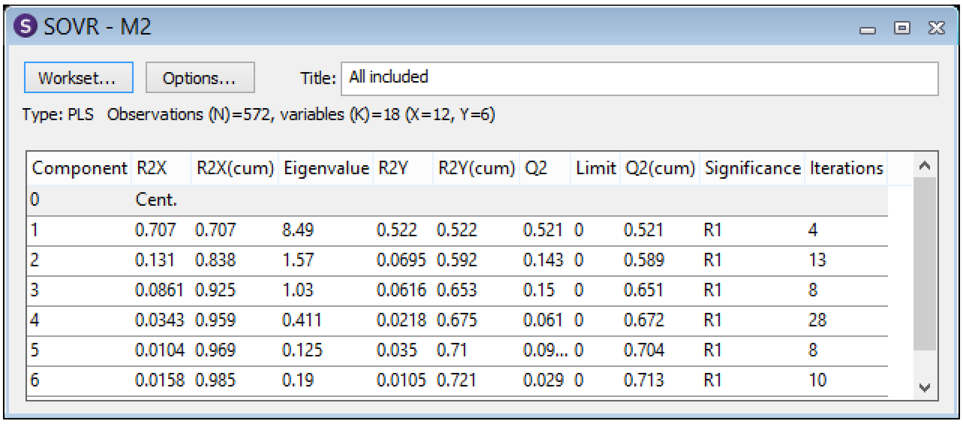
When marking observations the **Marked items** tab becomes available and active.

To create a contribution plot, click the relevant button in the **Drill down** group.

For more about creating contribution plots by marking in plots, see the Drill down contribution plots available subsection in the Marked Items tab section in Chapter 14, Plot and list contextual tabs.

13.2.6 Model window

The model window includes an overview of the model, the **Workset** and **Options** buttons, and displays a summary of the fit of the model with results for each component.



Title: All included

Type: PLS Observations (N)=572, variables (K)=18 (X=12, Y=6)

Component	R2X	R2X(cum)	Eigenvalue	R2Y	R2Y(cum)	Q2	Limit	Q2(cum)	Significance	Iterations
0	Cent.									
1	0.707	0.707	8.49	0.522	0.522	0.521	0	0.521	R1	4
2	0.131	0.838	1.57	0.0695	0.592	0.143	0	0.589	R1	13
3	0.0861	0.925	1.03	0.0616	0.653	0.15	0	0.651	R1	8
4	0.0343	0.959	0.411	0.0218	0.675	0.061	0	0.672	R1	28
5	0.0104	0.969	0.125	0.035	0.71	0.09...	0	0.704	R1	8
6	0.0158	0.985	0.19	0.0105	0.721	0.029	0	0.713	R1	10

The model window holds the following information about the model:

Item	Explanation
Title	Title of model.
Type	The model type used when fitting.
Observations (N)	Number of observations.
Variables (K)	Total number of variables
X	Number of variables as X (including expanded and lagged terms).
Y	Number of variables as Y.
Lagged	Number of lagged variables.
Expanded	Number of expansions.
Components	The list of components and their statistics and properties. For more see the Model summary of fit subsection later in this section.

13.2.6.1 Workset

Clicking **Workset** displays the workset associated with the model. Note that if you click **Workset**, edit the workset, and click **OK**, the model will be replaced by a new unfitted model. For more about the workset, see the Workset section in Chapter 7, Home.

13.2.6.2 Options

Clicking **Options** displays the **Model Options** dialog. For details, see the Model Options subsection in the Workset section in Chapter 7, Home.

13.2.6.3 Model summary of fit

The model window consists of a summary line for each component A of the model, starting with component 0 representing centering.

The table describes all columns available for each component.

Column header	Description
A	The component number.
R2X	Fraction of Sum of Squares (SS) of the entire X explained by the current component.
R2X (cum)	Cumulative SS of the entire X explained by all extracted components.
Eigenvalue	Eigenvalue of the X matrix, R2X * min(K,N).
R2Y	Fraction of Sum of Squares of all y-variables explained by this component.
R2Y (cum)	The cumulative SS of all the y-variables explained by the extracted components.
Q2	The fraction of the total variation of X (PC) and Y (PLS/OPLS/O2PLS) that can be predicted by the current component.

Column header	Description
Limit	The cross validation threshold for that component. When Q2 > Limit the component is significant.
Q2 (cum)	The cumulative Q2 for all the x-variables (PC) and y-variables (PLS/OPLS/O2PLS) for the extracted components.
Significance	Significance of the component according to cross validation rules: R1, R2, U, R5, NS, N3, N4. For details about the cross validation rules, see the Cross validation section in the Statistical appendix.
Iterations	Number of iterations till convergence.

13.2.6.4 Model window for OPLS and O2PLS models

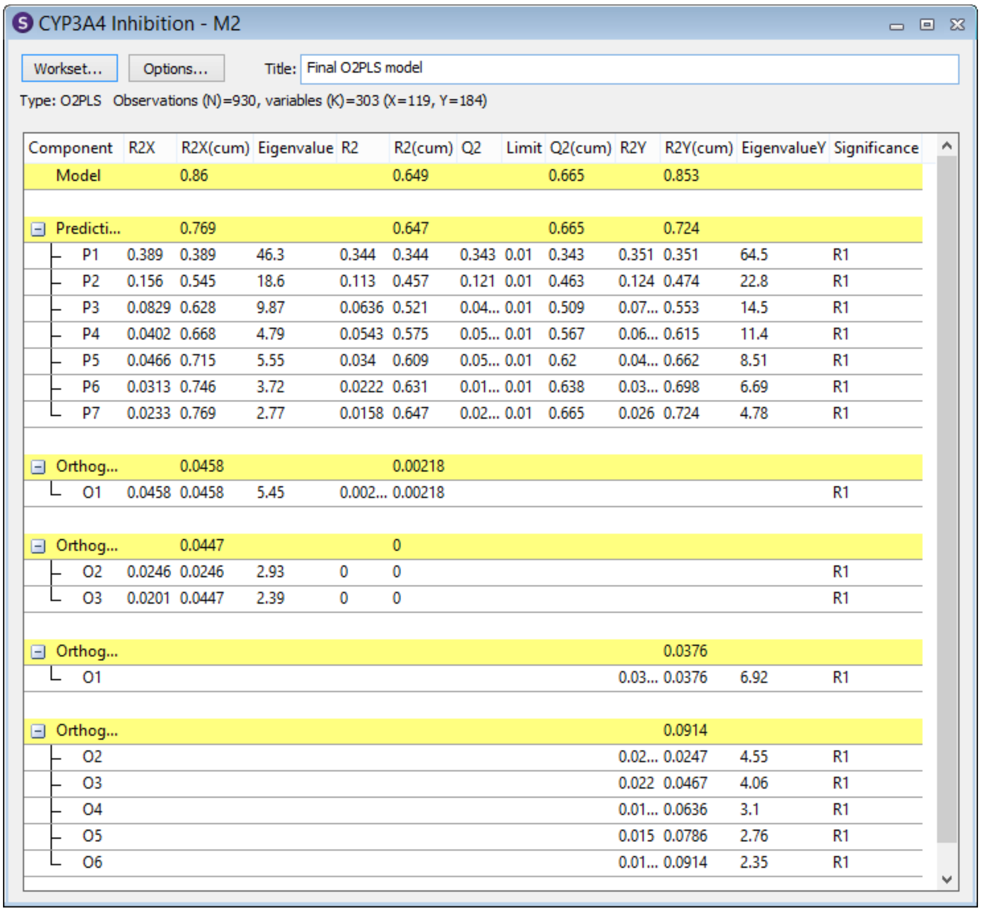
The **Model Window** corresponding to OPLS and O2PLS displays summary statistics related to the model. Components that capture variation found in both X and Y are denoted Predictive. Components that capture variation only found in X are denoted Orthogonal in X(OPLS). Components that capture variation only found in Y are denoted Orthogonal in Y(OPLS).

The OPLS model is based on the OPLS algorithm. The O2PLS model is based on the similar O2PLS algorithm, but in addition there is a PCA step. PCA is used after convergence of the O2PLS algorithm, to exhaust the E and F residual matrices from all remaining systematic variation. This yields the additional Orthogonal in X(PCA) and Orthogonal in Y(PCA) components.

The method underlying a certain orthogonal component is indicated in the name of the component in the **Model Window**.

Note: The model window for OPLS models displays, if existing, three types of components: Predictive, Orthogonal in X, Orthogonal in Y. Additionally, The model window for O2PLS displays, if existing, Orthogonal in X and Orthogonal in Y components estimated by PCA.

Figure 2. The Model Window for an O2PLS model with 7 predictive, 3 Orthogonal in X and 6 Orthogonal in Y components (a 7+3(1+2) +6(1+5) O2PLS model).



Title: Final O2PLS model

Type: O2PLS Observations (N)=930, variables (K)=303 (X=119, Y=184)

Component	R2X	R2X(cum)	Eigenvalue	R2	R2(cum)	Q2	Limit	Q2(cum)	R2Y	R2Y(cum)	EigenvalueY	Significance
Model		0.86			0.649			0.665		0.853		
⊟ Predicti...		0.769			0.647			0.665		0.724		
P1	0.389	0.389	46.3	0.344	0.344	0.343	0.01	0.343	0.351	0.351	64.5	R1
P2	0.156	0.545	18.6	0.113	0.457	0.121	0.01	0.463	0.124	0.474	22.8	R1
P3	0.0829	0.628	9.87	0.0636	0.521	0.04...	0.01	0.509	0.07...	0.553	14.5	R1
P4	0.0402	0.668	4.79	0.0543	0.575	0.05...	0.01	0.567	0.06...	0.615	11.4	R1
P5	0.0466	0.715	5.55	0.034	0.609	0.05...	0.01	0.62	0.04...	0.662	8.51	R1
P6	0.0313	0.746	3.72	0.0222	0.631	0.01...	0.01	0.638	0.03...	0.698	6.69	R1
P7	0.0233	0.769	2.77	0.0158	0.647	0.02...	0.01	0.665	0.026	0.724	4.78	R1
⊟ Orthog...		0.0458			0.00218							
O1	0.0458	0.0458	5.45	0.002...	0.00218							R1
⊟ Orthog...		0.0447			0							
O2	0.0246	0.0246	2.93	0	0							R1
O3	0.0201	0.0447	2.39	0	0							R1
⊟ Orthog...										0.0376		
O1									0.03...	0.0376	6.92	R1
⊟ Orthog...										0.0914		
O2									0.02...	0.0247	4.55	R1
O3									0.022	0.0467	4.06	R1
O4									0.01...	0.0636	3.1	R1
O5									0.015	0.0786	2.76	R1
O6									0.01...	0.0914	2.35	R1

The **Model Window** displays:

Section	Description	Component types
Model	Summarizes the model, showing the cumulative R2X, R2, Q2, and R2Y.	
Predictive	The Predictive section where the first row summarizes the predictive components in the model followed by a listing of each predictive component.	The predictive loading vectors are *p* for the X-block and *q* for the Y- block. The predictive score vectors are *t* for the X-block and *u* for the Y-block. In the figure above there are 7 components for *p*, *q*, *t* and *u*.
Orthogonal in X (OPLS)	The Orthogonal in X(OPLS) section where the first row summarizes the orthogonal components in the X model followed by a listing of each orthogonal in X component. The orthogonal in X components show the variation in X that is uncorrelated to Y.	The orthogonal in X(OPLS) loading vectors are *po* for the X-block and *so* for the Y-block. The orthogonal in X (OPLS) score vector is *to* for the X-block. In the figure above there is one orthogonal in X(OPLS) component. This means that the po[1], so[1], and to[1] vectors are the orthogonal in X(OPLS) vectors.
Orthogonal in X (PCA)	The Orthogonal in X(PCA) sections where the first row summarizes the orthogonal components in the X model followed by a listing of each orthogonal in X component. The orthogonal in X components show the variation in X that is uncorrelated to Y	The orthogonal in X(PCA) loading vectors are *po* for the X-block and *so* for the Y-block. The orthogonal in X (PCA) score vector is *to*. The orthogonal in X(PCA) components are extracted after the orthogonal in X(OPLS) components, and their relational order is indicated through the shared nomenclature. In the figure above there are two orthogonal in X(PCA) components. This means that the po[2], po[3], so[2], so[3], to[2] and to[3] vectors are the orthogonal in X(PCA) vectors
Orthogonal in Y (OPLS)	The Orthogonal in Y (OPLS) sections where the first row summarizes the orthogonal components in the Y model followed by a listing of each orthogonal in Y component. The orthogonal in Y components show the variation in Y that is uncorrelated to X.	The orthogonal in Y(OPLS) loading vectors are *r* for the X-block and *qo* for the Y-block. The orthogonal in Y (OPLS) score vector is *uo* for the Y block. In the figure above there is one orthogonal in Y(OPLS) component. This means that the r[1], qo[1], and uo[1] vectors are the orthogonal in Y(OPLS) vectors.
Orthogonal in Y (PCA)	The Orthogonal in Y (PCA) sections where the first row summarizes the orthogonal components in the Y model followed by a listing of each orthogonal in Y component. The orthogonal in Y components show the variation in Y that is uncorrelated to X	The orthogonal in Y(PCA) loading vectors are *r* for the X-block and *qo* for the Y-block. The orthogonal in Y (PCA) score vector is *uo* for the Y block. The orthogonal in Y(PCA) components are extracted after the orthogonal in Y(OPLS) components and their relational order is indicated through the shared nomenclature. In the figure above there are five orthogonal in Y(PCA) components. This means that the r[2]-r[6], qo[2]-qo[6], and uo[2]-uo[6] vectors are the orthogonal in Y(PCA) vectors.

The table columns are:

- Component - Component index.
- R2X - Fraction of X variation modeled in that component, using the X model.
- R2X(cum) - Cumulative R2X up to the specified component.
- Eigenvalue - The minimum number of observations (N) and X-variables multiplied by R2X, that is, min(N,K)*R2X.
- R2 - Fraction of Y variation modeled in that component, using the X model.
- R2(cum) - Cumulative R2 up to the specified component.
- Q2 - Fraction of Y variation predicted by the X model in that component, according to cross-validation.
- Q2(cum) - Cumulative Q2 up to the specified component.
- R2Y - Fraction of the Y variation modeled in that component, using the Y model.
- R2Y(cum) - Cumulative R2Y up to the specified component
- EigenvalueY - The minimum number of observations (N) and Y-variables multiplied by R2Y, that is, min(N,M)*R2Y.
- Significance – Significance level of the model component.

For more, see the OPLS/O2PLS - Orthogonal PLS modeling section in the Statistical appendix.

13.2.7 Notes

In the **Notes** pane you can record your own notes concerning the project and models. You can paste SIMCA plots (using the bitmap format) and lists. The notes contents are saved with the project file.

The notes-file can also be saved as .rft (Rich Text Format) and read directly by a word processor with all plots.

13.2.8 Observations pane

The **Observations** pane displays the observations included in the workset of the active model.

Right-clicking the pane opens the shortcut menu holding the following commands: **Include**, **Exclude**, **Set class**, **Select all**, and **Observation label**. These commands work as described in the Marked items section previously in this chapter.

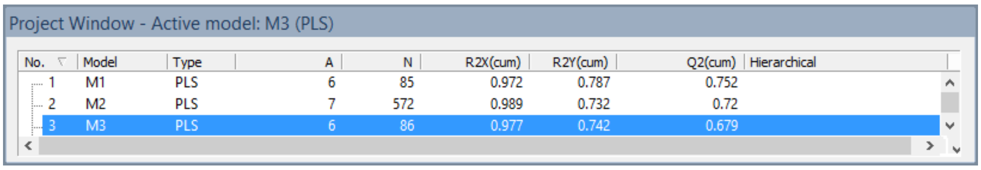
13.2.9 Project window

The project window displays a list of all models with their respective model information.

The model selected in the project window is the active model, displayed in the window caption (frame) both when displayed and when minimized. All plots created are created for the active model.

The project window is by default docked and can then only be minimized, not closed. To have the project window slide away after showing it, click **Auto Hide** so that it turns. See the Show subsection for details.

To have the project window as a regular window, see the Customizing the Project window subsection.



Project Window - Active model: M3 (PLS)

No.	Model	Type	A	N	R2X(cum)	R2Y(cum)	Q2(cum)	Hierarchical
1	M1	PLS	6	85	0.972	0.787	0.752	
2	M2	PLS	7	572	0.989	0.732	0.72	
3	M3	PLS	6	86	0.977	0.742	0.679	

The list of models by default displays the following information about each model:

Column header	Description
No.	Workset number. Workset numbers are assigned sequentially. When the model is a batch model the workset number also holds the abbreviation BM for Batch Model. With class models, the workset number also holds the abbreviation CM for Class Model.
Model	Automatic model name. The models are named Mxx with xx being a sequential number starting at 1
Type	Fit method used to fit the model.
A	Number of components.

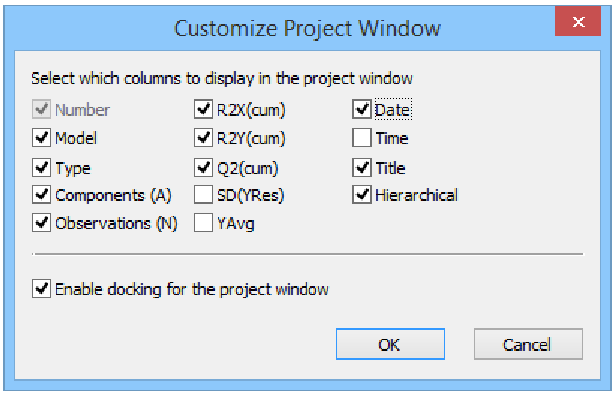
Column header	Description
R2X	Sum of Squares of all the x-variables explained by the extracted components.
R2Y	For PLS, Sum of Squares of all the y-variables explained by the extracted components.
Q2(Cum)	Cumulative cross validated R2.
SD(Y)	Standard deviation of Y (not displayed by default).
Date	Date when the model was fitted.
Time	Time when the model was fitted (not displayed by default).
Title	Title of the model entered by the user. By default all models have the title 'Untitled'.
Hierarchical	Displays B or T when the model is a Base or Top hierarchical model. A model using the scores or residuals of other models as variables is a hierarchical top model. Hierarchical models are described in detail in Chapter 10, Analyze.

13.2.9.1 Customizing the Project window

To select which columns to display in the **Project Window**, click **Customize** from the shortcut menu.

In the dialog that opens, select and clear as desired.

Note: For the project window to behave like a regular window, clear the **Enable docking for the project window** check box.



Customize Project Window

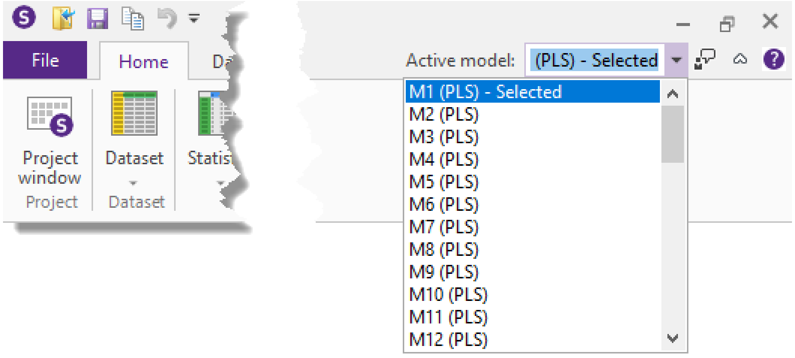
Select which columns to display in the project window

☑ Number ☑ R2X(cum) ☑ Date
☑ Model ☑ R2Y(cum) □ Time
☑ Type ☑ Q2(cum) ☑ Title
☑ Components (A) □ SD(YRes) ☑ Hierarchical
☑ Observations (N) □ YAvg

☑ Enable docking for the project window

13.2.9.2 Project window as regular window

When the project window behaves as a regular window, see Customizing the Project window, you can open it by clicking **Project window** to the far left on the **Home** tab. You can also, at all times, see and switch the current active model in the Active model box in the upper right corner.



13.2.9.3 Project Window shortcut menu

From the shortcut menu of the **Project Window** the following commands are available:

- **Open** - Opens the model window of the active model.
- **Edit Model x** - Opens the workset for the model, see the Editing the workset subsection in the Workset section in Chapter 7, Home.

- **New as Model x -** Opens a copy of the workset for the model, see the New workset as model subsection in the Workset section in Chapter 7, Home.
- **Change model title -** Opens the **Model Title** dialog, see the Changing the model title subsection later in this chapter.
- **Delete -** Deletes the active model, see the Deleting the model subsection in the Workset section in Chapter 7, Home.
- **Hierarchical base model**, **Non hierarchical base model -** Specifies the model as hierarchical/non hierarchical base model, see the Hierarchical models subsection in Chapter 8, Data.
- **Generate report -** Opens the report generator, see the Appending to, inserting in, or replacing existing report subsection in the Generate Report section in Chapter 5, File.
- **PLS-Tree plot** - Opens the PLS-Tree dendrogram, see the PLS-Tree resulting dendrogram subsection in Chapter 10, Analyze.
- **Add to report -** Adds the project window to the report, see the Add to Report subsection in the Generate Report section in Chapter 5, File.
- **Customize -** Opens the **Customize Project Window** dialog, see the Customizing the Project window subsection later in this section.
- **Model options** - Opens the **Model Options** of the active model, see the Model Options subsection in the Workset section in Chapter 7, Home.

13.2.9.4 Changing the model title

The model title is by default 'Untitled'. To change the model title:

1. With the:
    - **Model Window** open, type in the **Title** field, or
    - **Project Window** open, right-click the model, and click **Change model title**.
2. Enter the new model title and click **OK**.

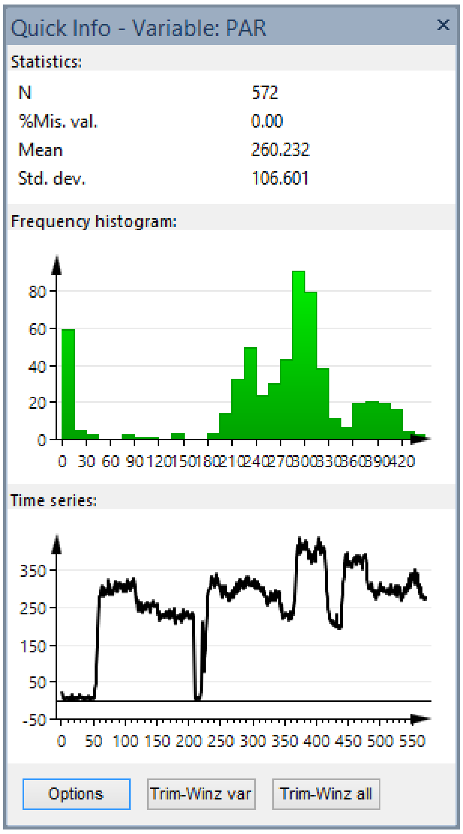
13.2.10 Quick info

The **Quick Info** pane displays overview information about marked items in an open plot, list, or spreadsheet. When displaying the Quick Info of variables after marking in a dataset spreadsheet, trimming and Winsorizing is also available.

A separate **Quick Info** pane is available in the workset dialog, tab **Spreadsheet**. Trim-Winsorizing in the workset applies to the model only, not the dataset. For more, see the Spreadsheet in the Workset dialog subsection in the Workset section in Chapter 7, Home.

To open the **Quick Info** pane:

- On the **View** tab, in the **Show** group, select the **Quick info** check box OR
- Right-click the dataset spreadsheet and click **Quick info**.



Quick Info - Variable: PAR

Statistics:

N	572
%Mis. val.	0.00
Mean	260.232
Std. dev.	106.601

13.2.10.1 Quick Info pane description

The **Quick Info** pane has the following content:

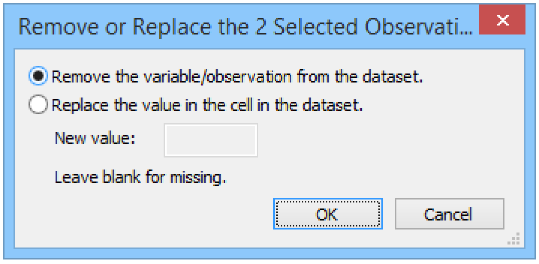
- Caption bar with the current item information including the type of item (variable/observation etc.), **Auto Hide**, and **Close**.
- **Statistics** section holding the statistics and optionally variable recipe when selected for display in **Options**. Default is to display **N** (number of items in the series), **% Mis. val.** (percent missing values), **Mean**, and **Std. dev.** (standard deviation).
- Selection of plots according to selection in **Options**. Default is to display the **Frequency histogram** and **Time series** plots.
- **Selection bar** if selected in **Options**. Default is to not display the **Selection bar**.
- **Options** button.
- **Trim-Winz var** and **Trim-Winz all**-buttons when the **Quick Info** is for variables.

The quick info plots and the buttons **Options**, **Trim-Winz var**, and **Trim-Winz all** are described in the subsections that follow.

13.2.10.2 Quick info plots and interactive delete or replace

Deleting an observation or variable, or changing the value of a selected cell, can be done interactively using the **Quick Info** pane **Time series** or **Spectrum** plot in the following manner:

1. Mark points in the **Time series** or **Spectrum** plot. The **Remove or Replace the x Selected Observations/Variables** dialog opens:



Remove or Replace the 2 Selected Observati...

● Remove the variable/observation from the dataset.

○ Replace the value in the cell in the dataset.

New value:

Leave blank for missing.

2. Select

   a. **Remove the variable/observation from the dataset** to delete the marked variables or observations OR

   b. **Replace the value in the cell in the dataset** and type the new value in the **New value** field, to replace.

3. Click **OK** to take action.

---

*Note: The **Remove or Replace** dialog automatically opens when marking points in the Quick Info **Time series** or **Spectrum** plots when the **Trim-Winz var** dialog is closed.*

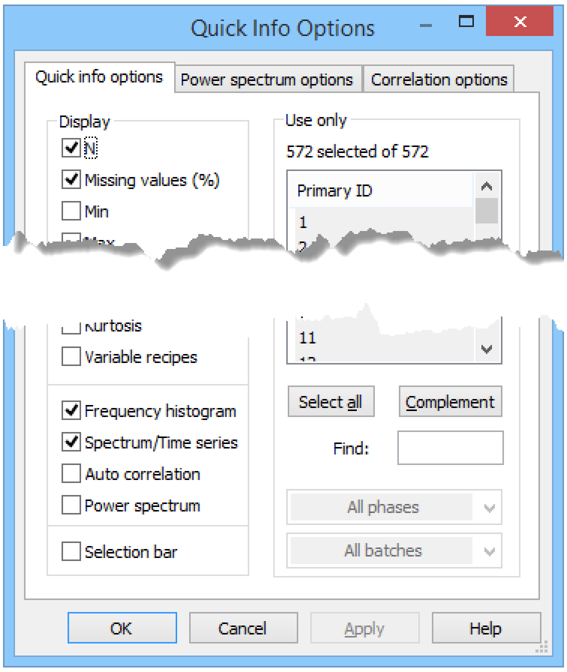
13.2.10.3 Quick Info Options button

The selected settings in the **Quick Info Options** dialog define what is displayed in the **Quick Info** pane.

Clicking the **Options** button opens the options dialog with the tabs **Quick info options**, **Power spectrum options**, and **Correlation options**. The content of these tabs is described in the subsections that follow.

13.2.10.3.1 Quick Info Options page

To open the **Quick Info Options** dialog, click the **Options** button.



Quick Info Options

Display

☑ N

☑ Missing values (%)

□ Min

□ Max

□ Kurtosis

□ Variable recipes

☑ Frequency histogram

☑ Spectrum/Time series

□ Auto correlation

□ Power spectrum

□ Selection bar

Use only

572 selected of 572

Primary ID

1

2

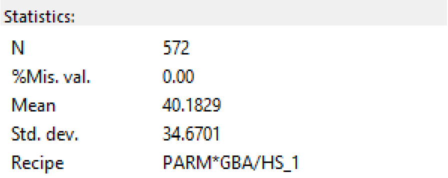
11

Statistics section

The first section under **Display** lists the statistics that can be displayed in the **Statistics** section of the **Quick Info** pane and an option named **Variable recipes**.

The available statistics are: **N**, **Missing value (%)**, **Min**, **Max**, **Min/Max**, **Mean**, **Median**, **Standard deviation**, **Std. dev./Mean**, **Skewness**, and **Kurtosis**.

The **Variable recipe** describes how a new generated variable was created. For example, after creating the variable named *PARM*GBA/HS_1* as the product of variable v5 multiplied with the ratio of variable v10 and variable v6, clicking that variable displays the formula in the statistics section.



Statistics:

N	572
%Mis. val.	0.00
Mean	40.1829
Std. dev.	34.6701
Recipe	PARM*GBA/HS_1

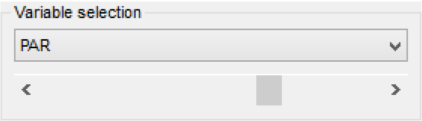
Selecting Quick Info pane plots

Select to display any or all of the 4 following plots:

1. **Frequency histogram** (default selected).
2. **Spectrum/Time series** (default selected).
3. **Auto correlation**.
4. **Power spectrum**.

Displaying the selection bar

The **Selection bar** is a **Variable selection** bar with a scrolling tool. Moving this tool allows moving in the dataset by emulating cursor movement. Above the scroll bar, the current variable is displayed in the **Variable selection** box. Use the **Variable selection** box or click the arrow-button to switch variables.



Selecting items to include

Under **Use only** on the right side of the pane is a list of observations (for **Quick Info** of variables) or variables (for **Quick Info** of observations). Use this function to select which observations or variables to include. By default all the observations or variables are included.

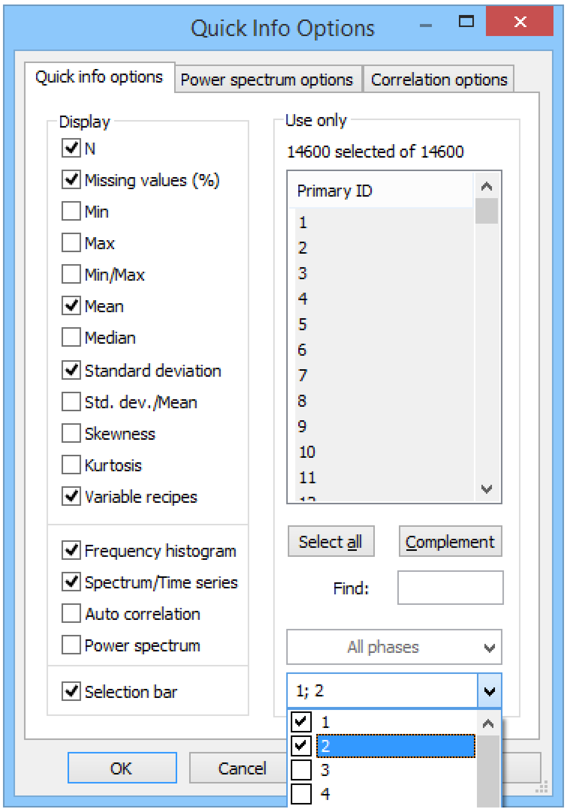
A **Find** feature is available to facilitate this task. Observations or variables may be selected by entering characters in the **Find** field. Wild card symbols **'?'**, and **'*'** are allowed in specifying observations or variables identifiers. For example “?LH*” selects observations or variables with names such as SLH2 or QLHSW, etc. Click the **Complement** button to display the complement of the selected variables or observations.

Note: *The **Find** utility in SIMCA is cASe inSEnitiVE.*

To display another or more identifiers, right-click the list and select it.

Selecting phases and batches for batch data

With batch data, select to display the Quick Info pane for all phases and batches or for a selection of phases and batches.



Quick Info Options

Quick info options | Power spectrum options | Correlation options

Display
- ☑ N
- ☑ Missing values (%)
- □ Min
- □ Max
- □ Min/Max
- ☑ Mean
- □ Median
- ☑ Standard deviation
- □ Std. dev./Mean
- □ Skewness
- □ Kurtosis
- ☑ Variable recipes
- ☑ Frequency histogram
- ☑ Spectrum/Time series
- □ Auto correlation
- □ Power spectrum
- ☑ Selection bar

Use only

14600 selected of 14600

Primary ID: 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11

Select all | Complement

Find:

All phases

1; 2
- ☑ 1
- ☑ 2
- □ 3
- □ 4

OK | Cancel

Select the phase and batches from the boxes positioned bottom right. Default is to use **All phases** and **All batches**. All statistics and plots will refer to the selected phases and batches.

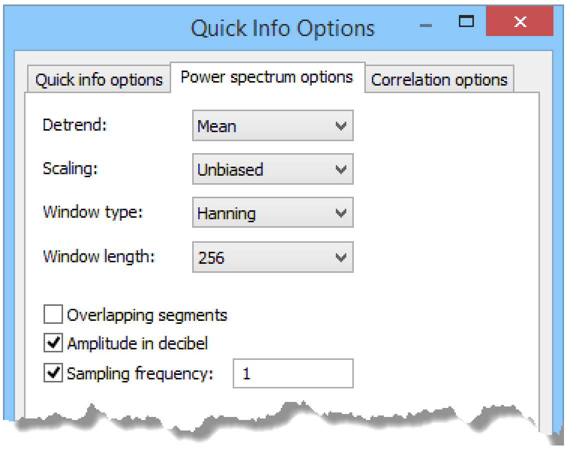
13.2.10.3.2 Power spectrum options page

The Power Spectrum Density (PSD) is the representation of the sequence x (t) in the frequency domain. The power spectrum is the square of the amplitude of the Fourier component at each frequency.

The frequency domain representation is particularly helpful to detect irregular cycles and pseudo periodic behavior, i.e. tendency towards cyclic movements centered on a particular frequency.

For more, see the Power spectrum density section in the Preprocessing appendix.

Note: *With a dataset that has been wavelet transformed and compressed variables wise, using* ***Data | Spectral filters****, the PSD observation wise refers to the reconstructed observations, when the* ***Reconstruct wavelets*** *check box is selected.*



Quick Info Options

Quick info options | Power spectrum options | Correlation options

Detrend: Mean

Scaling: Unbiased

Window type: Hanning

Window length: 256

- □ Overlapping segments
- ☑ Amplitude in decibel
- ☑ Sampling frequency: 1

The **Power spectrum options** tab includes the following options.

Detrending

The default is to detrend by removing the **Mean**. There are two more options:

- Removing the best linear fit by selecting **Linear** or
- Removing nothing by selecting **None**.

Scaling

Asymptotically **Unbiased** is the default scaling. Selecting **Peaks** estimates the heights of the original peaks.

Selecting window type

The default **Window type** is **Hanning**.

To select another window type, click the **Window type** box and select **Welsch** or **Bartlett**.

Selecting window length

The default **Window length** is the smallest of 256 or ½ the length of X (t), padded, to the nearest length 2^n, where n= integer, although always larger than or equal to 16.

Select another length from the **Window length** box.

Overlapping segments

The default is to not overlap the segments.

To overlap, select the **Overlapping segments** check box.

Scaling of the Y axis

The scale of the y-axis is default in Decibel.

To display the y-axis non transformed, clear the **Amplitude in decibel** check box.

Selecting sampling frequency

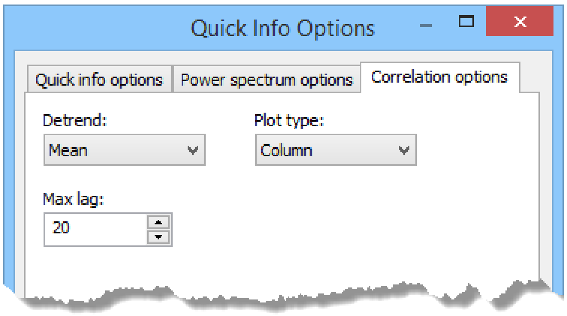
The output of the PSD is a vector of length = (window length)/2 +1. This is the scale of x if you have not entered a sampling frequency.
The sampling frequency is used as a scaling multiplier to properly scale the frequency axis, with the highest frequency being the Nyquist frequency = Fs/2. It has no effect on the PSD.
By default SIMCA assumes a sampling frequency of 1 and Fs/2=0.5 is displayed as the highest frequency.

13.2.10.3.3 Correlation options page

The auto correlation is a measure of dependence of adjacent observations and characterizes a time series or observation profile, in the time domain.

Note: With a dataset that has been wavelet transformed and with the ***Reconstruct wavelets*** *check box selected, the auto correlation is displayed in the reconstructed domain.*

For more, see the Auto and cross correlation of variables or observations section in the Preprocessing appendix.



Detrend: Mean

Plot type: Column

Max lag: 20

The **Correlations options** page includes the following options:

Detrending

The default is to detrend by removing the **Mean**. There are two more options:

- Removing the best linear fit by selecting **Linear** or
- Removing nothing by selecting **None**.

Maximum number of lags

The auto correlation is default computed up to lag L=30 or N/4 whichever is smaller.

To change the number of lags, enter a new number in **Max lag**.

Selecting plot type

Default is to display the auto correlation plot as a column plot.

To display it as a line plot, select **Line** in the **Plot type** box.

13.2.10.4 Preprocessing the dataset using Trim-Winsorizing

Trimming and Winsorizing is available for variables only. The **Trim-Winz var** and **Trim-Winz all** buttons are available when one or more variables are marked.

Trimming is cutting the upper and lower edges of the variables and replacing them by *missing values*.

Winsorizing is cutting the upper and lower edges of the variables and replacing the removed values by *new values*.

Note: Trimming or Winsorizing the dataset deletes all models that include the affected variables.

The **Trim-Winz var** and **Trim-Winz all** buttons are positioned bottom right in the **Quick Info** pane:

To Trim-Winsorize, click:

- **Trim-Winz var** to trim or Winsorize the marked variable.
- **Trim-Winz all** to trim or Winsorize all variables in the dataset or a selected subset by using the **Selected variables** page.

Note: When a number of values are equal, none of them will be changed if not all of them fall outside the limits.

Note: The details of the performed trim-Winsorizing are registered in the audit trail when the audit trail is turned on, and in Trimming overview.

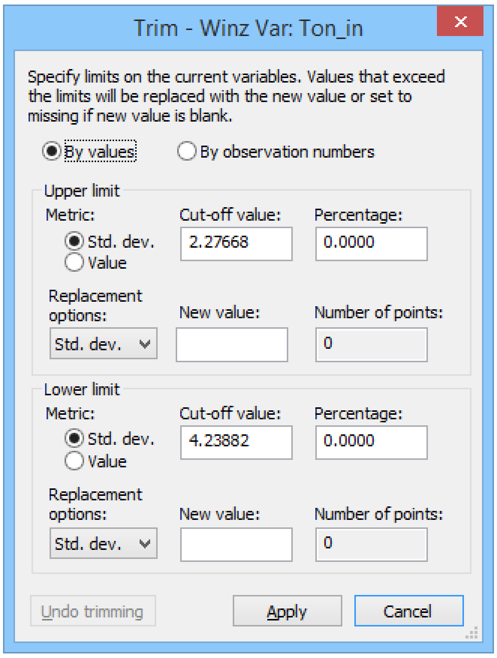
13.2.10.4.1 Trim-Winz Var dialog

The **Trim-Winz Var** dialog displays:

- **By** section where you can select either the **By values** option or the **By observation numbers** option. The trimming and Winsorizing **By values** is applied to values found ***outside*** the defined limits. Observations found within the limits remain untouched. Trimming and Winsorizing **By observation number** is applied to the items found ***inside*** the defined limits and the items found outside the limits remain untouched.
- **Upper limit** section – defines the upper limit including limit type, limit, optional new value, and new value type.
- **Lower limit** section – defines the lower limit including limit type, limit, optional new value, and new value type.
- **Undo trimming** button – resets the performed trimming or Winsorizing with the exception when selecting **Deleting obs**. **Deleting obs.** cannot be reset.
- **Apply** button – performs the defined trimming or Winsorizing. The statistics are updated and displayed for the changed dataset.
- **Cancel** button – cancels any unapplied trimming and closes the trim-Winz dialog.

*Note: The **Trim-Winz Var** dialog remains open after clicking **Apply** to facilitate trim-Winsorizing of another variable.*

More about the upper and lower limit sections follows.



Trim - Winz Var: Ton_in

Specify limits on the current variables. Values that exceed the limits will be replaced with the new value or set to missing if new value is blank.

● By values ○ By observation numbers

Upper limit

Metric: ● Std. dev. ○ Value

Cut-off value: 2.27668

Percentage: 0.0000

Replacement options: Std. dev.

New value:

Number of points: 0

Lower limit

Metric: ● Std. dev. ○ Value

Cut-off value: 4.23882

Percentage: 0.0000

Replacement options: Std. dev.

New value:

Number of points: 0

Defining upper and lower limits By values

The **Upper limit** and **Lower limit** sections are identical. To define the upper and lower limits **By values** follow these steps:

1. Under **Metric** select one of the options:
   a. **Std. dev.** to define and view the **Cut-off value** in robust standard deviation. The robust standard deviation is computed as the interquartile divided by 1.075.
   b. **Value** to define and view the **Cut-off value** as the real value.
2. In the **Cut-off value** or **Percentage** fields, enter the value defining the cut off. When entering a value in the **Cut-off value** field, the **Percentage** field is automatically updated and vice versa. After defining the limit, note that the number of points affected is displayed in the **Number of points** field.
3. Select what to do with the marked items by selecting one of the options available from the **Replacement options** menu, described in the table, and then click **Apply**.

Replacement options	New value	Result and example
Std. dev.	Number of robust standard deviations.	Entering for instance 2 means that the limit is 2*robust standard deviation where the robust standard deviation is calculated as the interquartile/1.075. To view the actual number that will be used when replacing: 1. Select Std. dev. under Metric. 2. Enter the number of standard deviations entered in the **New value** field, in the **Cut-off value** field. 3. Click **Value** under **Metric** to automatically display the standard deviations value in real values in the **Cut-off value** field.
Value	The actual value to replace with.	Enter the value '1' replaces all marked values with '1'. To replace with missing, leave **New value** blank.
Percent	Percentage value.	Replaces with the value at the entered percentage. To view the actual number that will be used when replacing: 1. Select **Value** under **Metric**.

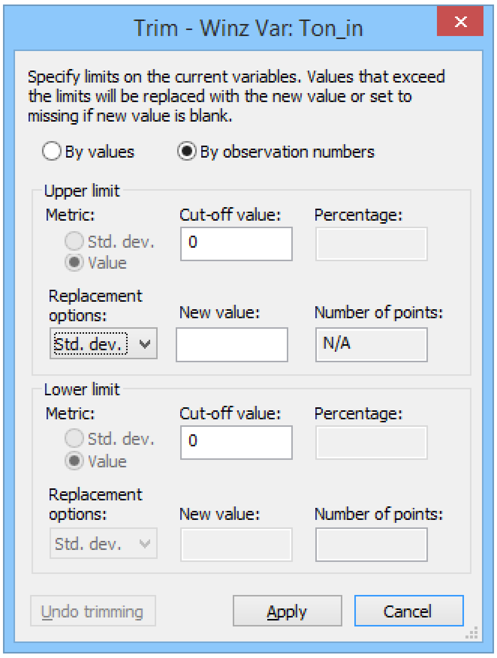
Replacement options	New value	Result and example
		2. Enter the percentage value entered in the **New value** field, in the **Percentage** field. The **Cut-off value** field is then updated to display the real value.
Last good value	No entry.	Valid with Time Series and defined as the last value (in time) of this variable that was inside the limit.
Delete obs	No entry.	Irretrievably deletes the observations from the dataset.

Note: When switching between displaying the limit in ***Std. dev.*** *and* ***Value*** *the* ***Cut-off value*** *field is updated automatically. That is, if the limit is the value 10, clicking* ***Std. dev.*** *automatically displays the corresponding value for standard deviations.*

Defining upper and lower limits By observation numbers

When selecting **By observation numbers** the fields available are the upper and lower limits, the **Replacement options** box and the **New value** field.

1. In the **Cut-off value** fields, enter the observation numbers defining the lower and upper limits for the observations to trim or Winsorize.
2. Select how to trim or Winsorize the marked items by clicking the arrow and selecting one of the items. For details, see table in the previous section Defining upper and lower limits By values.
3. Click **Apply**.



Trim - Winz Var: Ton_in

Specify limits on the current variables. Values that exceed the limits will be replaced with the new value or set to missing if new value is blank.

○ By values ● By observation numbers

Upper limit
Metric: ○ Std. dev. ● Value
Cut-off value: 0
Percentage:
Replacement options: Std. dev.
New value:
Number of points: N/A

Lower limit
Metric: ○ Std. dev. ● Value
Cut-off value: 0
Percentage:
Replacement options: Std. dev.
New value:
Number of points:

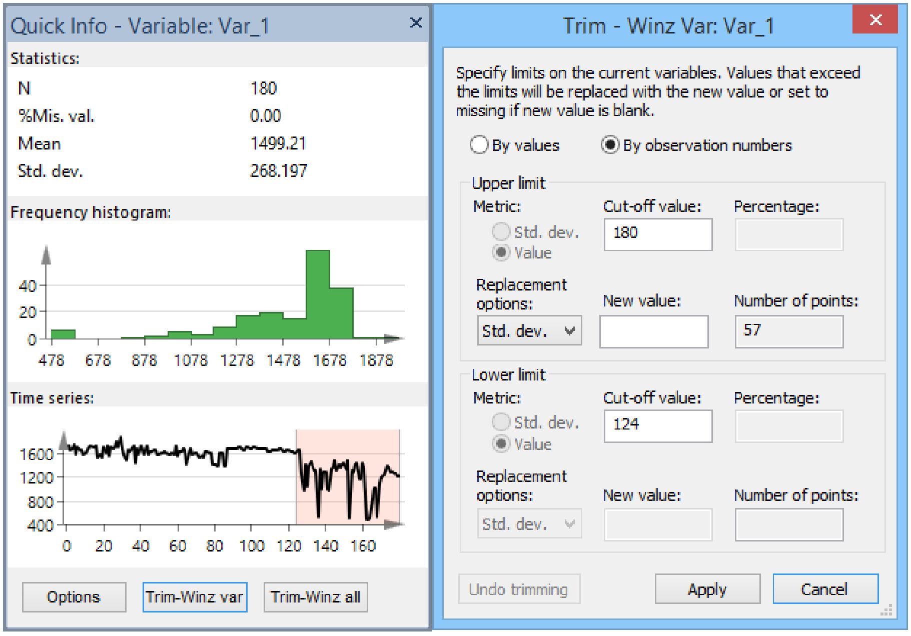
13.2.10.4.2 Trim-Winsorizing from Quick Info plot By values

When trimming or Winsorizing interactively **By values**, the area outside the marking will be affected.

To trim-Winsorize directly from the **Quick Info** plots **Frequency histogram** or **Time series**:

1. Click the **Trim-Winz var** button.
2. Select the **By values** option to mark an area according to the value.
3. In the histogram, vertically mark the area of the plot. Alternatively, in the time series plot, horizontally mark the area of the plot to keep. The area becomes white and the area outside the cut off limits becomes yellow. The **Trim-Winz Var** dialog is updated according to the marking displaying the cut-off values, percentages, and the number of

marked data points.



Quick Info - Variable: Var_1

Statistics:

N	180
%Mis. val.	0.00
Mean	1499.21
Std. dev.	268.197

Frequency histogram:

Time series:

Trim - Winz Var: Var_1

Specify limits on the current variables. Values that exceed the limits will be replaced with the new value or set to missing if new value is blank.

○ By values ● By observation numbers

Upper limit

Metric: ○ Std. dev. ● Value

Cut-off value: 180

Percentage:

Replacement options: Std. dev.

New value:

Number of points: 57

Lower limit

Metric: ○ Std. dev. ● Value

Cut-off value: 124

Percentage:

Replacement options: Std. dev.

New value:

Number of points:

4. In the **Replacement options** boxes select how to replace and if applicable enter a value in the **New value** fields.

5. Click **Apply**.

13.2.10.4.3 Trim-Winsorizing from Quick Info plot By observation numbers

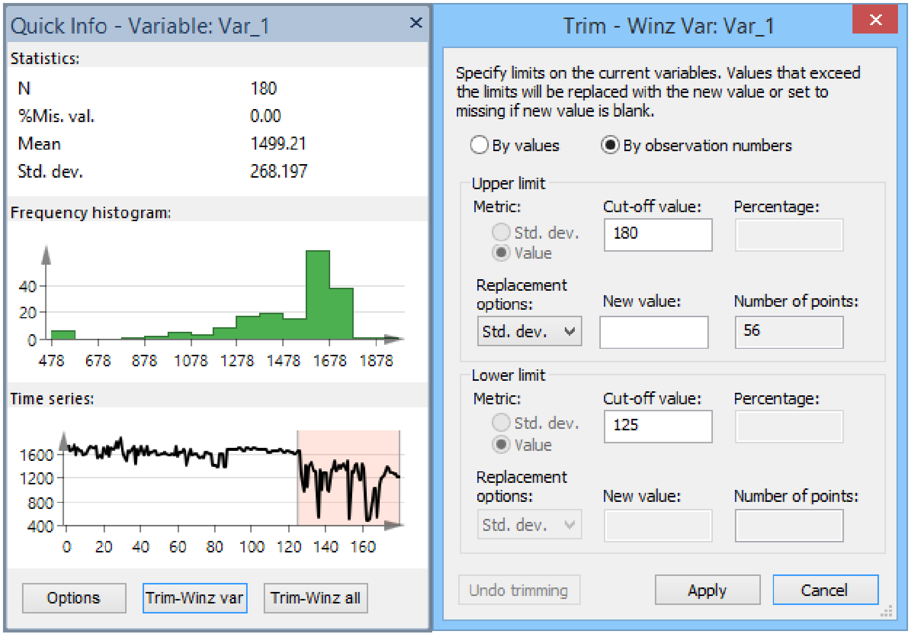
When trimming or Winsorizing interactively **By observation numbers**, the marked area will be affected.

To trim-Winsorize directly from the **Quick Info** plot **Time series**:

1. Click the **Trim-Winz bar** button.

2. Select the **By observation numbers** option to mark an area according to observation number.

3. Vertically mark the area of the plot to trim or Winsorize. The area becomes yellow and the area outside the limits remains white. The **Trim-Winz Var** dialog is updated according to the marking displaying the limits, percentages, and the number of marked data points.



Quick Info - Variable: Var_1

Statistics:

N	180
%Mis. val.	0.00
Mean	1499.21
Std. dev.	268.197

Frequency histogram:

Time series:

Trim - Winz Var: Var_1

Specify limits on the current variables. Values that exceed the limits will be replaced with the new value or set to missing if new value is blank.

○ By values ● By observation numbers

Upper limit

Metric: ○ Std. dev. ● Value

Cut-off value: 180

Percentage:

Replacement options: Std. dev.

New value:

Number of points: 56

Lower limit

Metric: ○ Std. dev. ● Value

Cut-off value: 125

Percentage:

Replacement options: Std. dev.

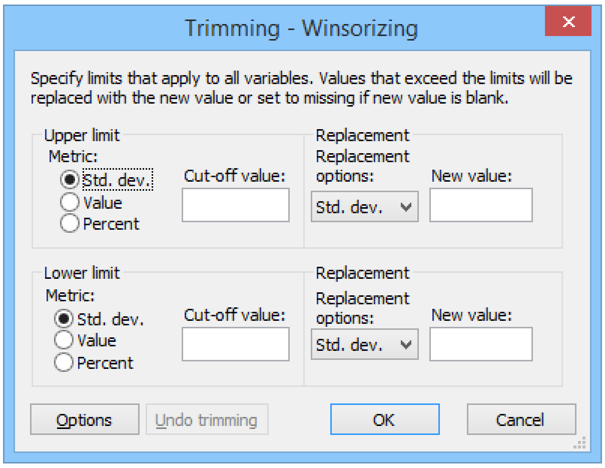
New value:

Number of points:

4. Click **Apply**.

13.2.10.4.4 Trim-Winz All dialog

Trimming - Winsorizing All is used with large datasets where it would be impractical to trim one variable at a time.



Trimming - Winsorizing

Specify limits that apply to all variables. Values that exceed the limits will be replaced with the new value or set to missing if new value is blank.

Upper limit
Metric: ● Std. dev. ○ Value ○ Percent
Cut-off value:
Replacement options: Std. dev.
New value:

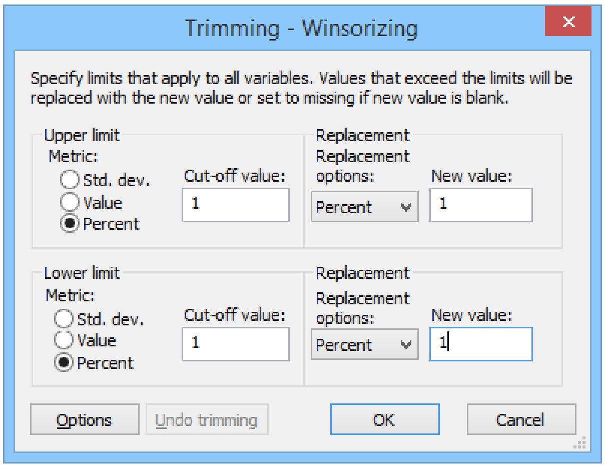
Lower limit
Metric: ● Std. dev. ○ Value ○ Percent
Cut-off value:
Replacement options: Std. dev.
New value:

To trim-Winsorize all variables at the same time:

1. In the **Upper limit** and **Lower limit** sections select the **Metric** to cut by: **Std. dev.**, **Value**, or **Percent**.
2. In **Cut-off value** field enter the value to trim or Winsorize by. Anything outside these limits will be affected in the trim-Winsorizing.
3. In the **Replacement options** box, select the metric or how to replace the affected values: **Std. dev.**, **Value**, **Percent**, **Last good value**, or **Delete obs.** When the selected replacement type is **Std. dev.**, **Value**, or **Percent** enter values in the **New value** field. For more, see the table in the Defining upper and lower limits By values subsection previously in this chapter.
4. Click **OK**.

Trim-Winsorizing all variables example

For example, to Winsorize the upper and lower 1% of the dataset and have the values above and below the 1% replaced by the values at 1%, the dialog should look as follows.



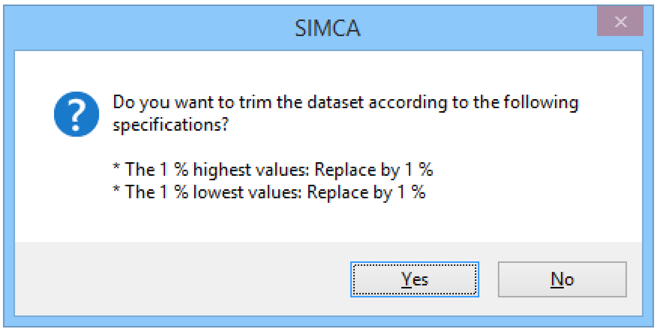
Trimming - Winsorizing

Specify limits that apply to all variables. Values that exceed the limits will be replaced with the new value or set to missing if new value is blank.

Upper limit
Metric: ○ Std. dev. ○ Value ● Percent
Cut-off value: 1
Replacement options: Percent
New value: 1

Lower limit
Metric: ○ Std. dev. ○ Value ● Percent
Cut-off value: 1
Replacement options: Percent
New value: 1

Click **OK** and the following message is displayed:



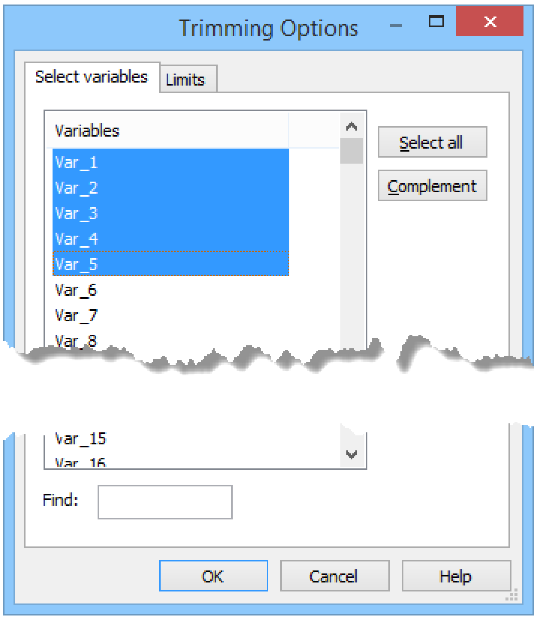
Do you want to trim the dataset according to the following specifications?

* The 1 % highest values: Replace by 1 %
* The 1 % lowest values: Replace by 1 %

13.2.10.4.5 Trim-Winsorizing a selection of variables

To trim-Winsorize a selection of variables at the same time:

1. Make the selections in the **Trim-Winz All** dialog as described in the Trim-Winz All dialog subsection previously in this chapter.
2. Click the **Options** button and select the desired subset of variables.
3. Click **OK**.



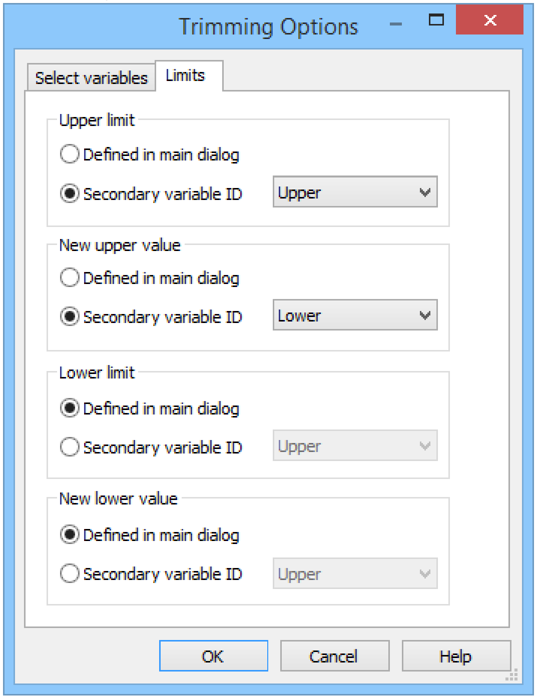
13.2.10.4.6 Trimming-Winsorizing using limits and values from secondary IDs

When using **Trim-Winz All**, limits and new values can be defined from variable secondary IDs.

Note: When selecting cut-off values or new values from secondary IDs, the corresponding fields in the main dialog become unavailable.

1. In the **Trim-Winz All** dialog, click the **Options** button.
2. Click the **Limits** tab.
3. There are four sections: **Upper limit**, **New upper value**, **Lower limit**, and **New lower value**. Under each section select one of the options:
   a. **Defined in main dialog** to define the limit or new value in the **Trim-Winz All** dialog.

b. **Secondary variable ID** and then select the secondary ID holding the cut-off values or new values.



Trimming Options

Select variables | Limits

Upper limit
○ Defined in main dialog
● Secondary variable ID: Upper

New upper value
○ Defined in main dialog
● Secondary variable ID: Lower

Lower limit
● Defined in main dialog
○ Secondary variable ID: Upper

New lower value
● Defined in main dialog
○ Secondary variable ID: Upper

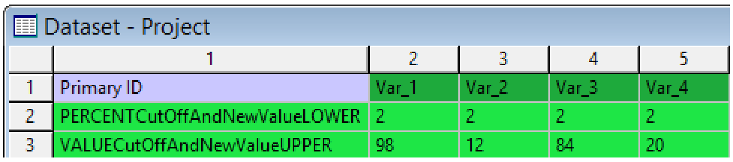
4. Click **OK**.

5. Select type metric of the cut-off-value and optional limits and new values – In the **Trimming-Winsorizing** dialog, the **Cut-off value** and **New value** fields specified by a secondary variable ID are unavailable. The **Metric** and **Replacement options** always have to be specified as well as values left with **Defined in main dialog** selected.

For info on how to add secondary IDs to the dataset, see the Adding secondary IDs subsection in the Dataset spreadsheet section in Chapter 7, Home.

13.2.10.4.7 Trim-Winsorizing using secondary ID example

In this example the dataset holds two secondary variable IDs named *PERCENTCutOffAndNewValueLOWER* and *VALUECutOffAndNewValueUPPER*. *PERCENTCutOffAndNewValueLOWER* contains the lower cut-off value and new lower value in percent, 2%. *VALUECutOffAndNewValueUPPER* contains the upper cut-off values and new values in actual values.



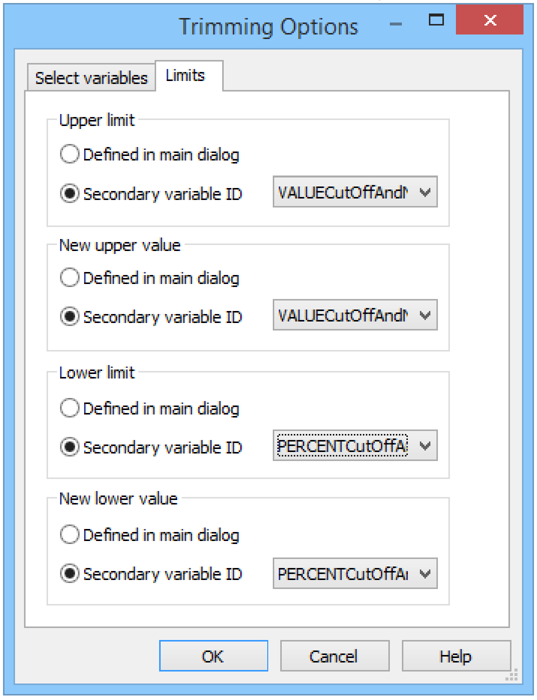
Dataset - Project

	1	2	3	4	5
1	Primary ID	Var_1	Var_2	Var_3	Var_4
2	PERCENTCutOffAndNewValueLOWER	2	2	2	2
3	VALUECutOffAndNewValueUPPER	98	12	84	20

To use the secondary IDs as limits and new values:

1. Click the **Options**-button, and then the **Limit** tab.

2. Select the IDs as shown in the dialog and click **OK**.



Trimming Options

Select variables | Limits

Upper limit
○ Defined in main dialog
● Secondary variable ID: VALUECutOffAndN

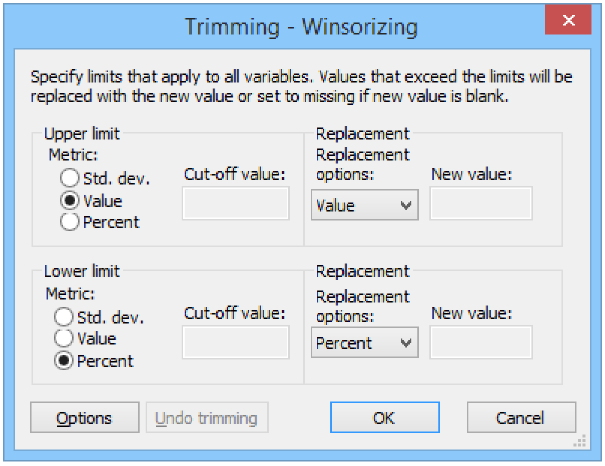
New upper value
○ Defined in main dialog
● Secondary variable ID: VALUECutOffAndN

Lower limit
○ Defined in main dialog
● Secondary variable ID: PERCENTCutOffA

New lower value
○ Defined in main dialog
● Secondary variable ID: PERCENTCutOffA

3. In the **Trim-Winz All** dialog:

- For the upper limit, select **Value** both as **Metric** and in the **Replacement options** box. This specifies to the Quick Info to interpret the **Upper limit** and **New upper value** from the secondary ID as values.
- For the lower limit, select **Percent** both as **Metric** and in the **Replacement options** box. This specifies to the Quick Info to interpret the **Lower limit** and **New lower value** from the secondary ID as percent.



Trimming - Winsorizing

Specify limits that apply to all variables. Values that exceed the limits will be replaced with the new value or set to missing if new value is blank.

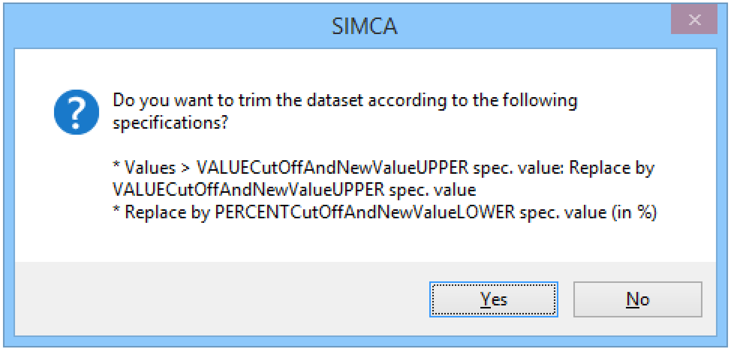
Upper limit
Metric:
○ Std. dev.
● Value
○ Percent
Cut-off value:

Replacement
Replacement options: Value
New value:

Lower limit
Metric:
○ Std. dev.
○ Value
● Percent
Cut-off value:

Replacement
Replacement options: Percent
New value:

4. Click **OK** and a summary message is displayed.



SIMCA

Do you want to trim the dataset according to the following specifications?

* Values > VALUECutOffAndNewValueUPPER spec. value: Replace by VALUECutOffAndNewValueUPPER spec. value
* Replace by PERCENTCutOffAndNewValueLOWER spec. value (in %)

13.2.11 Variables pane

The **Variables** pane displays the variables included in the workset of the active model.

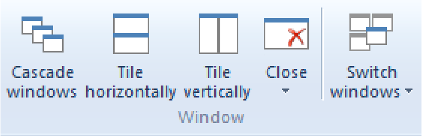
Right-clicking the pane opens the shortcut menu holding the following commands: **X**, **Y**, **Exclude**, **Select all**, and **Variable label**. These commands work as described in the Marked items subsection previously in this section.

13.2.12 Full screen

To maximize the plot area, leaving only the minimized ribbon and the plot area, on the **View** tab, click **Full screen**. To return to normal, again click **Full screen** or the ESC-button on your keyboard.

13.3 Window group

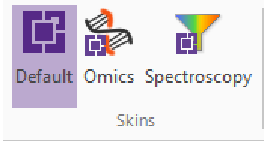
The **Window** group contains the regular window commands **Cascade**, **Tile horizontally**, **Tile vertically**, **Close** and **Switch windows**. The **Switch windows** menu lists the last 9 plots/lists/spreadsheets/windows plus **Arrange windows**.



13.4 Skins

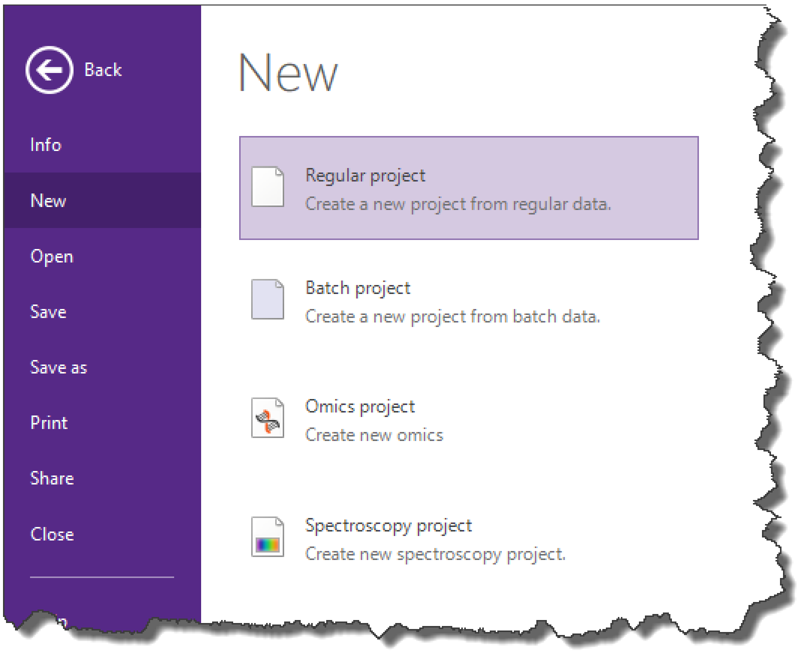
The skins available in SIMCA were developed to offer a simplified and customized interfaced designed for specific application areas. Compared to the regular SIMCA interface, some default settings, default plot options and shortcuts for typical routine operations were introduced to suit the application area data and normal model procedures within this community. The plot library, model types and calculations are identical to those performed in regular SIMCA.

The **Skins** group on the **View** tab is available when one or more skins have been installed and enabled in the Skins section in the SIMCA options page in the **File | Options** dialog.



After activating a skin, by clicking it on the **View** tab, creating a new project automatically opens the skin, after importing data, with all skin specific features available. For more about the respective skin, see the tutorials and quick guides at https://umetrics.com/downloads/simca after login.

With skins enabled, creating a new application specific project also activates that skin.



New

Regular project
Create a new project from regular data.

Batch project
Create a new project from batch data.

Omics project
Create new omics

Spectroscopy project
Create new spectroscopy project.

Note: If you have installed a skin but it is not displayed on the View tab, click **File | Options** and in the **Customize ribbon** section click **Reset**.

14Plot and list contextual tabs

14.1 Introduction

The features available in the **Plot** and **List** contextual tabs are context sensitive appearing when applicable. This means that the **Plot** contextual tab **Tools** becomes available when opening a plot and displays the features applicable to the active plot. Likewise the **List** contextual tab **Tools** becomes available when opening a list and displays the features applicable to the active list.

Marking in a plot or list opens the **Marked items** contextual tab.

The contextual tabs include features like:

- The tools: **Select**, **Zoom**, **Zoom out**, and **Highlight series**.
- The properties: **Color by**, **Size by**, etc.
- The **Create** and **Change type** features: **Scatter**, **Column**, **List**, **Sources of variation**, **Out of control** etc.
- The layout features: loading and saving of templates, show/hide header, footer, legend etc.
- After marking items: **Exclude**, **Include**, **Labels**, etc.

14.2 Mini-toolbar - format plot

The mini-toolbar is available to customize the attributes of the plot. By default the mini-toolbar is displayed when you click and then move the cursor northeast. When right-clicking the mini-toolbar is displayed above the shortcut menu.

By clicking an item, line, symbol, text, etc., you can change attributes such as line width, symbol type, color of a category, font in a text box, etc.

Note: When clicking a symbol or column, that symbol or column is marked and the mini-toolbar for marked items appears.

Features available when clicking in plots are described in the table.

Click in plot area	Mini-toolbar features in order of appearance
An empty area in the plot area.	Format Plot dialog, Properties dialog and zooming.
A symbol.	Symbol style, size and color for the marked symbol only. To change for all symbols in a series, use the legend.
A line.	**Format Plot** dialog, line width, style, and color of that specific line.
A column.	Color for the marked column only. To change for all columns in a series, use the legend.
A limit.	**Format Plot** dialog, line width, style, color and fill color of that specific line. The last button allows saving the current settings as default for the limit type.

Note: After marking in a plot and making a change using the mini-toolbar, a new series named **Custom** is created in the **Styles** node in the **Format Plot** dialog, allowing further modification of the marked group.

Features available when clicking in the legend are described in the table.

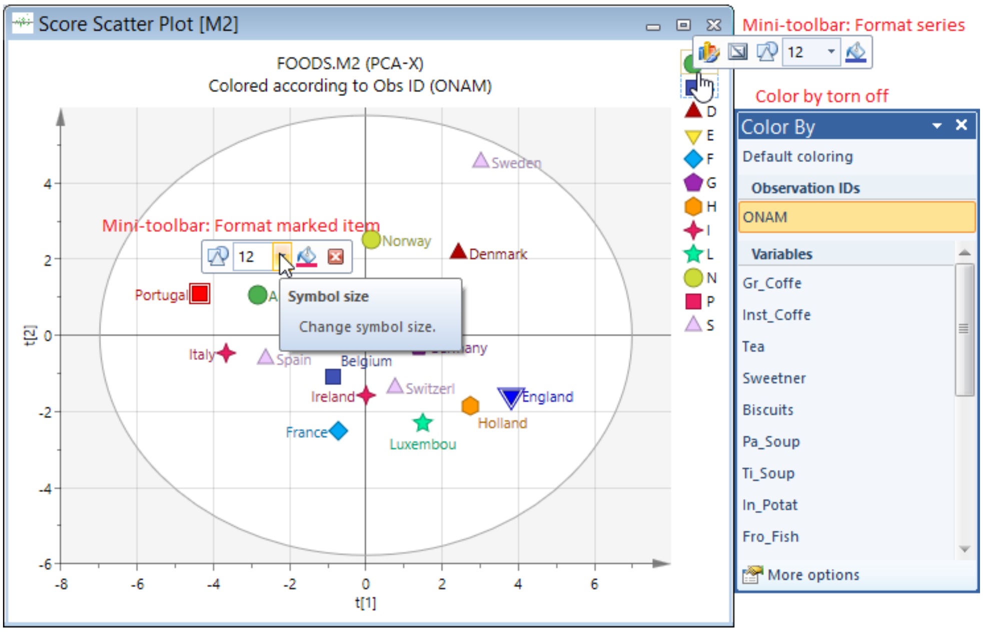
Click in legend	Mini-toolbar features in order of appearance
Symbol	**Format Plot** dialog, hide series, symbol style, size and color.
Line	**Format Plot** dialog, hide series, line width, style, and color of that specific line.
Column	**Format Plot** dialog, hide series, color.

Color after category coloring	**Format Plot** dialog, color.
Color with continuous coloring	**Format Plot** dialog, color 1 (start color), color 2 (end color).

Features available when clicking in a text box are described in the table.

Click in text box	Mini-toolbar features in order of appearance
Any text box (header, footer, axis title, etc.)	**Format Plot** dialog, hide selected, font face, font size, grow font, shrink font, bold, italic, font color and save as default style.

In the figure below both the legend mini-toolbar and the marking mini-toolbars are displayed. To the right is the **Color by** feature floating after being torn off.



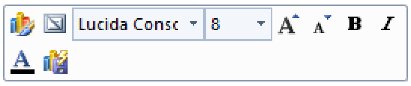
14.2.1 Mini-toolbar to customize plot text

You can use the mini-toolbar to interactively customize the text positioned outside the plot area.

14.2.1.1 Customize specific text

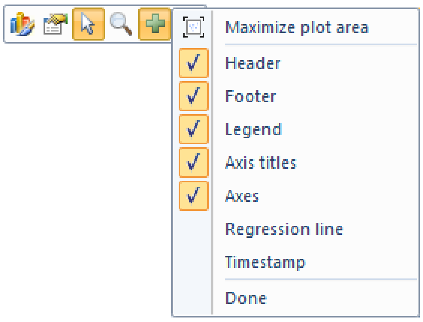
To customize a specific text, for instance the footer, right-click the text to customize and select how to customize the font or color. Clicking the last button saves the changes to the current template.

Note that the second button hides the footer.



14.2.1.2 Add or remove several texts

To add or remove several of the Add plot element features, right-click outside the plot area and click the green plus sign in the mini-toolbar.



14.2.2 Managing the mini-toolbar

The mini-toolbar is always displayed above the shortcut menu, but you can specify when you want to see it after clicking or marking in plots.

To hide the mini-toolbar that is displayed when marking:

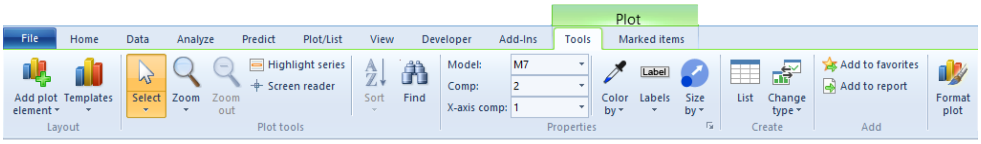
- Click the x in the mini-toolbar or
- Click the cogwheel in the mini-toolbar that shows above the shortcut menu and clear **Show mini-toolbar on selection**.

To hide the mini-toolbar that is displayed when clicking an item in a plot or in the legend without marking, click the cogwheel in the mini-toolbar that shows above the shortcut menu and clear **Show mini-toolbar**.

14.3 Tools tab

The **Tools** contextual tab holds:

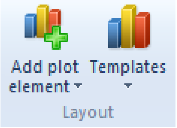
- The **Layout** group with **Add plot element** and **Templates**.
- The **Plot tools** group with the **Select** tool, **Zoom, Zoom out**, **Highlight series, Screen reader**, **Sort** and **Find**.
- The **Properties** group with **Model, Comp, Batch** etc. depending on open plot/list or window, **Color by**, **Labels**, and **Size by**.
- The **Create** group with **List** and **Change type** plus the conditional **Out of control**, **Sources of variation**, or **Merge list**.
- The **Add** group with **Add to favorites** and **Add to report**.
- **Format plot** that opens the **Format Plot** dialog.



Model: M7
Comp: 2
X-axis comp: 1

14.3.1 Layout group

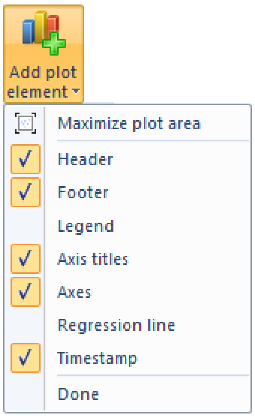
The **Layout** group holds features pertaining to how the plot is displayed. These features are described in the Add plot element and Templates sections that follow.



14.3.1.1 Add plot element

The **Add plot element** menu contains a number of features that can be turned on and off for the active plot.

- **Maximize plot area** - see the **Maximizing the plot area** later in this section.
- The **Header**, **Footer**, **Legend**, **Axis titles**, **Axes**, and **Timestamp** check boxes which are displayed if selected and hidden when cleared.
- **Regression line** - see the **Regression line** subsection later in this section.



14.3.1.1.1 Maximizing the plot area

Each plot displays a plot area and also a header and a footer.

To view only the plot area and not the header and footer, on the **Tools** tab, in the **Layout** group, click **Add plot element** | **Maximize plot area**.

To again view header and footer, click **Maximize plot area** again.

14.3.1.1.2 Regression line

The regression line and equation can be displayed for any 2D scatter or line plot in SIMCA.

Open a plot, for instance the Observed vs. predicted plot, and on the **Tools** tab, in the **Layout** group, click **Add plot element** | **Regression line**.

The attributes of the line and equation can be changed in **Format Plot**, in the pages **Region style**, **Font**, and **Label style**.

Add regression line to Quick Access Toolbar

In order to have the regression line available at a single click, add it to the Quick Access Toolbar as follows:

1. Click the arrow on the Quick Access Toolbar and click **More Commands**.
2. Select **Layout** under Choose commands from.
3. Mark **Regression line** and click **Add**.

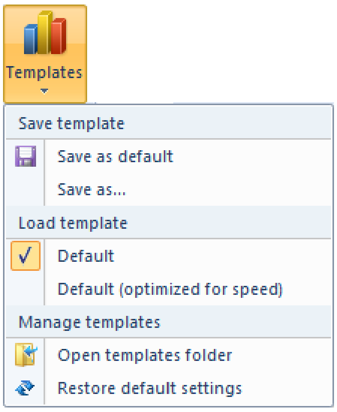
14.3.1.2 Templates

The **Templates** menu holds features pertaining to the formatting of plots.

The following features are available:

- **Save as default** and **Save as** described in Saving Format Plot template subsection.
- **Load template** described in Switching plot formatting templates subsection.
- **Open templates folder** - opens the folder holding the templates.
- **Restore default settings** described in Restoring to default plot formatting subsection.

The **Format Plot** is positioned to the far right on this tab, and is described in the Format Plot section later in this chapter.



14.3.1.2.1 Switching plot formatting templates

After having added customized plot formatting templates, these templates can be selected by clicking the relevant template under **Templates**.

After loading a new template, that template is applied to all open and future plots.

The template ***Default (optimized for speed)*** should be used when your project has so much data that the plotting becomes slow. In this template the most CPU consuming features have been turned off.

14.3.1.2.2 Saving format plot template

After customizing the plots using **Format Plot** you can save the settings of some attributes, such as fonts, gridlines, symbol type etc., to a template.

To save a template, with the plot open, click **Templates** | **Save as default**, or **Save as** and specify a name.

Note: Only the formatting available in the current plot is saved to the customized plot formatting configuration. All other formatting will remain default. This means that formatting of headers, footers etc. apply to all plot types (e.g. scatter, column, line) while default line color, default symbol shape are plot specific and need to be specified with that plot type open.

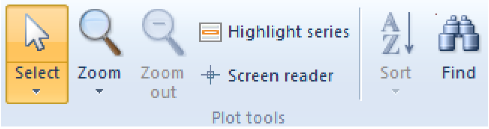
14.3.1.2.3 Restoring to default plot formatting

To restore to the default plot formatting template, click **Templates** | **Restore default settings**. This restores the **Default** plot template to the Umetrics default plot formatting and switches to it.

14.3.2 Plot tools group

The **Plot tools** group includes:

- Select tool - specifies the type of selection.
- **Zoom, Zoom out** - for zooming in and out in 2D plots.
- **Highlight series** - to quickly get an overview over how one series evolves or is distributed.
- **Screen reader** - displays the current coordinates in the hovered plot.
- Sort - to sort plots or lists as desired.
- Find - to search for items that fulfill certain criteria.



14.3.2.1 Select – Marking tool

The **Select** tool is used to select which type of marking to use.

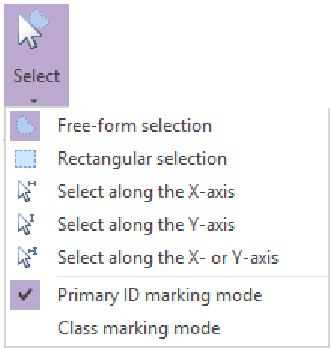
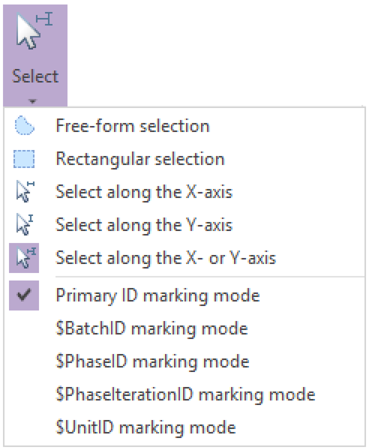
Click the small arrow below and then click the type of marker from the menu. The available marking types are:

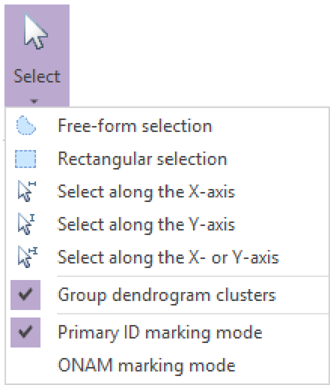
- **Free-form selection**: Allows marking to take any shape.

- **Rectangular selection**: Allows marking in a rectangular shape.
- **Select along the X-axis**: Marks as a vertical bar.
- **Select along the Y-axis**: Marks as a horizontal bar.
- **Select along the X or Y-axis**: Marks as a horizontal bar/vertical bar depending on which direction the cursor moves.
- **<ID> marking mode**: Marks all observations with the specific ID in common, for instance a batch. Using **Exclude** after marking an entire batch excludes the selected batch from the model or BEM, depending on which type of plot is was marked in. A new BM model is automatically generated with a BEM holding a PLS or OPLS model for each phase.
- **Group dendrogram clusters:** Available for an open **Dendrogram** and displays a horizontal line with which the resolution of the dendrogram is specified, and thereby the number of clusters. For more, see the Group dendrogram clusters marking tool subsection in Chapter 10, Analyze.

Note: The **Batch marking mode** is an on/off switch to marking entire batches instead of points. The marking type is still **Free-form selection, Rectangular selection** etc.

The table displays the available commands from the **Select plot items** tool.

Menu	Available for
 Select Free-form selection Rectangular selection Select along the X-axis Select along the Y-axis Select along the X- or Y-axis Primary ID marking mode Class marking mode	Regular project standard plots.
 Select Free-form selection Rectangular selection Select along the X-axis Select along the Y-axis Select along the X- or Y-axis Primary ID marking mode $BatchID marking mode $PhaseID marking mode $PhaseIterationID marking mode $UnitID marking mode	Batch evolution models standard plots.

Menu	Available for
	Dendrogram plots open in any project.

Note: *To keep the marked points marked, while marking new points, hold down CTRL. The marked points then belong to the same group of marked items.*

Deselecting/unmarking points

To deselect points in a plot, click a white area in the plot.

To deselect points in a list, mark the first row.

See also the Marked items tab section later in this chapter.

Displaying properties of the item

When positioning the cursor on an item in a plot, the marker behaves as a pointer and displays the name and coordinates of the observation or variable.

Creating contribution plots

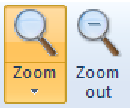
With any marker:

1. Double-click an observation in a score plot for instance. The contribution plot opens, comparing the variables of the selected observation to the average of all the observations in the workset. This plot indicates why the selected observation is different from the average.
2. Click the first observation, and then double click the second observation. The resulting contribution indicates why the first observation differs from the second.

For more about creating contribution plots, see the Contribution plot from plot section in Chapter 10, Analyze.

14.3.2.2 Zooming in

To zoom in a plot, click the **Zoom** tool in the **Plot tools** group.



Use the **Zoom** menu to select the type of zoom from the drop down menu:

- **Zoom in**: Magnifies a rectangular region
- **Zoom X**: Expands the x direction
- **Zoom Y**: Expands the y direction
- **Zoom subplot**: Magnifies a subplot in a multi-plot display.

Then mark the desired region, or subplot, of the plot to zoom.

Note: With any zooming type selected, double-clicking a subplot automatically zooms the subplot.

Zooming in a scatter 3D plot is described in the Zooming in 3D scatter plot subsection in the Score scatter 3D plot section in Chapter 7, Home.

14.3.2.2.1 Zooming out

Click **Zoom out** to revert zoom to original scale in the steps taken when zooming.

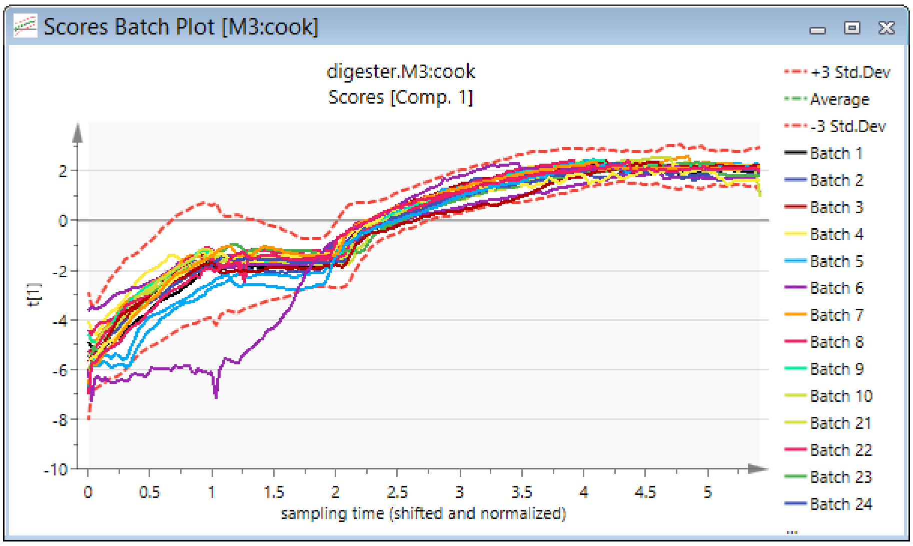
Zoom out is available for all lists and spreadsheets from the shortcut menu.

14.3.2.3 Highlight series

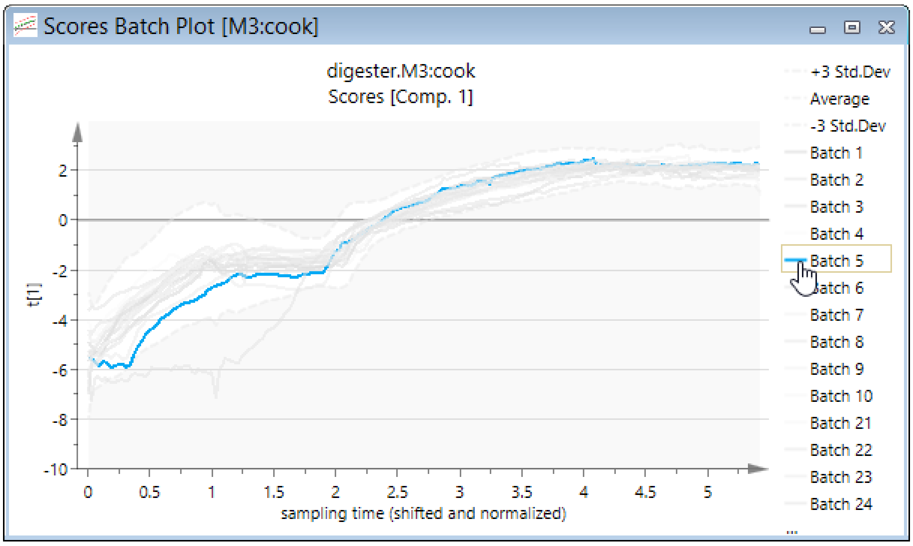
With **Highlight series** selected, hovering over one series in the legend, or in the plot, grays all series but the hovered one.

Highlight series

Scores batch control chart with 20 batches:

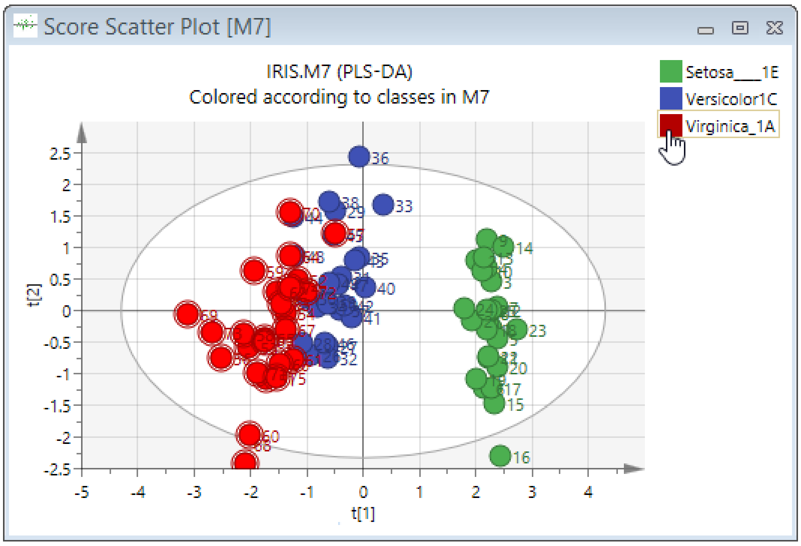


Scores batch control chart with 20 batches and Highlight series activated:



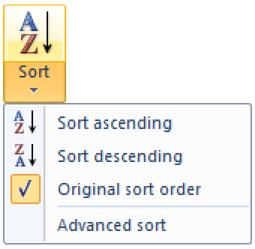
14.3.2.4 Selecting points using category in legend

All points in a color can be selected by clicking that color in the legend.



14.3.2.5 Sorting ascending or descending

All lists, the dataset spreadsheets, and column plots can be sorted ascending or descending.



14.3.2.6 Sorting lists

Sorting of the dataset spreadsheet is available both as sorting the presentation and as sorting the dataset. Sorting of the presentation is what is done if you just click **Sort** and not a menu item.

Note: Sorting is only available when one variable is marked.

To sort:

1. Mark the variable to sort by.
2. On the **Tools** tab click **Sort | Sort ascending** or **Sort descending**.
3. When sorting a dataset, in the **Sort Dataset** dialog that opens select:
    a. **Sort the list** to sort only the presentation of the data in this spreadsheet. This sorting will not delete the models, only sort the list. When creating a new workset, the original order of the observations will be used.
    b. **Sort the dataset** to sort the dataset the models are built from. With this option all models will be deleted. When creating a new workset, the new sorted order of the observations will be used.

Note: Read-only datasets cannot be sorted. Only the presentation can be sorted for batch evolution datasets.

14.3.2.7 Sorting column plot by value or ID

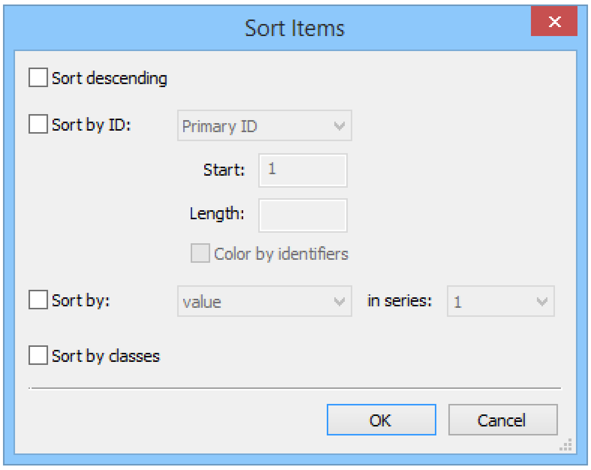
All column plots, including contributions, can be sorted by strings in the primary or secondary ID and/or by values. This allows displaying variables grouped as desired. The various groups will have different colors.

To sort a column plot by value:

- On the **Tools** tab, in the **Plot tools** group, click **Sort**.
- Alternatively, right-click the column plot and then click **Sort ascending** or **Sort descending**.

To sort a column plot by ID and/or value:

1. On the **Tools** tab, in the **Plot tools** group, click **Sort | Advanced sort**.
2. Select how to sort the data in the **Sort Items** dialog and then click **OK**.



Sort Items

□ Sort descending

□ Sort by ID: Primary ID

Start: 1

Length:

□ Color by identifiers

□ Sort by: value in series: 1

□ Sort by classes

The **Sort Items** dialog is described in the table below.

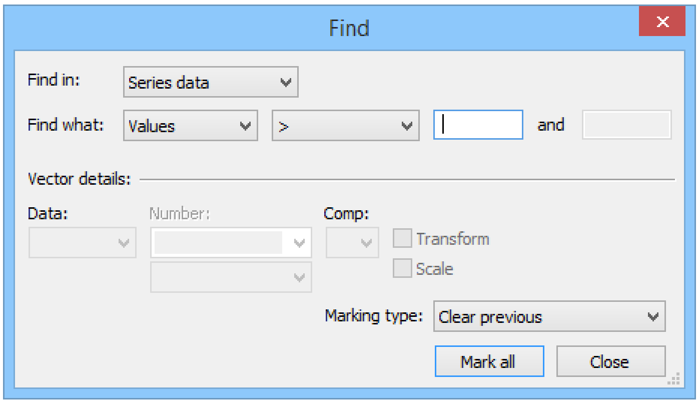
Option	Description	Default
Sort by ID	Select the **Sort by ID** check box to sort the column plot by the selected ID.	After selecting the **Sort by ID** check box, the primary ID is the default.
Start	To sort by a part of the ID, enter the start character position in the **Start** field.	'1' which means that the starting point is the first character.
Length	To sort by a part of the ID, enter the number of characters to use in the **Length** field.	By default the entire ID is used in the sorting, that is **Length** is <empty>.
Color by identifiers	Select the **Color by identifiers** check box to color the columns according the identifier selected to sort by.	Not selected.
Sort by	Selecting the **Sort by** check box and in the **Sort by** box select **value** or **absolute value** to sort the column plot accordingly. Selecting to sort by **absolute value** results in sorting according to size of the column, independent of whether it is positive or negative.	After selecting the **Sort by** check box, **value** is by default selected.
In series	When selecting the **Sort by** check box, the sorting has to be done using one of the series in the plot. When available you can select another series if desired.	After selecting the **Sort by** check box, the first series is by default selected.
Sort by classes	When there are classes specified in the workset, selecting the **Sort by classes** check box sorts the plot accordingly. For the **Dot plot** this means that the items in each bin are sorted by class.	Not selected.

14.3.2.8 Find

With an active plot, list or spreadsheet, **Find** enables finding items meeting selected criteria.

The **Find** dialog is opened by clicking **Find** in the **Plot tools** group on the **Tools** tab or by pressing CTRL+F.

Find



In the table, the available items in the **Find in**, **Find what**, and logical expression boxes are listed.

Find in	Searches in	Logical expressions
Identifiers	The text or values of the selected identifier, primary or secondary, or all identifiers. For batches the secondary identifiers include the batch level IDs **Phase**, **Maturity**, **Source**, and **Number**, and the batch project IDs **$BatchID** and **$PhaseID** when available.	For numerical identifiers: >, >=, <, <=, between, =, not equal. For text identifiers: begins with, ends with, contains, =, not equal.
All data	The vectors displayed on all axes. For the default score scatter plot, the search is done on both t1 and t2.	>, >=, <, <=, between, =, not equal.
Series data	The vectors that are selected as series. For 2D scatter, line, and column plots that means that the search is limited to the y-axis vectors while for the 3D scatter plot the search is limited to the z-axis vectors. For example, for the default score scatter plot, the search is limited to searching in the vector t2 found on the y-axis. For lists, this option is the same as **All data**.	>, >=, <, <=, between, =, not equal.
X-axis	The vector displayed on the x-axis. Available for plots only.	>, >=, <, <=, between, =, not equal.
Vectors	The selected vector in **Find what**. When selecting **Vectors** in **Find in**: • The **Find what** box contains all vectors available for the type of vector displayed in the active plot or list, e.g. if the plot displays t1 vs. t2, the available vectors are all vectors of data type Variables and scores. • The **Vector details** section becomes available enabling selection of model.	>, >=, <, <=, between, =, not equal.
Text	The list as if all entries where text and marks the matching cells. Available for lists and spreadsheets only.	begins with, ends with, contains, =, not equal.

Note: To search in a variable, in the **Find in** box select **Vectors** and in the **Find what** box select **XVar**. Then in the **X-terms** box in the **Vector details** section, select the desired variable.

14.3.2.8.1 Marking type

There are three marking types:

- **Clear previous** – clears the previous marking and marks according to the current criterion.
- **Union with previous** – marks the items that satisfy the current **OR** the previous criterion but not both.
- **Intersection with previous** – marks the items that satisfy both criteria, both the previous *AND* the current.

The default marking type is **Clear previous**.

Open the **Marked Items** pane (select the **Marked items** check box on the **View** tab) to see the items previously and currently marked. For more, see the Marked Items subsection in Chapter 13, View.

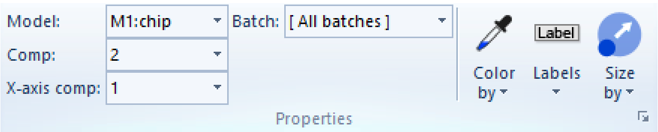
14.3.2.8.2 Using Find

Here follows a step by step example of using the **Find** function.

1. Open a plot or list.
2. Click **Find**.
3. In the **Find in** box, select the category of the attribute.
4. In the **Find what** box, select the attribute and then specify the criterion.
5. Click **Mark All** and all objects in the plot or list satisfying the criterion are marked.
6. Then switch criterion and select **Marking type** union or intersection with the previously marked objects. The intersection will select among the objects already marked those that satisfy both criteria. The union marks objects that satisfy either criterion but not both.

14.3.3 Properties group

The **Properties** group holds information and features concerning the active plot or list, allowing you to switch between models, components, variables, coloring, labeling, sizing etc. In this section the combo boxes in the Properties group are described.


Model: M1:chip
Comp: 2
X-axis comp: 1
Batch: [All batches]

Property available	**Description**
Model	The model of the current window. Lists all models in the project.
X-axis comp, Y-axis comp, Z-axis comp.	The component displayed on 1D, 2D, and 3D plots, such as **Score Line Plot**, **Score Scatter Plot**, and **Score Scatter 3D Plot**.
Comp	Component in the plot. Available for cumulative plots and DMod plots.
X-variable	Lists all x-variables in the active model with the displayed x-variables check boxes selected when more than one variable is displayed.
Y-variable	Lists all y-variables in the active model with the displayed y-variables check boxes selected when more than one y-variable is displayed.
Observations	Lists all observations in the active model, dataset, or predictionset with the displayed observations check boxes selected when more than one observation is displayed.
Batch	Displays all batches in the active model or predictionset with the currently displayed batches check boxes selected. All batches can be selected with one click by selecting the first check box **[All batches]**.

Some of the boxes in the **Properties** group can be accessed using keystrokes. For more, see the Switching components, batches, and models subsection after this section.

When the active plot is a coefficient plot created for a hierarchical top level model the **Resolve coefficients** check box is available on the **Tools** tab. For more, see the Coefficient Plot for hierarchical top level models subsection in Diagnostics & interpretation section in Chapter 7, Home.

The Properties dialog is opened by clicking the dialog box launcher in the **Properties** group on the **Tools** tab.

14.3.3.1 Switching components, batches, and models

Switching components on the plot axes, batches displayed, and model for the active plot is available using keystrokes shortcutting to the **Tools** tab, **Properties** group.

For **regular projects**, switch:

- Components on the Y-axis by pressing the **UP** and **DOWN** arrow keys.
- Components on the X-axis by pressing the **LEFT** and **RIGHT** arrow keys.
- Models by pressing the **PAGE UP** and **PAGE DOWN** keys.

For **batch projects**, in the batch control charts switch:

- Components on the Y-axis by pressing the **UP** and **DOWN** arrow keys.
- Batches by pressing the **LEFT** and **RIGHT** arrow keys.
- Phases (models) by pressing the **PAGE UP** and **PAGE DOWN** keys.

The active window and property bar are updated according to the changes.

14.3.3.2 Color by

Color by is available for plots displaying observations or variables.

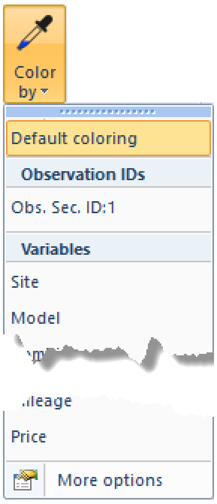
Note: Only a selection of coloring types is available from **Color by** on the **Tools** tab. The **Color** page in **Properties** contains more coloring options.

Available are for example:

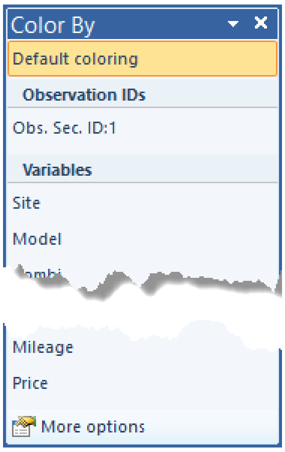
- **Default coloring -** all points are colored the same color.
- Color by **Observation ID/Variable ID -** the available secondary IDs are available.
- Color by **Variable** - for observation plots the variables of the included datasets are listed.
- Color by **Batches** - for batch control charts and other plots displaying batches.
- Color by **Classes** - for observation scatter plots where the model has classes specified.

14.3.3.3 Color by torn off

Color by can be torn off and docked by pulling the dotted part.

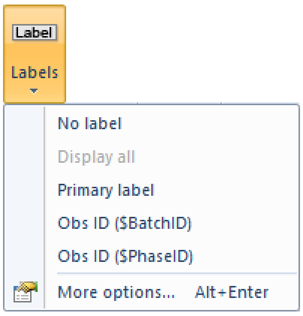


Color by torn off from the ribbon and floating.



14.3.3.4 Label types for plots

On the **Tools** tab, you can select the label type for the symbols in the current plot by clicking **Labels** in the **Properties** group.



In the **Properties** dialog for plots, in the **Label types** page, the labels to use as **Point label**, **Axis label**, and **Title label** can be specified.

To specify a **Point label**:

1. Select the primary or secondary identifiers in the **Use label** box.
2. Enter the character in the label to start with in the **Start** field.
3. Enter the number of characters to use in the **Length** field.

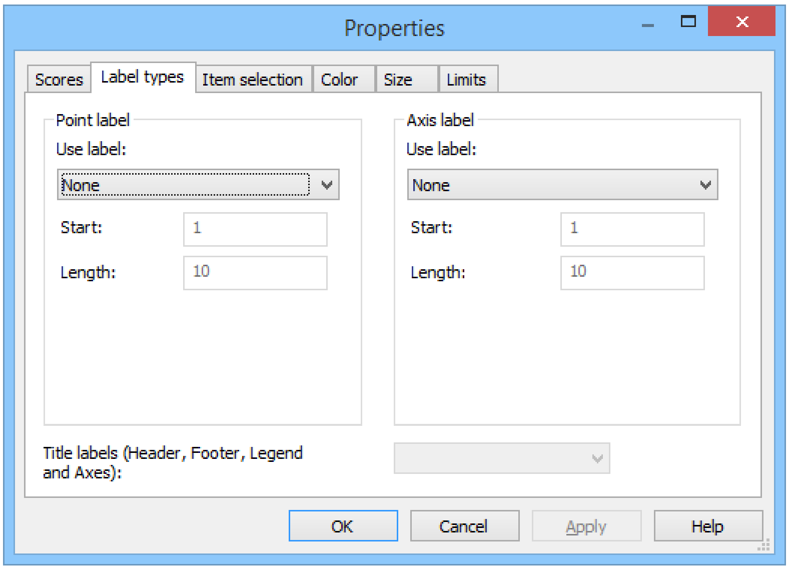
To specify an **Axis label**:

1. Select the primary or secondary identifiers in the **Use label** box.
2. Enter the character in the label to start with in the **Start** field.
3. Enter the number of characters to use in the **Length** field.

To specify the **Title labels**:

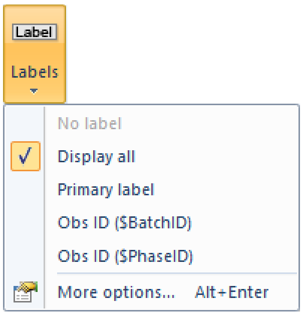
1. Click the **Title labels** box.
2. Select the desired variable ID.

Note: The variable ID selected in the **Title labels** box is displayed in all applicable headers, footers, legends, and axis labels.



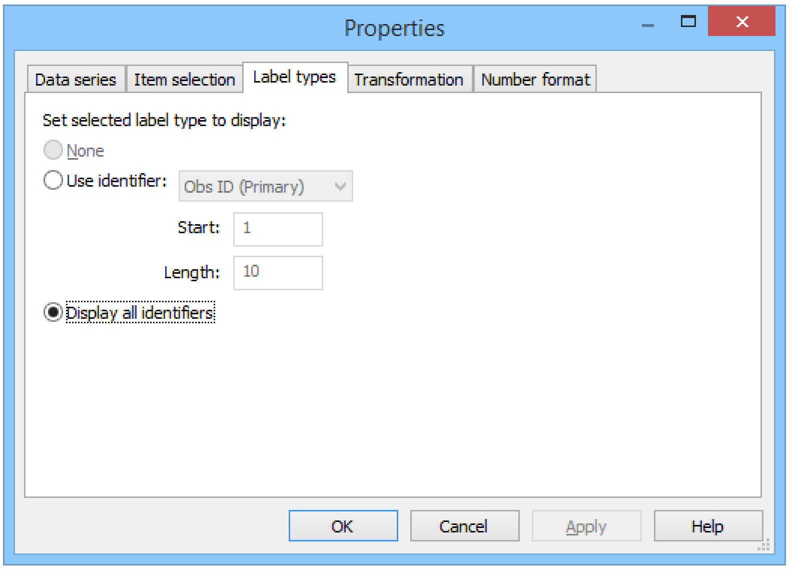
14.3.3.5 Label Types for lists

On the **Tools** tab, in the **Properties** group, you can select to **Display all labels** or a specific label in the list using **Labels**.



In the **Properties** dialog for lists, in the **Label types** page, the following options are available:

1. Displaying a specific ID by selecting **Use identifier** and
   a. Selecting an identifier in the list. By default the primary ID.
   b. Enter the character in start with in the **Start** field. By default 1.
   c. Enter the number of characters to use in the **Length** field. By default 10.
2. Selecting **Display all identifiers** resulting in displaying all available identifiers in their full length.



Properties

Data series | Item selection | Label types | Transformation | Number format

Set selected label type to display:

○ None

○ Use identifier: Obs ID (Primary)

Start: 1

Length: 10

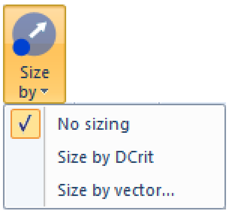
● Display all identifiers

OK | Cancel | Apply | Help

14.3.3.6 Size by

The plot marks of all scatter plots, both 2D and 3D, can be sized according to a selected vector. Additionally, all scatter plots of vectors of the type variables and scores can be enlarged when the observation is found outside the DCrit of DModX or DModXPS.

Sizing is available on the **Tools** tab, in the **Properties** group, by clicking **Size by**.



Size by

✓ No sizing

Size by DCrit

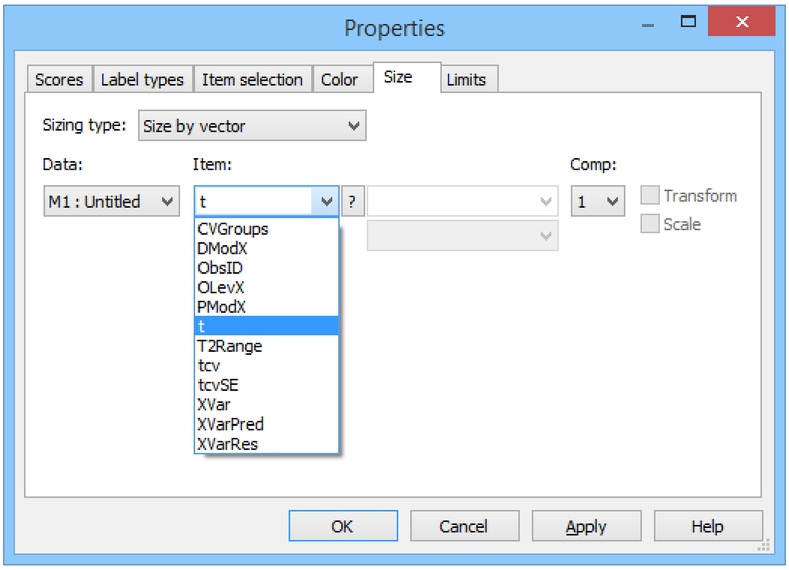
Size by vector...

14.3.3.6.1 Sizing by a vector

When selecting to **Size by vector**, the **Properties** dialog opens and all applicable vectors are available.

For instance, for a score plot, all vectors found with data type **Variables and scores** in the **Plot/List | Scatter** dialog are available.

When clicking **OK**, the size of the plot marks will be smaller or larger than the default plot mark depending on the value for the specific observation or variable in the selected vector.



Properties

Scores | Label types | Item selection | Color | Size | Limits

Sizing type: Size by vector

Data: M1 : Untitled

Item: t

Comp: 1

□ Transform

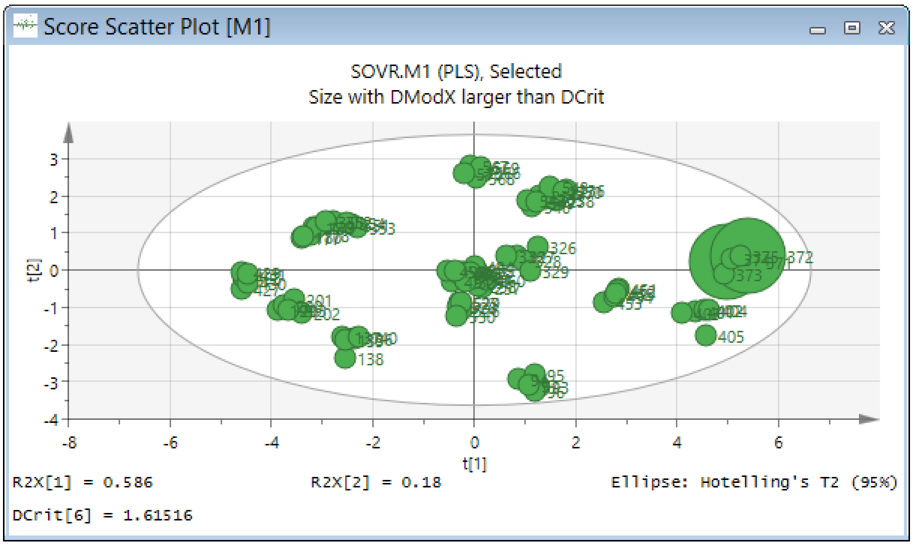
□ Scale

CVGroups
DModX
ObsID
OLevX
PModX
t
T2Range
tcv
tcvSE
XVar
XVarPred
XVarRes

OK | Cancel | Apply | Help

14.3.3.6.2 Enlarging when outside DCrit

When clicking **Size by | Size by DCrit**, all observations with DModX outside DCrit are enlarged proportionally to the distance to DCrit.



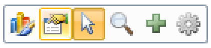
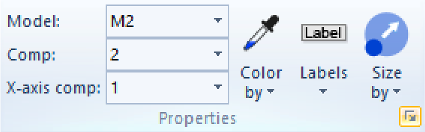
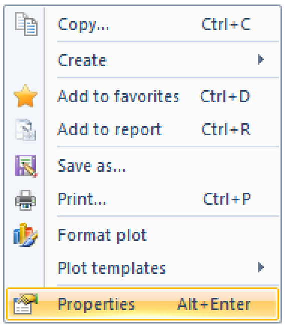
Size by DCrit is only available for plots displaying observations.

To shrink or enlarge all plot symbols, use Symbol style page in **Format Plot**.

14.3.3.7 Properties dialog

All plots and lists have a context sensitive **Properties** dialog. Many of the pages in this dialog are general and available for several plot types. These pages are described in this section. Other pages are plot specific and are therefore described in connection with the description of the plot.

The table describes the different ways to open the **Properties** dialog.

Open Properties by	Screenshot
Clicking the plot (in an area where there is no points) and clicking **Properties** in the mini-toolbar	
Clicking the dialog box launcher in the **Properties** group on the **Tools** tab	 Model: M2 Comp: 2 X-axis comp: 1 Color by Labels Size by Properties
Right-clicking the plot and clicking **Properties** from the shortcut menu.	 Copy... Ctrl+C Create Add to favorites Ctrl+D Add to report Ctrl+R Save as... Print... Ctrl+P Format plot Plot templates Properties Alt+Enter

The property pages described in this section are:

- Color
- Label types for plots - earlier in this section.
- Label types for lists - earlier in this section.
- Size - earlier in this section.

- Item selection
- Limits
- Components
- Select Y-variable
- Number format

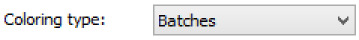
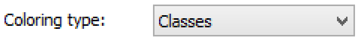
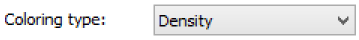
14.3.3.7.1 Color in the Properties dialog

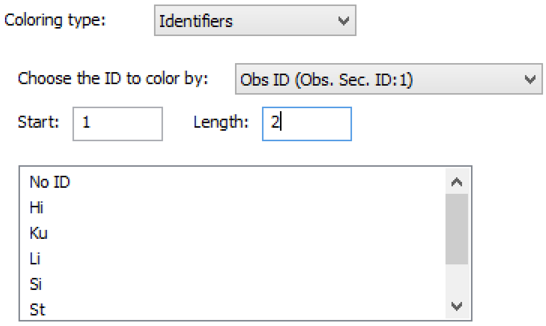
With all plots displaying variables or observations, the plot symbol, line, or column can be colored as described in the table, by clicking **Color by** on the **Tools** tab. Clicking **More options** opens the **Properties** dialog with the **Color** tab open. Here all coloring types for the active plot are available.

Note: When coloring a line plot, the connecting line when the line changes color starts with one color and gradually turns into the other. However, when a point in a line plot does not have a connecting line on either side, the plot mark of that point is displayed.

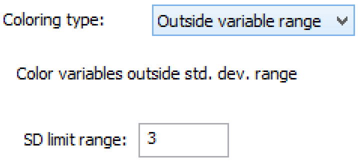
This table describes the coloring types available in the **Color** page and how to specify after selecting the respective coloring in the **Coloring type** box.

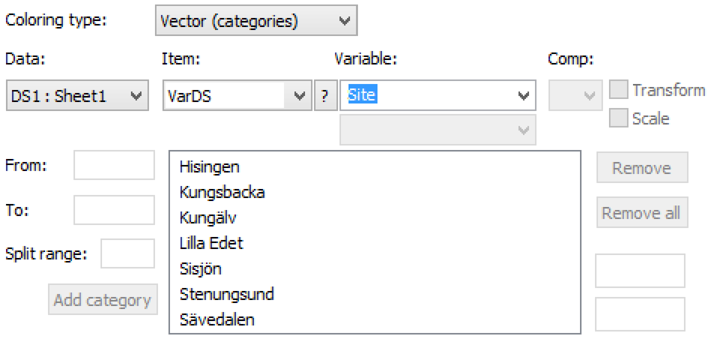
Note: The color of the classes/batches/categories etc. can be changed in **Format Plot**, **Styles**, **Category coloring**.

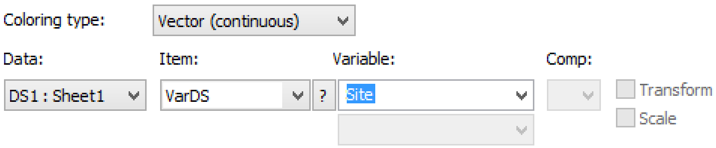
Color by	Action	Screen shot
Batches	Plots created for batch evolution models can be colored by **Batches**. When coloring by **Batches**, each batch is then assigned a color that it keeps independent of which batches are displayed in the plot.	 Coloring type: Batches
Classes	When classes are present in the plot, the observations are by default colored by **Classes**. To change the colors of the individual classes, use the legend mni-toolbar or **Format Plot, Styles, Category coloring**.	 Coloring type: Classes
Density	When a plot has many observations, coloring by **Density** (density function) is sometime useful.	 Coloring type: Density

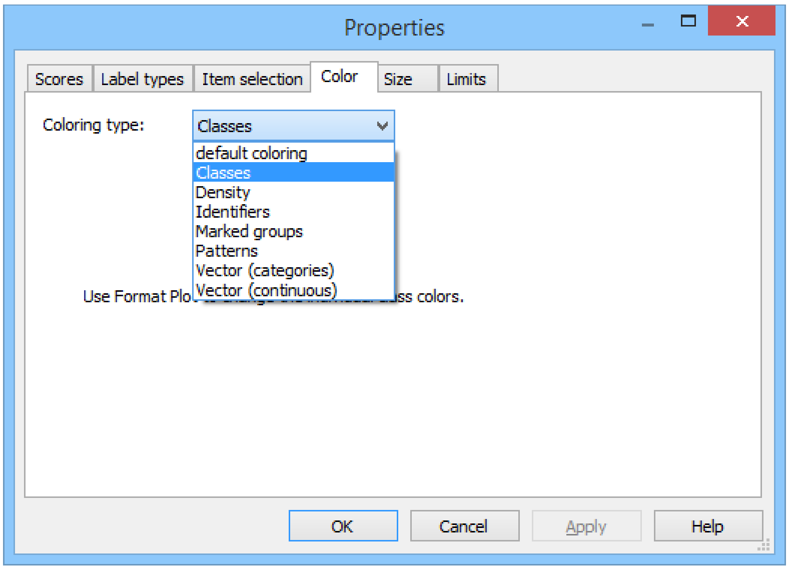
Color by	Action	Screen shot
	When coloring by **Density**, the plot marks are colored according to how many points are positioned close to them. This means that, using the automatic color scheme, a point with many points close is colored red while a point with few points close is colored blue. Available for plots displaying variables or observations. To change the start and end colors, use the legend mini-toolbar or **Format Plot**, **Styles**, **Coloring**.	
Identifiers	To color by **Identifier**: 1. Select the identifier in the **Choose the ID to color by** box. By default the first secondary ID is selected. 2. In the **Start** and **Length** fields enter values to specify which characters in the ID to use. Leaving the Length field empty includes all characters. Available for plots displaying variables or observations.	 Coloring type: Identifiers Choose the ID to color by: Obs ID (Obs. Sec. ID:1) Start: 1 Length: 2 No ID Hi Ku Li Si St

Color by	Action	Screen shot
	To change the color, use the legend mini-toolbar or **Format Plot**, **Styles**, **Category coloring**.	
Observation classes	When classes have been specified, each line of the XObs, YObs and Spectra plots can be colored by the class belonging of the observation.	
Observation identifiers	Each line of the XObs, YObs and Spectra plots can be colored by the observation ID. For how to specify, see the **Identifiers** description above.	
Observation vectors	Each line of the XObs, YObs and Spectra plots can be colored by an observation vector. For how to specify, see the **Vector (continuous)** description below.	
Marked groups	When observations are marked, you can color by **Marked groups**. When coloring by **Marked groups** the observations in the first group are displayed in one color, the observations in the second group in another color, etc. Available for plots displaying variables or observations and especially useful after marking using the **Group dendrogram clusters** tool.	For an example, see the HCA section in Chapter 10, Analyze.

Color by	Action	Screen shot
Models and predictions	Prediction plots can be colored by **Models and predictions**. This means that observations belonging to different models are colored in different colors and the observations that are not part of a model are colored in yet another color. Useful in the Coomans' plot.	
Outside variable range	Contribution plots can be colored depending on whether a variable is **Outside variable range** at the investigated point or points. Variables outside the standard deviation limit (by default 3) are colored orange. For variables where the limit cannot be calculated, that is, a maturity outside the average maturity range, the columns are colored gray.	 Coloring type: Outside variable range Color variables outside std. dev. range SD limit range: 3
Predictions	Observations that are part of the workset are colored in one color, and observations that are only part of the predictionset are colored in another color.	
Terms	Plots displaying variables can be colored by **Terms**. This results in that all types of terms (original X, expanded terms square, cross, cubic, etc.) are colored in different colors.	

Color by	Action	Screen shot
	Color by **Terms** is the default for the loading scatter plot.	
Variable classes	When variables have been assigned to blocks, use **Variable classes** to color these blocks.	
Vector (categories)	To color by **Categories**: 1. Select data source and variable in the **Data** respective **Item** boxes. Note here that both model terms and variables are available. 2. Optionally enter the desired number of groups in the **Split range** field. 3. Click the **Add category** button. 4. The range of the added categories can be modified by clicking the category and modifying the fields beneath the **Remove all** button.	 Coloring type: Vector (categories) Data: DS1 : Sheet1 Item: VarDS Variable: Site Comp: □ Transform □ Scale From: To: Split range: Add category Hisingen Kungsbacka Kungälv Lilla Edet Sisjön Stenungsund Sävedalen Remove Remove all

Color by	Action	Screen shot
	Note: To color by batch conditions or hierarchical variables, select that dataset in the **Data** box. To color by model results, select the model in **Data** and the vector in **Item**.	
Vector (continuous)	To color by **Vector (continuous)**, select data source and variable in the **Data** respective **Item** boxes. Note here that both model terms and variables are available in **Item**. **Note**: To color by batch conditions or hierarchical variables, select that dataset in the **Data** box. To color by model results, select the model in **Data** and the vector in **Item**.	 Coloring type: Vector (continuous) Data: DS1 : Sheet1 Item: VarDS Variable: Site Comp: □ Transform □ Scale



Properties

Coloring type: Classes

SIMCA by default remembers the selected coloring when opening the next plot. For more, see the Plot options subsection in the SIMCA options section in Chapter 5, File.

14.3.3.7.2 Item selection

The **Item selection** page in the **Properties** and **Plot/List** dialogs displays the items displayed in the current plot or list.

To remove some items from the current plot or list:

1. Mark the points in the plot.

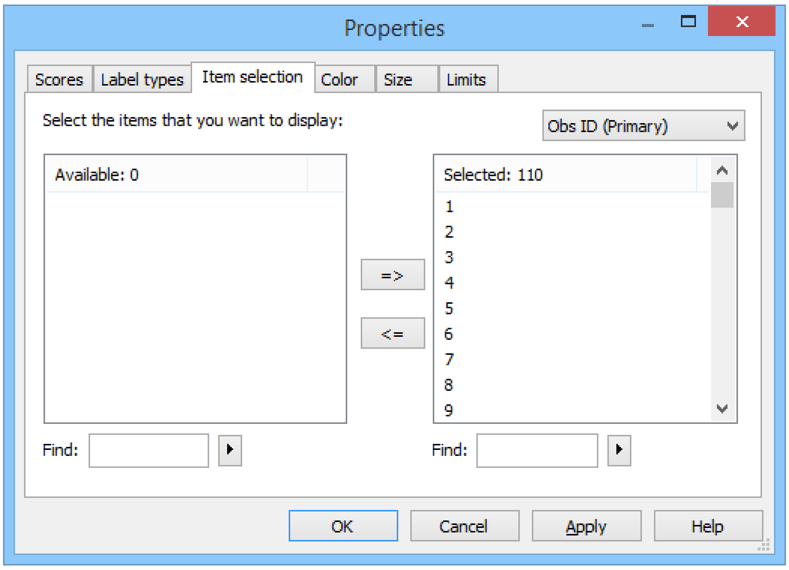
2. Click **Hide** on the **Marked items** tab.

As a result the **Item selection** page in the **Properties** dialog is updated accordingly.

The **Item selection** page displays the **Available** and **Selected** items. Removing and adding items from the current plot or list can also be done here.

1. Select the items in the **Selected** list.
2. Click **<=** to move them to the **Available** list.

To display a different identifier, select another ID by clicking the ID box.



Select the items that you want to display: Obs ID (Primary)

Available: 0

Selected: 110
1
2
3
4
5
6
7
8
9

Find:

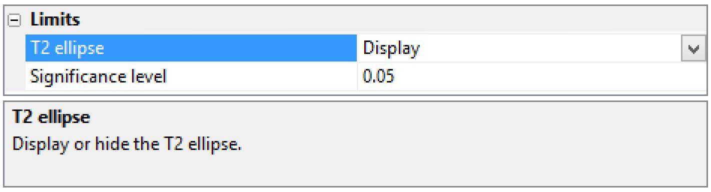
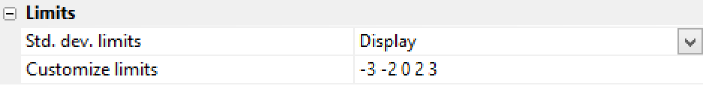
Find:

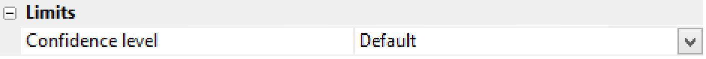
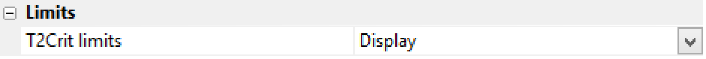
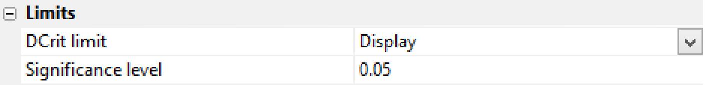
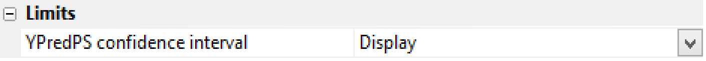
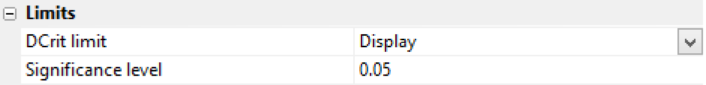
For more about the **Find** feature, see the Find feature in workset dialog subsection in the Workset section in Chapter 7, Home.

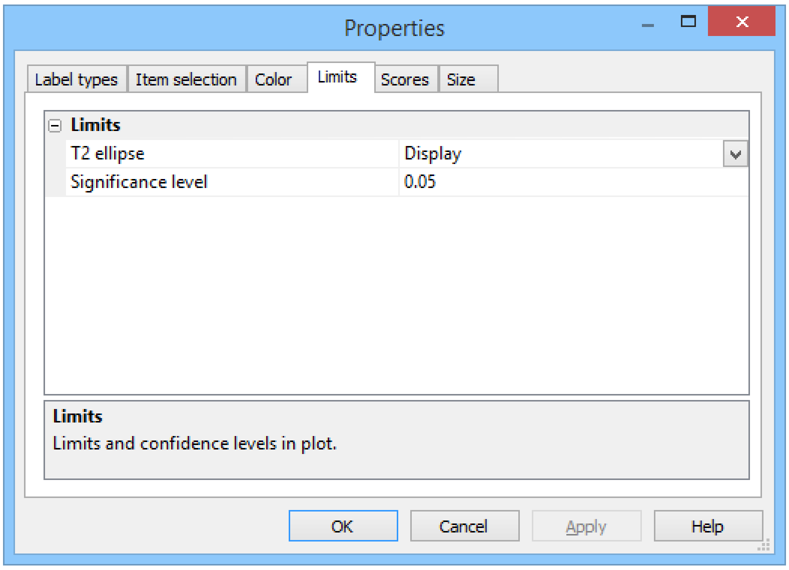
14.3.3.7.3 Limits

The **Limits** page enables customizing the displayed confidence intervals, limits, or ellipse.

The following plots have a **Limits** page in their **Properties** dialog for the described limits:

Plot	Limit	Option
Score Scatter Plot, 2D and 3D	Hotelling's T2 ellipse	**T2 Ellipse** box with: **Display** (default) and **Hide**. **Significance level** field with default value **0.05**.  **Limits** T2 ellipse: Display Significance level: 0.05 **T2 ellipse** Display or hide the T2 ellipse.
Score Line Plot	Standard deviation lines	**Std. dev. limits** box with: **Display** (default) and **Hide**. Customize limits field with the default -3 -2 0 2 3. Note that all limits inside the range -3 to 3 are by default colored in orange, and all outside in red. '0' represents the average.  **Limits** Std. dev. limits: Display Customize limits: -3 -2 0 2 3

Plot	Limit	Option
Score and Loading Column plots, Coefficient Plot, and VIP.	Jack-knifing uncertainty bars on the columns	**Confidence level** box with: **Default** (the setting in Model Options), **None** (to not display the error bars), **99%**, **95%**, and **90%**.  ⊟ **Limits** Confidence level: Default
Hotelling's T2Range	95% and 99% T2Crit	**T2Crit limits** box with: **Display** (default) and **Hide**.  ⊟ **Limits** T2Crit limits: Display
Distance to model	DCrit	**DCrit limit** box with: **Display** (default) and **Hide**. **Significance level** field with default value **0.05**.  ⊟ **Limits** DCrit limit: Display Significance level: 0.05
Y Predicted Column Plot	Jack-knifing uncertainty bars on the columns	YPredPS confidence interval box with: Display (default) and Hide.  ⊟ **Limits** YPredPS confidence interval: Display
Coomans' Plot	DCrit	**DCrit limit** boxes with: **Display** (default) and **Hide**.  ⊟ **Limits** DCrit limit: Display Significance level: 0.05



⊟ **Limits**

T2 ellipse: Display

Significance level: 0.05

Limits

Limits and confidence levels in plot.

14.3.3.7.4 Components in Properties

For a number of plots, the **Properties** dialog has a **Components** page.

Use this page to select for which components to display the plot.

For instance, selecting another component than **Last component** for the **Coefficient Plot** will display the plot cumulative including the selected component.

For the **Hotelling's T2Range Plot**, both the **From component** and **To component** has to be selected.

Note: When adding a plot to **Favorites** or the report, **Last component** is necessary if you plan to use the favorite for a model with a different number of components and want the last component to be used.

14.3.3.7.5 Select Y-variable

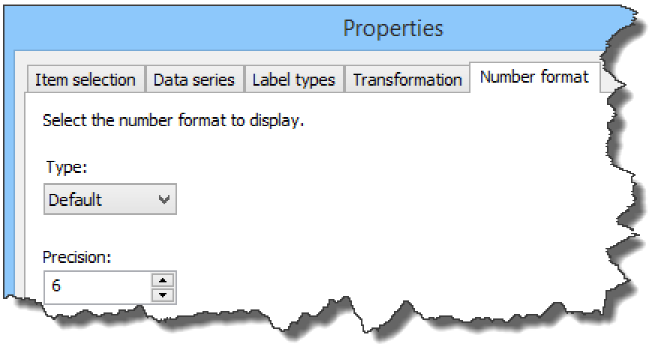
The **Coefficient Plot**, **Residual Normal Probability Plot**, **Observed vs. Predicted Plot**, and all **Y Predicted** plots found in the **Y PS** gallery on the **Predict** tab, are all displayed for one y-variable at a time. By default the plots are displayed for the first y-variable.

To switch to another y-variable in the plot use one of the following methods:

- Click the Y-variable box in the **Properties** group on the **Tools tab**, and select the desired y-variable.
- Right-click the plot, click **Properties**, click the **Select Y-variable** tab, and select the new variable in the **Select Y-variable** box.

14.3.3.7.6 Number format

Selecting the number format type and precision applies only to lists.



Select the number format to display.

Type: Default

Precision: 6

The available format types in the **Type** box are:

- **Default** - displaying the numbers in decimal format with the number of digits stated in the **Precision** box but leaving ending zeros hidden.
- **Exponential** - displaying the exponential format using the stated **Precision**.
- **Decimal** - displaying the number of decimals stated in the **Precision** box.

The values can be displayed using 1-6 digits. This is selectable in the **Precision** box.

14.3.4 Create group

In the **Create** group you can select to create another type of plot or list from the active plot.

The possible buttons are:

- **Out of control summary plot (OOC)** - described in the Out of control summary plot (OOC) subsection in this section.
- **Batch control chart** is available for the **Out of control summary plot** and displays the batches displayed in the OOC plot in a batch control chart.
- **Sources of variation plot** - described in the Sources of variation plot subsection in this section.
- **Merge list** - available for the dendrogram plots.
- **List** - Creates a list of the content of the current plot. For Dendrogram see the **Create list for the HCA dendrogram** subsection. See also the Creating lists subsection in the Marked Items tab section.
- **Change type** - described in the Change type subsection later in this section.

Note: The above commands are also available by clicking **Create** on the shortcut menu.

14.3.4.1 Out of Control Summary Plot (OOC)

The **Out of Control Summary Plot**, OOC plot, displays a normalized column plot for each batch that deviates from the limits in the current batch control chart, by integrating the area outside the selected limits, for the selected phase and component. The Y axis is in units of percent of the area outside the limits.

The Out of Control Summary (OOCSum) for all the vectors is always computed on aligned vectors.

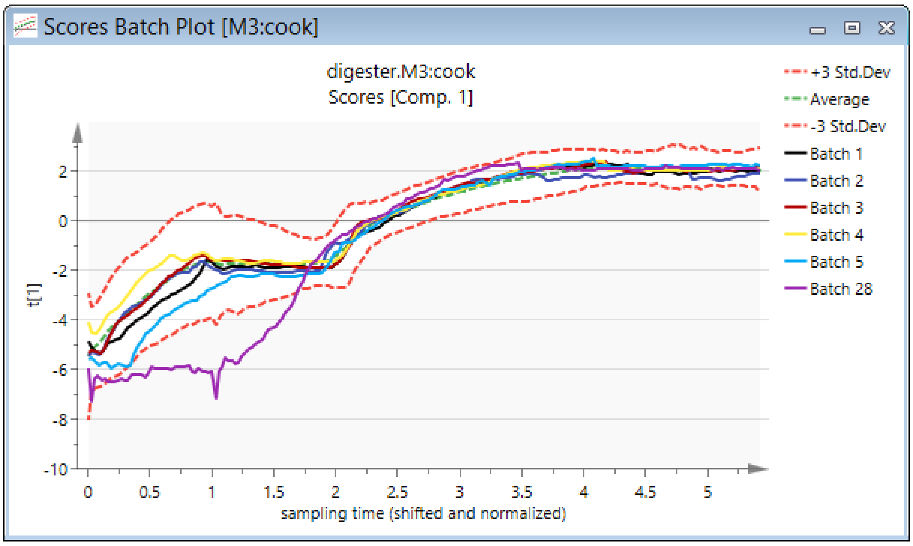
14.3.4.1.1 Creating the out of control summary plot

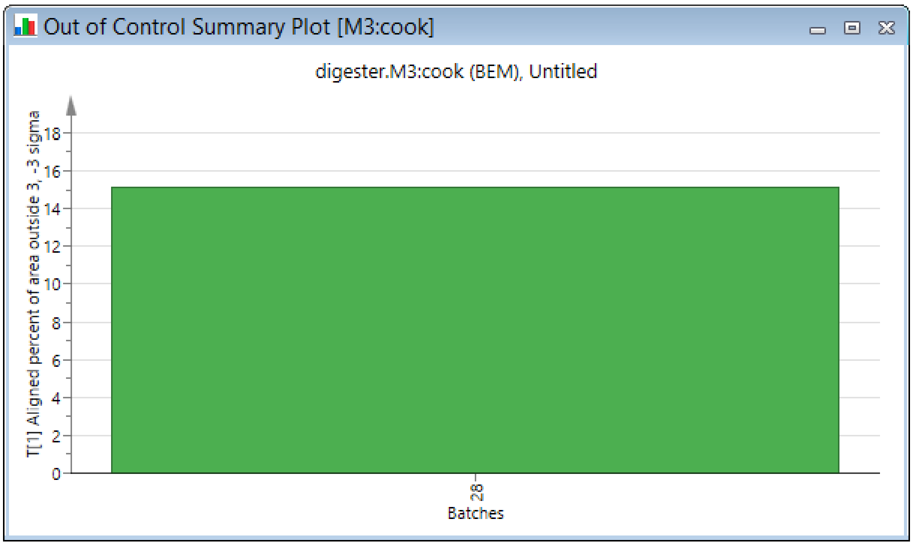
To open the **OOC** plot for the open batch control chart, on the **Tools** tab, in the **Create** group, click **Out of control summary**.

After creating the OOC plot you can recreate the batch control chart holding only the batches that were out of control by, clicking **Batch control chart**, in the **Create** group, on the **Tools** tab.

14.3.4.1.2 OOC plot example

From the batch control chart the **Out of Control Summary Plot** was created.





In the **Out of Control Summary Plot** above, batch 28 has 20% of its area outside the limits.

14.3.4.1.3 Creating Out of Control Summary Plot from Plot/List tab

The OOCSum vectors can be plotted and listed from the **Plot/List** tab by:

1. Clicking a plot type.
2. Selecting **Batch vectors** in the **Select data type** box.

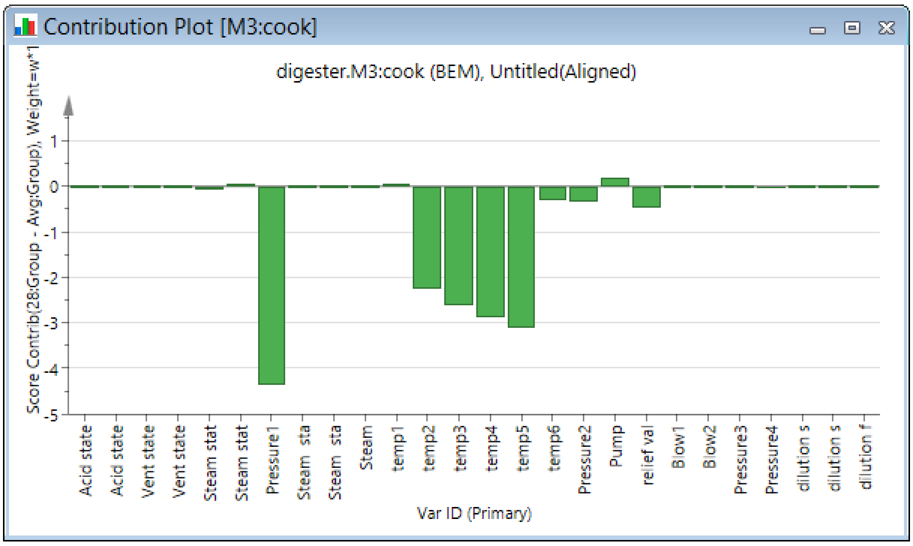
3. Adding the desired OOCSum vector.

See also the Batch vectors - Out of control summary subsection in the Statistical appendix.

14.3.4.1.4 Contribution plot from OOC plot

Double-click any batch column in the **Out of Control Summary Plot** to display its contribution plot.

Double-clicking a variable in the contribution plot opens the variable batch control chart.



14.3.4.2 Sources of variation plot

In batch level models it is useful to display the contribution and loading plots (or any other plot displaying variables) as line plots over time rather than column plots at every time point. Therefore the **Sources of variation plot** is the default loading and contribution plot for all BLM with one or more score or raw variables. The Sources of variation plot contains the exact same data as a loading or contribution plot would show. Instead of having the variable number on the x-axis, the maturity of the batch is used. This gives a better view of how the process variables relate to each other at different stages in the process.

For projects with phases, this plot is displayed showing all phases.

14.3.4.2.1 BLM with batch conditions

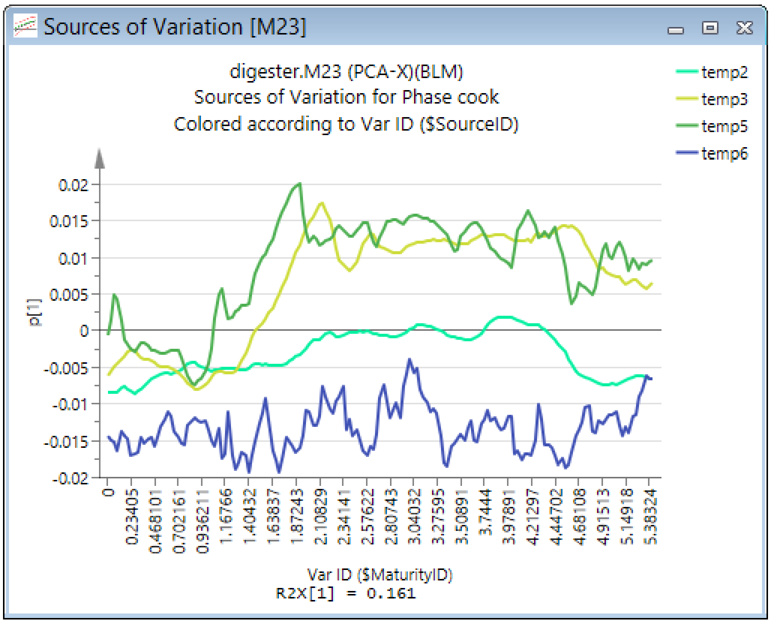
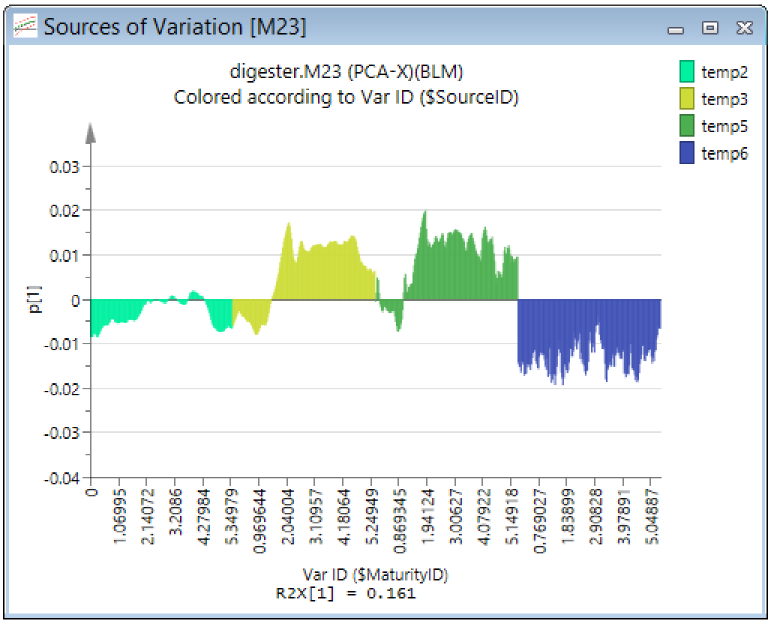
Variables without maturity, i.e. batch conditions, cannot be shown in Sources of variation plots. When the BLM contains batch conditions it can be useful to view the plot as a regular column plot too.

To switch the Sources of variation plot to a column plot, on the **Tools** tab, click **Change type** | **Column**. A normal loading plot can always be created from the **Loading** plot gallery, in the **Diagnostics & interpretation** group on the **Home** tab, by selecting one of the standard options.

Contribution plots in column form may be selected on the **Marked items** tab, in the **Drill down** group, by clicking **Column** in the comparison plot gallery.

14.3.4.2.2 BLM loading and contribution plots example

How to change between a Sources of variation plot and a column plot is described in the table. This example uses a loading plot, but is applicable for contribution plots as well.

Step	Illustration/description
1. On the **Home** tab, click **Loadings**.	 For a PCA loading sources of variation plot, the main systematic variation over time in the data for the selected variables is displayed. For a PLS/OPLS/O2PLS loading sources of variation plot, the variable loading over time, i.e. the variation over time that is related to the Y-variable is displayed. In a contribution sources of variation plot, how the variables over time differ between the selected batch and the average batch is displayed.
2. To transform to the column plot, on the **Tools** tab, click **Change type | Column**.	
3. To transform to the Sources of variation plot (from the column plot), on the **Tools** tab, in the **Create** group, click **Sources of variation**.	
4. To switch phases or displayed variables in the contribution plot open **Properties** and:	

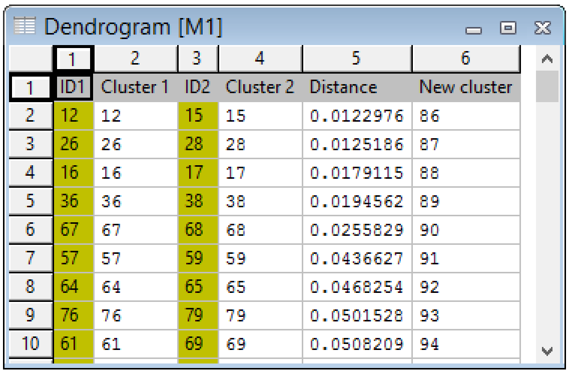
Step	Illustration/description
- click the desired phase in the **Select phase** box. - add to the **Selected** list the variables to display.	

14.3.4.3 Merge list for HCA dendrogram

With the HCA dendrogram open, **Merge list** is available in the **Create** group on the **Tools** tab.

Merge list

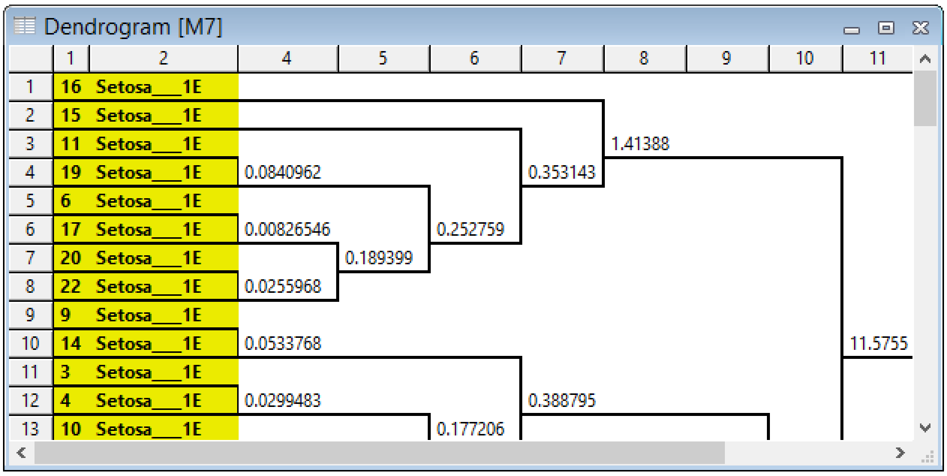
This command creates a list of the calculations behind the dendrogram.



	1	2	3	4	5	6
1	ID1	Cluster 1	ID2	Cluster 2	Distance	New cluster
2	12	12	15	15	0.0122976	86
3	26	26	28	28	0.0125186	87
4	16	16	17	17	0.0179115	88
5	36	36	38	38	0.0194562	89
6	67	67	68	68	0.0255829	90
7	57	57	59	59	0.0436627	91
8	64	64	65	65	0.0468254	92
9	76	76	79	79	0.0501528	93
10	61	61	69	69	0.0508209	94

14.3.4.4 Create list for the HCA dendrogram

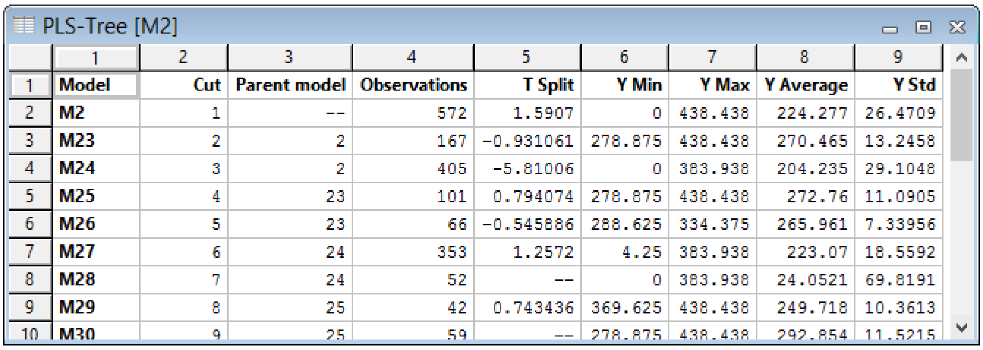
With the HCA dendrogram plot open, click **List** to display all clusters and the calculated distances.



	1	2
1	16	Setosa___1E
2	15	Setosa___1E
3	11	Setosa___1E
4	19	Setosa___1E
5	6	Setosa___1E
6	17	Setosa___1E
7	20	Setosa___1E
8	22	Setosa___1E
9	9	Setosa___1E
10	14	Setosa___1E
11	3	Setosa___1E
12	4	Setosa___1E
13	10	Setosa___1E

14.3.4.5 Create list for PLS-Tree

With the PLS-Tree dendrogram plot open, clicking **List**, creates a list displaying details about the PLS-Tree sub-models.



PLS-Tree [M2]

	1	2	3	4	5	6	7	8	9
1	Model	Cut	Parent model	Observations	T Split	Y Min	Y Max	Y Average	Y Std
2	M2	1	--	572	1.5907	0	438.438	224.277	26.4709
3	M23	2	2	167	-0.931061	278.875	438.438	270.465	13.2458
4	M24	3	2	405	-5.81006	0	383.938	204.235	29.1048
5	M25	4	23	101	0.794074	278.875	438.438	272.76	11.0905
6	M26	5	23	66	-0.545886	288.625	334.375	265.961	7.33956
7	M27	6	24	353	1.2572	4.25	383.938	223.07	18.5592
8	M28	7	24	52	--	0	383.938	24.0521	69.8191
9	M29	8	25	42	0.743436	369.625	438.438	249.718	10.3613
10	M30	9	25	59	--	278.875	438.438	292.854	11.5215

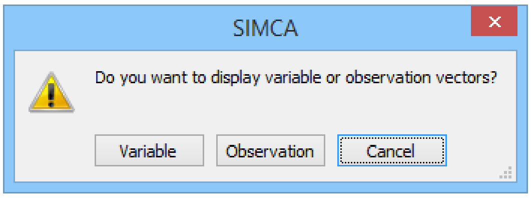
14.3.4.6 Change type

By clicking **Change type** on the **Tools** tab you can select to display the open plot or list as another plot type. When changing between the regular plot types the plot window is reused.

The possible plot types are:

- **Scatter -** Changes the current plot into a scatter plot.
- **Line -** Changes the current plot into a line plot.
- **Column -** Changes the current plot into a column plot.
- **Other plot types -** opens the **Create Plot** dialog described in the Creating plots subsection in the Marked Items tab section.

When the marking is not of an entire row or column in a spreadsheet, the following message is displayed. Select the vectors to be displayed in the list by clicking **Variable** or **Observation**.



SIMCA

Do you want to display variable or observation vectors?

Note: With any plot or list open you can create another plot or list using the same data by clicking **Create | Plot** on the shortcut menu.

14.3.5 Add to favorites

Clicking **Add to favorites** adds the active plot or list to the **Favorites** pane. For more, see the Favorites section earlier in this chapter.

14.3.6 Add to report

Clicking **Add to report** adds the active plot or list to the HTML Report. For more, see the Generate Report section in Chapter 5, File.

14.3.7 Format Plot

The most common attributes of the plot axes, plot area and of the header and footer can be customized directly in the plot using the mini-toolbar, or by opening the **Format Plot** dialog.

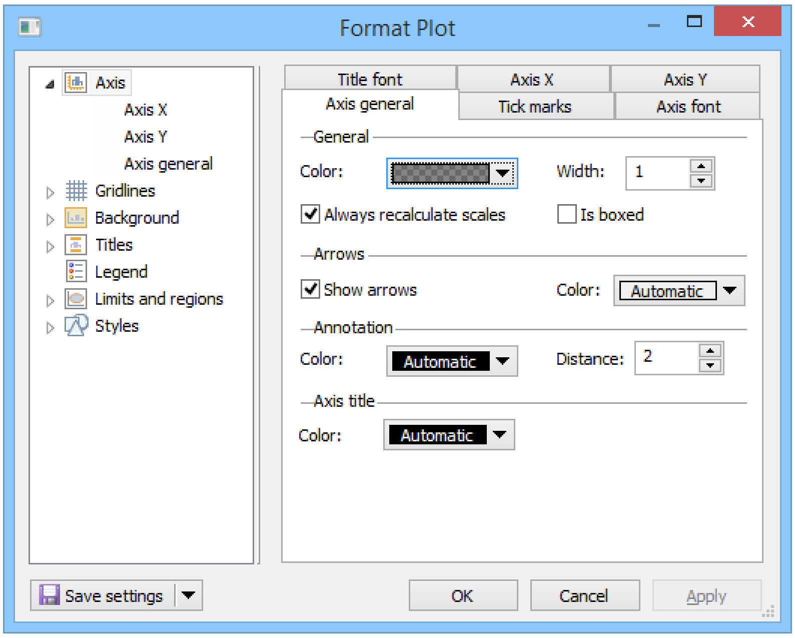
The mini-toolbar is displayed after clicking an item (header, footer, legend, symbol, column etc.) and moving the cursor northeast.

To open the **Format Plot** dialog use one of the following methods:

- On the **Tools** tab, click **Format plot** (to the far right).
- Double-click the plot area, header or footer, or axes in the plot.
- Right-click the plot and then click **Format plot**.

14.3.7.1 Axis

The properties under the **Axis** node apply to the selected axis: Axis X, Axis Y, Axis Y2 (second Y-axis) etc.



General
Color:
Width: 1
☑ Always recalculate scales
☐ Is boxed

Arrows
☑ Show arrows
Color: Automatic

Annotation
Color: Automatic
Distance: 2

Axis title
Color: Automatic

In the **Format Plot** dialog, **Axis** node, click:

- The respective axis to customize the scaling of the selected axis, annotation rotation etc.
- **Axis general** to access the following pages:
  1. **Axis general** to customize color, width and other properties of all axes.
  2. **Tick marks** to select how to display major and minor tick marks.
  3. **Axis font** to customize the font of the axis annotation.
  4. **Title font** to customize the font of all axis titles.

14.3.7.1.1 Changing the scale, tick mark label and the axis properties

Use the specific axis page under the **Axis** node to change the scale, tick mark label and axis properties of the selected axis.

14.3.7.1.2 Individual axes

The content for the individual axes is described in the table below:

Field/button	Displays	Result after entering a new value and clicking Apply
	Axis	
Show axis	Default selected.	If cleared, that axis is not displayed.
Minimum	Start point for the selected axis when the values are displayed in regular order. For time-variables the page is adjusted, see the Time axis topic.	The new start point is used for the selected axis.
Maximum	End point for the selected axis when the values are displayed in regular order.	The new end point is used for the selected axis.
Auto adjust scales for suitable limits and step size	Default selected.	If cleared, enables the **Step size** field.
Step size	Default disabled.	The entered value defines the major tick mark spacing for the selected axis.

Field/button	Displays	Result after entering a new value and clicking Apply
Reverse axis	Default cleared.	If selected, the scale is displayed with the highest number to the left and the lowest to the right.
	Annotation	
Rotation	Default No Rotation.	Selecting *90 degrees* displays the annotation turned 90 degrees.
	Title	
Show title	Default selected.	If cleared, the axis title is not displayed.
Title	The vector name.	The new title. Title changes cannot be saved.

Note that the distance between the tick marks is constant.

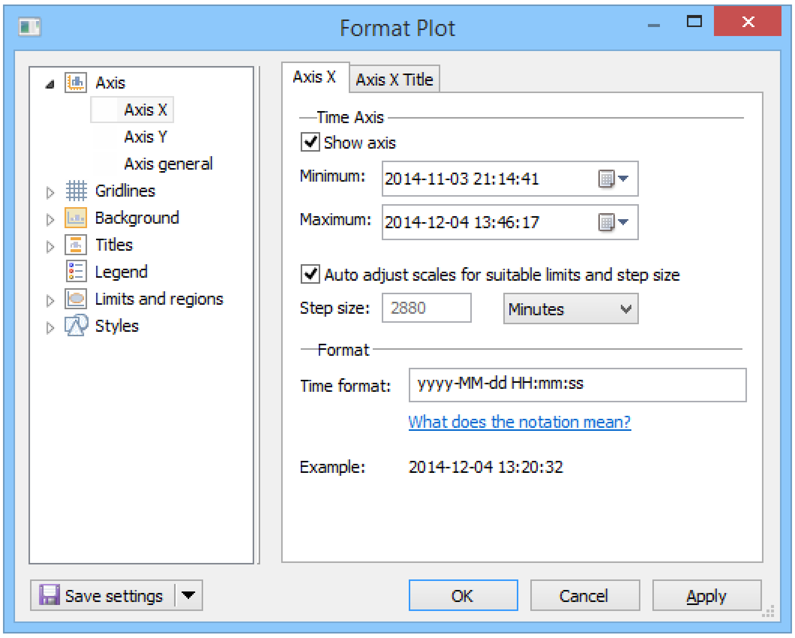
When you have more than one series in a plot, you can select to display more than one y-axis. For more, see the Multiple Y-axes subsection later in this chapter.

14.3.7.1.3 Time axis

The content for the **Axis X** and **Axis X title** pages for a time variable is described in the table below:

Field/button	Displays	Result after entering a new value and clicking Apply
Show axis	Default selected.	If cleared, that axis is not displayed.
Minimum	Start point in time units. Change by typing in the field.	The new start point is used for the selected axis.
Maximum	End point in time units. Change by typing in the field.	The new end point is used for the selected axis.
Auto adjust scales for suitable limits and step size	Default selected.	If cleared, enables the **Step size** field.
Step size	Default disabled.	The entered value defines the major tick mark spacing for the selected axis.
unit	The unit of the step size.	Switching between units updates the step size automatically.
	Axis X Title tab	
Rotation under Annotation	Default No Rotation.	Selecting *90 degrees* displays the annotation turned 90 degrees.
Show title under Title	Default selected.	If cleared, the axis title is not displayed.
Title	The vector name.	The new title. Title changes cannot be saved template.

Note that the distance between the tick marks is constant.



Time Axis

☑ Show axis

Minimum: 2014-11-03 21:14:41

Maximum: 2014-12-04 13:46:17

☑ Auto adjust scales for suitable limits and step size

Step size: 2880 Minutes

Format

Time format: yyyy-MM-dd HH:mm:ss

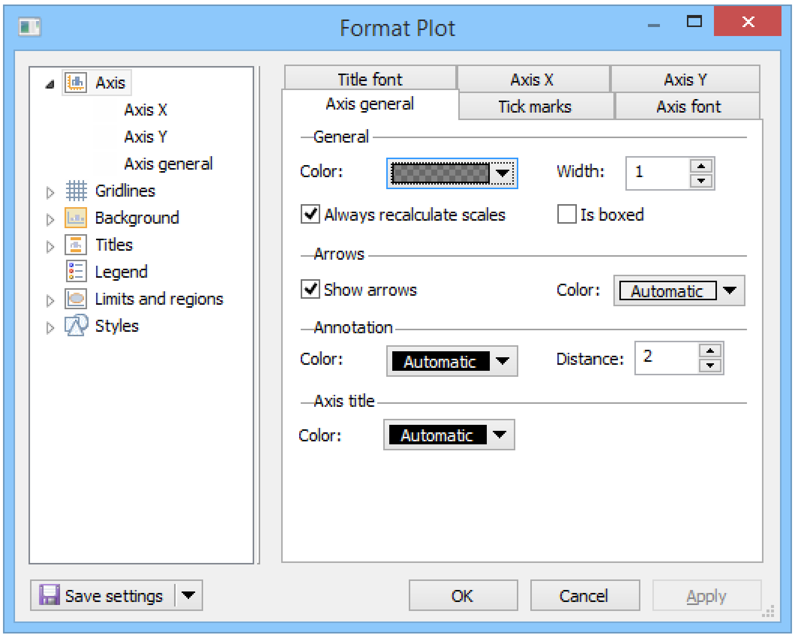
What does the notation mean?

Example: 2014-12-04 13:20:32

14.3.7.1.4 Axis general

In **Axis general** the following features are available and are applied for all axes:

- Axis **Color** and **Width**.
- **Always recalculate scales -** when selected it auto scales all axes. Clearing it makes the current ranges of the axes stick even if the vector displayed is switched.
- **Show arrows** - when selected the arrows are displayed at the end of the axes.
- Arrow **Color** - *Automatic* here means the same as the axis color.
- Annotation **Color** and **Distance** from axis.
- Axis title **Color**.



General

Color: ▨ Width: 1

☑ Always recalculate scales ☐ Is boxed

Arrows

☑ Show arrows Color: Automatic

Annotation

Color: Automatic Distance: 2

Axis title

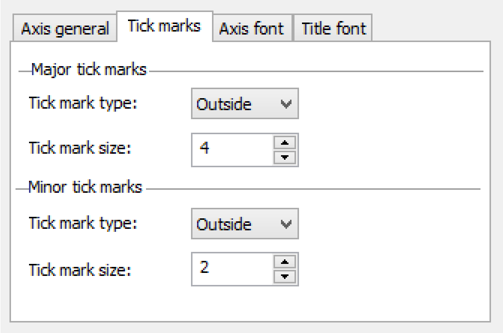
Color: Automatic

14.3.7.1.5 Tick marks

Use the **Tick marks** page to specify how the tick marks should be oriented and how long they should be.

Under **Major tick marks** and **Minor tick marks** the same boxes are available:

- **Tick mark type -** where **None** is no tick mark, **Outside** is to have the tick mark outside the axis, **Inside** is to have the tick mark inside the axis and **Cross** is to have the tick mark on both sides of the axis.
- **Tick mark size** is the length of the tick mark.



Major tick marks

Tick mark type: Outside

Tick mark size: 4

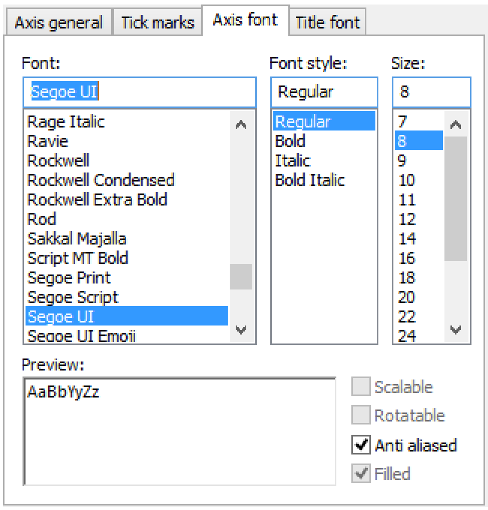
Minor tick marks

Tick mark type: Outside

Tick mark size: 2

14.3.7.1.6 Font

Use the respective font pages, to select the **Font**, **Font style**, **Size**, and **Effects** for the annotation, title, etc.



Font: Segoe UI

Rage Italic
Ravie
Rockwell
Rockwell Condensed
Rockwell Extra Bold
Rod
Sakkal Majalla
Script MT Bold
Segoe Print
Segoe Script
Segoe UI
Segoe UI Emoji

Font style: Regular

Regular
Bold
Italic
Bold Italic

Size: 8

7
8
9
10
11
12
14
16
18
20
22
24

Preview:

AaBbYyZz

□ Scalable
□ Rotatable
☑ Anti aliased
☑ Filled

Section	Description
Font	Displays the currently selected font. Click another font to switch.
Font style	Displays the current font style. Select to display the text **Regular** (default), **Bold**, **Italic**, or **Bold Italic**.
Size	Displays the current size. Select another size as desired.
Preview	Displays a preview of the expected text according to the selections above.
Anti aliased, Filled check boxes	Allows selecting to display the text **Anti aliased** and/or **Filled** or neither.

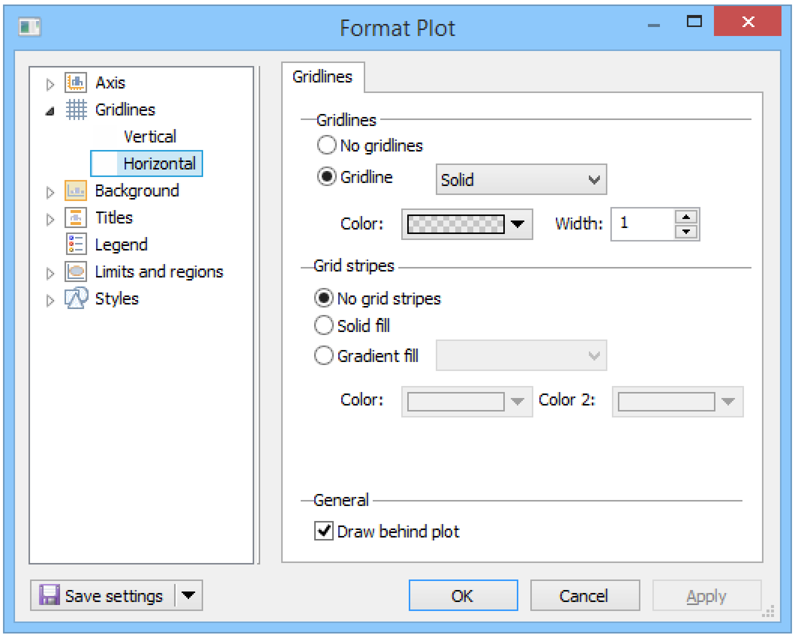
14.3.7.2 Gridlines

Use the **Gridlines** page to customize the gridlines and grid stripes. The gridlines are placed on the major tick marks. Grid stripes are the areas between the gridlines, where every second such area can be colored.

Note: Gridlines and grid stripes can be specified individually for **Vertical** and **Horizontal**. Specification using the node applies to both.

The following is available:

Option/Box/Field	Description
No gridlines	No gridlines are displayed when **No gridlines** is selected.
Gridline	When selecting **Gridline** you can select to display the lines *Solid*, *Dashed*, *Dotted*, *Dash dot*, or *Dash dot dot*.
Gridline Color	The color of the grid, by default gray.
Width	The width of the gridlines.
No grid stripes	No grid stripes are displayed when **No grid stripes** is selected.
Grid stripe **Solid fill**	When selecting **Solid fill** the grid stripes are displayed in the selected color.
Grid stripe **Color**	Displays the current color and allows selecting a new color.
Grid stripe Gradient fill	When selecting **Gradient fill** you can select to display the stripes Horizontal, Vertical, Forward diagonal, Backward diagonal, Radial, Horizontal bar, Vertical bar.
Grid stripe **Color 2**	Displays the current color and allows selecting a new second color for **Gradient fill**.
Draw behind plot	When selected (default) the grids are drawn behind all plot contents.



Gridlines

○ No gridlines

● Gridline: Solid

Color: Width: 1

Grid stripes

● No grid stripes

○ Solid fill

○ Gradient fill

Color: Color 2:

General

☑ Draw behind plot

14.3.7.3 Background

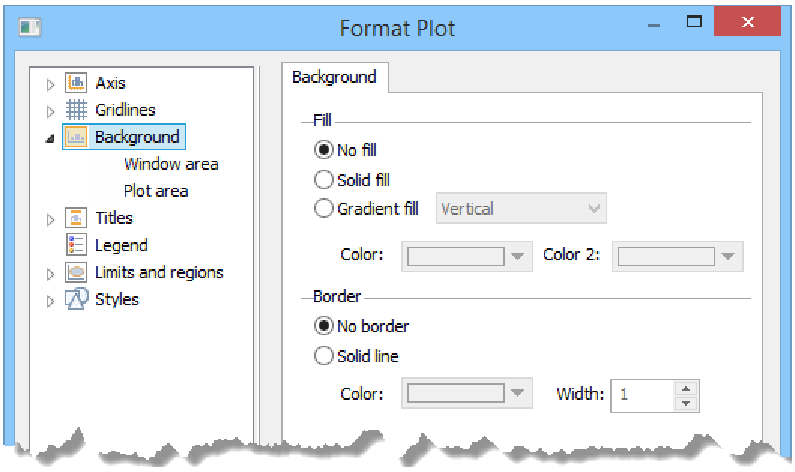
The **Background** node controls the attributes of the background displayed in the plot.

Note: The background fill and border can be specified individually for the **Window area** and **Plot area**. Specification using the node applies to both.

The table describes the available options:

Option/Box/Field	Description
	Fill
No fill	No background is displayed when **No fill** is selected.
Sold fill	When selecting **Solid fill** the background is displayed in the selected color.
Gradient fill	When selecting **Gradient fill** you can select to display the background Horizontal, Vertical, Forward diagonal, Backward diagonal, Radial, Horizontal bar, Vertical bar.
Color	Displays the current color and allows selecting a new color for the background.
Color 2	Displays the current color and allows selecting a new second color for **Gradient fill**.
	Border

Option/Box/Field	Description
No border	No border around the background area is displayed when **No border** is selected.
Solid line	When selecting **Solid fill**, the background is displayed in the selected color.
Color	Displays the current color and allows selecting a new color for the border.
Width	The width of the border.



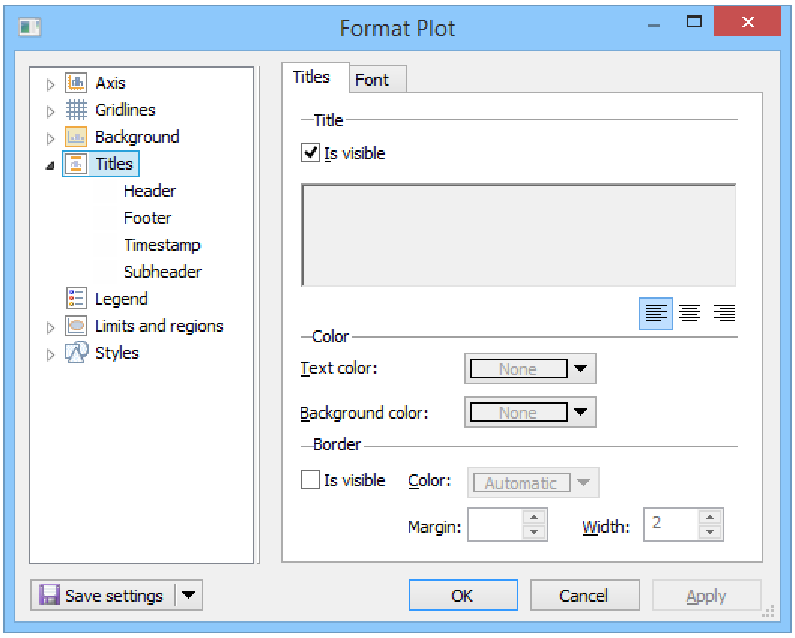
Fill
● No fill
○ Solid fill
○ Gradient fill Vertical
Color: Color 2:

Border
● No border
○ Solid line
Color: Width: 1

14.3.7.4 Titles

Use the **Format Plot** dialog to customize the items available in the **Titles** node. When customizing, the changes apply to the selected item, **Header/Footer/Timestamp/Subheader**.

Note: Changing color, font and size of the Header/Footer/Timestamp/Subheader can be done directly in the plot by clicking and using the mini-toolbar.



Title
☑ Is visible

Color
Text color: None
Background color: None

Border
□ Is visible Color: Automatic
Margin: Width: 2

On the **Titles** page:

- Select to hide or show by selecting or clearing the **Is visible** check box.
- Select where to display the title in the **Anchor** box, when applicable.
- Customize the text displayed by changing or typing in the field.
- Align the text right, center, or right by clicking the appropriate alignment button.

- Customize the color of the text in the **Text color** box.
- Customize the background color by clicking the **Background color** box.
- Select to display a border by selecting the **Is visible** check box in the **Border** section. With it selected you can customize **Color**, **Margin** (to the text) and **Width** of the border.

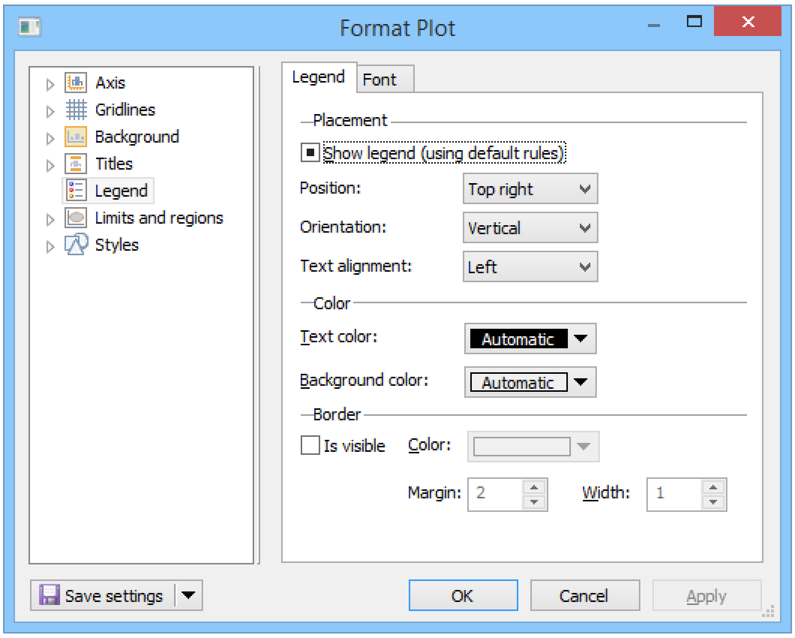
On the **Font** page you can select the **Font**, **Font style**, **Size**, and **Effects**. See also the Font subsection earlier in this chapter.

14.3.7.5 Legend

The **Legend** page controls the attributes of the legend, such as placement, color, and border.

The table describes the available options:

Option/Box/Field	Description
	Placement section
Show legend	The legend is displayed when the **Show legend** check box is selected. When this check box is in intermediate state, as in the screenshot here, this means that the legend is displayed according to internal rules. The rule is to show the legend with more than one series and less than 100.
Position	By default the legend is positioned *Top right*. To change from the default, click one of the available placement options.
Orientation	The orientation is by default *Vertical*. *Horizontal* is the other option.
Text alignment	Alignment of the text in the legend is by default *Left*. *Right* and *Center* are the other options.
	Color section
Text color	By default the text is black. To customize text color of the legend, click the **Text color** box.
Background color	The default background color is white. To select another color, click the **Background color** box.
	Border section
Is visible	By default the border is not displayed. To display the border around the legend, select the **Is visible** check box.
Color	To customize the border color of the legend, click the **Color** box in the **Border** section.
Margin	To specify the margin to the text, change the value in the **Margin** field.
Width	To increase or decrease the width, enter a new number in the **Width** field.


Format Plot

Placement

■ Show legend (using default rules)

Position: Top right

Orientation: Vertical

Text alignment: Left

Color

Text color: Automatic

Background color: Automatic

Border

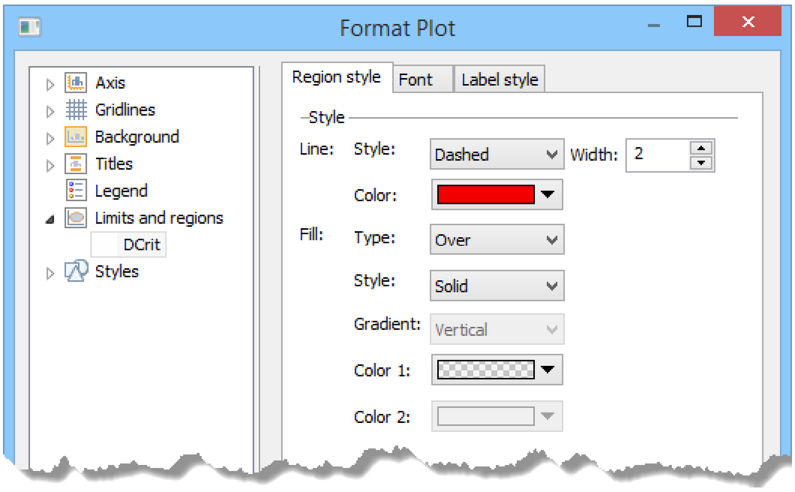
□ Is visible Color:

Margin: 2 Width: 1

14.3.7.6 Limits and regions

The selected limit or region can be customized in the **Region style** page.

Feature	Description
Line	
Style	Select between No line, Solid, Long dash, Dotted, Dash dot.
Width	Increase or decrease as desired.
Color	Displays the current color and allows selecting a new color.
Fill	
Type	Select to fill the area *Over* or *Under* the limit, or select *No fill.*
Style	Select the fill to be *Solid* or *Gradient.* Selecting *Solid* enables the **Color 1** box and selecting *Gradient* enables the **Gradient**, **Color 1** and **Color 2** boxes.
Gradient	When selecting **Gradient** you can select to display the fill Horizontal, Vertical, Forward diagonal, Backward diagonal, Radial, Horizontal bar, Vertical bar.
Color 1	Displays the current color and allows selecting a new color.
Color 2	Displays the current color and allows selecting a new color. Available when the **Style** is *Gradient.*
Font tab - see the Font topic.	
Label style - see the Labels topic.	



Style

Line: Style: Dashed Width: 2

Color: 🟥

Fill: Type: Over

Style: Solid

Gradient: Vertical

Color 1:

Color 2:

To not display the limit, see the Limits subsection in the Tools section previously in this chapter.

There are a number of limits available in plots in SIMCA, for instance the ellipse in the score scatter plot, the DCrit limit in the DModX plot etc. Additionally there are regions, such as the background of phases in batch control charts and models in hierarchical top model coefficient and contribution plots that are colored to differentiate between models.

The attributes of the limits and regions can be modified individually for each limit and region type under the **Limits and regions** node in the **Format Plot** dialog, in the respective **Region style** pages. The **Region style** page is described in this section.

For multi plots, **Control charts** and **Wavelet structure**, the limit pages are positioned last in the **Format Plot** dialog under *Plot 1, Plot 2, Plot 3*, etc.

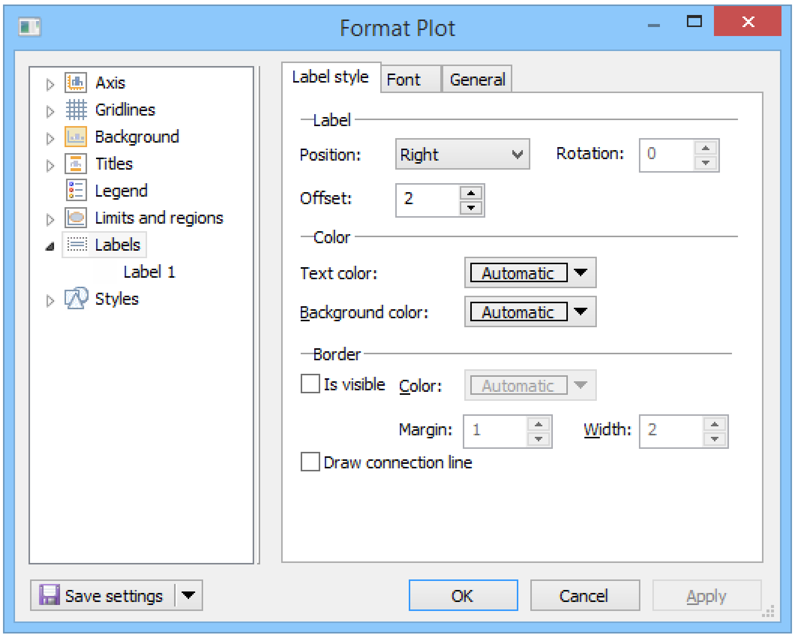
For batch control charts, the limit pages are positioned under **Styles**.

14.3.7.7 Label style

The **Labels** pages control the attributes of the displayed plot marks. Color, alignment, font and rotation apply to all labels in a given series.

The tabs available in the **Labels** node, **Label style**, **Font** and **General**, are described in the table.

Option/Box/Field	Description
Label section in Label styles	
Position	The default position of the label in reference to the point is *Right*. To position the label in another direction, click the **Position** box and make a new selection.
Offset	The offset defines the distance between the label and what it labels in the direction of the selected **Position**. To increase or decrease the distance between the label and item, enter a new value in the **Offset** field.
Rotation	The default rotation of the labels is *0*. To rotate the label, enter a new value in the **Rotation** field. Note that this field is unavailable when **Avoid overlapping labels** has been selected in the **General** tab.
Color section in Label styles	
Text color	Displays the current color of the text in the label and allows selecting a new color. *Automatic* displays the text in the same color as the symbol fill
Background color	The background color of the label is default transparent. To select a color, click the **Color** box and make the selection.
Border section in Label styles	
Is visible	By default, no border for the label is displayed. To display a border around the label select the **Is visible** check box.
Color	Displays the current color of the border and allows selecting a new color.
Margin	The margin between the text and the border can be customized in the **Margin** field.
Width	To increase or decrease the width, enter a new number in the **Width** field.
Draw connection line	**Draw connection line** is by default cleared. Selecting it will display a thin line between the label and its point.
Font tab - see the Font topic.	
General tab	
Avoid overlapping labels	With **Avoid overlapping labels** selected, point labels will try not to overlap each other. A high specified limit in the **Limit** field in combination with many labels can be quite time consuming.



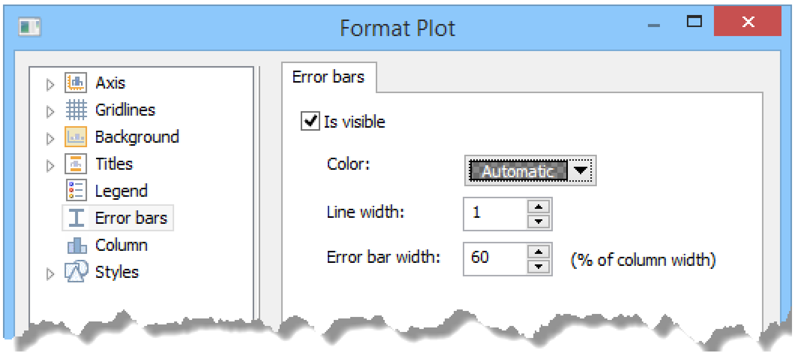
Position: Right
Rotation: 0
Offset: 2
Text color: Automatic
Background color: Automatic
□ Is visible Color: Automatic
Margin: 1
Width: 2
□ Draw connection line

14.3.7.8 Error bars

The **Error bars** page controls the attributes of the error bars displayed in the score, loading, coefficient, VIP, and Y PS column plots.

The settings available are:

- **Is visible** - hides the error bars when cleared.
- **Color** of the error bars - by default black. To display the error bars in any other color, click the **Color** box.
- **Line width** of the vertical and horizontal lines. To display wider error bars, enter a new number in the field.
- **Error bar width** is how wide the horizontal line is compared to the column. By default 60%.



☑ Is visible

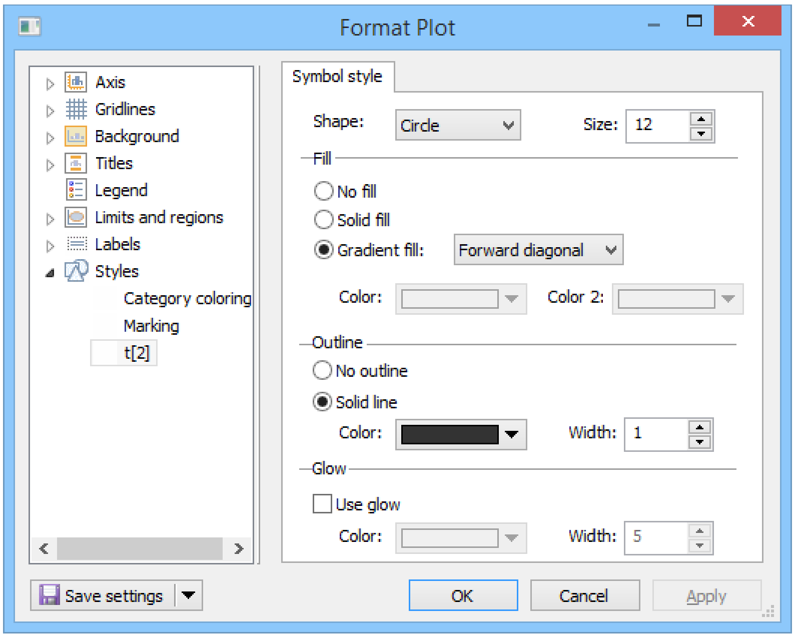
Color: Automatic

Line width: 1

Error bar width: 60 (% of column width)

14.3.7.9 Styles

In the **Styles** node the attributes of the series, *Category coloring* and for BCC plots also limits can be customized.



Shape: Circle Size: 12

Fill

○ No fill

○ Solid fill

● Gradient fill: Forward diagonal

Color: Color 2:

Outline

○ No outline

● Solid line

Color: Width: 1

Glow

□ Use glow

Color: Width: 5

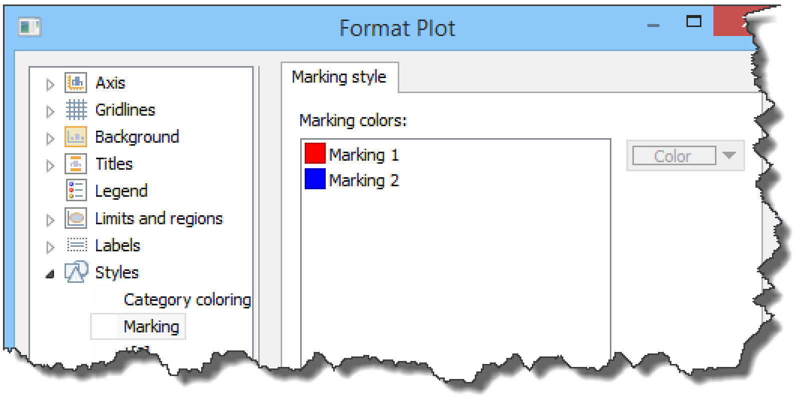
The available pages in the **Styles** node, different depending on which plot is open, are:

- Marking style
- Category coloring
- Symbol style
- Line style
- Column style
- Region style which includes Fill style.

- Options
- Y-axis
- Font

14.3.7.9.1 Marking style

In the **Marking style** page you can change the marking colors by marking and selecting a new color in the color box to the right.

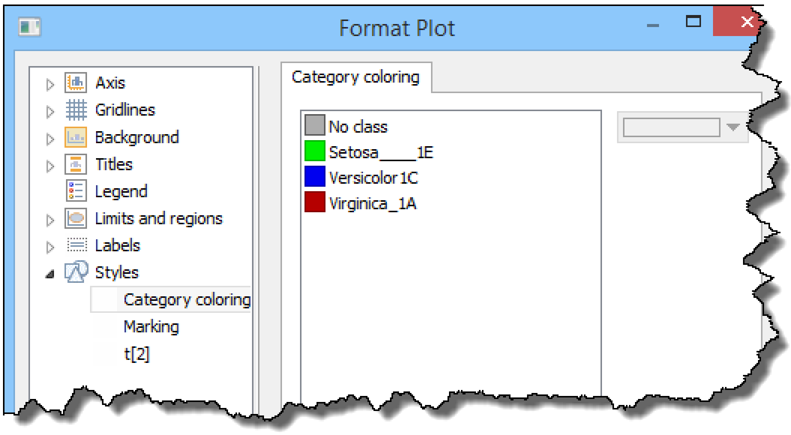


Marking colors:
🟥 Marking 1
🟦 Marking 2

14.3.7.9.2 Category coloring

Category coloring is available after applying a category coloring and the **Use different symbols on category colored values** check box in the **Options** page remains not selected.

In this page, the colors can be changed as desired by marking a category and changing the color in the menu to the right.



⬜ No class
🟩 Setosa____1E
🟦 Versicolor 1C
🟥 Virginica_1A

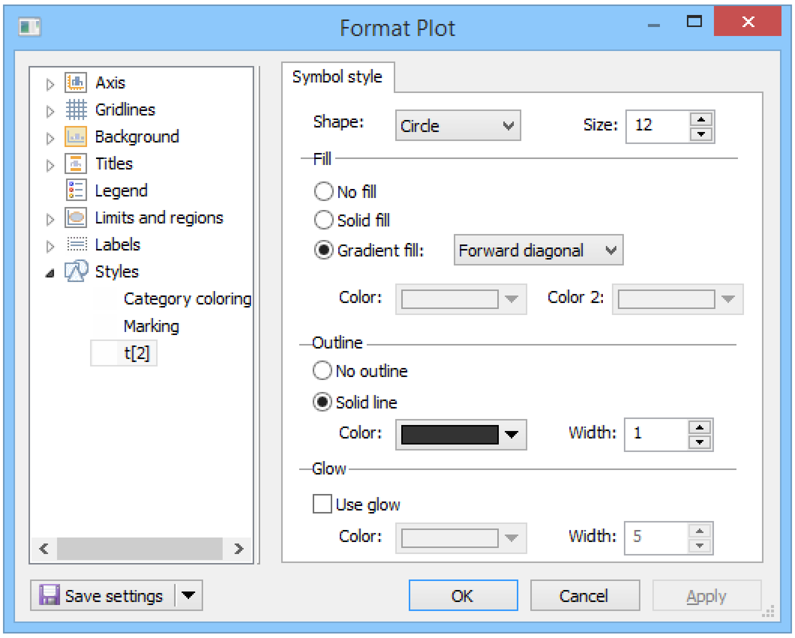
14.3.7.9.3 Symbol style

The **Symbol style** page controls the attributes of the symbols displayed in the plot.

The table describes the available options:

Option/Box/Field	Description
Shape	The shapes of the series can be changed by: 1. Marking a series. 2. Selecting a new shape in the **Shape** box. With *None* selected, no symbols are displayed.
Size	To increase or decrease the size, enter a new number in the **Size** field. After using the **Size by** feature, changing the value in **Size** affects the points proportionally.

Option/Box/Field	Description
	Fill
No fill	Results in symbols transparent inside the outline.
Solid fill	Displays the color selected in **Color**.
Gradient fill	Allows you to select to display the symbol with a gradient fill of type Horizontal, Vertical, Forward diagonal, Backward diagonal, Radial, Horizontal bar, Vertical bar.
Color	Displays the current color. To display another color, click the **Color** box, and then select a new color.
Color 2	Displays the current second color for **Gradient fill** and allows selecting a color.
	Outline
No outline	No outlining contour of the symbols.
Solid line	The outline of the symbol is displayed.
Color	Color of the outline. *Automatic* results in an outline in the same color as the symbol but in a darker shade.
Width	Width of the outline.
	Glow
Use glow	When selected an area outside the outline is colored for a glowing effect.
Color	Color of the glow.
Width	Width of the glow.



Shape: Circle
Size: 12

Fill

○ No fill
○ Solid fill
● Gradient fill: Forward diagonal

Color:
Color 2:

Outline

○ No outline
● Solid line

Color:
Width: 1

Glow

□ Use glow

Color:
Width: 5

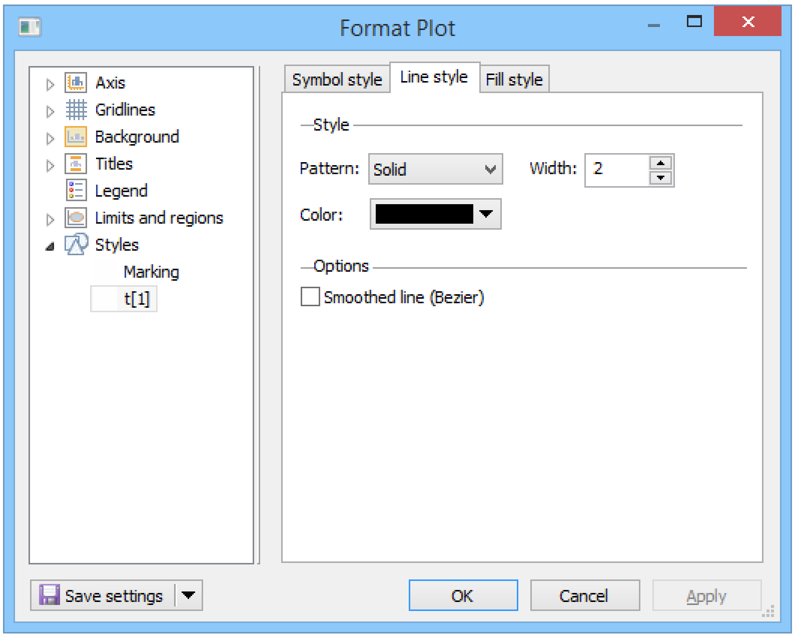
14.3.7.9.4 Line style

The **Line style** page controls the attributes of the lines displayed in the plot.

The table describes the available options:

Option/Box/Field	Description
Pattern	Change the pattern of the line by clicking the **Pattern** box and selecting another pattern. The available types are: *Solid*, *Long dash*, *Dotted*, and *Dash dot*.
Width	To increase or decrease the width, enter a new number in the **Width** field.
Color	To display another color, click the **Color** box, and then select a new color.
Smoothed line (Bezier)	Select **Smoothed line (Bezier)** to smooth out the edges of the line.

Note: Filling is available in the **Fill style** tab. See the Limits and regions subsection for details.



Style

Pattern: Solid Width: 2

Color: ■

Options

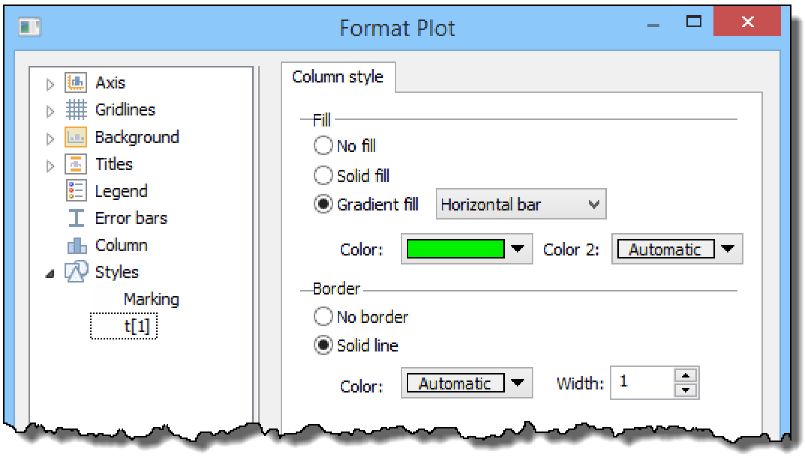
☐ Smoothed line (Bezier)

14.3.7.9.5 Column and Column style

The **Column** and **Column style** pages control the attributes of the columns displayed in the plot.

The **Column** page, found above the **Styles** node, displays the current **Column width** and allows adjusting it.

The **Fill** and **Border** options are described in the Symbol style subsection; **Border** is there named **Outline**.



Fill

○ No fill

○ Solid fill

● Gradient fill Horizontal bar

Color: 🟩 Color 2: Automatic

Border

○ No border

● Solid line

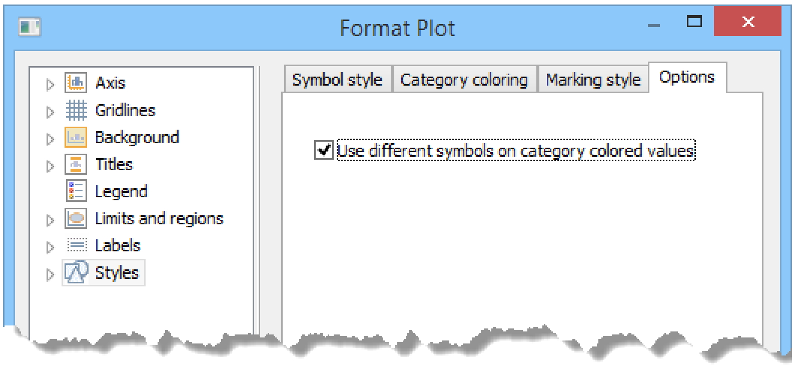
Color: Automatic Width: 1

14.3.7.9.6 Options page in Format Plot

Selecting the **Use different symbols on category colored values** check box will display different symbols for the different colors when coloring a plot.

This also has the effect that each color becomes a series in the **Format Plot** dialog and thus enables the **Symbol style** features.

Note: Symbols for continuous coloring are not affected by this option.



☑ Use different symbols on category colored values

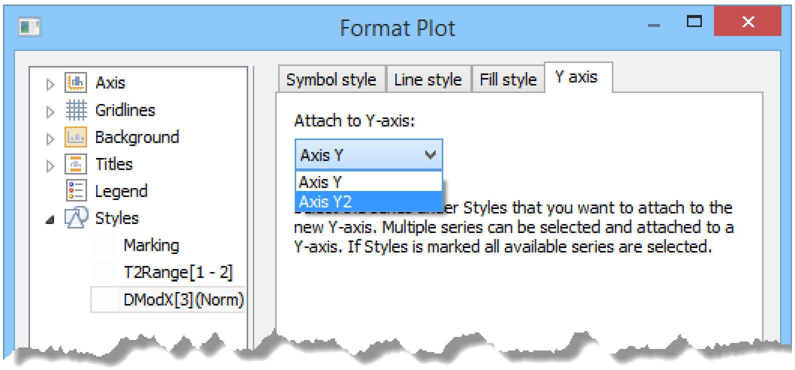
14.3.7.9.7 Multiple Y-axes

When you have more than one series in a plot, you can select to display more than one y-axis and linking it to one of the series.

To display multiple y-axes:

1. Click the **Styles** node and click the series you want on the second y-axis.
2. Click the **Y-axis** tab.
3. In the **Attach to Y-axis** box, select *Axis Y2.*

Steps 1 - 3 can be repeated for more series.



Attach to Y-axis: Axis Y

…er Styles that you want to attach to the new Y-axis. Multiple series can be selected and attached to a Y-axis. If Styles is marked all available series are selected.

14.3.7.10 Contour levels

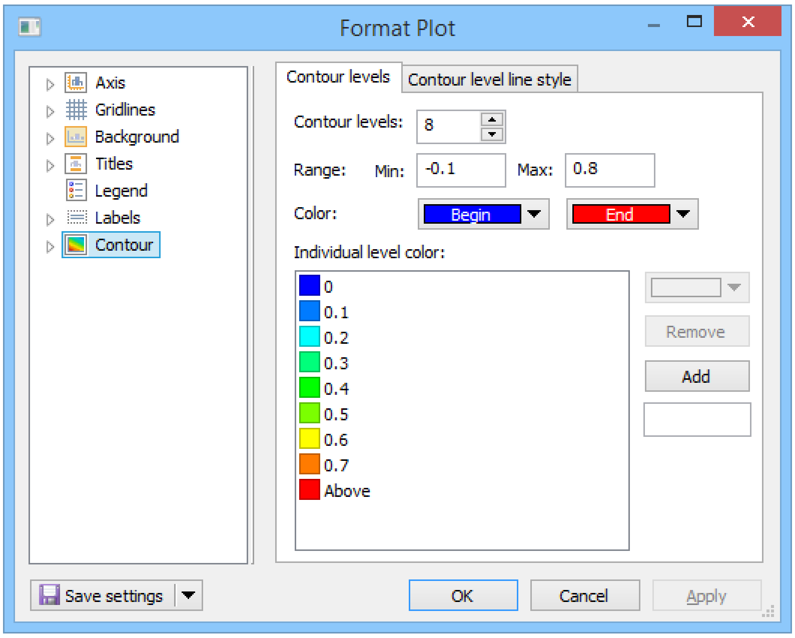
For the **Response contour** and **Response surface** plots the **Contour levels** page is available in **Format Plot**.

In the **Contour levels** page you can:

- Change the number of **Contour levels**.
- Increase/decrease the range by changing the **Min** and **Max** values.
- Change the coloring scheme in the **Begin** and **End color** boxes.
- Change the colors of individual levels by clicking a level and selecting a new color in the color box to the right of the **Individual level color** section.
- Remove a level by marking it and clicking the **Remove** button.
- Add a specific level by typing a value in the field under the **Add**-button and then clicking **Add**.

In the **Contour level line style** page you can:

- Select to not display the contour lines by clearing the **Show lines** check box.
- Change the **Pattern**, **Width** and **Color** of the contour lines by introducing changes in the respective boxes.



Contour levels: 8

Range: Min: -0.1 Max: 0.8

Color: Begin End

Individual level color:

🟦	0
🟦	0.1
🟦	0.2
🟩	0.3
🟩	0.4
🟩	0.5
🟨	0.6
🟧	0.7
🟥	Above

See also the Response contour plot options subsection in Chapter 12, Plot/List.

14.3.7.11 Multi plots

In SIMCA there are two multi plots: **Control charts** and **Wavelet structure**.

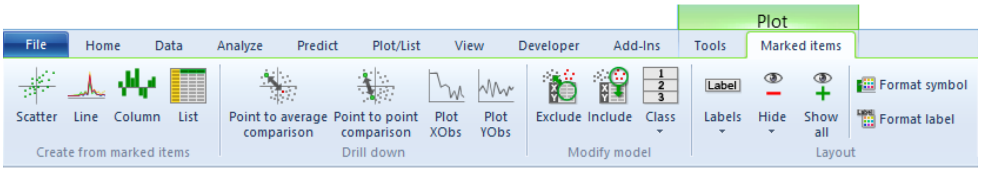
For these two plots there are **Plot** nodes beneath the **Styles** node, named *Plot 1, Plot 2, etc*.

In these plot specific nodes the **Sub title** of the individual plots can be entered but not saved to plot settings.

14.4 Marked items tab

The **Marked items** tab is automatically activated when marking in a plot. The groups available on the **Marked items** tab are:

- Create from marked items
- Drill down
- Modify model
- Layout



14.4.1 Create from marked items group

Display the selected items in another plot type or a list by clicking the desired plot/list icon in the **Create from marked items** group.

The Create from marked items group holds:

- **Scatter** - Creates a scatter plot of the currently selected items.
- **Line** - Creates a line plot of the currently selected items.
- **Column** - Creates a column plot of the currently selected items.
- **List** - Creates a list of the currently selected items. See also the Creating lists subsection in this section.

14.4.1.1 Creating plot from selection

To generate a new plot from marked points in the open plot, list, or spreadsheet:

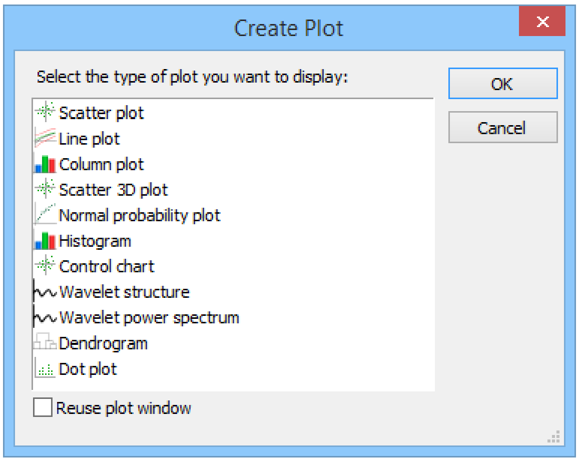
1. Mark
    - the points in a plot or
    - rows or columns in a list or spreadsheet.
2. On the **Marked items** tab, click the desired plot type (**Scatter**, **Line**, **Column**) in the **Create from marked items** group.

14.4.1.2 Creating special plots from selection

Extended functionality of the **Create from marked items** group is available from the shortcut menu and described here.

To generate a new plot from the open plot, list, or spreadsheet:

1. Mark
    - the points in a plot or
    - cells, rows, or columns in a list or spreadsheet.
    - nothing which is the same as marking all.
2. Right-click the plot, list, or selection and then click **Create | Plot**.
3. In the **Create Plot** dialog, click the desired plot type. The plot types available are: **Scatter plot**, **Line plot**, **Column plot**, **Scatter 3D plot**, **Normal probability plot**, **Histogram plot**, **Control chart**, **Wavelet structure**, **Wavelet power spectrum**, and **Dendrogram**.
4. To use the window of the current plot for the new plot, select the **Reuse plot window** check box.
5. Click **OK** to create the plot.



14.4.1.3 Creating list from selection

To generate a new list from marked points in the open plot, list, or spreadsheet:

1. Mark
    - the points in a plot or
    - rows or columns in a list or spreadsheet.
2. On the **Marked items** tab, in the **Create from marked items** group, click **List**.

14.4.1.4 Creating list extended

Extended functionality of the **List** feature is available from the shortcut menu and described here.

To create a list from the open plot, list, or spreadsheet:

1. Mark
    a. the points in a plot or
    b. cells, rows, or columns in a list or spreadsheet or
    c. nothing which is the same as marking all.
2. Right-click the plot, list, or selection and then click **Create | List**.

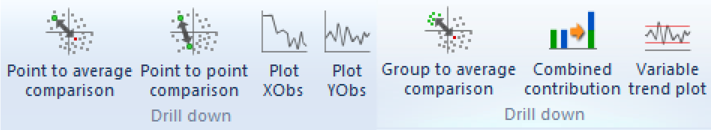
When selecting **Create list** with a dendrogram plot active, a special list is created. For more, see the Create list for the dendrogram subsection in the Tools tab section previously in this chapter.

14.4.2 Drill down group

Create comparison (contribution) plots and observations/variable line plots using the selected items by clicking a button in the **Drill down** group. The plots can also be created by clicking the **Create** command on the shortcut menu.

The possible plots are:

- **Plot XObs** and **Plot YObs** - described in the XObs and YObs line plots subsection in this section.
- **Variable trend plot** - available when a variable is marked in a plot or list, for instance in the loading column plot. For BEM this plot is the Variable BCC for the selected variable.
- **Contribution plot** - available after marking an observation. For more see the Creating plots from plots section in Chapter 14, Plot and list contextual tabs.
- **Combined contribution** - available after marking more than one column in a batch level contribution plot. For more see the Combined contribution plot in batch level models subsection in the Contribution plots section in Chapter 10, Analyze.


Point to average comparison
Point to point comparison
Plot XObs
Plot YObs
Drill down
Group to average comparison
Combined contribution
Variable trend plot
Drill down

14.4.2.1 Creating XObs and YObs line plots from selection

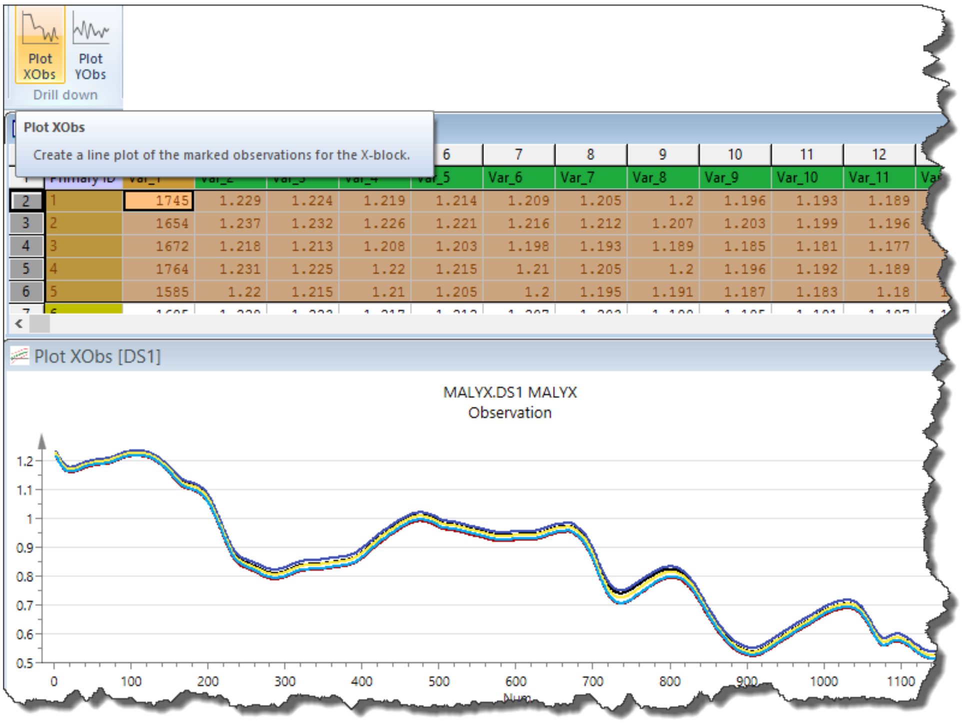
Plot XObs and **Plot YObs** are available from the **Marked items** tab.

To create XObs for the entire spectra, click **Spectra** on the **Data** tab.

To create a line plot of all or a selection of the observations:

1. Mark the observations.
2. Click **Plot XObs** or **Plot YObs** on the **Marked items** tab. **Plot YObs** is only available when there are y-variables defined in the dataset spreadsheet. Define y-variables either at import or by clicking the **Save as default workset** button in the **Workset** dialog, tab **Variables**, after specifying the y-variables.

Note: The first secondary variable ID is by default displayed on the x-axis when it is numerical.



Plot XObs

Create a line plot of the marked observations for the X-block.

						6	7	8	9	10	11	12
1	Primary ID	Var_1	Var_2	Var_3	Var_4	Var_5	Var_6	Var_7	Var_8	Var_9	Var_10	Var_11
2	1	1745	1.229	1.224	1.219	1.214	1.209	1.205	1.2	1.196	1.193	1.189
3	2	1654	1.237	1.232	1.226	1.221	1.216	1.212	1.207	1.203	1.199	1.196
4	3	1672	1.218	1.213	1.208	1.203	1.198	1.193	1.189	1.185	1.181	1.177
5	4	1764	1.231	1.225	1.22	1.215	1.21	1.205	1.2	1.196	1.192	1.189
6	5	1585	1.22	1.215	1.21	1.205	1.2	1.195	1.191	1.187	1.183	1.18

Note: *With spectral data, it is particularly useful to display the* ***XObs*** *plot of all observations.*

For details about coloring the line plot, see also the Color subsection in the Tools tab section earlier in this chapter.

14.4.2.2 Drill down contribution plots

When a time point or batch point deviates from the expected, a contribution plot displays which variables that have contributed to the deviation.

In the table, find a description on how to create the different types of contribution plots using the buttons on the **Marked items** tab.

The marking is done using **Free** from selection when not stated otherwise. Table 1 is valid for regular projects, batch level models, and for batch evolution models when **Batch marking mode** is *NOT* selected. Table 2 is valid when using **Batch marking mode** (only available for batch evolution models).

Table 1. Contribution plots for all types of projects when **Batch Marking Mode** is not the selected tool.

	Plot type	Action
1	One point compared to the average.	Mark a point and click Point to average comparison.
2	One point compared with another point.	Click one time point and then on the other. Click **Point to point comparison**.
3	A group of points compared to the average.	Mark all points in the group by circling them or by holding down the CTRL key and clicking the points. Then click **Group to average comparison**.
4	One point compared to a group of points.	Mark all points in the group by circling them and then click the single time point (without holding down the CTRL key). Click **Group to point comparison**.
5	A group of points compared to another group of points.	Mark all time points in the first group by circling them or by holding down the CTRL key and clicking the time points. Release the CTRL key before starting to mark the next group. Then mark all time points in the second group by circling them or by holding down the **CTRL** key and clicking the points. Click **Group to group comparison**.

Table 2. Contribution plots for batch evolution models when comparing entire batches (**Batch Marking Mode** the selected tool).

	Plot type	Action
1	One batch in a BEM compared to the group average.	1. Select **Batch marking mode** by clicking the **Select** marking tool. 2. Mark a point in the batch and note that all points of that batch are marked 3. Click Group to average comparison.
2	One batch compared with another batch.	1. Select Batch marking mode. 2. Mark a batch, and then mark another batch. 3. Click Group to group comparison.
3	A group of batches compared to the average.	1. Select Batch marking mode. 2. Mark at least one point in each batch by circling them or by holding down the CTRL key and clicking the points. 3. Click Group to group comparison.
4	One batch compared to a group of batches.	1. Select Batch marking mode. 2. Mark at least one point in each batch by circling them or by holding down the CTRL key and clicking the points. 3. Mark the single batch (without holding down the CTRL key). 4. Click Group to group comparison.
5	A group of batches compared to another group of batches.	1. Select Batch marking mode. 2. Mark at least one point in each batch by circling them or by holding down the CTRL key and clicking the points. 3. Release the CTRL key before starting to mark the next group. 4. Mark at least one point in each batch by circling them or by holding down the CTRL key and clicking the points 5. Click Group to group comparison.

For more about contribution plots, see the respective section Contribution plots in Chapter 10, Analyze and section Contribution PS in Chapter 11, Predict.

14.4.2.3 Drill down plots possible

The **Drill down** group becomes available after marking one or more points.

The table lists the different buttons possible in the **Drill down** group, for regular and BLM. For BLM the group can be a batch or a group of batches.

	Marked points in regular projects	Buttons available after marking
1	One or more observations in for instance a score plot. 1. One observation marked.	1. **Point to average comparison** – when clicked it displays the observation vs. average contribution plot, where the average is over all observations in the workset.
	2. A group of observations marked.	2. **Group to average comparison** – when clicked it displays the group vs. average contribution plot.
	3. One observation first marked and then a group.	3. **Point to group comparison** – when clicked it displays the observation vs. group contribution plot.
	4. A group first marked and then another group.	4. **Group to group comparison** – when clicked it displays the group vs. group contribution plot.
2	The above but for predicted observations (using the predictionset).	The above but for the predictionset.
3	One or more variables in any plot, for instance in a loading or a contribution plot.	**Variable trend plot** - when clicked displays a variable plot with one or more series.
4	One or more observations in any plot.	**Plot XObs** - when clicked displays a plot with one or more observation series.

Additionally, there is a number of drill down plots possible for batch evolution models after marking. These are listed in the table below. This table also lists a couple of special drill down plots created from BLM.

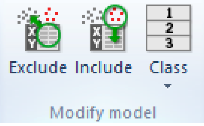
	Marked points in BEM/BLM	Buttons available after marking
1	BEM. With the **Batch marking mode** selected, one or more batches in for instance a score BCC. 1. One batch marked.	1. **Point to average comparison** – when clicked it displays the observation vs. average contribution plot, where the average is the average batch.
	2. A group of batches marked.	2. **Group to average comparison** – when clicked it displays the group vs. average contribution plot.
	3. One batch first marked and then a group.	3. **Point to group comparison** – when clicked it displays the observation vs. group contribution plot.
	4. A group of batches first marked and then another group.	4. **Group to group comparison** – when clicked it displays the group vs. group contribution plot.
2	Time points in BEM (marked with the **Batch marking mode** not selected). 1. One observation marked.	1. Point to average comparison
	2. A group of observations marked.	2. Group to average comparison
	3. An observation first marked and then a group.	3. Point to group comparison
	4. A group first marked and then another group.	4. Group to group comparison
3	A variable in a plot from a BEM.	**Variable trend plot** - displays a variable plot with control limits. This plot cannot display more than one variable at a time.
4	A point in a BLM score plot for a model built on score or raw variables.	**Point to average comparison** - displays a sources of variation contribution plot.
5	A score (t) contribution column in a BLM.	**Point to average comparison** - A BEM combined squared score contribution plot.
6	More than one score (t) contribution column in a BLM.	**Combined contribution** – displays a combined contribution plot.

14.4.3 Modify model

In the **Modify model** group, features that modify the unfitted model, or create a new unfitted modified model, are available.

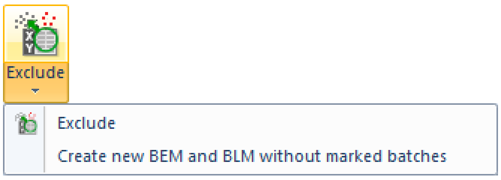
The available features are described in this section and are listed here:

- **Exclude** - described in the Excluding marked items subsection in this chapter.
- **Include** - described in the Including marked items subsection in this chapter.
- **Class** - described in the Assigning observations to classes subsection in this chapter.
- **Class | Create PLS-DA model/OPLS-DA model** - described in the Creating a PLS-DA or OPLS-DA model from plot marking subsection in this chapter.
- **Class | Create class models** - described in the Creating class models from plot marking subsection in this chapter.



14.4.3.1 Excluding marked items

Exclude observations, variables, expanded terms, lags, and batches, using the **Exclude** tool in the **Modify model** group on the **Marked items** tab.



14.4.3.1.1 Excluding observations or variables

To exclude observations, variables, expanded terms, or lags:

1. Open a plot, scores, loadings, VIP, etc.
2. Mark the items to exclude.
3. Click **Exclude**.
4. SIMCA builds a new workset, with the selected items excluded. The new unfitted model becomes the active model.
5. Repeat this operation as many times as needed; all exclusions are done in the unfitted model.

Note: *The variables or observations are removed only from the new workset and not from any of the plots.*

For how to exclude items using the **Variable**, **Observation**, or **Marked items** pane, see the Show section in Chapter 13, View.

14.4.3.1.2 Excluding batches in the batch evolution model

To exclude batches in a BEM:

1. Open a plot displaying the batch.
2. On the **Tools** tab, in the **Plot tools** group, click **Select | Batch marking mode**.
3. Click a point in the batch and note that all points in that batch are marked.
4. Click **Exclude**.

14.4.3.1.3 Excluding batches in batch level model creating new batch evolution model and batch level dataset

When marking batches in the BLM, clicking the arrow under the **Exclude** tool displays the options:

1. **Exclude** (default) and
2. **Create new BEM and BLM without marked batches**.

Selecting the second choice leads to the following:

1. SIMCA creates and fits a new BEM after excluding the marked batches.
2. SIMCA creates a new batch level dataset and a new BLM with the same batch condition datasets as before and the new reduced batch level datasets.

Note: None of the settings of the old BLM are applied to this new BLM. This means that any scaling, transformation, y-variables, excluded variables etc. must be specified.

This is very useful when outliers are found in the batch level model, and one needs to rebuild the BEM and BLM without the outlying batches.

14.4.3.1.4 Excluding in predictionsets

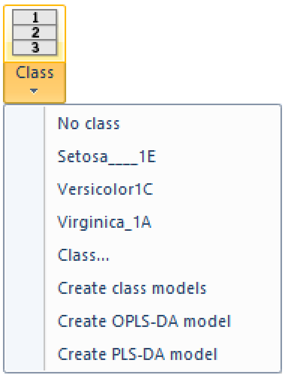
When the displayed observations are those of a predictionset, marking and excluding them excludes the observations from the predictionset.

14.4.3.2 Including marked items

Clicking **Include** creates a new model including only the marked items when there is no unfitted model. When there is an unfitted model, **Include** adds the marked items to the unfitted model.

14.4.3.3 Creating class or DA-model from selection

Create class models, **Create OPLS-DA model** and **Create PLS-DA model** are available when two (or more groups) are marked in any plot displaying observations. If only one class is marked, **Class** is available.



To assign observations to classes:

1. Mark the observations in a plot or list.
2. Click **Class**, either the button or the arrow, and select the class name or number if listed, or click **Class** and enter a new class name or number in the dialog.
3. Repeat this operation until you have selected all the observations you want in classes.
4. When you are done editing the active model, verify the model type, mark the CM and click **Autofit**.

To create class or DA-models:

1. Mark two groups of observations in a plot.
2. Click the **Class** arrow, and click **Create class models, Create OPLS-DA model** or **Create PLS-DA model**.
3. Click **Autofit** to fit the model.

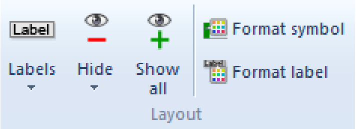
Note: All unassigned observations are excluded.

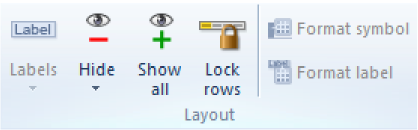
To create class models or a DA-model from a dendrogram plot:

1. Mark in the dendrogram plot so that the desired groups are displayed in different colors.
2. On the **Marked items** tab, click **Class | Create class models** or **Create OPLS-DA model** or **Create PLS-DA model**.

14.4.4 Layout group

The presentation of marked items in a plot can be manipulated by changing the label type, changing the formatting, etc. available from the **Layout** group on the **Marked items** tab. In this group you can also select to lock rows or columns of a list.



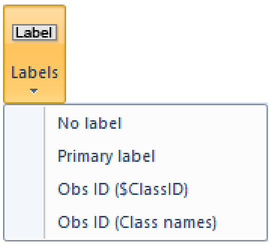


14.4.4.1 Changing/adding labels

With a large numbers of variables or observations in a plot it is useful to be able to have labels on selected items only.

1. Mark interesting points in the plot.
2. Click the **Labels** arrow on the **Marked items** tab and select the desired label type. All available labels are listed.

Note: If you want only labels on some items and there are labels on all items in the plot, remove them by clicking **Labels | No labels** on the **Tools** tab first and then use step 1 and 2.



14.4.4.2 Hiding marked/unmarked items

To hide the marked items, without removing them from the model, click **Hide**.

To hide the unmarked items, without removing them from the model, click **Hide | Hide unmarked items**.

To show hidden items, click the **Show all** button.

The above can also be done from the **Properties** dialog in the **Item selection** tab where hidden items also can be selected to be displayed again.

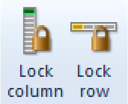
14.4.4.3 Locking rows or columns

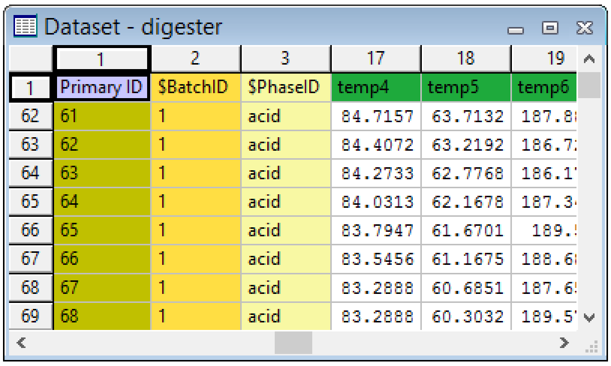
Locking rows and columns is available for all lists and spreadsheets when an entire row or column is marked in the spreadsheet. When locking rows or columns those rows or columns, and all to the left or above, are always displayed when scrolling the list.

To lock rows or columns:

1. Mark the columns or rows to lock in the list or spreadsheet by clicking the column or row number.
2. On the **Marked items** tab click **Lock columns/Lock rows**.

The locked rows or columns are displayed when scrolling to the right or down, see the example here.



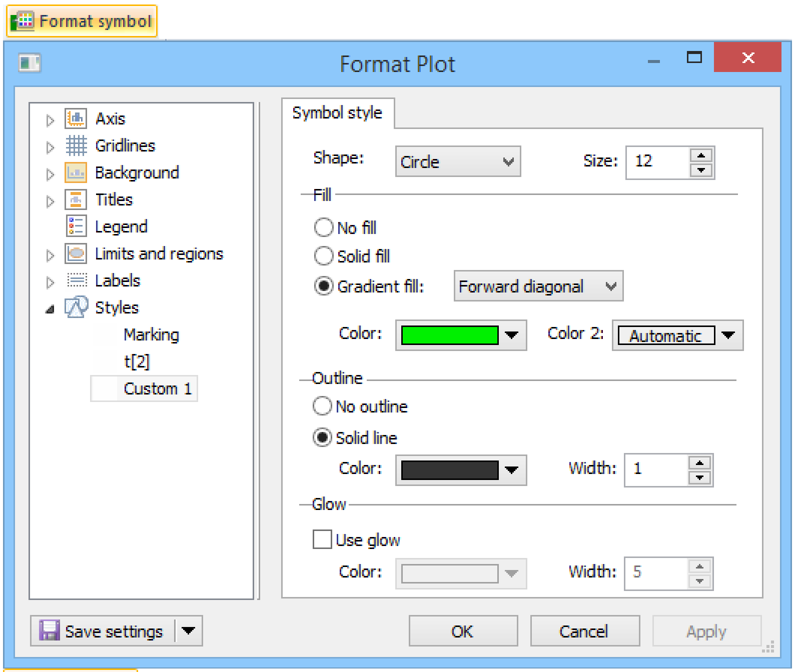


	1	2	3	17	18	19
1	Primary ID	$BatchID	$PhaseID	temp4	temp5	temp6
62	61	1	acid	84.7157	63.7132	187.8
63	62	1	acid	84.4072	63.2192	186.7
64	63	1	acid	84.2733	62.7768	186.1
65	64	1	acid	84.0313	62.1678	187.3
66	65	1	acid	83.7947	61.6701	189.
67	66	1	acid	83.5456	61.1675	188.6
68	67	1	acid	83.2888	60.6851	187.6
69	68	1	acid	83.2888	60.3032	189.5

14.4.4.4 Marked Values - changing attributes of selected items in a plot

To change the fonts, symbols, size, etc., of only the marked points in a plot, click **Format symbol** and **Format label** respectively in the **Layout** group on the **Marked items** tab. The **Format Plot** dialog is automatically opened with *Custom* under **Styles** or *Custom label* under **Labels** default selected.

Changing the properties of the *custom* series will only apply to the marked items. See also the Mini-toolbar - format plot section earlier in this chapter.



Shape: Circle Size: 12

Fill

○ No fill

○ Solid fill

● Gradient fill: Forward diagonal

Color: 🟩 Color 2: Automatic

Outline

○ No outline

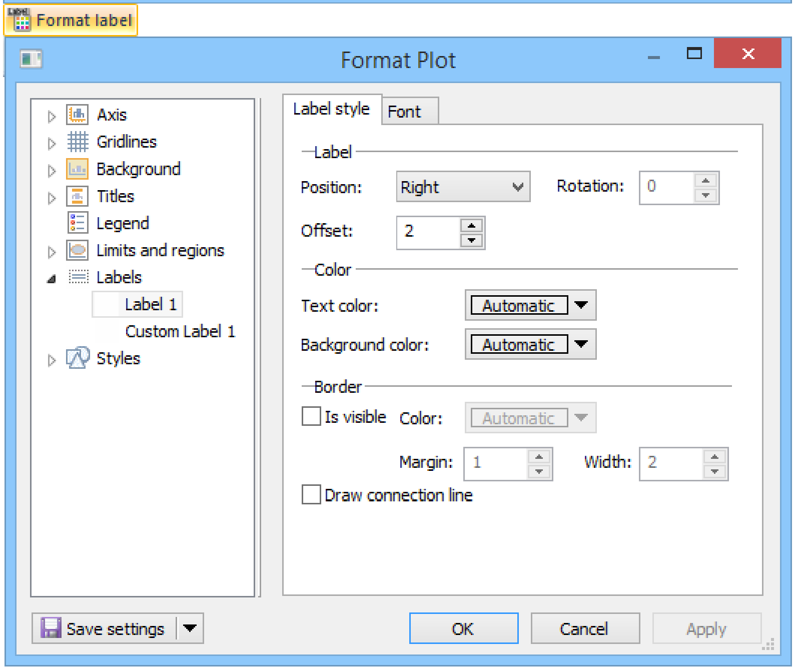
● Solid line

Color: ■ Width: 1

Glow

□ Use glow

Color: Width: 5



Label

Position: Right Rotation: 0

Offset: 2

Color

Text color: Automatic

Background color: Automatic

Border

□ Is visible Color: Automatic

Margin: 1 Width: 2

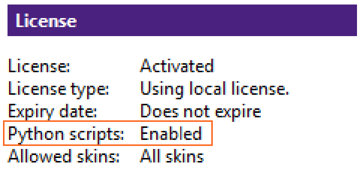
□ Draw connection line

15 Scripting

15.1 Python scripting in SIMCA

For up-to-date scripting information, see http://umetrics.com/products/scripting.

In SIMCA you can automate/facilitate tasks using Python scripts. In order to use Python scripts you must have a license that allows it. Click File | Help to see your license information.



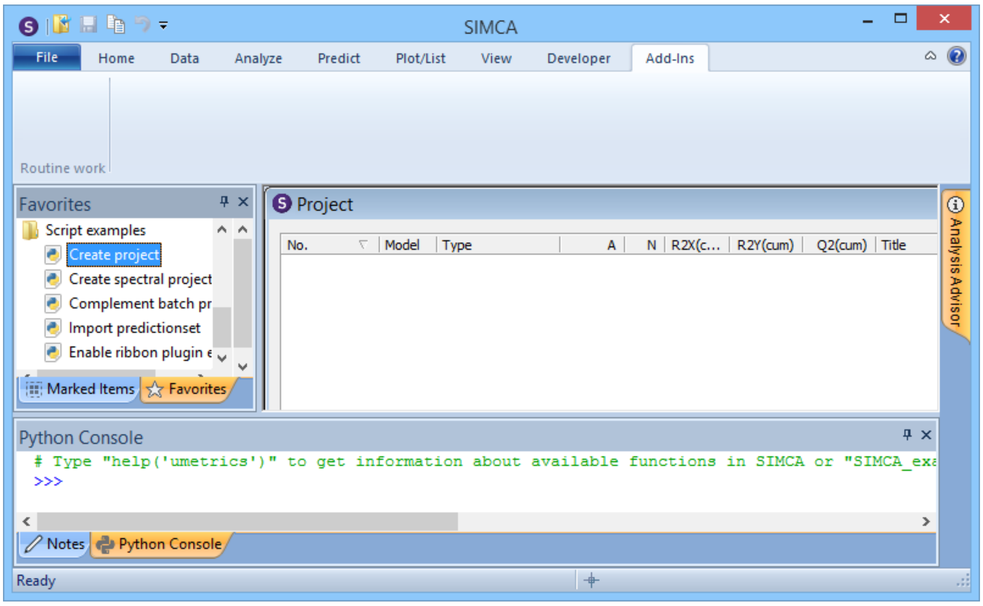
License

License:	Activated
License type:	Using local license.
Expiry date:	Does not expire
Python scripts:	Enabled
Allowed skins:	All skins

Much of the functionality relating to Python can be accessed from the **Developer** tab; see the Developer tab subsection next.

The Python interpreter is embedded in SIMCA and is accessible through the Python Console, script favorites and **Add-Ins** tab.

The descriptions that follow assume that you have some experience with Python. If you have little or no experience with Python we recommend that you follow one of the tutorials in found at http://umetrics.com/products/scripting.



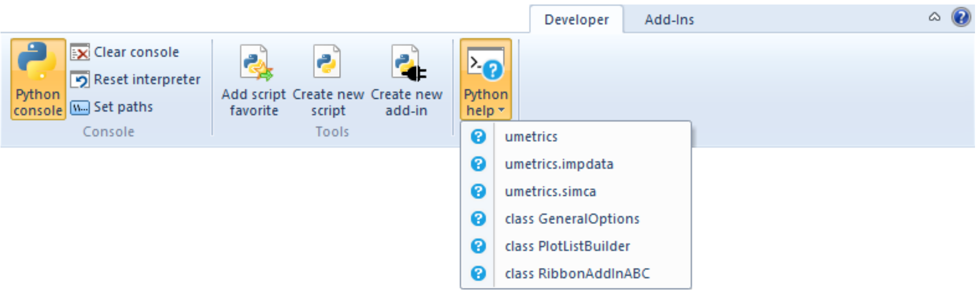
```
# Type "help('umetrics')" to get information about available functions in SIMCA or "SIMCA_exa
>>>
```

15.2 Developer tab

On the **Developer** tab you can;

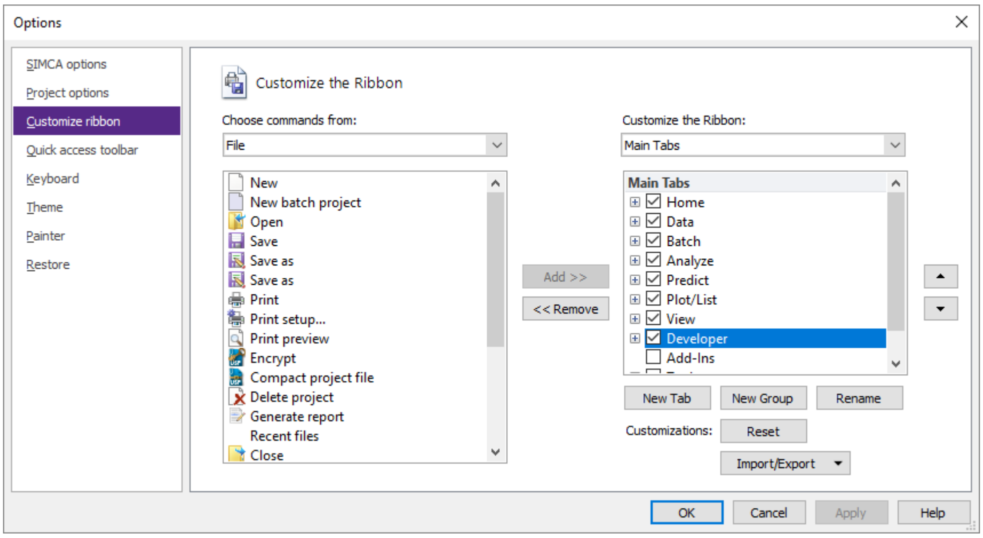
- Open the **Python console -** Opens as a pane at the bottom of the screen, see the Python console subsection next.
- **Clear console -** empties the contents of the pane.
- **Reset interpreter** - restores all environment variables and imports.
- **Set paths** - specify more/less directories that SIMCA searches for scripts to add to the Add-Ins tab.
- **Add script favorite** - Add a script to the Favorites pane.
- **Create new script** - Creates a new .py file with the necessary boiler plate code.
- **Create new add-in** - Creates a new .py file with the necessary boiler plate code. Add-ins are automatically available as buttons on the Add-ins tab.

- **Python help** - Opens the respective help file;
  - **umetrics** - general help.
  - **umetrics.impdata** - import of data.
  - **umetrics.simca** - SIMCA specific help.
  - **class GeneralOptions** - info about how to handle the available SIMCA options.
  - **class - PlotListBuilder** - how to create plots and lists.
  - **class RibbonAddInABC** - handling the Add-In tab.
  - **Browse the documentation for Python scripting** - opens the Umetrics scripting portal.



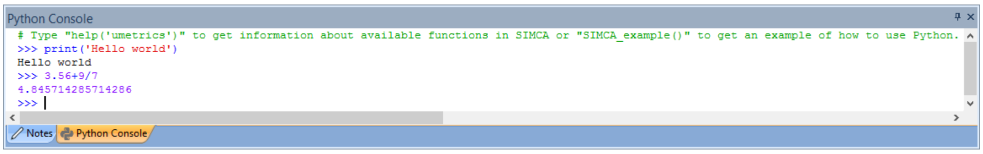
15.3 Open the Developer tab

If your license allows scripting but you cannot see the Developer tab, click **File | Options | Customize** and in the Customize the Ribbon list, select the **Developer** check box.



15.4 Python console

The console fills much the same function as the Python interactive interpreter and IDLE. Python commands can be executed directly in the console:



```
# Type "help('umetrics')" to get information about available functions in SIMCA or "SIMCA_example()" to get an example of how to use Python.
>>> print('Hello world')
Hello world
>>> 3.56+9/7
4.845714285714286
>>> |
```

Output from script favorites and add-ins will also be printed in the console.

15.5 Creating and accessing scripts

The easiest way to create a script is to click **Create new script** on the **Developer** tab. This will create a new .py file with the necessary boiler plate code.

After writing your scripts you can make them accessible in SIMCA in the Favorites pane but not on the Add-Ins tab.

To create a script accessible on the Add-Ins tab, click **Create new add-in**.

15.5.1 Script favorites

Python scripts can be added to the Favorites pane, either by dropping .py files in the pane or by right clicking and selecting **Add script favorites** and browsing for them.

When you click a script favorite, the script is executed.

15.5.2 Add-Ins

To create an add-in, click **Create new add-in** on the **Developer** tab. A new .py file is then created with the necessary boiler plate code.

Add-ins are more complex to write than scripts created using **Create new script** but gives you better control of how they look and behave.

Add-Ins are automatically added if the script file is located in one of the directories that Python searches for modules and contains both the on_command and get_button_name functions.

Directories to search in can be added or deleted by clicking **Set paths** on the **Developer** tab.

15.6 SIMCA functionality available in Python

For up-to-date scripting information, see http://umetrics.com/products/scripting.

SIMCA exposes functionality to Python that allows scripts to create projects and datasets, create new models, read supported data files, use spectral filters, select predictionsets and create plots and lists.

This functionality is exposed through a package called *umetrics* that can be imported in the usual way. The *umetrics* package in turn contains other packages, classes and methods as illustrated in the graph here.

The umetrics package is built into SIMCA and can only be used by scripts running inside SIMCA. There is no Python source code available since it is in fact written in C++.

16Statistical appendix

16.1 Introduction

This chapter contains brief background information and formulas for SIMCA. For more extensive reading, use the reference material.

The topics covered are:

- PCA - Principal Components modeling
- PLS - Partial Least Squares Projection to Latent Structures modeling
- OPLS/O2PLS - Orthogonal PLS modeling
- Cluster Analysis (CA), dendrograms, Hierarchical CA (HCA), PLS including Hierarchical Cluster Analysis - HCA and PLS-Trees
- Vectors available in SIMCA
- Formulas and descriptions
- Transform page criteria
- Scaling
- Cross validation
- PLS Time Series Analysis
- CV-ANOVA
- ROC background
- Fisher's Exact test
- Control Chart statistics
- S-plot

16.2 Fit methods background

A dataset is composed of N rows and K columns. The N rows are here called observations and the K columns are called variables.

Geometrically we can represent the observations as points in a multidimensional space where the variables define the axes. The lengths of the axes are determined by the scaling of the variables.

To calculate a model that approximates the dataset the following fit methods are available in SIMCA:

- Principal Components modeling - PC modeling.
- Partial Least Squares Projection to Latent Structures modeling - PLS modeling.
- Orthogonal PLS - OPLS and O2PLS modeling.

All other fit methods, available by clicking **Change model type** use one of the fit methods above, see the Model types available subsection in Chapter 7, Home.

16.2.1 PCA - Principal Components modeling

Principal Component Analysis is the technique for finding a transformation that transforms an original set of correlated variables to a new set of uncorrelated variables, called principal components. The components are obtained in order of decreasing importance, the aim being to reduce the dimensionally of the data.

The analysis can also be seen as an attempt to uncover approximate linear dependencies among variables.

PC modeling shows the correlation structure of your data matrix X, approximating it by a matrix product of lower dimension (**TP'**), called the principal components plus a matrix of residuals (**E**).

X = Xbar + TP' + E

where

Xbar contains X average.

T is a matrix of scores that summarizes the X-variables.

P is a matrix of loadings showing the influence of the variables.

E is a matrix of residuals; the deviations between the original values and the projections.

This geometrically corresponds to fitting a line, plane or hyper plane to the data in the multidimensional space with the variables as axes. The scaling of the variables specifies the length of the axes of this space. For more about scaling see the Scaling section later in this chapter.

SIMCA iteratively computes one principal component at a time, comprising a score vector $\mathbf{t_a}$ and a loading vector $\mathbf{p_a}$.

16.2.1.1 Number of model dimensions (A)

To get an overview of the dataset, a few (2 or 3) principal components are often sufficient.

However, if the PC model is used for modeling or for other predictions (e.g. principal properties), cross validation (CV) should be used for testing the significance of the principal components. In this way, the "significant" number of PC components, A, is obtained, which is essential in modeling.

It is also possible to use the eigenvalue limit (EV) for testing component significance by clearing the **Use cross validation when fitting** check box in **Model Options**, tab **Model**.

Eigenvalue limit (EV): A component is considered significant if its normalized eigenvalue is larger than 2.

Cross validation (CV) is described in the Cross validation section later in this chapter.

16.2.1.2 Reference PCA

1. Jackson, J.E. (1991), *A User's Guide to Principal Components*, John Wiley, New York. ISBN 0-471-62267-2.

16.2.2 PLS - Partial Least Squares Projection to Latent Structures modeling

When fitting a Partial Least Squares Projection to Latent Structures model, PLS finds the ***linear (or polynomial) relationship between*** a matrix Y (dependent variables) and a matrix X (predictor variables) expressed as:

Y = f(X) + E

The matrix X refers to the predictor variables and their squared and/or cross terms if these have been added. Active X variables or expansions participating in the model are sometimes referred to as **terms**. The function f(X) is usually a polynomial, possibly in the transformed variables.

Note: Cross terms should be added to the linear terms in X **only** when the data supports such terms, for instance after using a design to generate X.

PLS is most easily understood geometrically, where we see the matrices X and Y as **N** points in two spaces, the X-space with **K** axes, and the Y-space with **M** axes, **K** and **M** being the number of columns in X and Y.

PLS modeling consists of simultaneous projections of both the X and Y spaces on low dimensional hyper planes. The coordinates of the points on these hyper planes constitute the elements of the matrices T and U. The analysis has the following **objectives:**

- To well approximate the X and Y spaces
- To maximize the correlation between X and Y

The PLS model accomplishing these objectives can be expressed as:

X = Xbar + TP' + E

Y = Ybar + UC' + F

U = T + H (the inner relation)

where

Xbar contains X average.

Ybar contains Y average.

Note that the coefficients of the inner relation are 1.

In the PLS algorithm there are additional loadings, W, called weights. These express the correlation between U and X and are used to calculate T.

This modeling geometrically corresponds to fitting a line, plane or hyper plane to both the X and Y data represented as points in a multidimensional space, with the objective of well approximating the original data tables X and Y, and ***maximizing the covariance*** between the observation positions on the hyper planes.

SIMCA will iteratively compute one PLS component at a time, that is: one vector each of X-scores t, Y-scores u, weights w and c, and loadings p.

The PLS components are calculated in descending order of importance.

Vector	Description
T	Matrix of scores that summarizes the X variables.
P	Matrix of loadings showing the influence of the variables.
W	Matrix of weights expressing the correlation between X and U (Y).
U	Matrix of scores that summarizes the Y variables.
C	Matrix of weights expressing the correlation between Y and T (X).
E, F, H	Matrices of residuals.

16.2.2.1 Number of model dimensions (A)

The criterion used to determine the model dimensionality, (number of significant PLS components), is cross validation (CV). With CV, observations are kept out of the model development, then the response values (Y) for the kept out observations are predicted by the model, and compared with the actual values.

This procedure is repeated several times until every observation has been kept out once and only once.

16.2.2.2 Reference PLS

Wold, S., Sjöström, M., and Eriksson, L., (2001b), *PLS-Regression: A Basic Tool of Chemometrics*, Journal of Chemometrics, 58, 109-130.

16.2.3 OPLS/O2PLS - Orthogonal PLS modeling

16.2.3.1 OPLS - Orthogonal PLS modeling

A simple way to understand OPLS is to consider how PLS and OPLS differ in their handling of the variance of the X-matrix. PLS divides the variability in X in two parts (figure below), i.e., the systematic and residual parts. The systematic part is the sum of the variability in X that is correlated (predictive) to Y and the variability in X that is uncorrelated (orthogonal) to Y. Thus, whereas PLS divides the sum of squares of X in two parts, OPLS divides it in three parts. This yields good predictions and improved interpretability.

It should be noted that in the single-Y case, by theory, the OPLS model can only have one predictive component [Trygg and Wold, 2002]. Should a single-Y OPLS model comprise more than one component, all components beyond the first one reflect orthogonal variation. However, with multiple Y-variables there can be more than one predictive OPLS component.

For the single-y case only OPLS is available in SIMCA. The results from OPLS/O2PLS in SIMCA-P+ 12 are identical to the results using OPLS in SIMCA 13 and later.

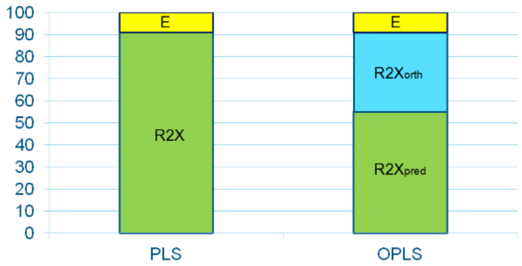


Figure: PLS (left) divides the variability in the X-matrix in two parts, the systematic variability and the residual variability. OPLS (right) further splits the systematic variability, R2X, in two parts, the part that is correlated (predictive) to Y and the part that is uncorrelated (orthogonal) to Y.

In the case of a single response variable, we can write the X-part of the OPLS model as

$X = 1x' + tp' + T_oP_o' + E$

and the OPLS model prediction of y as

$y = y' + tq' + f$

The multi-Y OPLS model can be expressed as follows:

$X = 1x' + TP' + T_oP_o' + E$

and the OPLS model prediction of Y as

$Y = 1y' + TQ' + F$

Where the matrix products TP' and TQ' hold the joint X/Y information overlap. The number of score vectors (in T and U) and loading vectors (in P' and Q') is determined using cross-validation.

Thus, in comparison with the single-y OPLS model, the main difference lies in the fact that there can be more than one predictive component in the multi-y OPLS model. The number of predictive components is regulated by the number of latent variables in the information overlap between X and Y, which in turn often is linked to the rank of Y.

16.2.3.2 O2PLS - Orthogonal PLS modeling

The O2PLS model can be written as follows:

$X = 1x' + TP' + ToPo' + E$

$Y = 1y' + UQ' + UoQo' + F$

Where the matrix products TP' and UQ' hold the joint X/Y information overlap. The number of score vectors (in T and U) and loading vectors (in P' and Q') is determined using cross-validation. In the example in the Model Window for OPLS and O2PLS models subsection in Chapter 13, View, there are seven components of this type (predictive components).

The number of components in the respective set of components is determined using cross validation.

For any part of the OPLS/O2PLS model, the percentages explained and predicted variances can be obtained from plots and lists in the software.

For more about the differences between OPLS/O2PLS and PLS, see the Conventional PLS compared with OPLS and O2PLS subsection.

16.2.3.3 Conventional PLS compared with OPLS and O2PLS

16.2.3.3.1 PLS

Conventional PLS applies to the two-block (X/Y) regression problem. It uses X to construct a model of Y, where the objective is to predict the latter from the former for new samples in the predictionset. In that sense, PLS is unidirectional, i.e., X → Y, but not vice versa.

When X is composed of e.g. spectroscopic data, process readings or measurements from bio-analytical platforms, there is a risk that systematic variation may reside in X which is not linearly correlated with Y. Such variability in X is usually called

Orthogonal in X [1]. Although the Orthogonal in X variation can be handled by a PLS model, it often makes model interpretation more difficult [2].

16.2.3.3.2 OPLS

The OPLS method is a recent modification of the PLS method [1-3], which is designed to handle variation in X that is orthogonal to Y. OPLS separates the systematic variation in X into two parts, one that is linearly related (and therefore predictive) to Y and one that is orthogonal to Y. The predictive variation of Y in X is modeled by the predictive components. The variation in X which is orthogonal to Y is modeled by the orthogonal components. This partitioning of the X-data provides improved model transparency and interpretability, and gives very similar predictive power. For OPLS with one Y the predictive model with the same number of components is identical to the same PLS model. Similarly to PLS, OPLS is a unidirectional method, where the scope is the relation X → Y.

16.2.3.3.3 O2PLS

O2PLS is a generalization of OPLS [4,5]. In contrast to PLS and OPLS, O2PLS is bidirectional, i.e. X ↔ Y. Additionally, with O2PLS it is possible to partition the systematic variability in X and Y into three parts, (i) the X/Y joint predictive variation, (ii) the variation in X orthogonal to Y (X-unique Variation), and (iii) the X-unrelated variation in Y (Y-unique Variation). The variation in X orthogonal to Y can be further divided into two parts; one part which is equivalent to the component in OPLS (*Orthogonal in X (OPLS)*) is a matrix effect that needs to be modeled to achieve the best possible prediction and interpretation. The second part (*Orthogonal in X (PCA)*) consists of structured variation that does not affect the prediction but can be interesting to study to further improve the interpretation of complex multivariate data. The X-unrelated variation in Y may be modeled in a similar way.

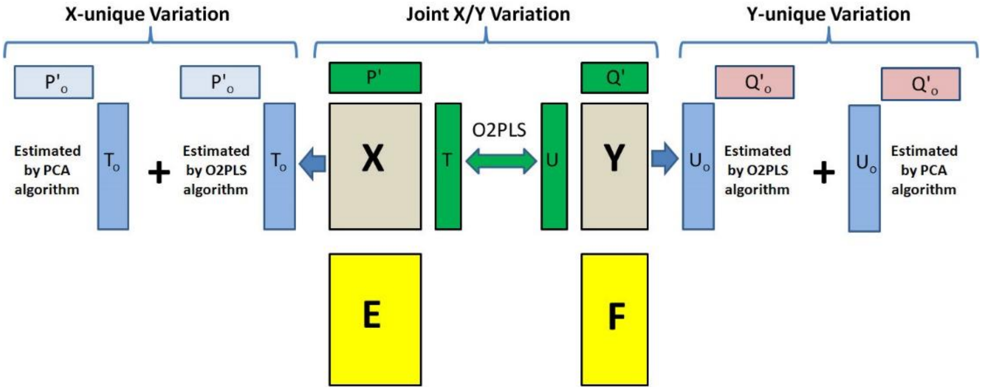

X-unique Variation
Joint X/Y Variation
Y-unique Variation
P'o
P'o
P'
Q'
Q'o
Q'o
Estimated by PCA algorithm
To
+
Estimated by O2PLS algorithm
To
X
T
O2PLS
U
Y
Uo
Estimated by O2PLS algorithm
+
Uo
Estimated by PCA algorithm
E
F

Figure 1. Overview of the O2PLS model relating two data tables to each other. Unique variation in X also named variation in X orthogonal to Y in the left-hand side of the Figure. The X/Y joint predictive variation (middle part of the Figure) describes the predictive variation between X and Y, the information overlap. The Unique variation in Y also named variation Orthogonal in Y in the right-hand side of the figure.

The ability to interpret the X/Y joint predictive variation separated from the non-correlated variation implies that the model interpretation is refined and simplified. Furthermore, it should be noted that for the single-y case the OPLS and O2PLS methods are identical. For such a model there can only be one predictive component expressing the joint X/Y predictive variation [4,5].

16.2.3.4 Combination with the hierarchical approach

Because of its ability to divide the information in X and Y into different parts, the O2PLS model is ideally suited for combining with the hierarchical modeling approach. This is of interest when working with multi-block process data and spectroscopic data [6,7]. The flexible structure of the O2PLS method also allows setting it up as a filter for peeling off any undesired systematic variability in your data.

16.2.3.5 Y-related profiles

The Y-related profiles are coefficients rotated displaying the pure profiles of the underlying constituents in X using the assumption of additive Y-variables.

The estimation includes a linear transformation of the coefficient matrix, $Bp(Bp^{T}Bp)^{-1}$, using only the predictive components to compute the coefficients (i.e., the components orthogonal to Y are not included in the computation of the Y-related profile).

16.2.3.6 References OPLS and O2PLS

1. Trygg, J., and Wold, S., (2002), *Orthogonal Projections to Latent Structures (OPLS)*, Journal of Chemometrics, 16, 119-128.
2. Trygg, J., (2004), *Prediction and Spectral Profile Estimation in Multivariate Calibration*, Journal of Chemometrics, 18, 166-172.
3. Eriksson, L., Johansson, E., Kettaneh-Wold, N., Trygg, J., Wikström, M., and Wold, S., Multi- and Megavariate Data Analysis, Part II, Method Extensions and Advanced Applications, Chapter 23, Umetrics Academy, 2005.
4. Trygg, J., (2002), *O2-PLS for Qualitative and Quantitative Analysis in Multivariate Calibration*, Journal of Chemometrics, 16, 283-293.
5. Trygg, J., and Wold, S., (2003), *O2-PLS, a Two-Block (X-Y) Latent Variable Regression (LVR) Method With an Integral OSC Filter*, Journal of Chemometrics, 17, 53-64.
6. Gabrielsson, J., Jonsson, H., Airiau, C., Schmidt, B., Escott, R., and Trygg, J., (2006), *The OPLS methodology for analysis of multi-block batch process data,* Journal of Chemometrics, 20, 362-369.
7. Eriksson, L., Dyrby, M., Trygg, J., and Wold, S., (2006), *Separating Y-predictive and Y-orthogonal variation in multi-block spectral data*, Journal of Chemometrics, 20, 352-361.
8. Galindo-Prieto, B., Eriksson, L., Trygg, J., Variable influence on projection (VIP) for orthogonal projections to latent structures (OPLS), Journal of Chemometrics, 28 (2014) 623-632.

16.3 Cluster Analysis (CA), dendrograms, Hierarchical CA (HCA), PLS-Tree

Large datasets are often clustered, grouped, and relationships between variables are often different in different groups (clusters). Cluster analysis tries to find a natural grouping (clustering) of a data set so that there is less variation (greater similarity) within the clusters, and more variation (less similarity) between the clusters. The difference between on the one hand CA, and on the other hand classification and discriminant analysis (CDA) is that in the latter the classes are *pre-defined* by the user, and each observation in the workset belongs to one of these classes. CA has no predefined classes, but after the analysis a set of clusters has been "found", and each observation belongs to one of these. In HCA and PT the "fineness" of the solution, i.e., number of clusters and the observation assignment, can be modified by moving the cursor up and down in the ***dendrogram*** (tree diagram).

CA is particularly useful in the analysis of large data sets, often called "Data Mining". The resulting groups, clusters, can lead to the generation of new ideas – exploratory data analysis – and often better models for parts of the data.

SIMCA has two approaches of hierarchical clustering.

1. HCA = hierarchical clustering, available on the **Analyze** tab, in the **Clustering** group, by clicking **HCA**, and
2. PT = PLS-Trees which is a new PLS-based clustering method developed by Sartorius Stedim Data Analytics (PLS-TREE™), available on the **Analyze** tab, in the **Clustering** group, by clicking **PLS-Tree**.

Note that much of what is described regarding dendrograms and coloring applies both to HCA and PLS-Trees. Hence, the reader is recommended to also read the following topics and sections:

- Hierarchical Cluster Analysis - HCA later in this section.
- HCA in Chapter 10, Analyze.
- PLS-Trees later in this section.
- PLS-Tree in Chapter 10, Analyze.

16.3.1 Hierarchical Cluster Analysis - HCA

In Hierarchical Clustering Analysis (HCA) a similarity or distance criterion is first specified by the user (default = "Ward", other option: Single Linkage). Then HCA basically starts with as many clusters as there are observations (N). The two closest clusters or observation points are merged, thereafter the two closest clusters or points are again merged, etc., until only one cluster remains. The result is shown by means of a ***dendrogram***. Open plots, e.g., score plots, are colored according to the clusters marked in the dendrogram. For more, see the HCA section in Chapter 10, Analyze.

16.3.1.1 Ward clustering

In *Ward* clustering the distance measure is a function that measures the error increase of the model when a pair of clusters are merged into one new cluster. The error function used in SIMCA is the classical error function which calculates the difference in the sum of sum of squares around the mean of each cluster before and after merging two clusters.

This type of clustering works well when the clusters are spherical.

16.3.1.2 Single linkage

In *single linkage* clustering, the distance between a pair of clusters is the Euclidean distance between the two observations (one in each cluster) closest to each other. This type of clustering works well when the clusters are warped filaments.

16.3.2 PLS-Trees

PLS-Trees is an approach similar to regression and classification trees [3], but using the first score vectors of PLS and PLS-DA instead of the original X-variables for splitting clusters into two.

Thus, the basic idea of a PLS-Tree is to start with a PLS model of the whole data set (the user must before specify what is X and Y, scaling, etc.), and then split the data along the sorted 1st score (**t**) of the PLS model. This split is made to optimize a criterion with three parts:

a. improving the variance of the score (**t**) so that when combined, the variance in the resulting two sub-groups is as small as possible, and

b. analogously for the variance of Y, and

c. do this so that the sizes of the two sub-groups are as equal as possible. Each of these three criteria is in advance given a relative weight by the user, and the criterion to be optimized is the combination of the three parts weighted by the user supplied weights. The user also specifies a minimal size of a cluster beyond which it cannot be further split.

The weight allows the user to focus on the clustering in the X-space, or in the Y-space, or in both, and to more or less focus on splitting into groups of approximately the same size.

Once the split is made and the criterion indicates an improvement, the split goes on with the two sub-groups, and thereafter with the resulting sub-groups of these, until all “branches” have been terminated due to either lack of improvement by further splitting, or that the clusters are reaching the minimal size.

The result is a hierarchical set of PLS models in a tree structure. Each model is an ordinary PLS model which can be further modified, investigated, displayed, and interpreted.

For details about coloring etc., see also the PLS-Tree and HCA dendrogram sections in Chapter 10, Analyze.

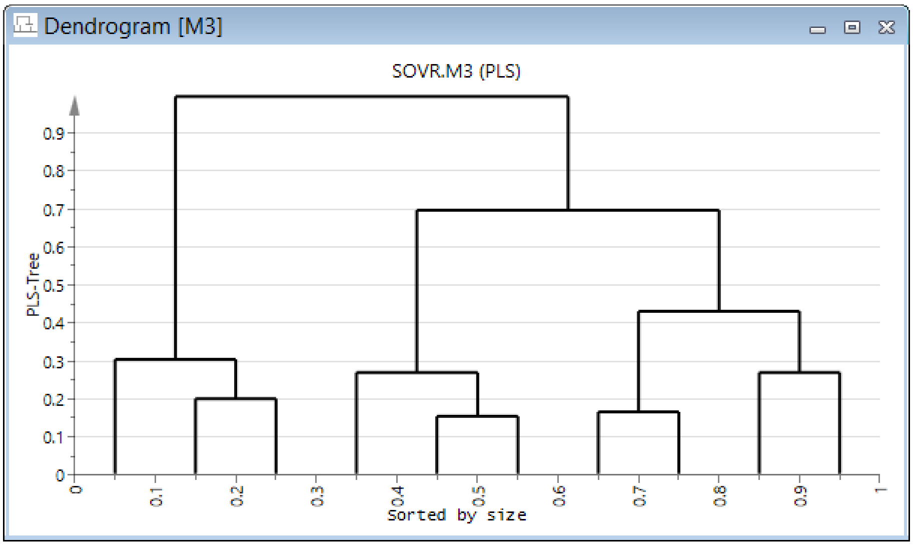


Figure. A typical PLS-Tree. Each branch of the tree corresponds to a PLS model fitted to a sub-set of observations.

16.3.2.1 Calculation of PLS-Trees

Cross validation is used to terminate the branches of the tree, and to determine the number of components of each cluster PLS model.

To accomplish a PLS-Tree the data matrices, X and Y, are first centered and scaled, as usual. A PLS analysis is made of X and Y. Thereafter, the first X-score, t1, is used as the dividing coordinate together with the Y-data (X and Y are sorted along t1). The point on t1 is searched that divides X and Y in two parts, 1 and 2, such that the following expression is minimized:

$\beta * (N_1 - N_2)^2/(N_1 + N_2)^2 + (1 - \beta) * [\alpha * ((V_{Y1} + V_{Y2})/ V_Y) + (1 - \alpha) * ((V_{t1} + V_{t2})/V_t)]$

In the expression above, V denotes variance,

α and β, A and B in SIMCA, are two adjustable parameters.

The parameters A and B both run between 0 and 1. They regulate how the PLS models are split (i.e., how the observations from one upper level PLS model are distributed among two lower level models) according to the score t1, the Y-variable(s) or the group size. The first parameter, **A**, sets the balance between the score t1 and the Y; the ***closer to zero*** the more weight is attributed to the **score t1**. The second parameter, **B**, takes into account the group size of the resulting clusters; the ***closer to zero*** the less important it becomes to have ***equal group sizes*** in the dendrogram. In summary, this means that a division along t1 is sought that minimizes the within groups variation and hence maximizes the between group differences in t1 and Y.

The approach results in the row-wise splitting of data into a tree structure (dendrogram) of PLS models, one split for each cluster (node in the dendrogram). The dendrogram with the associated PLS models is called a PLS-Tree. When Y comprises a discrete matrix with 1/0 columns corresponding to a number of predefined classes, the result is a PLS classification tree.

16.3.3 References cluster analysis

1. Kriegl, J.M., Eriksson, L., Arnhold, T., Beck, B., Johansson, E., and Fox, T., (2005), *Multivariate Modeling of Cytochrome P450 3A4 Inhibition*, European Journal of Pharmaceutical Sciences, 24, 451-463.
2. Eriksson, L., Johansson, E., Müller, M., and Wold, S., (2000c), *On the Selection of Training Set in Environmental QSAR When Compounds are Clustered*, Journal of Chemometrics, 14, 599-616.
3. Breiman, L., Friedman, J.H., Olshen, R.A., and Stone, C.J., (1984) *Classification and Regression Trees,* Wadsworth & Brooks / Cole Advanced Books & Software, Monterey, CA.
4. Everitt, B.S., Landau, S., Leese, M., (2001), *Cluster Analysis*, Fourth Edition Arnold Publishers, London.
5. Ward, J.H., (1963), *Hierarchical grouping to optimize an objective function*. J. Am. Stat. Assoc., 58, 236-244.

16.4 Vectors available in SIMCA

Modeling using PCA, PLS, OPLS, and O2PLS results in a number of vectors describing the model and its properties, and the residuals.

In the subsections that follow all vectors available in SIMCA are described. The vectors are divided in groups according to their data type in the **Plot/List** dialogs.

- For vectors such as variables, scores, and distance to model, see the Variables and scores vectors subsection.
- For vectors such as observations, loadings, and Q2VX, see the Observations and loadings vectors subsection.
- For vectors pertaining to a component such as Q2, R2X, or SDt see the Function of component vectors subsection.
- For lag vectors for models with lags defined in the workset, see the Function of lags vectors subsection.
- For aligned vectors for batch evolution models, see the Aligned vectors subsection.
- For Out Of Control vectors for models in batch evolution models, see the Batch vectors - Out of control summary subsection.

Some of the vectors are described with formulas in the Formulas and descriptions section later in this chapter.

Note: All vectors available for PLS are also available (with the same description) for OPLS and O2PLS unless otherwise stated. For OPLS and O2PLS these common vectors generally refer to the predictive side.

OPLS and O2PLS specific vectors are described in the Orthogonal PLS modeling subsection earlier in this chapter.

16.4.1 Variables and scores vectors

In the **Plot/List** tab dialogs, the vectors found in the **Items** box with data type **Variables and scores** are column vectors with the same shape as variables and scores, i.e., with one element per observation.

See the table for the vectors available and their description in alphabetical order. The rightmost column displays the plot/list/spreadsheet where the vector is available, when applicable, in bold text if the vector is displayed by default.

Vector	Description	Displayed
CVgroups	The cross-validation group that each observation is assigned to.	
Date/Time	Variable in the dataset specified as **Date/Time Variable** in the SIMCA import. For more see the Formatting variable as Date/Time subsection in Chapter 6, SIMCA import.	All line plots displaying observations, for instance: Home | Scores | Line
Date/Time-PS	Predictionset variable specified as **Date/Time Variable** in the SIMCA import. For more see the Formatting variable as Date/Time subsection in Chapter 6, SIMCA import.	All line plots displaying observations, for instance: Predict | Score PS | Line
DModX	Distance to the model in X space (row residual SD), after A components (the selected model dimension), for the observations used to fit the model. If you select component 0, it is the standard deviation of the observations with scaling and centering as specified in the workset, i.e., it is the distance to the origin of the scaled coordinate system. (A) = Absolute distance. (N) = Normalized distance. (M) = Mpow weighted residuals.	Home | DModX
DModXPS	Distance to the model in the X space (row residual SD), after A components (the selected dimension), for new observations in the predictionset. Displaying component 0, it is the standard deviation of the observations with scaling as specified in the workset times *v* (correction factor for workset observations, see the Absolute distance to the model of an observation in the workset subsection in the Statistical appendix), i.e., it is the distance to the origin of the scaled coordinate system.	Predict | DModX PS+
DModXPS+	Combination of DModXPS and tPS, when the latter is declared different from the workset observations.	Predict | DModX PS+
DModY	Distance to the model in the Y space (row residual SD) after A components (the selected model dimension) for the observations used to fit the model. If you select component 0, it is the standard deviation of the observations with scaling and centering as specified in the workset.	Line or Column under the DModY header in Home | DModX
DModYPS	Distance to the model in the Y space (row residual SD) after A components (the selected model dimension) for observations in the predictionset. If you select component 0, it is the standard deviation of the observations with scaling and centering as specified in the workset.	Line or Column under the DModY header in Predict | DModXPS
Num	Index number: 1, 2, 3 etc.	All lists displaying observations, for instance **Predict | Y PS | List**
ObsID	Numerical observation identifiers, primary, secondary, batch, or phase.	
OLevX	The leverage is a measure of the influence of a point (observation) on the PC model or the PLS model in the X space. The observations leverages are computed as the diagonal elements of the matrix H^0 after A dimensions. $H^0 = T[T'T]^{-1}T'$.	

Vector	Description	Displayed
OLevY	The leverage is a measure of the influence of a point (observation) on the PLS model in the Y space. The observations leverages are computed as the diagonal elements of the matrix H^y after A dimensions. $H^y = U[U'U]^{-1}U'$.	
ORisk	The observation risk is a sensitivity measure and indicates the "risk" (the influence) of including an observation in the workset. ORisk is based on the Y residual (in a PLS/OPLS/O2PLS model) for a selected observation. It is computed from the difference between the residual standard deviation of the selected Y, when the observation is and is not in the model.	
ORisk(pooled)	The pooled ORisk is analogous to ORisk but is valid across all Y variables in a PLS/OPLS/O2PLS model rather than an individual Y variable. It is computed from the difference between the pooled residual standard deviation of the Y variables, when the observation is and is not in the model.	
PModX	Probability of belonging to the model in the X space, for observations used to fit the model. Component 0 corresponds to a point model, i.e., the center of the coordinate system. Observations with probability of belonging of less than 5% are considered to be non-members, i.e., they are different from the normal observations used to build the model.	
PModY	Probability of belonging to the model in the Y space, for observations used to fit the model. Component 0 corresponds to a point model, i.e., the center of the coordinate system. Observations with probability of belonging of less than 5% are considered to be non-members, i.e., they are different from the normal observations used to build the model.	
PModXPS	Probability of belonging to the model in the X space, for new observations in the predictionset. Component 0 corresponds to a point model, i.e., the center of the coordinate system. Observations with probability of belonging of less than 5% are considered to be non-members, i.e., they are different from the normal observations used to build the model.	Predict | Prediction list
PModXPS+	The same as PModXPS but based on DModXPS+ instead of DModXPS.	Predict | Prediction list Predict | Classification list
PModYPS	Probability of belonging to the model in the Y space, for new observations in the predictionset. Component 0 corresponds to a point model, i.e., the center of the coordinate system. Observations with probability of belonging of less than 5% are considered to be non-members, i.e., they are different from the normal observations used to build the model.	
r	R is the projection of uo onto X. R contains non-zero entries when the score matrix Uo is not completely orthogonal to X. The norm of this matrix is usually very small but is used to enhance the predictions of X. Available for OPLS and O2PLS models.	Home | Loadings | Orth Y
SerrL	Lower limit of the standard error of the predicted response Y for an observation in the workset.	
SerrLPS	Lower limit of the standard error of the predicted response Y for a new observation in the predictionset. SerrLPS is always in original units, i.e., back transformed when Y was transformed, when displayed in the **Prediction List**.	Predict | Prediction list

Vector	Description	Displayed
SerrU	Upper limit of the standard error of the predicted response Y for an observation in the workset.	
SerrUPS	Upper limit of the standard error of the predicted response Y for a new observation in the predictionset. SerrUPS is always in original units, i.e., back transformed when Y was transformed, when displayed in the **Prediction List**.	Predict | Prediction list
t	Scores t, one vector for each model dimension, are new variables computed as linear combinations of X. They provide a summary of X that best approximates the variation of X only (PC model), and both approximate X and predict Y (PLS/OPLS/O2PLS model).	Home | Scores
T2Range	Hotelling's T2 for the selected range of components. It is a distance measure of how far away an observation is from the center of a model hyperplane. For OPLS/O2PLS the range is locked to using first predictive to last Orthogonal in X.	Home | Hotelling's T2
T2RangePS	Predicted Hotelling's T2 for the selected range of components. For OPLS/O2PLS the range is locked to using first predictive to last Orthogonal in X.	Predict | Hotelling's T2PS
tcv	X score t for the selected model dimension, computed from the selected cross validation round. For PLS/OPLS/O2PLS tcv contains one value per observation and for PCA one value per observation and cross validation round.	Analyze | CV scores
tcvSE	Jack knife standard error of the X score t computed from all rounds of cross validation.	
to	Orthogonal X score to of the X-part of the OPLS/O2PLS model, for the selected component. It summarizes the unique X variation, i.e., the X variation orthogonal to Y.	Home | Scores
tocv	Orthogonal X score to from the X-part of the OPLS/O2PLS model, for a selected model dimension, computed from the selected cross validation round.	
toPS	Predicted orthogonal X score to of the X-part of the OPLS/O2PLS model, for the observations in the predictionset	Predict | Scores PS
toPScv	Matrix of cross validated predicted scores ToPS for the predictionset. Available for OPLS and O2PLS models.	
tPS	Predicted X score t, for the selected model dimension, for the observations in the predictionset.	Predict | Score PS
tPScv	Predicted X score t, for the selected model dimension, computed from the selected cross validation round.	
tPScvSE	Jack knife standard error of the X score t, for the observations in the predictionset, computed from all rounds of cross validation.	
u	Scores u, one vector for each model dimension, are new variables summarizing Y so as to maximize the correlation with the X scores t.	Analyze | Inner relation
ucv	Y score u for the selected model dimension, computed from the selected cross validation round.	
uo	Orthogonal Y score uo of the Y-part of the OPLS/O2PLS model, for the selected component. It summarizes the unique Y variation, i.e., the Y variation orthogonal to X.	Home | Scores | Orth Y
uocv	Orthogonal Y score uo of the Y-part of the OPLS/O2PLS model, computed from the selected cross validation round.	

Vector	Description	Displayed
VarDS	Variable from the selected dataset, in original units. Available after selecting a DS in the **Data** box.	
VarID	Variable Identifier.	
VarPS	X variable from the predictionset. Can be displayed in transformed or scaled units.	
XVar	X variable from the workset. Can be displayed in transformed or scaled units.	
XVarPred	A reconstructed variable from the workset. For PLS and PCA models, an X variable from the workset is reconstructed as X=TP'. For OPLS models XVarPred represents the X-values predicted from the given Y-values.	
XVarPredPS	A reconstructed variable from the predictionset. For PLS and PCA models, an X variable from the predictionset is reconstructed as X=TPS * P'. For OPLS models XVarPredPS represents the X-values predicted from the given Y-values.	
XVarPS	X variable from the predictionset. Can be displayed in transformed or scaled units.	Predict | Prediction list
XVarRes	X variable residuals for observations in the workset, in original units. Can be displayed in transformed or scaled units.	
XVarResPS	X variable residuals for observations in the predictionset, in original units. Can be displayed in transformed or scaled units.	
XVarResPSSt	X variable residuals for observations in the predictionset, in standardized units (divided by the residual standard deviation). Can be displayed in transformed or scaled units.	
XVarResSt	X variable residuals for observations in the workset, in standardized units (divided by the residual standard deviation). Can be displayed in transformed or scaled units.	
XVarResYRelated	X variable residuals where the systematic variation orthogonal to Y has been removed. Available for OPLS and O2PLS.	
YPred	Predicted values of Y variables for observations in the workset, in original units, i.e., back-transformed when transformations are present. Can be displayed in transformed or scaled units.	Home | Observed vs. predicted
YPredcv	Predicted values of the fitted Ys for observations in the workset, computed from the cross validation procedure.	
YPredPS	Predicted values for Y variables for observations in the predictionset, in original units, i.e. back transformed when transformations are present. Can be displayed in transformed or scaled units.	Predict | Y PS Predict | Prediction list
YPredErrcv	Prediction error of the fitted Ys for observations in the workset, computed from the cross validation procedure.	
YPredPSConfInt- YPredPSConfInt+	Lower/upper limit for the confidence interval of predicted Ys from the predictionset. The limit is calculated from the cross validation and the confidence level specified in model options.	
YPredPScv	Predicted values of the modeled Ys for observations in the predictionset, computed from the cross validation procedure.	
YPredPScvSE	Jack knife standard error of the prediction of Y for observations in the predictionset, computed from all rounds of cross validation.	
YVar	Y variable from the workset. Can be displayed in transformed or scaled units.	Home | Observed vs. predicted

Vector	Description	Displayed
YVarPS	Y variable from the predictionset. Can be displayed in transformed or scaled units.	Predict | Y PS
YVarRes	Y variable residuals for observations in the workset, in original units. Can be displayed in transformed or scaled units.	
YVarResSt	Y variable residuals for observations in the workset, in standardized units (divided by the residual standard deviation). Can be displayed in transformed or scaled units.	
YVarResPS	Y variable residuals for observations in the predictionset, in original units. Can be displayed in transformed or scaled units.	
YVarResPSSt	Y variable residuals for observations in the predictionset, in standardized units (divided by the residual standard deviation). Can be displayed in transformed or scaled units.	

16.4.2 Observations and loadings vectors

In the **Plot/List** tab dialogs the vectors found in the **Items** box with data type **Observations and loadings** are row vectors with the same "shape" as an observation, i.e., with one row per variable.

See the table for the vectors available and their description in alphabetical order. The rightmost column displays the plot/list/spreadsheet where the vector is available, when applicable, in bold text if the vector is displayed by default.

Vector	Description	Displayed
Batch VIP	The Batch Variable Importance plot (Batch VIP) is available for batch level models and displays the overall importance of the variable on the final quality of the batch. With phases, the plot displays the importance of a variable by phase. With a PLS model, the Batch VIP displays the plot for one y-variable at a time, with a column per variable and per selected phase. Note: The Batch VIP is only available for scores batch level datasets.	Batch | Variable importance plot
c	For every dimension in the PLS model there is a c vector. It contains the Y loading weights used to linearly combine the Y's to form the Y score vector u. This means the c vector actually expresses the correlation between the Y's and the X score vector t.	Home | Loadings
c(corr)	Y loading weight c scaled as a correlation coefficient between Y and u.	Home | Loadings Analyze | Biplot
ccv	Y loading weight c for a selected model dimension, computed from the selected cross validation round.	
ccvSE	Jack-knife standard error of the Y loading weight c computed from the rounds of cross validation.	
co	Orthogonal Y loading weights co combine the Y variables (first dimension) or the Y residuals (subsequent dimensions) to form the scores Uo. These orthogonal Y loading weights are selected so as to minimize the correlation between Uo and T, thereby indirectly between Uo and X. Available for OPLS and O2PLS models.	
cocv	Orthogonal Y loading weights co from the Y-part of the model, for a selected model dimension, computed from the selected cross validation round. Available for OPLS and O2PLS models.	
Coeff	PLS/OPLS/O2PLS regression coefficients corresponding to the unscaled and uncentered X and Y. This vector is cumulative over all components up to the selected one.	Home | Coefficients

Vector	Description	Displayed
CoeffC	PLS/OPLS/O2PLS regression coefficients corresponding to the unscaled but centered X and unscaled Y. This vector is cumulative over all components up to the selected one.	Home | Coefficients
CoeffCS	PLS/OPLS/O2PLS regression coefficients corresponding to centered and scaled X, and scaled (but uncentered) Y. This vector is cumulative over all components up to the selected one.	Home | Coefficients
CoeffCScv	PLS/OPLS/O2PLS regression coefficients corresponding to the centered and scaled X and the scaled (but uncentered) Y computed from the selected cross validation round.	
CoeffCScvSE	Jack-knife standard error of the coefficients CoeffCS computed from all rounds of cross validation.	
CoeffMLR	PLS/OPLS/O2PLS regression coefficients corresponding to the scaled and centered X but unscaled and uncentered Y. This vector is cumulative over all components up to the selected one.	Home | Coefficients
CoeffRot	Rotated PLS/OPLS/O2PLS regression coefficients corresponding to the unscaled and uncentered X and Y. This vector is cumulative over all components up to the selected one.	Home | Coefficients
MPowX	The modeling power of variable X is the fraction of its standard deviation explained by the model after the specified component.	
Num	Index number: 1, 2, 3 etc.	
ObsDS	Observation in the dataset, selected in the **Data box,** in original units.	
ObsPS	Observation in the current predictionset, in original units. There is only one current predictionset at a time although many can be specified.	
p	Loadings of the X-part of the model. With a PCA model, the loadings are the coefficients with which the X variables are combined to form the X scores, t. The loading, p, for a selected PCA dimension, represent the importance of the X variables in that dimension. With a PLS model, p expresses the importance of the variables in approximating X in the selected component.	Home | Loadings
p(corr)	X loading p scaled as a correlation coefficient between X and t.	Home | Loadings Analyze | Biplot
pc	X loading p and Y loading weight c combined to one vector.	Home | Loadings
pc(corr)	X loading p and Y loading weight c scaled as correlation coefficients between X and t (p) and Y and u (c), and combined to one vector.	Home | Loadings Analyze | Biplot
pccvSE	Jack-knife standard error of the combined X loading p and Y loading weight c computed from all rounds of cross validation.	
pcv	X loading p for a selected model dimension, computed from the selected cross validation round.	
pcvSE	Jack-knife standard error of the X loading p computed from all rounds of cross validation.	
po	Orthogonal loading po of the X-part of the OPLS/O2PLS model. po expresses the unique variability in X not found in Y, i.e., X variation orthogonal to Y, in the selected component.	Home | Loadings Home | Loadings | Orth X
po(corr)	Orthogonal loading po of the X-part of the OPLS/O2PLS model, scaled as the correlation coefficient between X and to, in the selected component.	

Vector	Description	Displayed
pocv	Orthogonal loading po of the X-part of the OPLS/O2PLS model, for a selected model dimension, computed from the selected cross validation round.	
poso	Orthogonal loading po of the X-part and the projection of to onto Y, so, combined to one vector. Available for OPLS and O2PLS.	Home | Loadings Home | Loadings | Orth X
pq	X loading weight p and Y loading weight q combined to one vector. Available for OPLS and O2PLS.	Home | Loadings Home | Loadings | Pred X-Y
q	Loadings of the Y-part of the OPLS/O2PLS model. q expresses the importance of the variables in approximating Y variation correlated to X, in the selected component. Y variables with large q (positive or negative) are highly correlated with t (and X).	Home | Loadings Home | Loadings | Pred X-Y
qcv	Y loading q for a selected model dimension, computed from the selected cross validation round. Available for OPLS and O2PLS models.	
Q2VX, Q2VY	Predicted fraction, according to cross validation, of the variation of the X (PCA) and Y variables (PLS/OPLS/O2PLS), for the selected component.	Home | Summary of fit | Component contribution
Q2VXcum, Q2VYcum	Cumulative predicted fraction, according to cross validation, of the variation of the X variables (PCA model) or the Y variables (PLS/OPLS/O2PLS model).	Home | Summary of fit
qo	Orthogonal loading qo of the Y-part of the OPLS/O2PLS model. qo expresses the unique variability in Y not found in X, i.e., Y variation orthogonal to X, in the selected component.	Home | Loadings | Orth Y
qocv	Orthogonal loading qo of the Y-part of the OPLS/O2PLS model, for a selected model dimension, computed from the selected cross validation round.	
qor	qo and r combined to one vector. Available for OPLS and O2PLS.	Home | Loadings | Orth Y
r	R is the projection of uo onto X. R contains non-zero entries when the score matrix Uo is not completely orthogonal to X. The norm of this matrix is usually very small but is used to enhance the predictions of X. Available for OPLS and O2PLS.	Home | Loadings | Orth Y
R2VX	Explained fraction of the variation of the X variables, for the selected component.	Home | Summary of fit | Component contribution
R2VXAdj	Explained fraction of the variation of the X variables, adjusted for degrees of freedom, for the selected component.	Home | Summary of fit | Component contribution
R2VXAdjcum	Cumulative explained fraction of the variation of the X variables, adjusted for degrees of freedom.	Home | Summary of fit | X/Y overview
R2VXcum	Cumulative explained fraction of the variation of the X variables.	Home | Summary of fit | X/Y overview
R2VY	Explained fraction of the variation of the Y variables, for the selected component.	Home | Summary of fit | Component contribution
R2VYAdj	Explained fraction of the variation of the Y variables, adjusted for degrees of freedom, for the selected component.	Home | Summary of fit | Component contribution
R2VYAdjcum	Cumulative explained fraction of the variation of the Y variables, adjusted for degrees of freedom.	Home | Summary of fit | X/Y overview
R2VYcum	Cumulative explained fraction of the variation of the Y variables.	Home | Summary of fit | X/Y overview
RMSEcv	Root Mean Square Error, computed from the selected cross validation round.	Analyze | RMSECV

Vector	Description	Displayed
RMSEE	Root Mean Square Error of the Estimation (the fit) for observations in the workset.	
RMSEP	Root Mean Square Error of the Prediction for observations in the predictionset.	Predict | Y PS | Scatter Predict | Y PS | Line
S2VX	Residual variance of the X variables, after the selected component, scaled as specified in the workset.	
S2VY	Residual variance of the Y variables, after the selected component, scaled as specified in the workset.	
so	So is the projection of to onto Y. So contains non-zero entries when the score matrix To is not completely orthogonal to Y. The norm of this matrix is usually very small but is used to enhance the predictions of Y. Available for OPLS and O2PLS models.	Home | Loadings | Orth X
VarID	Numerical variable identifiers, primary or secondary.	All lists displaying variables, for instance **Home | Coefficients | List**
VIP	Variable Influence on the Projection. It provides the influence of every term in the matrix X on all the Y's. Terms with VIP>1 have an above average influence on Y. This vector is cumulative over all components up to the selected one.	Home | VIP
VIPcv	VIP computed from the selected cross validation round.	
VIPcvSE	Jack-knife standard error of the VIP computed from all rounds of cross validation.	
VIPorth	Orthogonal variable importance for the projection, VIPorth, summarizes the importance of the variables explaining the part of X orthogonal to Y. Terms with VIP > 1 have an above average influence on the model.	
VIPpred	Predictive variable importance for the projection, VIPpred, summarizes the importance of the variables explaining the part of X related to Y. Terms with VIP > 1 have an above average influence on the model.	
w	X loading weight that combine the X variables (first dimension) or the X residuals (subsequent dimensions) to form the scores t. This loading weight is selected so as to maximize the correlation between t and u, thereby indirectly between t and Y. X variables with large w's (positive or negative) are highly correlated with u (and Y).	Home | Loadings
w*	X loading weight that combines the original X variables (not their residuals in contrast to w) to form the scores t. In the first dimension w* is equal to w. w* is related to the correlation between the X variables and the Y scores u. $W^* = W(P'W)^{-1}$ X variables with large w* (positive or negative) are highly correlated with u (and Y).	Home | Loadings
w*c	X loading weight w* and Y loading weight c combined to one vector.	Home | Loadings
w*ccvSE	Jack-knife standard error of the combined X loading weight w* and Y loading weight c computed from all rounds of cross validation.	
w*cv	X loading weight w*, for a selected model dimension, computed from the selected cross validation round.	
w*cvSE	Jack-knife standard error of the X loading weight w* computed from all rounds of cross validation.	

Vector	Description	Displayed
wcv	X loading weight w, for a selected model dimension, computed from the selected cross validation round.	
wcvSE	Jack-knife standard error of the X loading weight w computed from all rounds of cross validation.	
wo	Orthogonal loading weight wo of the X-part of the OPLS/O2PLS model. It combines the X residuals to form the orthogonal X score to. This loading weight is selected so as to minimize the correlation between to and u, thereby indirectly between to and Y.	
wocv	Orthogonal loading weight wo of the X-part of the OPLS/O2PLS model, for a selected model dimension, computed from the selected cross validation round.	
Xavg	Averages of X variables, in original units. If the variable is transformed, the average is in the transformed metric.	
XObs	X variables for the selected observation in the workset in original units. Can be displayed in transformed or scaled units.	
XObsPred	Reconstructed observations as X=TP' from the workset. Can be displayed in transformed or scaled units.	
XObsPredPS	Reconstructed observations as X=TP' from the predictionset. Can be displayed in transformed or scaled units.	
XObsRes	Residuals of observations (X space) in the workset, in original units. Can be displayed in transformed or scaled units.	
XObsResPS	Residuals of observations (X space) in the predictionset, in original units. Can be displayed in transformed or scaled units.	
Xws	Scaling weights of the X variables.	
YRelatedProfile	Displays the estimated pure profiles of the underlying constituents in X under the assumption of additive Y-variables. Estimation includes a linear transformation of the Coefficient matrix, $Bp(Bp^TBp)^{-1}$, where Bp is the Coefficient matrix using only the predictive components to compute the Coefficient matrix (i.e., the components orthogonal to Y are not included in the computation of Bp). Available for OPLS and O2PLS models.	Analyze | Y-related profiles
Yavg	Averages of Y variables, in original units. If the variable is transformed, the average is in the transformed metric.	
YObs	Y variables for the selected observation in the workset in original units. Can be displayed in transformed or scaled units.	
YObsRes	Residuals of observations (Y space) in the workset, in original units. Can be displayed in transformed or scaled units.	
YObsResPS	Residuals of observations (Y space) in the predictionset, in original units. Can be displayed in transformed or scaled units.	
Yws	Scaling weights of the Y variables.	

16.4.3 Function of component vectors

For the **Plot/List** tab dialogs the vectors found in the **Items** box with data type **F(component)** are available per component. Some statistics apply to the whole matrix; others are for selected variable, for each component.

See the table for the vectors available and their description in alphabetical order. The rightmost column displays the plot/list/spreadsheet where the vector is available, when applicable, in bold text if the vector is displayed by default.

Vector	Description	Displayed
Eig	Eigenvalues of the X matrix.	View | Model window

Vector	Description	Displayed
Iter	Number of iterations of the algorithm till convergence.	View | Model window
Num	Index number: 1, 2, 3 etc.	
Q2	Fraction of the total variation of the X block (PCA) or the Y block (PLS) that can be predicted by each component.	View | Model window
Q2(cum)progression	Cumulative Q2 for the extracted components, showing the progression of cumulative values for each added orthogonal component in the OPLS/O2PLS model, e.g. 1+0, 1+1, 1+2. Available for OPLS/O2PLS models with 1+x+0 components.	Home | Summary of fit
Q2cum	Cumulative Q2 for the extracted components.	View | Model window Home | Summary of fit
Q2VX, Q2VY	Predicted fraction, according to cross validation, of the variation of the X (PCA) and Y variables (PLS/OPLS/O2PLS), for the selected component.	Home | Summary of fit | Component contribution
Q2VXcum, Q2VYcum	Cumulative predicted fraction, according to cross validation, of the variation of the X variables (PCA model) or the Y variables (PLS/OPLS/O2PLS model).	Home | Summary of fit | X/Y overview
R2(cum)progression	Cumulative fraction of Y variation, showing the progression of cumulative values for each added orthogonal component in the OPLS/O2PLS model, e.g. 1+0, 1+1, 1+2. Available for OPLS/O2PLS models with 1+x+0 components.	Home | Summary of fit
R2VX	Explained fraction of the variation of the X variables, for the selected component.	Home | Summary of fit | Component contribution
R2VXAdjcum	Cumulative explained fraction of the variation of the X variables, adjusted for degrees of freedom.	Home | Summary of fit | X/Y overview
R2VXcum	Cumulative explained fraction of the variation of the X variables.	Home | Summary of fit | X/Y overview
R2VY	Explained fraction of the variation of the Y variables, for the selected component.	Home | Summary of fit | Component contribution
R2VYAdjcum	Cumulative explained fraction of the variation of the Y variables, adjusted for degrees of freedom.	Home | Summary of fit | X/Y overview
R2VYcum	Cumulative explained fraction of the variation of the Y variables.	Home | Summary of fit | X/Y overview
R2X	Fraction of the total variation of the X block that can be explained by each component.	View | Model window Home | Summary of fit
R2XAdj	Explained fraction of the variation of the X block, adjusted for degrees of freedom, for the selected component.	Home | Summary of fit
R2XAdjcum	Cumulative explained fraction of the variation of the X block, adjusted for degrees of freedom.	
R2Xcum	Cumulative explained fraction of the variation of the X block.	View | Model window Home | Summary of fit
R2Y	Fraction of the total variation of the Y block that can be explained by each component.	View | Model window Home | Summary of fit
R2YAdj	Explained fraction of the variation of the Y block, adjusted for degrees of freedom, for the selected component.	Home | Summary of fit
R2YAdjcum	Cumulative explained fraction of the variation of the Y block, adjusted for degrees of freedom.	
R2Ycum	Cumulative explained fraction of the variation of the Y block.	View | Model window Home | Summary of fit

Vector	Description	Displayed
RMSEcv	Root Mean Square Error, computed from the selected cross validation round.	Analyze | RMSECV
RMSEcv-progression	Root Mean Square Error showing the progression of RMSEcv values for each added orthogonal component in the OPLS/O2PLS model, e.g. 1+0, 1+1, 1+2. Available for OPLS/O2PLS models with 1+x+0 components.	Analyze | RMSECV
S2X	Variance of the X block. For component number A, it is the residual variance of X after component A.	
S2Y	Variance of the Y block. For component number A, it is the residual variance of Y after component A.	
SDt	Standard deviation of the X scores, T.	
SDu	Standard deviation of the Y scores, U.	
SSX	Sum of squares of the X block. For component number A, it is the X residual Sum of Squares after component A.	
SSY	Sum of squares of the Y block. For component number A, it is the Y residual Sum of Squares after component A.	
YPredErrcvSE	Jack-knife standard error of the prediction error of the fitted Ys for observations in the workset, computed from the cross validation rounds.	

16.4.4 Function of lags vectors

For the **Plot/List** tab dialogs vectors found in the **Items** box with data type **F(lags)** are available as functions of lags.

See the table for the vectors available and their description in alphabetical order.

Vector	Description
CoeffCScvSELag	Jack-knife standard error on the coefficients as a function of lag, computed from all cross validation rounds.
CoeffCSLag	Coefficients (for scaled and centered data) of a lagged variable x, for a selected Y as a function of lags.
Num	Index number: 1, 2, 3 etc.
pLag	X loading p of a lagged variable X, as a function of lags.
VIPLag	VIP of a lagged variable X as a function of lags.
VIPorthLag	VIPorth of a lagged variable X as a function of lags
VIPpredLag	VIPpred of a lagged variable X as a function of lags
wLag	X loading weight w of a lagged variable as a function of lags
w*Lag	X loading weight w* of a lagged variable as a function of lags

16.4.5 Aligned vectors

In the **Plot/List** tab dialogs the vectors found in the **Items** box with data type **Aligned vectors** are available for vectors aligned to median length. The average or standard deviation of the vector can be displayed, and selected batches.

Aligned vectors are available for batch evolution models.

Note: All aligned vectors are named '(Aligned)' in addition to the vector name.

See the table for the vectors available and their description in alphabetical order. The rightmost column displays the plot/list/spreadsheet where the vector is available.

Vector	Description	Displayed
DModX	DModX vector aligned to median length. See DModX description previously.	Batch | DModX BCC.
DModXPS	DModXPS vector aligned to median length. See DModXPS description previously.	Batch | DModX PS BCC.
Num	Index vector: 1, 2, 3 etc.	
t	t vector aligned to median length. See t description previously.	Batch | Scores BCC.
T2Range	T2Range vector aligned to median length. See T2Range description previously.	Batch | Hotelling's T2 BCC.
T2RangePS	T2RangePS vector aligned to median length. See T2RangePS description previously.	Batch | Hotelling's T2PS BCC.
Time/Maturity	Time or Maturity variable determining the end point of a Batch/Phase and used as Y in the observation level models. This variable is used to align Batch/Phase to the median length.	All aligned batch control charts.
toPS	toPS vector aligned to median length. See toPS description previously.	Batch | Scores PS BCC.| Orth scores
tPS	tPS vector aligned to median length. See tPS description previously.	Batch | Scores PS BCC.
tPS	tPS vector aligned to median length. See tPS description previously.	Batch | Scores PS BCC.
XVar	XVar vector aligned to median length. See XVar description previously.	Batch | Variable BCC.
XVarPS	XVarPS vector aligned to median length. See XVarPS description previously.	Batch | Variable PS BCC.
YPred	YPred vector aligned to median length. See YPred description previously.	Batch | Observed vs. time/maturity BCC.
YPredPS	YPredPS vector aligned to median length. See YPredPS description previously.	Batch | Observed vs. time/maturity PS BCC.
YVar	YVar vector aligned to median length. See YVar description previously.	Batch | Observed vs. time/maturity BCC.
YVarPS	YVarPS vector aligned to median length. See YVarPS description previously.	Batch | Observed vs. time/maturity PS BCC.

16.4.6 Batch vectors

In the **Plot/List** tab dialogs the vectors found in the **Items** box with data type **Batch vectors** are the Out of Control Summary vectors, **OOCSum**, for all vectors displayed in the batch control charts. That is: DModX, DModXPS, T2Range, T2RangePS, t, tPS, XVar, XVarPS, YPred, and YPredPS. The OOCSum vectors are all named as the mother vector with the suffix **AlignedOOCSum**.

The **OOCSum** for a given vector is the ratio of the area of the vector outside the control limits to the total area inside the limits, for each batch. The **OOCSum** is then expressed as a percent of the area inside the limits. With no part of the batch outside the limits, OOCSum=0.

OOCSum is always computed on aligned vectors, both for workset and predictionset vectors.

The **OOCSum** vector is default displayed using the default limits.

Change the limits as desired under **High limit** and **Low limit** after adding the series.

Vector	Description
DModXAlignedOOCSum	For a plot of DModX vs. Maturity for a batch in the workset the out of control (OOC) sum is the area outside the control limits expressed as a percentage of the total area. The summation is made relative to a DModX vector aligned to median length.

Vector	Description
DModXPSAlignedOOCSum	For a plot of DModX vs. Maturity for a batch in the predictionset the out of control (OOC) sum is the area outside the control limits expressed as a percentage of the total area.
T2RangeAlignedOOCSum	For a plot of T2Range vs. Maturity for a batch in the workset the out of control (OOC) sum is the area outside the control limits expressed as a percentage of the total area. The summation is made relative to a T2Range vector aligned to median length.
T2RangePSAlignedOOCSum	For a plot of T2Range vs. Maturity for a batch in the predictionset the out of control (OOC) sum is the area outside the control limits expressed as a percentage of the total area. The summation is made relative to a T2RangePS vector aligned to median length.
TAlignedOOCSum	For a plot of scores (t) vs. Maturity for a batch in the workset the out of control (OOC) sum is the area outside the control limits expressed as a percentage of the total area. The summation is made relative to a t vector aligned to median length.
TOAlignedOOCSum	For a plot of orthogonal scores (to) vs. Maturity for a batch in the workset the out of control (OOC) sum is the area outside the control limits expressed as a percentage of the total area. The summation is made relative to a to (orthogonal score) vector aligned to median length.
TOPSAlignedOOCSum	For a plot of predicted orthogonal scores (to) vs. Maturity for a batch in the predictionset the out of control (OOC) sum is the area outside the control limits expressed as a percentage of the total area. The summation is made relative to a toPS vector aligned to median length.
TPSAlignedOOCSum	For a plot of scores (t) vs. Maturity for a batch in the predictionset the out of control (OOC) sum is the area outside the control limits expressed as a percentage of the total area. The summation is made relative to a tPS vector aligned to median length.
XVarAlignedOOCSum	For a plot of an X-variable vs. Maturity for a batch in the workset the out of control (OOC) sum is the area outside the control limits expressed as a percentage of the total area. The summation is made relative to an XVar vector aligned to median length.
XVarPSAlignedOOCSum	For a plot of an X-variable vs. Maturity for a batch in the predictionset the out of control (OOC) sum is the area outside the control limits expressed as a percentage of the total area. The summation is made relative to an XVarPS vector aligned to median length.
YPredAlignedOOCSum	For a plot of YPred vs. Maturity for a batch in the workset the out of control (OOC) sum is the area outside the control limits expressed as a percentage of the total area. The summation is made relative to an YPred vector aligned to median length.
YPredPSAlignedOOCSum	For a plot of YPred vs. Maturity for a batch in the predictionset the out of control (OOC) sum is the area outside the control limits expressed as a percentage of the total area. The summation is made relative to an YPredPS vector aligned to median length.

16.5 Formulas and descriptions

Fitting a PCA, PLS, OPLS, or an O2PLS model generates all the vectors listed in the Vectors available in SIMCA section earlier in this chapter. This section describes and provides formulas for a selection of those vectors. The descriptions for PLS vectors are also true for the vectors created when fitting OPLS/O2PLS models unless otherwise stated. When fitting with OPLS/O2PLS a few additional vectors are calculated and these are listed in the same tables.

All vectors that have a 'Y' in the name refer to PLS/OPLS/O2PLS models.

SIMCA will iteratively compute one component at a time, that is: one vector each of X-scores **t**, Y-scores **u** (for PLS/OPLS/O2PLS), weights **w** and **c** (for PLS/OPLS/O2PLS), and loadings **p**.

The components are calculated in descending order of importance.

16.5.1 Prediction vectors

After fitting a model, this model can be used for predictive purposes for a given set of observations.

The following vectors are described in this section:

- R2Y, R2X, R2Yadj, R2Xadj
- R2V and R2Vadj

- Q2 and Q2V
- Q2(cum) and Q2V(cum)
- Leverages
- RSD of observations and variables
- Modeling power - MPowX
- Hotelling's T2
- Missing values correction factor
- Score and loading vectors
- Distance to the model
- Variable importance, VIP
- Standard Error on the predicted values
- Coefficients

16.5.2 R2Y, R2X, R2Yadj, R2Xadj

R^2Y and R^2X display the fraction of the sum of squares for the selected component, SS explained.

R^2Yadj, R^2Xadj display the variance explained in the model, that is, SS explained corrected for degrees of freedom

16.5.3 R2V and R2Vadj

For every variable in the model, the fraction of SS (R^2V) or variance (R^2Vadj) explained can be displayed. This is computed for both the current component and accumulated over all PC or PLS components. For response variables Y, this corresponds to R^2 (the multiple correlation coefficient), the goodness of fit.

16.5.4 Q2 and Q2V

Q^2: The fraction of the total variation of X or Y that can be predicted by a component, as estimated by cross-validation.

Q^2 is computed as:

$Q^2 = (1.0 - PRESS/SS)$

Q^2V: The fraction of the variation of a variable, e.g. x_k or y_m, that can be predicted by a component, as estimated by cross-validation.

Q^2V is computed as:

$Q^2VX = (1.0 - PRESS/SS)_k$

$Q^2VY = (1.0 - PRESS/SS)_m$

where Q^2VX is available for both PCA and PLS, but Q^2VY only for PLS.

When using SIMCA with cross validation, Q^2 and the limit are displayed in the model window and the significance column informs if the component is significant or not and according to which rule.

For details about the cross validation rules, see the Cross validation section later in this chapter.

16.5.5 Q2(cum) and Q2V(cum)

The cumulative Q^2 for the extracted components is computed as:

$Q^2(cum) = (1.0 - \Pi(PRESS/SS)_a)$

where

[a = 1, ...A]

$\Pi(PRESS/SS)_a$ = the product of PRESS/SS for each individual component a.

When a component is insignificant the value *PRESS/SS* is truncated for that component to –0.1, when that value is smaller than –0.1.

The cumulative Q^2V of a variable is similarly computed as:

$Q^2V(cum) = (1.0 - \Pi(PRESS/SS)_{ka})$

where

[a = 1, ...A]

When responses have large values of $Q^2V(cum)$ accumulated over all dimensions, the model for this variable is good. An accumulated value larger than about 0.5 can be considered large.

16.5.6 Leverages

The leverage is a measure of the ***influence*** of a point (observation) on the PC or PLS model. Leverage (OLev) is proportional to Hotelling's T^2. Observations with high leverages can exert a large influence on the model. A high leverage observation falling near a component axis reinforces the model. A high leverage observation lying far away from a component line causes a rotation of the model.

SIMCA computes the observations leverages in the X and Y spaces as the diagonal elements of the matrices H_0 and H_y, respectively:

$H_0 = T(T'T)^{-1}T'$

$H_Y = U(U'U)^{-1}U'$

16.5.7 RSD of observations and variables

The residual standard deviation (RSD) can be computed for observations and variables. The RSD of an observation in the X or Y space (rows in E and F) is proportional to the observation distance to the hyper plane of the PLS model in the corresponding space (DModX and DModY).

The RSD of an X variable (columns in E) relates to its relevance in the PC or PLS model. The RSD of a Y variable (columns in F) is a measure of how well this response is explained by the PLS model.

16.5.8 Relevance of variables

The importance of a variable in a PC model is indicated by the size of its explained Sum of Squares (R^2X) or variance (R^2Xadj).

A variable is relevant if its modeling power = 1.0. Variables with low modeling power, i.e., around (A/K) are of little relevance (A = number of model dimensions, K= number of variables).

16.5.8.1 Modeling power - MPowX

The modeling power of a variable is defined as its explained standard deviation:

$Mpow_k = 1.0 - SV_k/SV_{0k}$

where

SV_k = residual standard deviation (RSD) of variable x_k.

SV_{0k}= initial standard deviation of variable k. SV_{0k}= 1.0 if the variable has been autoscaled.

16.5.9 Hotelling's T2

T2Range is basically calculated as the sum over the selected range of components of the scores in square divided by their standard deviations in square, provided the variables were centered. Hence, T2Range is the distance in the model plane (score space) from the origin, in the specified range of components. This means that the same component is selected as 'From' and 'To' components, the plot displays the Hotelling's T2 for that component.

For OPLS and O2PLS the range is locked to 'From' the first predictive 'To' the last orthogonal in x.

The Hotelling's T^2 for observation i, based on A components is:

$T_i^{\ 2} = \Sigma\ ((t_{ia} - t_{avg})^2 / s_{ta}^{\ 2})$

where the summation is done over the range of the selected components,

s^2_{ta} = Variance of t_a according to the class model.

$T_i^2 * (N - A) / A(N - 1)$

is F distributed with A and N-A degrees of freedom.

N = Number of observations in the workset.

A = Number of components in the model or the selected number of components.

Hence if

$T_i^2 > A(N - 1) / (N - A) * F_{critical}$ (p=0.05)

then observation **i** is outside the 95% confidence region of the model.

16.5.9.1 Ellipse in score plot

The confidence region for a two dimensional score plot of dimension a and b is an ellipse with axis:

$\sqrt{(s^2_{ta\ or\ b} *F(2,N-2,\alpha) * 2 * ((N -1)/(N-2)))}$

The significance level is by default 0.05. On the **File** tab, click **Options** | **Project** and in the **Fit** tab change the default level if desired.

To not display the ellipse, see the Limits and regions and Limits subsections in Chapter 14, Plot and list contextual tabs.

16.5.10 Missing values correction factor

The NIPALS algorithm has been modified for data containing missing values. A limit has been introduced on the correction factor used with missing values. This stabilizes both the algorithm and the solution. A value of 3.0 for the limit on the correction factor for both the scores and the loadings has generally been found to be appropriate.

16.5.11 Missing values and PCA

A very important problem in industrial applications of PCA, such as multivariate statistical process control applications, is the estimation of scores when the observation vector has missing data. SIMCAs approach to score calculations for such incomplete observations are based on methods described in Nelson, P.R.C., Taylor, P.A., MacGregor, J.F., *Missing Data Methods in PCA and PLS: Score Calculations with Incomplete Observation, Chemometrics and Intelligent Laboratry Systems*, 35, 45-65, 1996.

SIMCA uses different approaches to compute t and tPS for incomplete observations and if the proportion of missing data is large there can be numerical differences between t and tPS.

The basic PCA and PLS model is generated by the NIPALS algorithm. It consists of a number of steps that iterate to convergence. Each one of those steps is a projection between a vector (e.g. score vector t) and each column in X, hence p=X't/(t't).

For example in PCA, missing data elements that exist in a column in X are handled separately in the projection step, that is, p(i)=X(i)'t/(t't) where the missing elements are set to 0 in the calculations in both the X(i) vector as well as the t vector. This corresponds to a linear regression calculation where the missing elements are positioned exactly on the regression line (i.e. they have no influence). This vector-vector projection way of handling missing data is done the same way for calculating the scores t, but now using the individual rows in X and the loading vector p.

16.5.12 Score and loading vectors

The score and loading plots available for plotting are described below.

Note that the score and loading plots complement each other. The position of an observation in a given direction in a score plot is influenced by variables lying in the same direction in the loading plot.

All of these score plots described here will reveal:

- Groups
- Trends

- Outliers
- Similarity

16.5.12.1 T scores (X): t1 vs. t2, ...

T score plots are windows in the X space displaying the observations as situated on the projection plane or hyper plane.

With a 2-dimensonal score plot SIMCA draws the elliptical confidence interval based on Hotelling's T^2.

16.5.12.2 U scores (Y): u1 vs. u2, ...

U score plots are windows in the Y space, displaying the observations as situated on the projection plane or hyper plane.

16.5.12.3 T vs. U scores (X&Y): t1 vs. u1, ...

T vs U score plots display the observations in the projected X(T) and Y(U) space, and show how well the Y space correlates to the X space.

16.5.12.4 P loadings (X): p1 vs. p2,...

P loading plots show the importance of the X variables in the approximation of the X matrix.

16.5.12.5 W loadings (X): w1 vs. w2, ...

W loading plots display the correlation between the X variables, in the first dimension, or the residuals of the X variables in subsequent dimensions, and the Y or Y residuals scores U(Y).

The **w**'s are the weights that combine the X variables (first dimension) or the residuals of the X variables (subsequent dimensions) to form the scores t. These weights are selected so as to maximize the covariance between T and U, thereby indirectly T and Y.

X variables with large w's (positive or negative) are highly correlated with U(Y).

Variables with large w's are situated far away from the origin (on the positive or negative side) on the plot.

16.5.12.6 W* loadings (X): w*1 vs. w*2, ...

For every PLS dimension the **W***'s are the weights that combine the original X variables (not their residuals as with w) to form the scores t.

W^* is computed as follows:

$W^* = W(P'W)^{-1}$

From this formula we can see that w^* is equal to w in the first dimension.

Also, when P is equal to W (for all dimensions), W^* is equal to W because W'W (and P’W) is equal to 1.

16.5.12.6.1 Relation of W* to the PLS regression coefficients

For a given response Y, the PLS regression coefficients are (for the model Y = XB):

$B = W(P'W)^{-1}C'$

or

$B = W^*C'$ and $Y = XW^*C'$

Hence, W^* is directly related to the PLS regression coefficients.

16.5.12.7 C loadings (Y): c1 vs. c2, ...

C loading plots display the correlation between the Y variables and T(X). The **c**'s are the weights that combine the Y variables with the scores **u**, so as to maximize their correlation with X. Y variables with ***large*** **c's** are highly correlated with T(X).

16.5.12.8 WC or W*C loadings (X&Y): wc1 vs. wc2, ...

WC or W*C loading plots show ***both*** the X-weights (**w or w***) and Y-weights (**c**), and thereby the correlation structure between X and Y. One sees how the X and Y variables combine in the projections, and how the X variables relate to Y.

16.5.12.9 TPS scores (X): tPS1 vs. tPS2, ...

The plots on the **Predict** tab classify (new) observations in the predictionset with respect to a PC or PLS model and predicts responses (values of Y variables) for (new) observations (PLS).

For a given set of observations, SIMCA computes the predicted scores: tPS. With missing data in the new observation (denoted by z below), these scores are calculated by means of PLS and the model below, according to Nelson, Taylor, and MacGregor (see reference list).

z = P*tPS + e

16.5.13 Distance to the model

This section describes the different distances to the model available in SIMCA for observations in the workset or in the predictionset.

- Absolute distance to the model of an observation in the workset
- Normalized Distance to the model of an observation in the workset
- Distance to the model of new observations in the predictionset
- MPow weighted distance to the model
- Critical distance to the model
- Membership significance level

16.5.13.1 Absolute distance to the model of an observation in the workset - DModX, DModY(Absolute)

For observations in the workset, SIMCA computes the observation distance to the model in the X space, DModX, and in the Y space, DModY (for PLS models). These distances are equivalent to X and Y residual standard deviations, respectively.

16.5.13.1.1 DModX absolute

DModX of an observation in the workset (i.e., that was part of the model) is computed as:

s_i= sqrt(Σe_{ik}^2 / (K - A))* v

The summation is made over the X variables (k) and $\mathbf{e_{ik}}$ are the X-residuals of observation i.

v is a correction factor (function of the number of observations and the number of components) and is slightly larger than one.

This correction factor takes into account the fact that the distance to the model (DModX) is expected to be slightly smaller for an observation that is part of the workset since it has influenced the model.

16.5.13.1.2 DModY absolute

DModY of an observation in the workset (i.e., that was part of the model) is computed as:

s_i= sqrt(Σf_{im}^2/ M)

The summation is made over the Y variables (m) and f_{im} are the Y residuals of observation i.

16.5.13.1.3 DModY absolute for OPLS/O2PLS

DModY of an observation in the workset, when the fit method is OPLS/O2PLS is computed as:

s_i= sqrt(Σf_{im}^2/ M) * v

The summation is made over the Y variables (m) and f_{im} are the Y residuals of observation i.

16.5.13.2 Normalized distance to the model of an observation in the workset - DModX, DModY (Normalized)

The normalized distance to the model is the observation absolute DModX or DModY divided by the pooled RSD of the model, s_0, in the X space and in the Y space.

The pooled RSD for the X space is calculated as:

s_0= √($\Sigma\Sigma e_{ik}^2$/((N - A - A_0)*(K - A)))

$\mathbf{A_0}$ = 1 if model is centered, 0 otherwise.

16.5.13.2.1 DModX normalized

DModX normalized = s_i/s_0

where

s_i is the absolute DModX.

s_0 is the pooled RSD for the X space.

The pooled RSD for the Y space is calculated as:

$s_0 = \sqrt{}(\Sigma\Sigma f_{im}^2/ ((N - A - A_0)*M)))$

16.5.13.2.2 DModY normalized

DModY normalized = s_i/s_0

where

s_i is the absolute DModY.

s_0 is the pooled RSD for the Y space.

16.5.13.3 Absolute distance to the model of new observations in the predictionset - DModXPS, DModYPS (Absolute)

The absolute distance to the model DModXPS of a new observation is computed as the observation RSD:

$s_i = \sqrt{}sqrt(\Sigma e_{ik}^2 / (K - A))$

The difference in the formula in comparison with the calculation of DModX is that the correction factor in not present.

The distance to the model in the Y space, DModYPS, of a new observation (i.e., that was not part of the model) is computed in the same way as DModY, that is, for an observation that was part of the model:

$s_i = \sqrt{}(\Sigma f_{im}^2/ M)$

16.5.13.4 Normalized distance of a new observation to the model - DModXPS, DModYPS (Normalized)

The normalized distance to the model is the observation absolute DModXPS or DModYPS divided by the pooled RSD of the model (not the predictionset) s_0:

Normalized DModXPS = s_i/s_0

where

$s_0 = \sqrt{}(\Sigma\Sigma e_{ik}^2/ ((N - A - A_0)*(K - A)))$

Normalized DModYPS = s_i/s_0

where

$s_0 = \sqrt{}(\Sigma\Sigma f_{im}^2/ ((N - A - A_0)*M)))$

A_0 = 1 if model is centered, 0 otherwise.

16.5.13.5 Distance to the model augmented - DModXPS+ (Absolute) or (Normalized)

With predictions, the distance to the model can be augmented with a term measuring how far outside (d) the acceptable model domain the projection of the observation falls. The result is called DModXPS+. Hence, for an observation in the predictionset (hence the “PS” label), this is:

$DModXPS+ = [DModXPS^2 + d^2]^{1/2}$

where

$d = \sum d0_i^2 * S2X_i/(SDt(i))^2$

for components i = 1 to A.

d0 is the distance between the score value t and the score limit for component i for an observation in the predictionset. If t is within the limits, d0 is zero. The score limits are:

Upper limit: Max(t) + SDt/2

Lower Limit: Min(t) - SDt/2

$S2X_i$ is the residual variance.

Here the distance from the projected point of the observation to the model domain is re-expressed in the same units as the residuals by multiplication by the RSD of the workset (s0) and division by the pooled standard deviation of the score vectors in which the projected point is outside the acceptable interval.

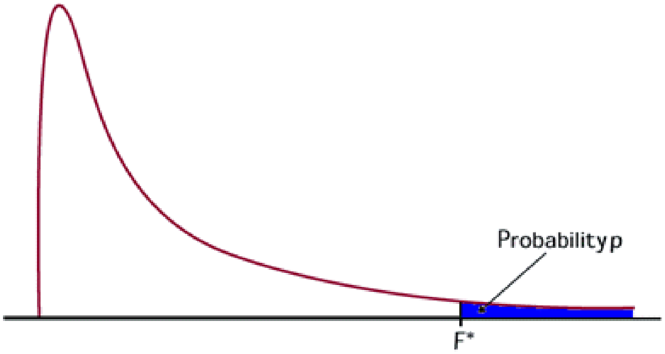
The DModXPS+ can be expressed in absolute or normalized, and weighted by the modeling power, just like DModXPS.

16.5.13.6 MPow weighted distance to the model - DModX, DModXPS, DModXPS+ (Abs/Norm and weighted)

With MPow weighted DModX/DModXPS/DModXPS+, that is, distance to the model for the X-block weighted by the modeling power, the observation RSD is computed with weighted residuals, where the weights are the modeling powers of the variables.

16.5.13.7 Critical distance to the model

The critical limit for the distance to model measure (DCrit) is calculated by taking the square root of an inverse cumulative F-distribution function. The three input parameters for this function are the significance level and the degrees of freedom of the numerator and the denominator of the F-distribution. In this case, the numerator is the degrees of freedom of the observations in the training set (DF_obs) and the denominator is the degrees of freedom of the model (DF_mod). DCrit is equal to the value F* in the figure below where the blue area is the probability p that an observation will be outside the DCrit limit. For example, if the significance level is set to 0.95, typically 95% of the observations would have a DModX value below DCrit. The exact shape and scale of the curve is determined by the degrees of freedom. The F* value can be extracted from statistical tables of the F-distribution.



In SIMCA, the value of the degrees of freedom for the model is calculated as:

DF_mod = √((N - C - A)*(K - A))

where

N = number of observations

C = 1 if all X variables are centered, else 0

A = number of components

K = number of X variables

(*DF_mod* cannot be smaller than 1)

The value of the degrees of freedom for the observations is calculated as:

If *K* > *DF_mod*

DF_obs = (M + Q – A) / CORR

else

DF_obs = (M – A) / CORR

where

M = the smallest value of *[K, 100, DF_mod]*

Q = square root of (K-DF_mod)

CORR = N / (N - C - A)

(*N - C - A* and *DF_obs* cannot be smaller than 1).

The expressions above result in a normalized DCrit value. If the critical limit is to be presented in absolute values, DCrit is multiplied by the residual variance in X.

16.5.13.8 Membership significance level

As default, observations with a probability of class membership less than 5% are considered non-members.

16.5.14 Variable importance, VIP

For PLS, SIMCA computes the influence on Y of every term (x_k) in the model, called VIP (variable importance in the projection). VIP is the sum over all model dimensions of the contributions VIN (variable influence). For a given PLS dimension, **a**, $(VIN)_{ak}^2$ is equal to the squared PLS weight $(w_{ak})^2$ of that term, multiplied by the explained SS of that PLS dimension.

The accumulated (over all PLS dimensions) value,

$VIP_{ak}^2 = \Sigma(VIN)_k^2$

where the summation is made over a = 1 to A.

This value is then divided by the total explained SS by the PLS model and multiplied by the number of terms in the model.

The final VIP is the square root of that number.

The formula can also be expressed as:

$$VIP_{PLS} = \sqrt{K \times \left(\frac{\left[\sum_{a=1}^{A}(W_a^2 \times SSY_{comp,a})\right]}{SSY_{cum}}\right)}$$

Thus the Sum of squares of all VIP's is equal to the number of terms in the model hence the average VIP is equal to 1. One can compare the VIP of one term to the others. Terms with large VIP, larger than 1, are the most relevant for explaining Y.

For OPLS, SIMCA computes three VIP vectors according to;

$$PRED\_VIP_{OPLS} = \sqrt{K_p \times \left(\frac{\left[\sum_{a=1}^{A_p}\left(P_a^2 \times SSX_{comp\ ,a}\right)\right]}{SSX_{cum}} + \frac{\left[\sum_{a=1}^{A_p}\left(P_a^2 \times SSY_{comp\ ,a}\right)\right]}{SSY_{cum}}\right)}$$

$$ORTH\_VIP_{OPLS} = \sqrt{K_o \times \left(\frac{\left[\sum_{a_o=1}^{A_o}\left(Po_{a_o}^2 \times SSX_{comp\ ,ao}\right)\right]}{SSX_{cum}} + \frac{\left[\sum_{a_o=1}^{A_o}\left(Po_{a_o}^2 \times SSY_{comp\ ,ao}\right)\right]}{SSY_{cum}}\right)}$$

$$TOT\_VIP_{OPLS} = \sqrt{\frac{K}{2} \times \left(\begin{array}{c}\frac{\left[\sum_{a_o=1}^{A_o}\left(Po_{a_o}^2 \times SSX_{comp\ ,ao}\right)\right]}{SSX_{cum}} + \frac{\left[\sum_{a=1}^{A_p}\left(P_a^2 \times SSX_{comp\ ,a}\right)\right]}{SSX_{cum}} + \\ \frac{\left[\sum_{a_o=1}^{A_o}\left(Po_{a_o}^2 \times SSY_{comp\ ,ao}\right)\right]}{SSY_{cum}} + \frac{\left[\sum_{a=1}^{A_p}\left(P_a^2 \times SSY_{comp\ ,a}\right)\right]}{SSY_{cum}}\end{array}\right)}$$

In the expressions above,

- $PRED\_VIP_{OPLS}$ represents the VIP value for the predictive components in an OPLS model,
- $ORTH\_VIP_{OPLS}$ corresponds to the VIP value for the orthogonal components in an OPLS model, and

- TOT_VIP_{OPLS} represents the total sum of VIP for both predictive and orthogonal parts of an OPLS model.

Furthermore, predictive components are represented by a and orthogonal components by a_o. Analogously, A_p is the total number of predictive components and A_o is the total number of orthogonal components. K is the total number of variables. The sum of squares (SS) has the subscript *comp* for the explained SS of ath component and the subscript *cum* for the cumulative (i.e. total) explained SS by all components in the model.

16.5.15 Standard error and jack-knifing uncertainties

SIMCA computes standard errors on the predicted Y values in two different ways:

- According to Höskuldsson resulting in the Serr vectors.
- From Jack-knifing resulting in error bars in plots.

16.5.15.1 Standard error according to Höskuldsson - Serr

The variance of the prediction (Yhat) for a given response y at a point X_0 according to Höskuldsson, is computed as:

$V(Yhat) = (1/N + t_0\ (T'T)^{-1}\ t_0'\ )\sigma^2$

where

t_0 are the scores t of observation X_0

σ^2 is the y error variance estimated from the Sum of Squares of the residuals of y divided by the degrees of freedom for PLS, i.e. ($N - A - A_0$).

A = number of PLS components and A_0 is 1 or 0, depending on whether y is centered or not.

Confidence intervals can be computed from the standard error by multiplying by a t (distribution) value with the appropriate degrees of freedom.

16.5.15.2 Jack-knifing (JK) uncertainties

Jack-knifing is a method for finding the precision of an estimate, by iteratively keeping out parts of the underlying data, making estimates from the subsets and comparing these estimates.

In both PCA and PLS, the set of multiple models resulting from the cross-validation is used to calculate jack-knifing uncertainty measures (standard errors and confidence intervals) of scores, loadings, PLS-regression coefficients, predicted Y-values, and VIP. These are displayed by default in column plots, and can also be listed by right-clicking the plot and clicking **Create list**.

Right-clicking a column plot and clicking **Properties**, clicking the **Limits** tab, and then selecting **None** as confidence limit provides the means to remove the confidence intervals if desired.

The standard formula of JK is used (see e.g., B. Efron and G. Gong).

16.5.15.2.1 Reference Jack-knifing

1. Efron, B., and Gong, G., (1983), A Leisurely Look at the Bootstrap, the Jack-knife, and Cross-validation, American Statistician, 37, 36-48.

16.5.16 Coefficients

The PLS model parameters are used to re-express the Y variables as multiple regression models of the X variables:

$Y = XB$

where

X refers to the X matrix, including squared and/or cross terms if those were added

Y is the matrix of responses.

The values of the regression coefficients depend on the scaling of X and Y.

Note*: These coefficients are usually* **not** *independent unless X has been generated by a statistical design.*

The types of coefficients available are described in the subsections that follow.

For the OPLS/O2PLS specific Y-Related profiles, see the Y-Related profiles subsection earlier in this chapter.

16.5.16.1 Scaled and centered coefficients - CoeffCS

CoeffCS are the coefficients when X is scaled and centered and Y is scaled. These coefficients are used for interpreting the influence of the variables X on Y.

The scaling weights are those selected in the workset, usually to give the X and Y variables unit variance (autoscaling).

The centered and scaled coefficients are expressed according to the following formula:

$y * ws_m = ybar * ws_m + b_k(x_k - xbar_k) * ws_k + ...$

$... + b_{kk}(z_k^2 * ws_k^2 - m_{kk}) * v_k + ...$

$... + b_{jk}(z_j * z_k * ws_j * ws_k - m_{jk}) + v_{jk} + ...$

where

$z_k = (x_k - xbar_k)$

ws_m = Scaling weights of response y_m

ws_k = Scaling weights of variable x_k

m_{kk} = Average of z_k^2

m_{jk}= Average of $z_j * z_k$

v_k = Scaling weight of z_k^2

v_{ij}= Scaling weight of $z_i * z_j$

16.5.16.2 Coefficients MLR - CoeffMLR

CoeffMLR are the coefficients when Y is unscaled and uncentered and X is scaled and centered and the second centering and scaling of the squared and cross terms has been removed.

$y = b_0 + b_k(x_k - xbar_k) * ws_k + ...$

$... + b_{kk}(z_k^2 * ws_k^2) + ...$

$... + b_{ik}(z_i * z_k * ws_i * ws_k) + ...$

where

$z_k = (x_k - xbar_k)$

ws_k = Scaling weights of variable x_k

These coefficients correspond to the multiple regression coefficients.

16.5.16.3 Coefficients unscaled - Coeff

The coefficients when X and Y are unscaled and uncentered are expressed as follows:

$y_m = b_0 + b_1x_1 + \dots + b_kx_k + b_{11}x_1^2 + b_{12}x_1x_2 + \dots$

The unscaled coefficients should be used only for computations, for example contour plots, but are difficult to interpret because of the differences in units between the raw variables.

Note: When x was transformed in the model it also needs to be transformed when used in the equation.

16.5.16.4 Rotated coefficients

When working with spectral data, it is often desirable to estimate the pure spectral profile as they relate to Y.

The PLS coefficients as relating to centered and scaled data are expressed as

$B = W(P'W)^{-1}C'$

The rotated coefficients are obtained by the transformation of the **B** matrix into the pure constituent profile estimates, $\mathbf{K}_{PLS}$.

$K_{PLS} = B(B^TB)^{-1}$

This corresponds to a projection of the X space into the B space, in order to estimate the pure constituents profile from Y, in other word a direct calibration.

Rotating the coefficients is warranted not only with spectral data, but in any situation, similar to indirect calibration, where Y is assumed to contribute additively to the variation in X.

16.5.16.5 Reference rotated coefficients

1. Trygg, J., (2004), *Prediction and Spectral Profile Estimation in Multivariate Calibration*, Journal of Chemometrics, 18, 166-172.

16.5.16.6 Coefficients with Y unscaled uncentered, X unscaled centered - CoeffC

The coefficients when Y is unscaled and uncentered, and X is unscaled but centered, are computed as follow:

$y = ybar + b_k(x_k - xbar_k\ ) + ...$

$... + b_{kk}(z_k^2 - m_{kk}) + ...$

$... + b_{jk}(z_j * \ \ z_k - m_{jk}) + ...$

where the terms are defined as for the other coefficients.

Note: CoeffC cannot be selected in the **Properties** dialog of the **Coefficient Plot** only in the **Plot/List** tab dialogs.

16.5.17 RMSEE, RMSEP and RMSECV

A popular plot to interpret the performance of a regression model is the scatter plot showing the relationship between the observed Y and the predicted Y. Such a plot can be constructed both for the workset observations and the predictionset observations, provided that the observed Y is known for the latter group.

By using the regression line tool in SIMCA, the resulting R2 of the regression line can be used to quantify the strength of the association between the observed Y and the predicted Y for the workset observations. The closer to unity the stronger the association. The drawback of the obtained association measure, however, is that neither it (R2) nor its residual correspondence (1-R2) relate to the measurement unit of the observed Y.

It is possible to obtain a performance measure that relates to the unit of the observed Y, which is denoted Root Mean Square Error of Estimation (RMSEE). RMSEE is computed as $\sqrt{}(\sum(Yobs-Ypred)^2/(N-1-A))$, where Yobs-Ypred refers to the fitted residuals for the observations in the workset. RMSEE measures the fit of the model. An analogous parameter for the predictionset is denoted Root Mean Square Error of Prediction (RMSEP). RMSEP is computed as $\sqrt{}(\sum(Yobs-Ypred)^2/N)$, where Yobs-Ypred refers to the predicted residuals for the observations in the predictionset. RMSEP measures the predictive power of the model.

An alternative predictivity measure for the model is available through summarizing the cross-validation residuals of the observations in the workset. The predictivity measure obtained is called Root Mean Square Error from cross-validation (RMSECV). RMSECV can be regarded as an intermediary to RMSEE and RMSEP, as it applies to the workset (as does RMSEE) but indicates predictive power (as does RMSEP). The RMSEE, RMSEP and RMSECV values are listed at the bottom of plots wherever these parameters are applicable.

RMSECV is available as a separate plot in the **Analysis** group on the **Analyze** tab, allowing the evolution of RMSECV across the model components to be displayed.

For OPLS and O2PLS models with 1+x+0 components, the RMSEcv plot is displayed showing the progression. For more see the RMSECV plot subsection in Chapter 10, Analyze.

16.6 Transform page criteria

In the **Transform** page in the **Workset** dialog the **Min/Max** and **Skewness** values are colored red when a transformation is recommended.

The criteria are:

- **Min/Max** is colored red when 0 <= Min/Max < 0.1.
- **Skewness** is colored red when sTest < -2 or 2 < sTest

where

sTest = Skewness/(√(6.0*dN*(dN-1.0)/((dN-2.0)*(dN+1.0)*(dN+3.0))))

Skewness is the skewness value listed in the variable list.

dN = number of non missing values in the variable and has to be equal to or larger than 3.

16.6.1 Automatic transformation criteria

When using the **Transform** button to automatically log transform when appropriate, the criteria used to decide if a log transform is needed is the same criteria as used for coloring Skewness and Min/Max red, with the following additions:

- When calculating **Min/Max** the Min value used is the smallest not counting 0.
- The number of non-missing values has to be larger than 4 and larger than 0.1*number of rows in the dataset.

C2 is calculated as follows:

1. If all values are positive: C2=0.
2. If there are values that are 0 or negative: C2=abs(smallest non-zero value)/2.
3. If there are negative values: Add abs(smallest non-zero value) to C2 calculated in step 2.

16.7 Scaling

The results of both PC and PLS modeling are scale dependent. Selecting the scaling of the variables is therefore an important step in fitting projection models such as PC or PLS.

The SIMCA default for all selected variables is a unit variance base weight and a block scaling factor of 1 (no block scaling). For more, see the Scaling variables section in Chapter 7, Home.

This section describes the computation of autoscaling, block scaling, the scaling weight, the scaling of expanded terms, transformed variables, lagged variables, variables in classes, scaling after reselecting observations, and calculation of the scaling weight.

16.7.1 Autoscaling

If one has no prior information about the importance of the variables, autoscaling all variables to unit variance (UV) is recommended. This is equivalent to making all of the variable axes have the same length, which is, giving all of the variables equal importance.

If one has prior information about the importance of the variables, it may be desirable to scale some variables up or down, by modifying their unit variance weights.

16.7.2 Block scaling

Block-wise scaling is warranted when a data table contains several types (blocks) of variables, with a highly different number of variables in each block. Block-wise scaling allows each block to be thought of as a unit and to be given the appropriate variance which is smaller than if each variable was autoscaled to unit variance.

In such cases you can select to scale a block, i.e., a number of variables of the same type, such that the whole block has

√(Kblock)

or

√(√(Kblock))

variance, where Kblock is the number of variables in the block.

16.7.3 Scaling weight calculation

The final scaling weight (Xws or Yws) is the product of:

- Base weight, usually Unit Variance.
- Block scaling weight.

- Modifier (default = 1; used to scale variables up or down relative to the base scaling weight).

When the variable is not blocked (block scaling weight = 1) and when the modifier is equal to 1, the scaling weight is equal to the base weight.

16.7.4 Scaling of expanded terms

Expanded variables, i.e. squares, cross or cubic terms are displayed in the **Scale** page. You can block scale expanded terms and/or change their modifier, but you cannot change the base type as it is inherited from the mother variable.

Note: *Whenever you change the base type of the mother variables, the scaling of both lagged variables and expanded terms is re-computed accordingly.*

16.7.4.1 Computation

To compute expanded variables, all mother variables are first always centered (even if mother variables in themselves are uncentered) and then scaled as specified by the base type of the mother variables.

16.7.4.2 *Scaling and centering of the expanded term after computation*

Expanded variable are scaled using the scaling base type of the mother variables.

For cross terms, if mother variables have different scaling types, the expanded term inherits the scaling type of the majority, or for 2 factor interactions the highest ranking scaling type.

The hierarchy of scaling types is as follow:

- **Centered** and then **Noncentered**.
- **UV**, **Pareto**, and then **None**.

16.7.5 Scaling weights for transformed variables

When variables are transformed, the scaling weights are those of the transformed variables.

If you later further transform a variable, the scaling weight is re-computed according to the base type.

If you transform a variable after selecting base type **Freeze**, the scaling weight is not recomputed. It is frozen with the status of the variable and the current selection of observations at the time you selected **Freeze** as base type.

16.7.6 Scaling of variables with classes

When you have grouped observations in classes, and fitted a PC or PLS class model, the scaling weights of the variables are computed using the observations in the class. If a variable has zero variance within the class observations, this variable is not excluded but is given a scaling weight based on the observations of the whole workset.

16.7.7 Scaling of lagged variables

The lagged variables, by default, inherit the scaling weight (and transformation) of the mother variables, but always centers the variable. It is strongly recommended not to change the scaling weight of lagged variables.

16.7.8 Scaling after changing the observation selection

The scaling weights of all variables, except those with base type **Frozen**, are recomputed when you change the selection of observation.

The scaling weights of variables with a frozen base type are not computed when the selection of observations is changed after **Freeze** was selected as base type.

16.8 Cross validation

16.8.1 Cross validation for PCA

The cross validation works as follows:

1. Parts of the X data are kept out of model development.
   SIMCA uses the approach of Krzanowski [1] where in two sub rounds, data are first kept out observation-wise (row-wise) to get a set of loading vectors, and second data are kept out variable-wise (column-wise) to get a set of score vectors.

2. The kept out parts are then predicted by the model.
3. The predictions of the kept out parts are compared with the actual values.
4. 1-3 is repeated until all parts have been kept out once and only once.

PRediction Error Sum of Squares - PRESS

The prediction error sum of squares (PRESS) is the squared differences between observed and predicted values for the data kept out of the model fitting. The prediction of the (i, k) element in scaled and centered form is the ith score value multiplied by the kth loading value, where both have been estimated in a CV round when this element was kept out.

This procedure is repeated several times until every data element has been kept out once and only once. The final PRESS then has contributions from all data.

For each component consecutively, SIMCA computes the overall PRESS/SS, where SS is the residual sum of squares of the previous component. SIMCA also computes $(PRESS/SS)_k$ for each X variable (x_k).

Data kept out observation and variable wise

A special (proprietary) PC estimation is used in the CV rounds to minimize the tendency for the present component to partly rotate into later components.

16.8.2 Cross validation for PLS, OPLS and O2PLS

The cross validation works as follows:

1. Rows of the X/Y-data are kept out of model development
2. The kept out parts are then predicted by the model.
3. The predictions of the kept out parts are compared with the actual values.
4. 1-3 is repeated until all parts have been kept out once and only once.

PRediction Error Sum of Squares - PRESS

The prediction error sum of squares (PRESS) is the squared differences between observed and predicted values for the Y-data kept out of the model fitting. The prediction of the (i, m) element in scaled and centered form is the ith score value multiplied by the mth loading value, where both have been estimated in a CV round when this element was kept out.

This procedure is repeated several times until every data element has been kept out once and only once. The final PRESS then has contribution from all data.

16.8.2.1 PLS Specific

For each component consecutively, SIMCA computes the overall PRESS/SS, where SS is the residual sum of squares of the previous component. This type of cross validation is usually named partial cross validation. SIMCA also computes $(PRESS/SS)_m$ for each Y variable (x_m).

16.8.2.2 OPLS and O2PLS Specific

The OPLS and O2PLS cross-validation is performed as follows:

1. The number of predictive or joint X/Y components is estimated; this number may be adjusted using rule R2 after calculating all predictive and orthogonal components.
2. The number of orthogonal components in X and Y are decided.

For these steps, rule R1 is used to determine the significance of the components.

For all included components, SIMCA computes the overall Q2=1-PRESS/SS, where SS is the sum of squares of Y. This type of cross validation is called full cross validation. SIMCA also computes $(Q2)_m$ for each Y variable.

The cross validation for the Orthogonal in X(PCA) and the Orthogonal in Y(PCA) is performed as for the regular PCA above.

16.8.3 Reference cross validation

1. Eastment, H. and Krzanowski, W., *Crossvalidatory choice of the number of components from a principal component analysis*, Technometrics 24 (1982) 73-77.

2. Martens, H and Naes, T., *Multivariate Calibration*, 1989.

16.8.4 Cross validation rules - Significant component

When calculating the PCA orthogonal components of O2PLS, the cross validation rules for PCA apply.

16.8.4.1 Rule 1: R1

A component is significant according to **Rule 1 when**

Q^2 > Limit

where

Limit = 0 for PLS models with more than 100 observations.

Limit = 0.05 for PLS models with 100 observations or less.

Limit = 0.01 for OPLS and O2PLS.

Limit depends on the number of components for PCA. The limit increases with subsequent components to account for the loss in degrees of freedom.

The significance limit for each component is displayed in the **Model Window**.

16.8.4.2 Rule 2: R2 for PCA

A component is significant according to **Rule 2 when**

Q^2V> Limit for at least

- 20% of the x-variables when K > 25.
- sqrt(K)*log10(max(10, K-20)) when K $\leq$ 25.

K = number of x-variables.

Q^2V is Q^2 for individual variables.

Provided the eigenvalue > 1.5 or K < 30.

16.8.4.3 Rule 2: R2 for PLS, OPLS and O2PLS

A component is significant according to **Rule 2 when**

Q^2V> Limit for at least

- 20% of the y-variables when M $\geq$ 25.
- sqrt(M) when M < 25.

M = number of y-variables.

Q^2V is Q^2 for individual variables.

16.8.4.4 Rule 3: U and R5

With PCA when a component is insignificant it is first labeled U (Undecided). If the next component is significant and has a similar eigenvalues (tolerance of 5%) as the previous one, then both component together are considered significant. The U of the undecided component is changed to R5.

16.8.5 Cross validation rules - Non significant component

The significance column of the model summary for a “non significant” component is marked **NS**, **N3**, or **N4**. When calculating the PCA orthogonal components of O2PLS, the cross validation rules for PCA apply.

16.8.5.1 N3

The component is not significant when the remaining data for that component have insufficient degrees of freedom. For PCA, SIMCA stops when the number of extracted components is larger than N/2 or K/2 whichever is smaller.

16.8.5.2 N4

The component is not significant according to rule 4 when the explained variance for X (PC) / Y (PLS) is less than 1% and no variable has more than 2% (PC) / 3% (PLS) explained variance.

16.8.5.3 NS

The component is not significant according to rule 1 or rule 2 and N3 and N4 do not apply.

NS is only displayed when the component is computed with cross validation.

Note*: N3 and N4 are always displayed when applicable, irrespective of whether cross validation was used or not.*

16.8.6 Cross validation rules for batches

The cross validation rules for batch evolution models fitted with PLS are different from other types of models since the objective here is to extract as much of X as possible.

The cross validation rules are:

- Minimum of 3 components, if R2X = 85 % continue if next component R2X > 7% and then next component if R2X > 5%.
- As many as needed to reach R2X of 85% not exceeding N/2.
- K/2 or 15 comp (K=Number of variables) whichever smaller and stop when R2X of a component is less than 3%.

For batch evolution models fitted with OPLS the cross validation rules are the same as for a regular OPLS model.

16.8.6.1 Rule 1: RB1

As long as 85% has NOT been reached and a component explains more than 5% of R2X, it is considered significant and labeled RB1.

16.8.6.2 Rule 2: RB2

As long as 85% has NOT been reached and a component explains 3 - 5% of R2X, it is considered significant and labeled RB2.

16.8.6.3 NB1 - stopping rule

NB1, stopping rule, is the label when the number of component exceeds one of the following:

- N/2
- K/2
- 15

16.8.6.4 NS - Not Significant

The component explains less than 3% of R2X and is considered not significant. The label is NS.

16.9 PLS time series analysis

Processes often have a “memory”, i.e., the state of the process at time **t** is influenced by the state at earlier times, i.e., **t-1**, **t-2**, **t-3**, ..., etc. To model such processes with “memory”, Box-Jenkins time series models, ARMA, and ARIMA models (autoregressive / integrated / moving average), have been widely used in process modeling and control. A time series model is basically formulated as an ordinary regression model, but including also *lagged* variables, possibly in both X and Y:

$Y_{t,m} = b_{0m}X_t + b_{1m}X_{t-1} + b_{2m}X_{t-2} + \ldots + c_{1m}Y_{t-1} + c_{2m}Y_{t-2} + \ldots + e_t$

The main problem with this model formulation has been that the predictor variables ($X_{t,}$ X_{t-1}, etc.) usually are very collinear and also noisy. Multiple regression with its assumptions of independence and preciseness of the predictors is therefore difficult to use for the model estimation.

With PLS, however, collinear and noisy predictor variables do not cause any particular problems, so the model can be directly estimated on the form above. Technically, this is done in SIMCA by creating an expanded predictor matrix, $\mathbf{X}^*$, that contains the appropriate selection of the original variables, plus ***lagged*** variables, i.e., time shifted one, two, or any selected time units.

The PLS analysis of the relationship between $\mathbf{X}^*$ and the pertinent **Y** is straightforward, and will give the ordinary PLS parameters, X and Y-scores **t** and **u**, weights **w** and **c**, and regression coefficients, **b**. These can be plotted and interpreted in the same way as with ordinary PLS models. Additionally, plots of weights (**w**) and coefficients (**b**) for the different lags of a single variable are of interest for the identification of the most important lag.

In this way time series analysis is incorporated in the same framework of modeling as ordinary data analysis of “non-dynamic” data, reducing the complexity and difficulties involved.

16.9.1 References PLS time series

1. Efron, B., and Gong, G., (1983), *A Leisurely Look at the Bootstrap, the Jack-knife, and Cross-validation*, American Statistician, 37, 36-48.

2. Eastment, H. and Krzanowski, W., (1982), *Crossvalidatory choice of the number of components from a principal component analysis*, Technometrics 24 73-77.

3. Höskuldsson, A., *PLS regression methods.* J. Chemometrics, 2, (1988) 211-228.

4. Nelson, P.R.C., Taylor, P.A., MacGregor, J.F., *Missing Data Methods in PCA and PLS: Score Calculations with Incomplete Observation*, Chemometrics and Intelligent Laboratory Systems, 35, 45-65, 1996.

16.10 CV-ANOVA

CV-ANOVA, ANalysis Of VAriance testing of Cross-Validated predictive residuals, is a diagnostic tool for assessing the reliability of PLS, OPLS and O2PLS models. It is implemented for single-Y and multiple-Y models for the relation X → Y. The diagnostic is based on an ANOVA assessment of the cross-validatory (CV) predictive residuals of a PLS, OPLS or O2PLS model. The advantages of using the CV-residuals are that no extra calculations are needed and that this procedure secures reasonably independent data and variance estimates.

Formally, ANOVA is a method to compare two models by the size of their residuals when fitted to the same data [1, 2, 3, 4]. In the regression context, the two models compared are:

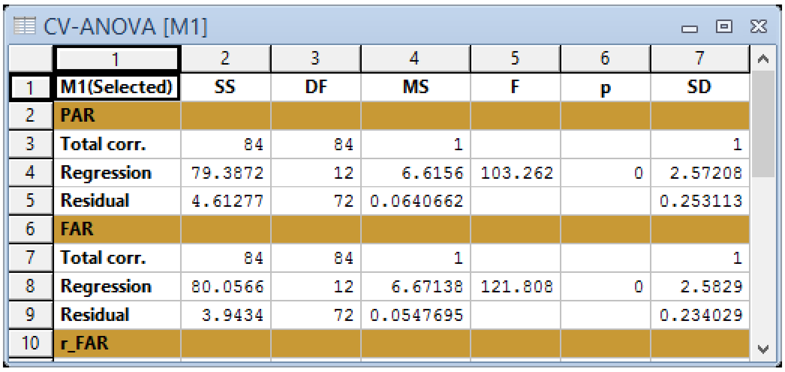
y_i = constant + d_i (1)

y_i = constant + bx_i + e_i (2)

The ANOVA is then made on the size of the sum of squares, SS(d) and SS(e), noting that they are not independent since the data underlying them (y) are the same. In the current context, this means that we test whether the (PLS/OPLS/O2PLS) model has significantly smaller cross validated predictive residuals than just the variation around the global average. In summary, the CV-ANOVA provides a significance test (hypothesis test) of the null hypothesis of equal residuals of the two compared models.

16.10.1 The ANOVA table

The output of the CV-ANOVA is given in a tabulated format using the conventional ANOVA lay-out (see illustration below).



CV-ANOVA [M1]

	1	2	3	4	5	6	7
1	M1(Selected)	SS	DF	MS	F	p	SD
2	PAR						
3	Total corr.	84	84	1			1
4	Regression	79.3872	12	6.6156	103.262	0	2.57208
5	Residual	4.61277	72	0.0640662			0.253113
6	FAR						
7	Total corr.	84	84	1			1
8	Regression	80.0566	12	6.67138	121.808	0	2.5829
9	Residual	3.9434	72	0.0547695			0.234029
10	r_FAR						

In the ANOVA table, the following numbers are displayed:

Vector	Type	Description
SS	Total corr (Total corrected)	SS of the Y of the workset corrected for the mean.

Vector	Type	Description
	Regression	Fraction of Total Corrected SS accounted for by the model, estimated via the cross validation principle.
	Residual	Difference between Total Corrected and Regression SS, i.e., the fraction of Total Corrected unaccounted for by the model.
DF	Total corr, Regression, residual	The number of degrees of freedom (DF). This is an approximate number based on the experience that PLS needs half the components to reach the same explanation of Y as principal components regression.
MS	Total corr, Regression, residual	By dividing each SS by the respective DF, the corresponding mean squares (MS), or variances, are obtained.
F		The F-test, based on the ratio MS Regression/MS Residual, formally assesses the significance of the model.
p		The p-value indicates the probability level where a model with this F-value may be the result of just chance. The common practise is to interpret a p-value lower than 0.05 as pointing to a significant model.
SD	Standard deviation.	Square root of MS.

The great benefit of CV-ANOVA is its user-friendliness. It brings the results of cross-validation to a familiar standard ANOVA format. Thus, CV-ANOVA can be seen as a formal test of the significance of the Q2YCV using the F-distribution. CV-ANOVA is fast and has a minimal additional computation time beyond the one of the standard cross validation.

The correctness of the CV-ANOVA requires that all experiments are independent. If there are replicated experiments or experiments from a time series the Degrees of Freedom will be difficult to estimate and that will give dubious results from the CV-ANOVA.

16.10.2 References CV-ANOVA

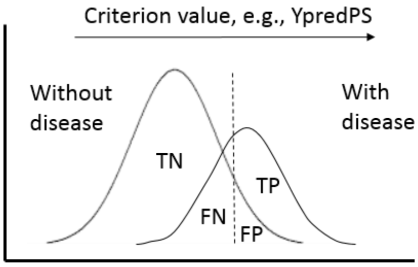
1. Box, G.E.P., Hunter, W.G., and Hunter, J.S. (1978). *Statistics for experimenters*. Wiley, New York. 2nd Edition, Wiley 2006.
2. Ståhle, L., and Wold, S., (1989), *Analysis of variance (ANOVA)*, Chemometrics and Intelligent Laboratory Systems, 6, 259-272.
3. Ståhle, L., and Wold, S., (1990), *Multivariate analysis of variance (MANOVA)*, Chemometrics and Intelligent Laboratory Systems, 9, 127-141.
4. Eriksson, L., Trygg, J., and Wold, S., *CV-ANOVA for significance testing of PLS and OPLS models*, submitted for publication 2008.

16.11 ROC - Receiver Operating Characteristic

A receiver operating characteristic curve, a ROC curve, is a graphical summary of the performance of a binary classifier. In SIMCA, a plot of a ROC curve can be created for class and discriminant analysis (DA) models.

In the following description of ROC the point of departure is a two-class PLS-DA or OPLS-DA model. When you consider the prediction results of such a discriminant analysis model for two classes – let´s say one class (population) with a disease and the other class (population) without the disease -- you will rarely observe a perfect separation between the two classes in terms of their YPredPS. Usually, the distribution of the test results will overlap, as shown in the figure below.

In the figure below, a moving threshold for classification or discrimination among the two classes is indicated. For every possible threshold you select to discriminate between the two classes, there will be some observations with the disease correctly classified as positive (TP = True Positive fraction), but some observations with the disease will be classified negative (FN = False Negative fraction). On the other hand, some observations without the disease will be correctly classified as negative (TN = True Negative fraction), but some observations without the disease will be classified as positive (FP = False Positive fraction).



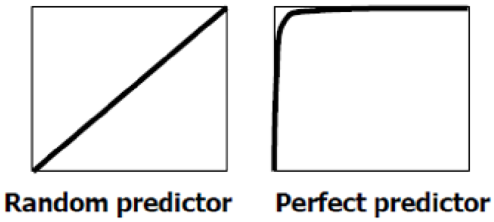
The different fractions (TP, FP, TN, FN) can be summarized to obtain the True Positive Rate (aka Sensitivity) and True Negative Rate (aka Specificity) of the classifier:

TPR = TP/(TP+FN)
TNR = TN/(TN+FP)

Thus, TPR (or Sensitivity) represents the probability that a test result will be positive when the disease is present and TNR (or Specificity) corresponds to the probability that a test result will be negative when the disease is not present.

The ROC curve is created by plotting the true positive rate (TPR) versus the false positive rate (FPR = 1 - TNR) at various threshold settings of the criterion parameter (PModXPS for class models and YPredPS for DA models); threshold settings are retrieved from the current predictionset. Thus, in other words, the ROC curve visualizes the classifier's Sensitivity versus 1 – Specificity.

Every point on the ROC curve represents a pair sensitivity/specificity values corresponding to a particular decision threshold. For a DA model YPredPS is used for thresholding and for a set of class models PModXPS is used for thresholding. Regardless of model type and thresholding parameter, a classifier with a perfect discrimination has a ROC curve that passes through the upper left corner (100% sensitivity, 100% specificity). Conversely, a ROC curve close to the 1:1 diagonal represents a very poor classifier.



Furthermore, when using normalized units the area under the curve (AUC) represents a quantitative performance measure of the classifier. It varies from 0.5 (random predictor) to 1.0 (perfect predictor).

16.12 Fisher's exact test

Fisher's exact test is derived from the probability of the particular classification result and all outcomes more extreme than the one observed. For a 2x2 contingency table the probability of a particular outcome is given by the formula below.

2 x 2 Table	Column 1	Column 2	Row Totals
Row 1	a	b	a + b
Row 2	c	d	c + d
Column Total	a + c	b + d	N

p = ((a + b)!(c + d)!(a + c)!(b + d)!)/(a! + b! + c! + d! + n!)

Where ! means factorial (the product of all numbers down to 1).

All probabilities more extreme than the observed pattern are computed and summed to give the probability of the table occurring by chance.

Fisher's probability is displayed in the Misclassification Table.

16.12.1 References Fisher's exact test

1. Fisher, R.A., (1922), *On the interpretation of χ2 from contingency tables, and the calculation of P*. Journal of the Royal Statistical Society 85(1):87-94.

2. Fisher, R.A., (1954), *Statistical Methods for research workers,* Oliver and Boyd.

3. Fisher, R.A., and MacKenzie, W., (1923), *Studies in Crop Variation. II. The manurial response of different potato varieties*, Journal of Agricultural Science, 13, 311-320.

16.13 Control chart statistics

This section describes the statistics described in the footers of the plots in the subsections:

- Nomenclature and notation
- Target and Standard deviation

16.13.1 Nomenclature and notation in control charts

In the control charts there are a number of statistics displayed in the footer of the plot. This subsection describes the statistics, the data source for the statistics, the standard deviation types calculated, and the model specific statistics.

See the table for a description of the statistics.

Statistic	Description
UCL	Upper Control Limit
LCL	Lower Control Limit
S	process standard deviation
Target	aim of the process
SAvg	average of standard deviation of subgroup
RAvg	average range of subgroup

In the table the available **data sources** *used to estimate S or Target are listed:*

There are a number of methods for estimating the standard deviation leading to different **types of standard deviations**. The different standard deviations are described in the table.

Method	Description
SAvg (within)	subgroup standard deviation estimated as the average standard deviation of the subgroups
SAvg (between)	between group standard deviation estimated as the **MSSD**
S	ordinary standard deviation when the sample size is 1
S(Target)	standard deviation estimated around the user entered target.

The **model specific statistics** available are described in the table. Model specific here means that they are calculated using the multivariate model.

Vector	Description
R2X[1]	Fraction of sum of squares for the first component.
Mxx-DCrit[last component]	critical distance in the DModX plot.
1 – R2X(cum)[last component]	1 – cumulative fraction of sum of squares up to the last component.

16.13.2 Target and standard deviation

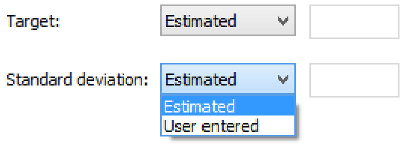
With all control charts, the **Target** and **Standard deviation** can be **Estimated** from the workset or **User entered**.

In the plots the following standard deviations and targets are displayed:

- **S(Mxx)** = process standard deviation over all observations in the model.
- **SAvg(within)** and **SAvg(between)** see the **Control limits…** sections in the sections for the respective plots. Displayed for >1 subgroups.

- **S(UE)** = user entered standard deviation. Displayed after selecting **User entered** in the **Standard deviation** box.
- **Target(Mxx)** = overall average when there are no subgroups. With subgroups, the average of the averages of the subgroups.
- **Target(UE)** = user entered target. Displayed instead of Target(Mxx) after selecting **User entered** in the **Target** box.

Note: When displaying plots with items from the predictionset, the estimated target and standard deviation values are computed from the workset of the selected model.


Target: Estimated

Standard deviation: Estimated

16.14 S-plot background

The S-plot is an easy way to visualize an OPLS discriminant analysis model of two classes. It has mainly been used to filter out putative biomarkers from “omics” data e.g. NMR, GC/MS and LC/MS metabolomics data.

In the S-plot both magnitude (intensity) and reliability is visualized. In spectroscopic data the peak magnitude is important as peaks with low magnitude are close to the noise level and thus have a higher risk for spurious correlation. The meaning of high reliability means high effect and lower uncertainty for putative biomarker.

The axes that are plotted in the S-plot from the predictive component are p1 vs p(corr)1, representing the magnitude (modeled covariation) and reliability (modeled correlation) respectively.

16.14.1 Reference S-plot

Wiklund, S., Johansson, E., Sjöström, L., Mellerowicz, E.J., Edlund, U., Shockcor, J.P., Gottfries, J., Moritz, T., and Trygg, J., (2008), *Visualization of GC/TOF-MS-Based Metabolomics Data for Identification of Biochemically Interesting Compounds Using OPLS Class Models,* Anal. Chem. 80, 115-122.

Note: The vector 'Cov(tp,X)' is named p[1] and the vector 'Corr(tp,X) is named p(corr)[1] in SIMCA.

16.15 Observation risk

Observation risk *(ORisk*) is a measure of the sensitivity of the results of a workset observation in the Y space measured as a change in the Y residuals when the observation is in the workset or not.

Observation risk is computed for each individual y-variable and for all y-variables together. The column plot displays the observation risk for each y-variable and for the pooled y-variables, as different series.

ORisk = 1 is displayed as a reference line. When ORisk for an observation equals 1, this means that the predicted result for the observation is the same whether the observation is included in the model or not.

ORisk(pooled), the rightmost columns, can be larger than or smaller than the ORisk of individual y-variables. This is due to a correction factor added to prevent DModY, when the observation is in the model, from becoming too small.

A plot displaying observation risk can be created by selecting the vector *ORisk* or *ORisk(pooled)* in one of the standard plots on the **Plot/List** tab.

17Preprocessing appendix

17.1 Preprocessing available in SIMCA

There are a number of transformations, or filters, available in SIMCA.

Transformations

In the **Plot/List** tab dialogs, clicking the **Transformation** tab offers: **Auto correlation**, **Cross correlation**, **Power spectrum**, **Wavelet coefficients**, **EWMA**, **Histogram**, **Normalize**, **R2X**, and Dot plot.

Time series filters

The following time series filters are available on the **Data** tab, **Filters** group, **Time series filters**: **Wavelet compress time series (WCTS)** and **Wavelet denoising/decimation (WDTS)**.

Spectral Filters

The following spectral filters, applied observation wise, are available on the **Data** tab, **Filters** group, **Spectral filters**:

Filter name in dialog	**Full name**
Derivative	1st , 2nd & 3rd Derivative
MSC	Multiplicative Signal Correction
SNV	Standard Normal Variate
Row center	Row Center
Savitzky-Golay	Savitzky-Golay
EWMA	Exponentially Weighted Moving Average
Wavelet compression	Wavelet Compression Spectral (WCS)
Wavelet denoising	Wavelet Denoise Spectral (WDS)
OSC	Orthogonal Signal Correction

This chapter describes the following:

- Auto and cross correlation of variables or observations
- Power Spectrum Density
- Wavelet transformations
- Filtering and calibration
- Derivatives
- Multiplicative Signal Correction (MSC)
- Standard Normal Variate (SNV)
- EWMA background
- Wavelet compression or de-noising of signals
- Orthogonal Signal Correction (OSC)

17.2 Auto and cross correlation of variables or observations

The auto correlation of a vector x is a measure of the dependence between adjacent observations.

In the time domain, for time series, the properties of ARMA processes are characterized by their auto correlation functions.

The ***auto covariance*** of a vector x is defined as the **Auto-covariance** of lag L of the vector y:

$c_{yy}(L) = 1/N(\Sigma(y_t - y_{avg})(y_{t+L} - y_{avg}))$

where Σ: t=1 to N-L, for L = 0, 1, 2, etc.

The ***auto correlation*** of a vector x is defined as the **Auto-correlation** of lag L of the vector y:

$r_L = c_{yy}(L) / c_{yy}(0)$, $c_{yy}(0) = 1/N(\Sigma\ (y_t - y_{avg})^2)$ variance of y_t

Note that $r_L = r_{-L}$

Similarly the ***cross covariance*** of two vectors x and y are defined as the cross covariance of lag L between x and y:

c_xy(L) = 1/N Σ(x_t - x_avg)(y_t+L - y_avg);   t = 1,2,..,N-L, L = 0,1,2,...

For negative L this is:

c_xy(L) = 1/N Σ(y_t - y_avg)(x_t-L - x_avg);   t = 1,2,..,N+L, L = 0,-1,-2,...

Similarly the ***cross correlation*** of two vectors x and y are defined as the cross correlation of lag L between x and y:

r_xy(L) = c_xy(L)/(s_x s_y),

where s_x and s_y are the standard deviations of x and y.

SIMCA estimates the auto/cross correlation using the FFT (Fast Fourier Transform).

Centering and detrending are optional in SIMCA.

Note: When excluding observations in time series data, the auto and cross correlation transformations are approximate as the excluded observations are not replaced by missing values.

17.2.1 Reconstruction of wavelet compressed data

With a dataset that has been wavelet transformed and compressed variable wise using **Data | Spectral filters**, the time series plot and the auto correlation observation wise refer to the reconstructed observations.

To display the auto correlation in the wavelet domain:

1. Click **File | Options** and click **Project options**.
2. Under **General**, select *Yes* in the **Reconstruct wavelet** box.
3. Use the **Plot/List** tab to recreate the plot.

In Quick info, observations in the wavelet domain are always reconstructed.

17.2.2 References auto and cross correlation

1. Box, G.E.P., Jenkins, G.M., and Reinsel, G.C., (1994), *Time Series Analysis - Forecasting and Control*, 3rd edition, Prentice-Hall, Inc., Englewood Cliffs, NJ. Pages 29-33, Page 411-415.
2. Press, W., Flannery, B., Teukolsky, S., and Vetterling, W., Numerical Recipes in C, Cambridge University Press.

17.3 Power spectrum density

The power spectrum density (PSD) is the representation of the sequence x (t) in the frequency domain. The power spectrum is the square of the amplitude of the Fourier component at each frequency.

The frequency domain representation is particularly helpful to detect irregular cycles and pseudo periodic behavior, i.e. tendency towards cyclic movements centered on a particular frequency.

SIMCA uses the Welsch's non-parametric method to estimate the PSD.

Note*: With a dataset that has been wavelet transformed and compressed variables wise, (using* ***Data | Spectral filters****), the PSD observation wise refers to the reconstructed observations, when the reconstruct option is on.*

17.3.1 Reference power spectrum

1. Belsley, D., Kuh, E., and Welsch, R., (1980), *Identifying Influential Data and Sources of Collinearity*, John Wiley, New York.

17.4 Wavelet transformations

17.4.1 Introduction

Wavelet transformation is a linear transformation, similar to the Fourier transform and its trademarks are good compression and de-noising of complicated signals. Wavelets look like small oscillating waves, and they have the ability to analyze a signal according to scale, i.e. inverse frequency. The size of the analyzing window in wavelet transform varies with different scales, and it is this small but still very important property, along with the fact that wavelet functions are local in both time and frequency, that makes the wavelet transform so useful.

17.4.2 Overview of the wavelet transform

The wavelet transform analyzes signals locally without prejudice to scale. This is possible because a basis function is employed, called the ‘mother’ wavelet, with a certain scale, i.e. window width. The mother wavelet is then stretched or compressed to create other scales, changing the width of the window, as can be seen in figure 1. Using a narrow wavelet for detecting the sharp features, and a broader wavelet for detecting the more general features, means that you see both the forest and the trees. The mother wavelet is local in time* and frequency, making wavelets useful not only for compression but also for removing noise and for feature extraction.

*(time, wavelength, wave number, etc.)

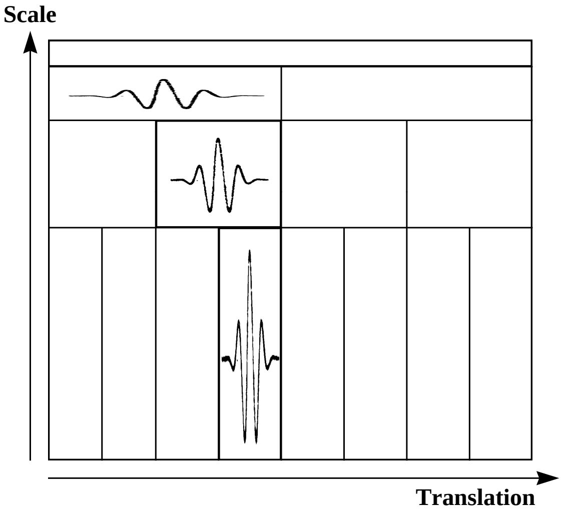


Figure. Changing the width of the wavelet function makes it possible to analyze different scales.

17.4.3 Wavelet theory

A very brief introduction will be given here. For a more complete theory description, the interested reader is referred to the reference list at the end of this section. Wavelets belong to the absolutely squared integrable function space L^2. The wavelet transform is simply the dot product between the signal $f(t) \in L^2(\Re)$ and the wavelet functions $\Psi_{m,n}(t)$.

Discrete Wavelet transform:

$$\rangle f(t), \Psi_{m,n}(t) \langle = \int_{-\infty}^{\infty} f(t)\Psi_{m,n}(t)dt$$

Mother wavelet:

$$\Psi_{m,n}(t) = 2^{-m/2}\psi(2^{-m}t - n)$$

where

m = Scale (Dilation), *n* = Translation in time.

One of the mathematical restrictions that apply to the wavelet is the admissibility condition:

$$C_{\Psi} = \int_{-\infty}^{\infty} \frac{\left|\hat{\Psi}(\omega)\right|^2}{|\omega|} d\omega < \infty$$

for finite energy

$$\hat{\Psi}(\omega) = 0 \; for \, \omega \leq 0$$

where ω= Frequency $\hat{\Psi}(\omega)$ = FT on wavelet function.

17.4.4 Multiresolution analysis, MRA

In 1986, a fast wavelet transformation technique called multiresolution analysis was presented by Mallat. The signal needs to be of length 2n, where n is an integer. This poses no problems, because the signal can be padded to the nearest 2n. In multiresolution analysis, another function called the scaling function is introduced, which acts as a starting point in the analysis and makes it possible to compute wavelet coefficients fast. From the wavelet and scaling function respectively, filter coefficients are derived and used in the transformation, and are implemented as finite impulse response (FIR) filters. These filter coefficients are put in a filter coefficient matrix of size k*k, where k is the length of the signal to be analyzed, and a pyramid algorithm is used. The filter coefficients are normalized to make sure that the energy on each scale is the same, and the normalizing constant is **1/sqrt(2)**. Energy is defined as the squared sum of all the coefficients. The scaling filter S is located on the first k/2 rows, and the wavelet filter D is located on the last k/2 rows. The filter matrix is constructed by moving the filter coefficients two steps to the right when moving from row to row, requiring k/2 rows to cover the signal. The number of filter coefficients depends on what wavelet function is being used. The wavelet filter coefficients can be derived from the scaling filter coefficients.

Wavelet coefficient (c-i+1) = $(-1)^i$ *Scaling coefficient (i), i=1,2,...,c* where c is the number of filter coefficients. The Daubechies-4 wavelet function has the following four **scaling** filter coefficients:

[(1 + √3)/4, (3 + √3)/4, (3 - √3)/4, (1 - √3)/4]

and **wavelet** filter coefficients:

[(1 - √3)/4, (3 - √3)/4, (3 + √3)/4, (1 + √3)/4]

Reconstruction of the original signal from the wavelet coefficients is straightforward, because the normalized orthogonal wavelet filters are used, $W^T W=I$ where *W* is the normalized filter coefficient matrix and *I* is the identity matrix. Simply transpose the filter matrix and reverse the procedure.

For a signal of length 2^n the filtering procedure is performed n times, creating n levels of different scales, separated with a factor two. The wavelet filter produces the detailed part, and those are the wavelet coefficients. The scaling filter creates an approximate description of the signal, and those coefficients are used for representing the signal at the next scale, see figure 2. When reaching the highest scale, only one scaling coefficient is produced, and it is related to the average value of the original signal. It is now possible to reconstruct the original signal using the average value and the wavelet coefficients. The size of the transformed signal is the same as the original signal, if the average value is taken into account. This method is fast, approximately *2*c*k* calculations are necessary for a complete transformation [11], where *c* is the number of filter coefficients and *k* is the original length of the signal.

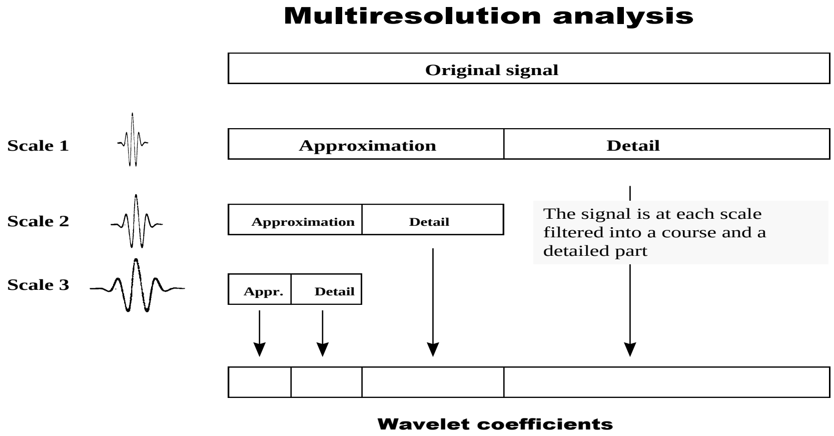


Figure 2. The fast multiresolution analysis results in a coefficient vector of the same size as the analyzed signal.

17.4.4.1 Example of MRA using the orthogonal Haar wavelet

Let us show an example how multiresolution analysis works by using the simplest orthogonal wavelet, the Haar wavelet. The filter coefficients for the scaling function is [1,1], and for the wavelet function [1,-1].

We start off with the original signal of length 2^3= 8, see figure 3. The normalized filter coefficient matrix is of size 8*8. The scaling filter coefficients are placed on the first half of the matrix, and the wavelet filter coefficients are placed on the second half of the rows, as described earlier.

1. Filtering the original signal with the filter matrix produces a signal of the same length as the filtered signal, where the coefficients on the right half represent the details in the signal at the given scale.
2. These coefficients are the wavelet coefficients, and they are removed and saved.
3. The remaining coefficients represent an approximate description of the original signal and are used to represent the original signal at the next scale. With the signal being half the length of the original signal, the filters are automatically up-scaled by a factor two, i.e. changing the width of the filter.
4. The coarse signal is then filtered with a reduced filter matrix. The procedure from the last scale is repeated, removing the right half of the coefficients as wavelet coefficients and using the other half to represent the signal at the next scale.
5. With an even more reduced filter matrix, the filtered output signal of length two consists of one wavelet coefficient and also the normalized average value of the original signal.
6. Both of these are put in the wavelet coefficient vector. Now, the fast wavelet transformation is done, and the wavelet coefficient vector can be used for a complete reconstruction of the original signal, by transposing the normalized filter coefficient matrix and reversing the filtering operations previously done. It is important to realize that the sum of the coarse and the detailed signal at a certain scale matches the signal on the scale below, if this is not the case we would not be able to recover the original signal.

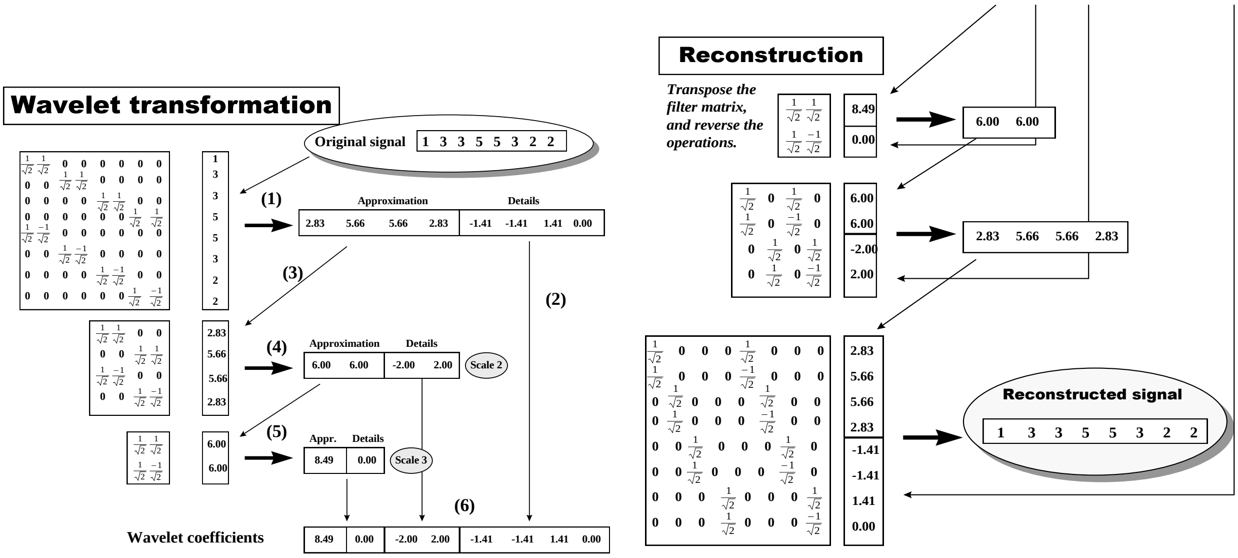


Figure 3. Describes the technique that MRA uses for retrieving the wavelet coefficients, and how reconstruction of the original signal is performed.

We have seen how MRA works on a signal, so let us try to understand how to interpret the different wavelet coefficients. In the Haar example we had a signal with length 2^3 = 8. As was shown in figure 5, the first scale in MRA gave 2^{3-1} = 4 wavelet coefficients. These coefficients contain the highest frequency details of the original signal, usually represented by white noise, and reside in the right half of figure 4. The second scale produce 2^{3-2} = 2 coefficients and those coefficients represent lower frequency details than scale 1, and are placed next to the coefficients from scale 1.

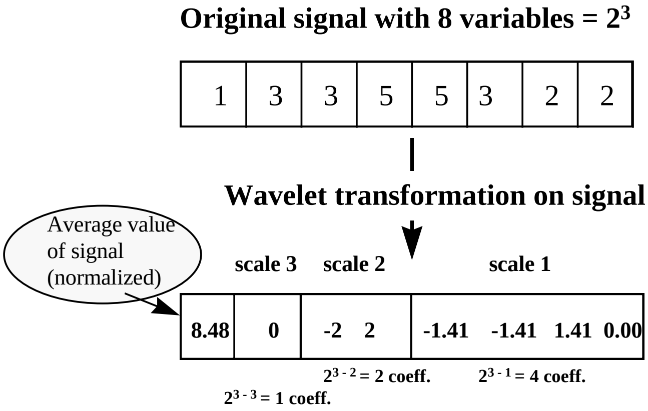
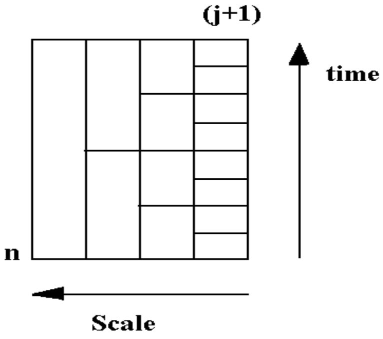


Figure 4. Description of the wavelet coefficient vector.

Now it is easy to understand that as we move further to the left, information about lower and lower frequencies in the original signal is detected. For example when compressing NIR-spectra, since they are usually smooth, most of the wavelet coefficients in the upper scales will be large, whereas all wavelet coefficients in the lower scales representing higher frequencies will be close to zero.

17.4.4.2 Best Basis

The MRA assumes that lower frequencies contain more important information than higher frequencies. With MRA only the low pass filter is iterated, creating a logarithmic tree. For many signals, in particular time series data, this is not always a good assumption. Hence, for compression of non-smooth signals, one uses ***the best basis*** decomposition. A selected signal (the average spectra, or a representative response Y) is decomposed using the wavelet packet. This means that at every node, the signal is sent to the low pass-high pass filter bank. This creates a 2-D matrix (n*(j+1)), where each column represents a new scale (j). The first column is the original signal (average spectra, or Y). This matrix is called a packet table and represents the complete dyadic tree structure.



An additive measure of information, called entropy by Coifman and Wickerhauser, is calculated for each block (node) in the packet table. Entropy is calculated as

!Sum(p. * (logp))

where p are the normalized coefficients (divided by the norm of the original signal), squared, in the block (node). Hence, the entropy is related to the sum of squares.

The best-basis algorithm is used to pick out the “best” basis from the entire possible basis in the packet table. Here “best” means the one that minimizes the entropy of the signal.

SIMCA uses this best basis, determined on the target signal, to calculate the wavelet transform (coefficients) of the X matrix, for spectra and the X and Y block for time series.

The compression is performed by extracting only a selected number of significant coefficients.

17.4.5 Wavelet families

The wavelet families available in SIMCA are the orthogonal and the biorthogonal wavelet families.

17.4.5.1 Orthogonal wavelet families

The orthogonal wavelet families are:

- The **Beylkin** wavelet places roots for the frequency response function close to the Nyquist frequency on the real axis. The length of the associated FIR filter is equal to 18. This wavelet gives good frequency localization but causes dephasing.
- The **Coiflet** wavelets of order 2N are designed to give the wavelet function 2N odd vanishing moments and the scaling function (2N –1) odd vanishing moments. These wavelets have good compression properties.
- The **Daubechies** wavelets maximize the smoothness of the "scaling function" by maximizing the rate of decay of its Fourier transform. The order of the wavelets is 2N. They have N odd vanishing moments and their support is of length 2N-1. These wavelets have good overall properties.
- The **Symmlets** are the "least asymmetric" compactly supported wavelets with maximum number of vanishing moments. Other properties are similar to the Daubechies wavelets.

Note*: All orthogonal wavelets are asymmetrical and hence their associated filters are not linear phase.*

17.4.5.2 Biorthogonal wavelet families

With Biorthogonal wavelets one uses two sets of wavelets and scaling functions, one set for the decomposition and the other set for the reconstruction.

In SIMCA the Biorthogonal wavelets are referred to as ”**biorNr**” and of order **”Nd”**. **Nr** is the reconstruction order and **Nd** is the decomposition order

The reconstruction wavelets have a support width of **(2Nr +1)** and the decomposition wavelets have a support width of **(2Nd +1)**.

Note*: Biorthogonal wavelets are symmetrical and their associated filters are linear phase.*

17.4.5.3 Criteria in selecting a wavelet

The support (width) of the wavelet function determines the speed of convergence to 0 when the time or the frequency goes to infinity.

The support quantifies both the time and frequency localization. You want short support for better time localization and long support for better frequency localization.

The symmetry of the wavelet function is needed to avoid dephasing in image and sound analysis. Only the biorthogonal wavelets are symmetrical.

The **number of odd vanishing moments** of the wavelet function determines how well the wavelet compresses a signal.

The regularity of the wavelet function is useful to achieve smoothness of the reconstructed signal.

17.4.6 Wavelet compression or de-noising of signals

SIMCA uses, as default, the Discrete Wavelet Transform (DWT) and the MRA algorithm. We have found that for NIR spectra, which are usually smooth signal, the Daubechies–4 works very well for both compression and reconstruction. You can select to use the “best basis” decomposition instead of DWT (for signals with high frequency content) and select other orthogonal or biorthogonal wavelet. With Best Basis we recommend that you use a wavelet with short support as the objective is to achieve good time localization. Select a biorthogonal wavelet if having no dephasing is important.

17.4.6.1 Wavelet denoising vs. compression

The objective with denoising is to remove noise. The objective with compression is to compress the dataset removing some frequencies. These objectives are very similar and the results are in most cases very similar.

The steps performed when wavelet compressing a dataset, are described in the subsections that follow in this section. The steps performed in wavelet denoising are very similar to compression in all steps performed, with the exception that after compressing the spectra with denoising, the wavelet compressed X matrix is transformed back to the original domain before creating the new project. This means that with denoising no reconstruction is available, nor necessary, since the denoised dataset is in the original domain.

17.4.6.2 Steps in wavelet compression of spectra using variance

In SIMCA the raw spectra (observations) are padded to the nearest length 2^n, n = integer.

Each spectrum, in the dataset, is transformed, with the selected wavelet using DWT or best basis as computed on the target signal (average spectra).

17.4.6.2.1 Wavelet compressing the signal using variance

The wavelet compression of the signal using Variance is done as follows:

1. With DWT:
    a. The variance spectrum of the coefficient matrix (training set) in the wavelet domain is calculated.
    b. The positions of a selected number of the largest variance coefficients are located, and those columns are extracted from the wavelet coefficient matrix into a compressed data matrix.
2. With Best Basis:
    a. The Sum of Squares of the selected signal (the average spectra) in the wavelet domain is calculated.
    b. The positions of a selected number of the largest Sum of Squares coefficients are located, and those columns are extracted from the wavelet coefficient matrix.
3. The original positions of the extracted coefficients are saved. These are used both in future compression of spectra, and in the reconstruction of loadings, or scores etc.
4. A new project is created with the compressed dataset.

17.4.6.2.2 Reconstructing the wavelet signal using variance

Reconstruction to the original loadings, coefficients, etc., is done as follows:

1. The coefficients are placed in their original position in the wavelet vector, and all other positions are filled with zeros.
2. The inverse wavelet transformation is performed.

The following picture illustrates the steps in the data compression of spectra when DWT is used.

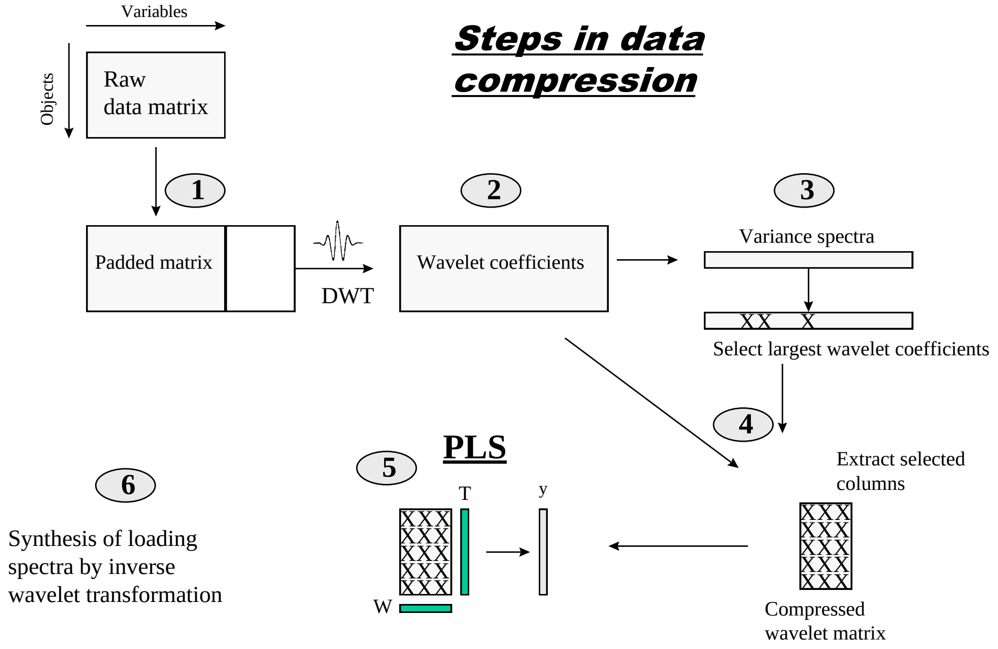

Variables
Objects
Raw data matrix
Steps in data compression
1
2
3
Padded matrix
DWT
Wavelet coefficients
Variance spectra
XX X
Select largest wavelet coefficients
4
PLS
5
6
Extract selected columns
T
y
XXX
W
Synthesis of loading spectra by inverse wavelet transformation
Compressed wavelet matrix

Figure 5. Overview of the different steps taken in the data compression and regression analysis.

17.4.6.3 Steps in wavelet compression of spectra using the detail levels

In SIMCA the raw spectra (observations) are padded to the nearest length 2^n, n = integer.

Each spectrum, in the dataset, is transformed, with the selected wavelet using DWT.

17.4.6.3.1 Wavelet compressing the signal using detail levels

With DWT, the percentage of Sum of Squares of the coefficient matrix in the wavelet domain, for each detail level (scale), is calculated. The lowest level (scale) contains the highest frequencies.

In the Wavelet Compression wizard in SIMCA, select the details to include and a new project is created with the compressed dataset consisting of the wavelet coefficients from the selected detail levels. For more about the actual steps in SIMCA, see the Wavelet Compression Spectral – WCS section in Chapter 8, Data.

This compression method is recommended for smooth signals, when most of the high frequencies are noise.

17.4.6.3.2 Reconstructing the wavelet signal using detail levels

When reconstructing to the original loading, coefficients, etc., the inverse wavelet transform with the coefficients of the details removed (set to 0), is performed.

17.4.6.4 PLS wavelet compression of time series

The objective with time series is to compress the X and Y blocks column wise, reducing the number of observations, while keeping the relationship between the Y and X blocks. The model in the compressed form should be as predictive as the model in the original data. The wavelet transform of time series focuses on one response, Y, with the objective to achieve a parsimonious representation of this signal, while keeping all of the information related to the relationship between X and Y. With several y-variables, one should first do a PCA selecting only a group of positively correlated y-variables to be compressed together. One y-variable is selected as the most representative, and becomes the target signal.

17.4.6.4.1 Steps in wavelet compression of time series using sum of squares

The raw data (X and Y variables), are padded to the nearest length 2^n, n = integer, and mean centered.

Each variable, in the dataset, is transformed, using DWT or the best basis, as computed on the target signal Y.

Wavelet compressing the time series signal using sum of squares

The wavelet compression of the time series signal, using Sum of Squares, is done as follows:

1. With Best Basis and DWT, the sum of squares of the selected signal Y, is calculated in the wavelet domain.
2. The positions of a selected number of the largest sum of squares coefficients are located, and those columns extracted from the wavelet coefficient matrix X and Y.
3. The original positions of the extracted coefficients are saved and used in future compression of time series.
4. A new project is created with the compressed dataset.

In summary, each series (the selected X and Y) are wavelet transformed, and the coefficients are kept which preserves the specified “focus variable” y. The same coefficients are kept for all variables (all X and Y).

No reconstruction of loading, coefficients etc. is necessary, in the compressed project, due to the fact that the relationship between variables has not been altered.

17.4.6.4.2 Steps in wavelet compression of time series using detail levels

The raw data (X and Y variables), are padded to the nearest length 2^n, n = integer, and mean centered.

Each variable, in the dataset, is transformed, using DWT.

Wavelet compressing the time series signal using detail levels

The wavelet compression of the time series signal, using Detail levels, is done as follows:

1. With DWT, the percentage of the sum of squares, of the selected signal Y, for each detail level (scale) is calculated. The lowest level (scale) contains the highest frequencies.
2. Select the detail levels to include and a new project is created with the compressed dataset (X and Y) containing only the coefficients from the selected detail levels.

No reconstruction of loadings, coefficients etc. is necessary, in the compressed project, due to the fact that the relationship between variables has not been altered.

This compression method is recommended for smooth Y signals, when most of the high frequencies are noise.

Note*: Use detail level selection to perform "Multiscale" analysis of time series.*

17.4.7 References for wavelets

1. Mittermayr, C.R., Nikolov, S.G., Hutter, H., and Grasserbauer, M., (1996), *Wavelet denoising of Gaussian peaks: a comparative study*, Chemometrics Intell. Lab. Syst., 34, 187-202.
2. Barclay, V.J., Bonner, R.F., and Hamilton, I.P., (1997), *Application of Wavelet Transforms to Experimental Spectra: Smoothing, Denoising, and Data Set Compression*, Anal.Chem., 69, 78-90.
3. Alsberg, B.K., Woodward, A.M., and Kell, D.B., (1997), *An Introduction to Wavelet Transforms for Chemometricians: A Time-Frequency Approach*, Chemometrics Intell. Lab. Syst., 37, 215-239.
4. Walczak, B. and Massart, D.L., (1997), *Noise Suppression and Signal Compression using the Wavelet Packet Transform*, Chemometrics Intell. Lab. Syst., 36, 81-94.
5. Bos, M. and Vrielink, J.A.M., (1994), *The wavelet transform for pre-processing IR spectra in the identification of mono- and di-substituted benzenes*, Chemometrics Intell. Lab. Syst., 23, 115-122.
6. Walczak, B., Bogaert, B., and Massart, D.L., (1996), *Application of Wavelet Packet Transform in Pattern Recognition of Near-IR Data*, Anal. Chem., 68, 1742-1747.
7. Hubbard, B.B., (1995), *The world according to wavelets*, A K Peters, Wellesley, MA.
8. Daubechies, (1992), *Ten Lectures on wavelets*, SIAM, Philadelphia, PA.
9. Kaiser, G., (1994), *A Friendly Guide to Wavelets*, Birkhäuser, Boston, MA.
10. Mallat, S.G., (1989), *A Theory for Multiresolution Signal Decomposition: The Wavelet Representation*, IEEE Transactions on Pattern Analysis and Machine Intelligence, v.11 n.7, p.674-693, July 1989.
11. Trygg, J., and Wold, S., (1998), *PLS Regression on Wavelet Compressed NIR Spectra*, Chemometrics and Intelligent Laboratory Systems, 42, 209-220.
12. Wickerhauser, M.V., (1994), *Adapted Wavelet Analysis from Theory to Software*, AK Peters.
13. Bakshi, B.R., (1998), *Multiscale PCA with Application to Multivariate Statistical Process Monitoring*, AIChE Journal, 44, 7, 1596-1610.

17.5 Filtering and calibration

Base line correction, signal correction, and the like are special cases of *filtering*, where a signal (e.g., a NIR spectrum) is made to look "better" by passing it through a "filter" = mathematical function.

In calibration, one can quantitatively specify at least one objective with filtering, namely that the filtering should NOT remove information about Y from the spectra. Here Y is what we calibrate against, e.g., concentrations.

One can often formulate the filtering as a projection (PCA or PLS-like). The X block is the (N x K) matrix of unfiltered, uncorrected, set of digitized spectra, while E is the (N x K) matrix of "filtered" spectra, T a (N x A) matrix of scores, and P' a (K x A) matrix of "filters", loadings. N and K are the numbers of samples and variables of the "training set" (calibration set).

$X = TP' + E$

If T can be made *orthogonal* against Y, we are not removing information from X that is linearly related to Y. With this simple insight, we can now develop filters, base-line corrections, signal corrections, etc., with this orthogonal constraint.

17.6 Derivatives

A rapid and often utilized method for reducing scatter effects for continuous spectra consists of using derivatives [Naes et al., 2002]. The first derivative spectrum is the slope at each point of the original spectrum. It peaks where the original spectrum has maximum slope and it crosses zero where the original has peaks. The second derivative spectrum is a measure of the curvature at each point in the original spectrum. Usually, this derivative spectrum is more similar to the original spectrum and has peaks approximately as the original spectrum, albeit with an inverse configuration [Naes et al., 2002]. The effect of the first derivative is usually to remove an additive baseline (“offset”), whereas the effect of the second derivative also involves removal of a linear baseline.

The third derivative spectrum is a measure of the “wigglyness” of the original spectrum. Alternatively, the third derivative spectrum can be understood as the slope at each point in the second derivative spectrum, much in the same way as the second derivative spectrum indicates the slope at each point of the first derivative spectrum, and the latter the slope at each point of the original spectrum.

A problem with the above approach is that differencing may reduce the signal and increase the noise, thus producing very noisy derivative spectra. Realizing this risk Savitzky and Golay (SG) proposed an improvement based on a smoothing approach [Savitzky and Golay, 1964]. SG-derivatives are based on fitting a low degree polynomial function (usually of quadratic or cubic degree) piece-wise to the data, followed by calculating the first derivative and second derivative from the resulting polynomial at points of interest. SIMCA supports the SG-derivative option.

17.6.1.1.1 References for derivatives

1. Naes, T., Isaksson, T., Fearn, T., and Davies, T., (2002), *A User-friendly Guide to Multivariate Calibration and Classification*, NIR Publications, Chichester, UK. ISBN: 0-95286662-5.
2. Savitzky, A., and Golay, M.J.E., (1964), *Smoothing and Differentiation by Simplified Least Squares Procedures*, Analytical Chemistry, 36, 1627-1632.

17.7 Multiplicative Signal Correction (MSC)

The empirical fact that the regression of spectral values (of related samples), against the mean spectral values is approximately linear, is the primary motivation for the MSC correction.

The MSC correction is defined as follows:

Each observation (spectra) $\mathbf{x}_{i,}$ is “normalized” by regressing it against the average spectrum ($m_k = \Sigma x_{ik}/n$).

$x_{ik} = a_i + b_i m_k + e_{ik}$

This gives the MSC corrected spectra:

$x_{ik,\text{ corrected}} = (x_{ik} - a_i)/b_i$

17.7.1 References for MSC

1. Martens, H. and Naes, T., *Multivariate Calibration*. Wiley, N.Y., 1989.
2. Geladi, P., MacDougall, D., and Martens, H., (1985), *Linearization and Scatter-correction for Near-infrared Reflectance Spectra of Meat*, Applied Spectroscopy, 3, 491-500.

17.8 Standard Normal Variate (SNV)

The standard normal variate transformation of Barnes et al is defined by:

$x_{ik} = [(x_{ik} - \bar{x}_i) / \sqrt{(\Sigma(x_{ik} - \bar{x}_i)^2)}] * \sqrt{(K-1)}$

where k = (1,.....K) gives the wavelength and i = the sample index $\bar{x}_i = \Sigma i x_i/K$

17.8.1 Reference for SNV

1. Barnes, R.J., Dhanoa, M.S., and Lister, S.J., (1989), *Standard Normal Variate Transformation and De-trending of Near-Infrared Diffuse Reflectance Spectra*, Applied Spectroscopy, 43, 772-777.

17.9 EWMA background

There are two types of EWMA calculations; the filter version and the predictive version. The filter EWMA is default for spectral filters, control charts and plot/list transformation, according to the default setting in **EWMA type** in **File | Options**, **SIMCA options** page, <u>**Plot** section</u>.

Filter EWMA is given by

$\hat{y}_t = (1 - \lambda)\hat{y}_{t-1} + \lambda y_t$

Predictive EWMA is given by

$$\hat{y}_t = (1 - \lambda)\hat{y}_{t-1} + \lambda y_{t-1}$$

$\hat{y}_t$ is the EWMA value of observation/subgroup at time point t.

$\hat{y}_1$is set to the Target (default the average if target is not specified).

17.9.1 Generate variables and EWMA

In generate variables there are two EWMA recipes available:

- *EWMAf(…)* for filter EWMA. This type is unavailable in SIMCA 14 and earlier.
- *EWMAp(…)* for predictive EWMA. This is the only type available in SIMCA 14 and earlier.

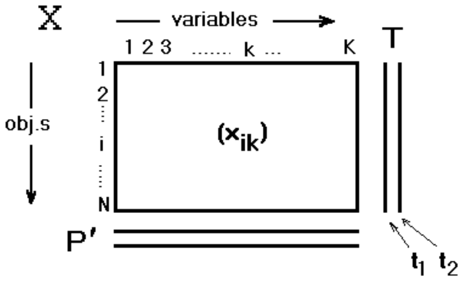
17.10 Orthogonal Signal Correction (OSC)

OSC is a PLS-related solution, which removes only so much of X as is unrelated (orthogonal) to Y.

The OSC algorithm performs the following steps:

Step	Description	Formula
1.	Specifies a starting "loading" or "correction" vector, **p'** In the first dimension this can be a row of 1's (corresponding to additive correction), or the loading of the first principal component of X (uncentered), or, in the second dimension, **p'** can be the average spectrum (multiplicative signal correction), or the second principal components loading etc.	
2	Calculates a "score vector", **t**, in the ordinary "NIPALS" way.	t = Xp/p'p
3	Orthogonalizes t to Y.	t_{new} = $(1 - Y(Y'Y)^{-1}Y')t$
4	Calculates a weight vector, w, that makes Xw = t_{new}. This is done by a PLS estimation giving a generalized inverse = $(X'X)^{-}$	w = $(X'X)^{-}t_{new}$
5	Computes a new loading vector.	p' = $t_{new}'X/(t_{new}'t_{new})$
6	Subtracts the "correction" from X, to give the "filtered" X. One can then, optionally, continue with the next "component", then another one, etc., until satisfaction. Usually two components should suffice, but with non-linear corrections three are sometimes warranted.	X_{new} = $X - t_{new}\,p'$

This approach is based on the fact that as long as the steps of the PLS NIPALS iterative algorithm are retained, the weight vector **w** can be modified in any way to encompass constraints, smoothness, or, as here, the objective that t = Xw is orthogonal to Y. This was shown by Höskuldsson (1988).



$\mathbf{p_1'}$ = [11111111 ....   111]

$\mathbf{p_2'}$ = [column averages   ]

$\mathbf{t_{1i}}$ **and** $\mathbf{t_{2i}}$ **are** $\mathbf{a_i}$ **and** $\mathbf{b_i}$

Sartorius Stedim Data Analytics recommends using OPLS/O2PLS instead of OSC as the OSC filter is prone to overfit and may give results that are too optimistic. The OPLS/O2PLS approach provides more realistic results and separates orthogonal variation from predictive variation in a single model.

17.10.1 Reference for OSC

1. Wold, S., Antti, H., Lindgren, F., and Öhman, J., (1998a), *Orthogonal Signal Correction of Near-Infrared Spectra*, Chemometrics and Intelligent Laboratory Systems, 44, 175-185.

18 References

This section holds references for multivariate data analysis. The appendices sections list numbered section specific references. These references are available in the reference list here too.

18.1 References for multivariate analysis

Albano, C., Dunn, III, W.J., Edlund, U., Johansson, E., Nordén, B., Sjöström, M., and Wold, S., (1978), *Four Levels of Pattern Recognition*, Analytica Chimica Acta, 103, 429-443.

Alsberg, B.K., Woodward, A.M, and Kell, D.B., (1997), *An Introduction to Wavelet Transforms for Chemometricians: A Time-Frequency Approach*, Chemometrics and Intelligent Laboratory Systems, 37, 215-239.

Andersson, G., Kaufmann, P., and Renberg, L, (1996), *Non-Linear Modelling with a Coupled Neural Network – PLS Regression System*, Journal of Chemometrics, 10, 605-614.

Andersson, P., Haglund, P., Tysklind, M., (1997a), *The Internal Barriers of Rotation for the 209 Polychlorinated Biphenyls*, Environmental Science and Pollution Research, 4, 75-81.

Andersson, P., Haglund, P., and Tysklind, M., (1997b), *Ultraviolet Absorption Spectra of all 209 Polychlorinated Biphenyls Evaluated by Principal Component Analysis*, Fresenius Journal of Analytical Chemistry, 357, 1088-1092.

Andersson, G., (1998), *Novel Nonlinear Multivariate Calibration Methods*, Ph.D. Thesis, The Royal Institute of Technology, Stockholm, Sweden.

Andersson, P.M., Sjöström, M., and Lundstedt, T., (1998), *Preprocessing Peptide Sequences for Multivariate Sequence-Property Analysis*, 42, 41-50.

Andersson, P.M., Sjöström, M., Wold, S., and Lundstedt, T., (2001), *Strategies for Subset Selection of Parts of an In-house Chemical Library*, Journal of Chemometrics, 15, 353-369.

Andersson, P.M., and Lundstedt, T., (2002), *Hierarchical Experimental Design Exemplified by QSAR Evaluation of a Chemical Library Directed Towards the Melanocortin 4 Receptor*, Journal of Chemometrics, 16, 490-496.

Andersson, M., Svensson, O., Folestad, S., Josefson, M., and Wahlund, K.G., (2005), *NIR Spectroscopy on Moving Solids Using a Scanning Grating Spectrometer – Impact on Multivariate Process Analysis*, Chemometrics and Intelligent Laboratory Systems, 75, 1-11.

Andre, M., (2003), *Multivariate Analysis and Classification of the Chemical Quality of 7-aminocephalosporanic-acid Using Near-infrared Reflectance Spectroscopy*, Analytical Chemistry, 75, 3128-3135.

Antti, H., Bollard, M.E., Ebbels, T., Keun, H., Lindon, J.C., Nicholson, J.K, and Holmes, E., (2002), *Batch Statistical Processing of 1H-NMR-derived Urinary Spectral Data*, Journal of Chemometrics, 16, 461-468.

Antti, H., Ebbels, T.M.D., Keun. H.C., Bollard, M.A., Beckonert, O., Lindon, J.C., Nicholson, J.K., and Holmes, E., (2004), *Statistical Experimental Design and Partial Least Squares Regression Analysis of Biofluid Metabonomic NMR and Clinical Chemistry Data for Screening of Adverse Drug Effects*, Chemometrics and Intelligent Laboratory Systems, 73, 139-149.

Atif, U., Earll, M., Eriksson, L., Johansson, E., Lord, P., and Margrett, S., (2002), *Analysis of Gene Expression Datasets Using Partial Least Squares Discriminant Analysis and Principal Component Analysis*. In: Martyn Ford, David Livingstone, John Dearden and Han Van de Waterbeemd (Eds.), Euro QSAR 2002 Designing Drugs and Crop Protectants: processes, problems and solutions. Blackwell Publishing, ISBN 1-4051-2561-0, pp 369-373.

Austel, V., (1995), *Experimental Design*, In: Mannhold, R., Krogsgaard-Larsen, P., and Timmerman, H., (Eds.), Methods and Principles in Medicinal Chemistry, Vol 2, VCH, Weinheim, Germany, pp. 49-62.

Bakshi, B.R., (1999), *Multiscale Analysis and Modelling Using Wavelets*, Journal of Chemometrics, 13, 415-434.

Barclay, V.J., Bonner, R.F., and Hamilton, I.P., (1997), *Application of Wavelet Transforms to Experimental Spectra: Smoothing, Denoising, and Data Set Compression*, Anal. Chem., 69, 78-90.

Barnes, R.J., Dhanoa, M.S., and Lister, S.J., (1989), *Standard Normal Variate Transformation and De-trending of Near-Infrared Diffuse Reflectance Spectra*, Applied Spectroscopy, 43, 772-777.

Baroni, M., Clementi, S., Cruciani, G., Kettaneh-Wold, S., and Wold, S., (1993a), *D-Optimal Designs in QSAR*, Quantitative Structure-Activity Relationships, 12, 225-231.

Baroni, M., Constatino, G., Cruciani, G., Riganelli, D., Valigi, R., and Clementi, S., (1993b), *Generating Optimal PLS Estimations (GOLPE): An Advanced Chemometric Tool for Handling 3D-QSAR Problems,* Quantitative Structure-Activity Relationships, 12, 9-20.

Barnett, V., and Lewis, T., (1994), *Outliers in Statistical Data*, John Wiley & Sons, Chichester, England.

Belsley, D., Kuh, E,. and Welsch, R., (1980), *Identifying Influential Data and Sources of Collinearity*, John Wiley, New York.

Berglund, A., and Wold, S., (1997a), *INLR, Implicit Non-Linear Latent Variable Regression*, Journal of Chemometrics, 11, 141-156.

Berglund, A., DeRosa, M.C., and Wold, S., (1997b), *Alignment of Flexible Molecules at Their Receptor Site Using 3D Descriptors and Hi-PCA*, Journal of Computer-Aided Molecular Design, 11, 601-612.

Berglund, A., and Wold, S., (1999), *A Serial Extension of Multi Block PLS*, Journal of Chemometrics, 13, 461-471.

Berglund, A., Kettaneh, N., Uppgård, L.L., Wold, S., Bandwell, N., and Cameron, D.R., (2001), *The GIFI Approach to Non-Linear PLS Modelling*, Journal of Chemometrics, 15, 321-336.

Berntsson, O., Danielsson, L.G., Johansson, M.O., and Folestad, S., (2000), *Quantitative Determination of Content in Binary Powder Mixtures Using Diffuse Reflectance Near Infrared Spectrometry and Multivariate Analysis*, Analytica Chimica Acta, 419, 45-54.

Berntsson, O., (2001), *Characterization and Application of Near Infrared Spectroscopy for Quantitative Process Analysis of Powder Mixtures*, PhD Thesis, KTH, Stockholm, Sweden, ISBN 91-7283-074-3.

Bharati, M.H., Liu, J.J., and MacGregor, J.F., (2004), *Image Texture Analysis: Methods and Comparisons*, Chemometrics and Intelligent Laboratory Systems, 72, 57-71.

Blanco, M., Coello, J., Iturriaga, H., Maspoch, S., and Pagès, J., (2000), *NIR Calibration in Non-linear Systems: Different PLS Approaches and Artificial Neural Networks*, Chemometrics and Intelligent Laboratory Systems, 50, 75-82.

Blum, D.J.W., and Speece, R.E., (1990), *Determining Chemical Toxicity to Aquatic Species*, Environmental Science and Technology, 24, 284-293.

Bos, M. and Vrielink, J.A.M., (1994), *The wavelet transform for pre-processing IR spectra in the identification of mono- and di-substituted benzenes*, Chemometrics Intell. Lab. Syst., 23, 115-122.

Box, G.E.P., Hunter, W.G., and Hunter, J.S., (1978), *Statistics for Experimenters*, John Wiley & Sons, Inc., New York.

Box, G.E.P., Jenkins, G.M., and Reinsel, G.C., (1994), *Time Series Analysis - Forecasting and Control*, 3rd edition, Prentice-Hall, Inc., Englewood Cliffs, NJ.

Breiman, L., Friedman, J.H., Olshen, R.A., and Stone, C.J., (1984) *Classification and Regression Trees,* Wadsworth & Brooks / Cole Advanced Books & Software, Monterey, CA.

Bro, R., (1996), *Håndbog i Multivariabel Kalibrering*, KVL, Copenhagen, Denmark.

Bro, R., (1999), *Exploratory Study of Sugar Production Using Fluorescence Spectroscopy and Multi-way analysis*, Chemometrics and Intelligent Laboratory System, 46, 133-147.

Burnham, A.J., Viveros, R., and MacGregor, J.F., (1996), *Frameworks for Latent Variable Multivariate Regression*, Journal of Chemometrics, 10, 31-45.

Burnham, A.J., MacGregor, J.F, and Viveros, R., (1999), *A Statistical Framework for Multivariate Latent Variable Regression Methods Based on Maximum Likelihood,* Journal of Chemometrics, 13, 49-65.

Burnham, A.J., MacGregor, J., and Viveros, R., (2001), *Interpretation of Regression Coefficients Under a Latent Variable Regression Model*, Journal of Chemometrics, 15, 265-284.

Buydens, L.M.C., Reijmers, T.H., Beckers, M.L.M., and Wehrens, R., (1999), *Molecular Data Mining: a Challenge for Chemometrics*, Chemometrics and Intelligent Laboratory Systems, 49, 121-133.

Börås, L., Sjöström, J., and Gatenholm, P., (1997), *Characterization of Surfaces of CMTP Fibers Using Inverse Gas Chromatography Combined with Multivariate Data Analysis*, Nordic Pulp & Paper Research Journal, 12, 220-224.

Carlson, R., Lundstedt, T., and Albano, C., (1985), *Screening of Suitable Solvents in Organic Synthesis. Strategies for Solvent Selection*, Acta Chemica Scandinavica, B39, 79-91.

Carlson, R., (2004), *Designs For Explorative Experiments in Organic Synthetic Chemistry*, Chemometrics and Intelligent Laboratory Systems, 73, 151-166.

Carlson, R., and Carlson, J.E., (2005), *Design and Optimization in Organic Synthesis – Second Revised and Enlarged Edition*, Data Handling in Science and Technology, Elsevier, ISBN: 0-444-51527-5.

Cho, R.J., Campbell, M.J., Winzeler, E.A., Steinmetz, L., Conway, A., Wodicka, L., Wolfsberg, T.G., Gabrielian, A.E., Landsman, D., Lockhart, D.J., and Davis R.W., (1998), *A Genome-wide Transcriptional Analysis of the Mitotic Cell Cycle*, Molecular Cell, 2, 65-73.

Cocchi, M., and Johansson, E., (1993), *Amino Acids Characterization by GRID and Multivariate Data Analysis*, Quantitative Structure-Activity Relationships, 12, 1-8.

Connor, K., Safe, S., Jefcoate, C.R., and Larsen, M., (1995), *Structure-Dependent Induction of CYP2B by Polychlorinated Biphenyl Congeners in Female Sprague-Dawley Rats*, Biochemical Pharmacology, 50, 1913-1917.

Coomans, D., Broeckaert, I., Derde, M.P., Tassin, A., Massart, D.L., and Wold, S., (1984), *Use of a Microcomputer for the Definition of Multivariate Confidence Regions in Medical Diagnosis Based on Clinical Laboratory Profiles*, Computational Biomedical Research, 17, 1-14.

Cronin, M.T.D, and Schultz, T.W., (2003), *Pitfalls in QSAR*, Journal of Molecular Structure (Theochem), 622, 39-51.

Cramer, R.D., Pattersson, D.E., and Bunce, J.D., (1988), *Comparative Molecular Field Analysis (CoMFA). I. Effects of Shape on Binding of Steroids to Carried Proteins*, Journal of American Chemical Society, 110, 5959.

Cruciani, G., Baroni, M., Carosati, E., Clementi, M., Valigi, R., and Clementi, S., (2004), *Peptide Studies by Means of Principal Properties of Amino Acids Derived from MIF Descriptors*, Journal of Chemometrics, 18, 146-155.

Dahl, K.S., Piovoso, M.J., and Kosanovich, K.A., (1999), *Translating Third-order Data Analysis Methods to Chemical Batch Processes*, Chemometrics and Intelligent Laboratory Systems, 46, 161-180.

Daubechies, (1992), *Ten Lectures on wavelets*, SIAM, Philadelphia, PA.

Davis, O.L., and Goldsmith, P.L., (1986), *Statistical Methods in Research and Production*, Longman, New York.

Dayal, B., MacGregor, J.F., Taylor, P.A., Kildaw, R., and Marcikic, S., (1994), *Application of Feedforward Neural Networks and Partial Least Squares Regression for Modelling Kappa Number in a Continuous Kamyr Digester*, Pulp and Paper Canada, 95, 26-32.

DeAguiar, P.F., Bourguignon, B., Khots, M.S., Massart, D.L., and Phan-Than-Luu, R., (1995), *D-Optimal Designs*, Chemometrics and Intelligent Laboratory Systems, 30, 199-210.

Dearden, J., (1985), *Partitioning and Lipophilicity in Quantitative Structure-Activity Relationships,* Environmental Health Perspectives, 61, 203-228.

De Jong, S., (1993), *PLS Fits Closer Than PCR*, Journal of Chemometrics, 7, 551-557.

De Jong, S., Wise, B.M., and Ricker, N.L., (2001), *Canonical Partial Least Squares and Continuum Power Regression*, Journal of Chemometrics, 15, 85-100.

Deneer, J.W., Sinninge, T.L., Seinen, W., and Hermens, J.L.M., (1987), *Quantitative Structure-Activity Relationships for the Toxicity and Bioconcentration Factor of Nitrobenzene Derivatives Towards the Guppy (Poecilia reticulata)*, Aquatic Toxicology, 10, 115-129.

Deneer, J.W., van Leeuwen, C.J., Seinen, W., Maas-Diepeveen, J.L., and Hermens, J.L.M., (1989), *QSAR Study of the Toxicity of Nitrobenzene Derivatives Towards Daphnia Magna, Chlorella Pyrenoidosa and Photobacterium Phosphoreum*, Aquatic Toxicology, 15, 83-98.

Denham, M.C., (1997), *Prediction Intervals in Partial Least Squares*, Journal of Chemometrics, 11, 39-52.

Dhanoa, M.S., Lister, S.J., Sanderson, R., and Barnes, R.J., (1994), *The Link Between Multiplicative Scatter Correction (MSC) and Standard Normal Variate (SNV) Transformation of NIR Spectra*, Journal of Near Infrared Spectroscopy, 2, 43-47.

Drewry, D.H., and Young, S.S., (1999), *Approaches to the Design of Combinatorial Libraries*, Chemometrics and Intelligent Laboratory Systems, 48, 1-20.

Duarte, I., Barros, A., Belton, P.S., Righelato, R., Spraul, M., Humper, E., and Gil, A.M., (2002), *High-resolution Nuclear Magnetic Resonance Spectroscopy and Multivariate Analysis for the Characterization of Beer*, Journal of Agricultural and Food Chemistry, 50, 2475-2481.

Dunn, III, W.J., (1989), *Quantitative Structure-Activity Relationships (QSAR)*, Chemometrics and Intelligent Laboratory Systems*,* 6, 181-190.

Dyrby, M., Petersen, R.V., Larsen, J., Rudolf, B., Nørgaard, L., Engelsen, S.B., (2004), *Towards On-line Monitoring of the Composition of Commercial Carrageenan Powders*, Carbohydrate Polymers, 57, 337-348.

Efron, B., and Gong, G., (1983), *A Leisurely Look at the Bootstrap, the Jack-knife, and Cross-validation*, American Statistician, 37, 36-48.

Elg-Kristoffersson, K., Sjöström, M., Edlund, U., Lindgren, Å., and Dolk, M., (2002) *Reactivity of Dissolving Pulp: Characterisation Using Chemical Properties, NMR Spectroscopy and Multivariate Data Analysis*, Cellulose, 9, 159-170.

Ergon, R., (1998), *Dynamic System Multivariate Calibration by System Identification Methods*, Modelling Identification and Control, 19, 77-97.

Eriksson, L., Dyrby, M., Trygg, J., and Wold, S., (2006), *Separating Y-predictive and Y-orthogonal variation in multi-block spectral data*, Journal of Chemometrics, 20, 352-361.

Eriksson, L., Jonsson, J., Sjöström, M., Wikström, C., and Wold, S., (1988), *Multivariate Derivation of Descriptive Scales for Monosaccharides*, Acta Chemica Scandinavica, 42, 504-514.

Eriksson, L., Jonsson, J., Hellberg, S., Lindgren, F., Sjöström, M., Wold, S., Sandström, B., and Svensson, I., (1991), *A Strategy for Ranking Environmentally Occurring Chemicals. Part V: The Development of two Genotoxicity QSARs for Halogenated Aliphatics*. Environmental Toxicology and Chemistry, 10, 585-596.

Eriksson, L., Sandström, B.E., Tysklind, M., and Wold, S., (1993), *Modelling the Cytotoxicity of Halogenated Aliphatic Hydrocarbons. Quantitative Structure-Activity Relationships for the IC50 to Human HeLa Cells*, Quantitative Structure-Activity Relationships, 12, 124-131.

Eriksson, L., and Hermens, J.L.M., (1995a), *A Multivariate Approach to Quantitative Structure-Activity and Structure-Property Relationships,* In: The Handbook of Environmental Chemistry, (Ed.) J. Einax, Vol2H, Chemometrics in Environmental Chemistry, Springer Verlag, Berlin.

Eriksson, L., Hermens, J.L.M., Johansson, E., Verhaar, H.J.M. and Wold, S., (1995b), *Multivariate Analysis of Aquatic Toxicity Data with PLS*, Aquatic Sciences, 57, 217-241.

Eriksson, L., and Johansson, E., (1996), *Multivariate Design and Modelling in QSAR*, Chemometrics and Intelligent Laboratory Systems, 34, 1-19.

Eriksson, L., Johansson, E., Müller, M., and Wold, S., (1997), *Cluster-based Design in Environmental QSAR*, Quantitative Structure-Activity Relationships, 16, 383-390.

Eriksson, L., Johansson, E., Tysklind, M., and Wold, S., (1998), *Pre-processing of QSAR Data by Means of Orthogonal Signal Correction*, The QSAR and Modelling Society, Newsletter 1998, www/pharma-ethz.ch./qsar.

Eriksson, L., Andersson, P., Johansson, E., Tysklind, M., Sandberg, M., and Wold, S., (1999a), *The Constrained Principal Property Space in QSAR – Directional and Non-Directional Modelling Approaches*, Proceedings 12th European Symposium on QSAR, August 1998, Copenhagen, Denmark.

Eriksson, L., Johansson, E., Kettaneh-Wold, N., Wikström, C., and Wold, S., (1999b), *Design of Experiments – Principles and Applications*, Umetrics AB.

Eriksson, L., Trygg, J., Johansson, E., Bro, R., and Wold, S., (2000a), *Orthogonal Signal Correction, Wavelet Analysis, and Multivariate Calibration of Complicated Process Fluorescence Data*, Analytica Chimica Acta, 420, 181-195.

Eriksson, L., Johansson, E., Lindgren, F., and Wold, S., (2000b), *GIFI-PLS: Modeling of Non-Linearities and Discontinuities in QSAR*, Quantitative Structure-Activity Relationships, 19, 345-355.

Eriksson, L., Johansson, E., Müller, M., and Wold, S., (2000c), *On the Selection of Training Set in Environmental QSAR When Compounds are Clustered*, Journal of Chemometrics, 14, 599-616.

Eriksson, L., Hagberg, P., Johansson, E., Rännar, S., Whelehan, O., Åström, A., and Lindgren, T., (2001), *Multivariate Process Monitoring of a Newsprint Mill. Application to Modelling and Predicting COD Load Resulting from Deinking of Recycled Paper*, Journal of Chemometrics, 15, 337-352.

Eriksson, L., Johansson, E., Lindgren, F., Sjöström, M., and Wold, S., (2002), *Megavariate Analysis of Hierarchical QSAR Data*, Journal of Computer-Aided Molecular Design, 16, 711-726.

Eriksson, L., Jaworska, J., Worth, A.P., Cronin, M.T.D., McDowell, R.M., and Gramatica, P., (2003), *Methods for Reliability and Uncertainty Assessment and for Applicability Evaluations of Classification- and Regression-based QSAR,* Environmental Health Perspectives, 11, 1361-1375.

Eriksson, L., Arnhold, T., Beck, B., Fox, T., Johansson, E., and Kriegl, J.M., (2004a), *Onion Design and its Application to a Pharmaceutical QSAR Problem*, Journal of Chemometrics, 18, 188-202.

Eriksson, L., Antti, H., Gottfries, J., Holmes, E., Johansson, E., Lindgren, F., Long, I., Lundstedt, T., Trygg, J., and Wold, S., (2004b), *Using Chemometrics for Navigating in the Large Data Sets of Genomics, Proteomics and Metabonomics*, Analytical and Bioanalytical Chemistry, 380, 419-429.

Eriksson, L., Antti, H., Holmes, E., and Johansson, E., (2005), in: Robertson, D. (Ed.), Modern Safety Assessment Methods of Compounds and Biomarkers: Metabonomics and Evaluation, *Chapter 8: Multi- and Megavariate Data Analysis: Finding and Using Regularities in Metabonomics Data*, Marcel Dekker/CRC Press, ISBN: 0-8247-2665-0.

Eriksson, L., Damborsky, J., Earll, M., Johansson, E., Trygg, J., and Wold, S., (2004c), *Three-block Bi-focal PLS (3BIF-PLS) and its application in QSAR*, SAR and QSAR in Environmental Research, 5/6, 481-499.

Eriksson, L., Gottfries, J., Johansson, E., and Wold, S., (2004d), *Time-resolved QSAR: an Approach to PLS Modelling of Three-way Biological Data*, Chemometrics and Intelligent Laboratory Systems, 73, 73-84.

Eriksson, L., Johansson, E., Kettaneh-Wold, N., Trygg, J., Wikström, M., and Wold, S., Multi- and Megavariate Data Analysis, Part II, Method Extensions and Advanced Applications, Chapter 23, Umetrics Academy, 2005.

Eriksson, L., Wold, S., and Trygg, J., (2006), *Multivariate Analysis of Congruent Images (MACI)*, Chemometrics and Intelligent Laboratory Systems, In press.

Eriksson, L., Trygg, J., and Wold, S., *CV-ANOVA for significance testing of PLS and OPLS models*, submitted for publication 2008.

Esbensen, K., and Geladi, P., (1989), *Strategy of Multivariate Image Analysis (MIA)*, Chemometrics and Intelligent Laboratory Systems, 7, 67-86.

Espina, J.R., Shockcor, J.P., Herron, W.J., Car, B.D., Contel, N.R., Ciaccio, P.J., Lindon, J.C., Holmes, E., and Nicholson, J.K., (2001), *Detection of In-vivo Biomarkers of Phospholipidosis Using NMR-based Metabonomic Approaches*, Magnetic Resonance in Chemistry, 39, 559–565.

Eastment, H. and Krzanowski, W., (1982), *Crossvalidatory choice of the number of components from a principal component analysis*, Technometrics 24 73-77.

Etemad, K., and Chellappa, R., (2004), *Discriminant Analysis for Recognition of Human Face Images*, Journal of Optical Society of America, 14, 1724-1733.

Everitt, B.S., Landau, S., Leese, M., (2001), *Cluster Analysis*, Fourth Edition Arnold Publishers, London.

Fisher, R.A., (1922), *On the interpretation of $\chi 2$ from contingency tables, and the calculation of P*. Journal of the Royal Statistical Society 85(1):87-94.

Fisher, R.A., and MacKenzie, W., (1923), *Studies in Crop Variation. II. The manurial response of different potato varieties*, Journal of Agricultural Science, 13, 311-320.

Fisher, R.A., (1936), *The use of Multiple Measurements in Taxonomic Problems*, Ann. Eugenics, 7, 179-188.

Fisher, R.A., (1954), *Statistical Methods for research workers,* Oliver and Boyd.

Flåten, G.R., and Walmsley, A.D., (2004), *A Design of Experiment Approach Incorporating Layered Designs for Choosing the Right Calibration Model*, Chemometrics and Intelligent Laboratory Systems, 73, 55-66.

Frank, I.E., and Friedman, J.H., (1993), *A Statistical View of Some Chemometrics Regression Tools*, Technometrics, 35, 109-135.

Frank, I., (1995), *Modern Nonlinear Regression Methods*, Chemometrics and Intelligent Laboratory Systems, 27, 1-19.

Gabrielsson, J., Lindberg, N.O., and Lundstedt, T., (2002), *Multivariate Methods in Pharmaceutical Applications*, Journal of Chemometrics, 16, 141-160.

Gabrielsson, J., Jonsson, H., Airiau, C., Schmidt, B., Escott, R., and Trygg, J., (2006), *The OPLS methodology for analysis of multi-block batch process data,* Journal of Chemometrics, 20, 362-369.

Gallagher, N.B., Shaver, J.M., Martin, E.B., Morris, J., Wise, B.M., Windig, W., (2004), *Curve Resolution for Multivariate Images with Applications to TOF-SIMS and Raman*, Chemometrics and Intelligent Laboratory Systems, 73, 105-117.

Gallop, M.A., Barrett, R.W., Dower, W.J., Fodor, S.P.A., and Gordon, E.M., (1994), *Applications of Combinatorial Technologies to Drug Discovery. 1. Background and Peptide Combinatorial Libraries*, Journal of Medicinal Chemistry, 37, 1233-1251.

Gauchi, J.P., and Chagnon, P., (2001), *Comparison of Selection Methods of Explanatory Variables in PLS Regression with Application to Manufacturing Process Data*, Chemometrics and Intelligent Laboratory Systems, 58, 171-193.

Geladi, P., MacDougall, D., and Martens, H., (1985), *Linearization and Scatter-correction for Near-infrared Reflectance Spectra of Meat*, Applied Spectroscopy, 3, 491-500.

Geladi, P., Isaksson, H., Lindqvist, L., Wold, S., and Esbensen, K., (1989), *Principal Component Analysis of Multivariate Images*, Chemometrics and Intelligent Laboratory Systems, 5, 209-220.

Geladi, P., (1992), *Some Special Topics in Multivariate Image Analysis*, Chemometrics and Intelligent Laboratory Systems, 14, 375-390.

Gillet, V.J., (2002), *Reactant- and Product-based Approaches to the Design of Combinatorial Libraries*, Journal of Computer-Aided Molecular Design, 16, 371-380.

Giraud, E., Luttmann, C., Lavelle, F., Riou, J.F., Mailliet, P., and Laoui, A., (2000), *Multivariate Data Analysis using D-optimal Designs, Partial Least Squares, and Response Surface Modelling, A Directional Approach for the Analysis of Farnesyltransferase Inhibitors*, Journal of Medicinal Chemistry, 43, 1807-1816.

Goodford, P., (1996), *Multivariate Characterization of Molecules for QSAR Analysis,* Journal of Chemometrics, 10, 107-117.

Gordon, E.M., Barret, R.W., Dower, W.J., Fodor, S.P.A., and Gallop, M.A., (1994), *Applications of Combinatorial Technologies to Drug Discovery. 2. Combinatorial Organic Synthesis, Library Screening Strategies, and Future Directions*, Journal of Medicinal Chemistry, 37, 1385-1401.

Gottfries, J., Blennow, K., Wallin, A., and Gottfries, C.G., (1995), *Diagnosis of Dementias Using Partial Least Squares Discriminant Analysis*, Dementia, 6, 83-88.

Gottfries, J., Depui, H., Fransson, H., Jongeneelen, M., Josefsson, M., Langkilde, F.W., and Witte, D.T., (1996), *Vibrational Spectrometry for the Assessment of Active Substance in Metoprolol Tablets: A Comparison Between Transmission and Diffuse Reflectance Near-Infrared Spectrometry*, Journal of Pharmaceutical and Biomedical Analysis, 14, 1495-1503.

Gottfries, J., Sjögren, M., Holmberg, B., Rosengren, L., Davidsson, P., and Blennow, K., (2004), *Proteomics for Drug Target Discovery*, Chemometrics and Intelligent Laboratory Systems, 73, 47-53.

Grainger, D.J., (2003), *Megavariate Statistics Meets High Data-density Analytical Methods: The Future of Medical Diagnostics*, IRTL Reviews 1, 1-6.

Granberg, R., (1998), *Solubility and Crystal Growth of Paracetamol in Various Solvents,* Ph.D. Thesis, Royal Institute of Technology, Stockholm, Sweden.

Gunnarsson, I., Andersson, P., Wikberg, J., and Lundstedt, T., (2003), *Multivariate Analysis of G Protein-coupled Receptors*, Journal of Chemometrics, 17, 82-92.

Gustafsson, A., (1993), *QFD and Conjoint Analysis – The Key to Customer Oriented Products*, Ph.D. Thesis, Linköping University, Linköping, Sweden.

Hammett, L.P., (1970), *Physical Organic Chemistry*, 2nd edn., McGraw-Hill, New York.

Hand, D.J., (1998), *Data Mining: Statistics and More?*, American Statistician, 52, 112-188.

Hansch, C., and Leo, A.J., (1970), *Substituent Constants for Correlation Analysis in Chemistry and Biology*, Wiley, New York.

Hartnett, M.K., Lightbody, G., and Irwin, G.W., (1999), *Identification of State Models Using Principal Components Analysis*, Chemometrics and Intelligent Laboratory Systems, 46, 181-196.

Hellberg, S., (1986), *A Multivariate Approach to QSAR*, Ph.D. Thesis, Umeå University, Umeå, Sweden.

Hellberg, S., Sjöström, M., and Wold, S., (1986), *The Prediction of Bradykinin Potentiating Potency of Pentapeptides. An Example of a Peptide Quantitative Structure-Activity Relationship*, Acta Chemica Scandinavica, B40, 135-140.

Hellberg, S., Eriksson, L., Jonsson, J., Lindgren, F., Sjöström, M., Skagerberg, B., Wold, S., and Andrews, P., (1991), *Minimum Analogue Peptide Sets (MAPS) for Quantitative Structure-Activity Relationships,* International Journal of Peptide and Protein Research, 37, 414-424.

Hermens, J.L.M., (1989), *Quantitative Structure-Activity Relationships of Environmental Pollutants.* In: Hutzinger, O., (Ed.), Handbook of Environmental Chemistry, Vol 2E, Reactions and Processes. Springer-Verlag, Berlin, 1989, pp. 111-162.

Hubbard, B.B., (1995), *The world according to wavelets*, A K Peters, Wellesley, MA.

Hunter, J.S., (1986), *The Exponentially Weighted Moving Average*, Journal of Quality Technology, 18, 203-210.

Höskuldsson, A., *PLS regression methods*. J. Chemometrics, 2, (1988) 211-228.

Höskuldsson, A., (1996), *Prediction Methods in Science and Technology*, Thor Publishing, Copenhagen, Denmark.

Höskuldsson, A., (1998), *The Heisenberg Modelling Procedure and Application to Nonlinear Modelling*, Chemometrics and Intelligent Laboratory Systems, 44, 15-30.

Höskuldsson, A., (2001), *Causal and Path Modelling*, Chemometrics and Intelligent Laboratory Systems, 58, 287-311.

Indahl, U.G., and Naes, T., (1998), *Evaluation of Alternative Spectral Feature Extraction Methods of Textural Images for Multivariate Modeling*, Journal of Chemometrics, 12, 261-278.

Jackson, J.E. (1991), *A User's Guide to Principal Components*, John Wiley, New York.
ISBN 0-471-62267-2.

Janné, K., Pettersen, J., Lindberg, N.O., and Lundstedt, T., (2001), *Hierarchical Principal Component Analysis (PCA) and Projection to Latent Structure Technique (PLS) on Spectroscopic Data as a Data Pretreatment for Calibration*, Journal of Chemometrics, 15, 203-213.

Jellum, E., Björnsson, I., Nesbakken, R., Johansson, E., and Wold, S., (1981), *Classification of Human Cancer Cells by means of Capillary Gas Chromatography and Pattern Recognition Analysis*, Journal of Chromatography, 217, 231-237.

Johansson, D, and Lindgren, P., (2002), *Analysis of Microarray Data Using a Multivariate Approach*, Masters Thesis in Bioinformatics, Umeå University, Umeå, Sweden.

Johansson, D., Lindgren, P., and Berglund, A., (2003), *A Multivariate Approach Applied to Microarray Data for Identification of Genes with Cell Cycle-Coupled Transcription*, Bioinformatics, 19, 467-473.

Jonsson, J., Eriksson, L., Hellberg, S., Sjöström, M., and Wold, S., (1989a), *Multivariate Parametrization of 55 Coded and Non-Coded Amino Acids*, Quantitative Structure-Activity Relationships, 8, 204-209.

Jonsson, J., Eriksson, L., Hellberg, S., Sjöström, M., and Wold, S., (1989b), *A Multivariate Approach to Saccharide Quantitative Structure-Activity Relationships Exemplified by Two Series of 9-Hydroxyellipticine Glycosides*, Acta Chemica Scandinavica, 43, 286-289.

Jonsson, J., Eriksson, L., Hellberg, S., Lindgren, F., Sjöström, M., and Wold, S., (1991), *A Multivariate Representation and Analysis of DNA Sequence Data*, Acta Chemica Scandinavica, 45, 186-192.

Jonsson, J., (1992), *Quantitative Sequence-Activity Modelling (QSAM),* Ph. D. Thesis, Umeå University, Umeå, Sweden.

Jonsson, J., Norberg, T., Carlsson, L., Gustafsson, C., and Wold, S., (1993), *Quantitative Sequence-Activity Models (QSAM) – Tools for Sequence Design*, Nucleic Acids Research, 21, 733-739.

Jonsson, P., Sjöström, M., Wallbäcks, L., and Antti, H., *Strategies for Implementation and Validation of On-line Models for Multivariate Monitoring and Control of Wood Chips Properties*, Journal of Chemometrics, 18, 203-207.

Kaiser, G., (1994), *A Friendly Guide to Wavelets*, Birkhäuser, Boston, MA.

Kassidas, A., MacGregor, J.F., and Taylor, P.A., (1998), *Synchronization of Batch Trajectories Using Dynamic Time Warping*, AIChE Journal, 44, 864-875.

Kettaneh-Wold, N., MacGregor, J.F., Dayal, B., and Wold, S., (1994), *Multivariate Design of Process Experiments (M-DOPE)*, Chemometrics and Intelligent Laboratory Systems, 23, 39-50.

Kettaneh, N., Berglund, S., and Wold, S., (2005), *PCA and PLS with Very Large Data Sets*, Computational Statistics & Data Analysis, 48, 69-85.

Kim, K.H., (1993), *Non-linear Dependence in Comparative Molecular Field Analysis*, Journal of Computer-Aided Molecular Design, 7, 71-82.

Kimura, T., Miyashita, Y., Funatsu, K., and Sasaki, S., (1996), *Quantitative Structure-Activity Relationships of the Synthetic Substrates for Elastase Enzyme Using Nonlinear Partial Least Squares Regression*, Journal of Chemical Information and Computer Science, 36,185-189.

Kjaer Pedersen, D., Martens, H., Pram Nielsen, J., Engelsen, S.B., (2002), *Near-infrared Absorption and Scattering Separated by Extended Inverted Signal Correction (EISC): Analysis of Near-infrared Transmittance Spectra of Single Wheat Seeds*, Applied Spectroscopy, 56, 1206-1214.

Kourti, T., (2002), *Process Analysis and Abnormal Situation Detection: From Theory to Practice*, IEEE Control Systems Magazine, October 2002, 10-25.

Kourti, T., (2003), *Multivariate Dynamic Data Modeling for Analysis and Statistical Process Control of Batch Processes*, *Start-ups and Grade Transitions*, Journal of Chemometrics, 17, 93-109.

Kriegl, J.M., Eriksson, L., Arnhold, T., Beck, B., Johansson, E., and Fox, T., (2005), *Multivariate Modeling of Cytochrome P450 3A4 Inhibition*, European Journal of Pharmaceutical Sciences, 24, 451-463.

Kristal, B.S., (2002), *Practical Considerations and Approaches for Entry-level Megavariate Analysis.*.

Kubinyi, H., (1990), *Quantitative Structure-Activity Relationships and Molecular Modelling in Cancer Research*, Journal Cancer Research & Clinical Oncology, 116, 529-537, 1990.

Könemann, H., (1981), *Quantitative Structure-Activity Relationships in Fish Studies. Part 1: Relationship for 50 Industrial Pollutants*, Toxicology, 19, 209-221.

Larsson, U., Carlson, R., and Leroy. J., (1993), *Synthesis of Amino Acids with Modified Principal Properties. 1. Amino Acids with Fluorinated Side Chains*, Acta Chemica Scandinavica, 47, 380-390.

Leardi, R., (2001), *Genetic Algorithms in Chemistry and Chemometrics: A Review*, Journal of Chemometrics, 15, 559-569.

Lewi, P.J., (1995), *Spectral Mapping of Drug-Test Specificities*, In: H. van de Waterbeemd (Ed.), Chemometric Methods in Molecular Design*,* VCH, Weinheim.

Lied, T.T., Geladi, P., and Esbensen, K.H., (2000), *Multivariate Image Regression (MIR): Implementation of Image PLSR – First Forays*, Journal of Chemometrics, 14, 585-598.

Lindberg, N.O., and Gabrielsson, J., (2004), *Use of Software to Facilitate Pharmaceutical Formulation – Experiences from a Tablet Formulation*, Journal of Chemometrics, 18, 133-138.

Linderholm, J., and Lundberg, E., (1994), *Chemical Characterization of Various Archaeological Soil Samples using Main and Trace Elements Determined by Inductively Coupled Plasma Atomic Emission Spectrometry,* Journal of Archaeological Science, 21, 303-314.

Lindgren, F., and Geladi, P., (1992), *Multivariate Spectrometric Image Analysis – An Illustrative Study with two Constructed Examples of Metal Ions in Solution*, Chemometrics and Intelligent Laboratory System, 14, 397-412.

Lindgren, Å., Sjöström, M., and Wold, S., (1996), *Quantitative Structure-Effect Relationships for Some Technical Nonionic Surfactants*, JAOCS, 7, 863-875.

Lindgren, Å., (2000), *Use of Multivariate Methods and DOE to Improve Industrial-Scale Production Quality of a Cellulose Derivative*. Journal of Chemometrics, 14, 657-665.

Linusson, A., Gottfries, J., Lindgren, F., and Wold, S., (2000), *Statistical Molecular Design of Building Blocks for Combinatorial Chemistry*, Journal of Medicinal Chemistry, 43, 1320-1328.

Linusson, A., (2000), *Efficient Library Selection in Combinatorial Chemistry*, Ph.D. Thesis, Umeå University, Umeå, Sweden.

Linusson, A., Gottfries, J., Olsson, T., Örnskov, E., Folestad, S., Nordén, B., and Wold, S., (2001), *Statistical Molecular Design, Parallel Synthesis, and Biological Evaluation of a Library of Thrombin Inhibitors*, Journal of Medicinal Chemistry, 44, 3424-3439.

Lockhart, D.J., and Winzeler, E.A., (2000), *Genomics, Gene Expression and DNA Arrays*, Nature, 405, 827-836.

Long, I., Andersson, P., Siefert, E., and Lundstedt, T., (2004), *Multivariate Analysis of Five GPCR Receptor Classes*, Chemometrics and Intelligent Laboratory Systems, 73, 95-104.

Louwerse, D.J., Tates, A.A., Smilde, A.K., Koot, G.L.M., and Berndt, H., (1999), *PLS Discriminant Analysis with Contribution Plots to Determine Differences Between Parallel Batch Reactors in the Process Industry*, Chemometrics and Intelligent Laboratory Systems, 46, 197-206.

Lowe, G., (1995), *Combinatorial Chemistry*, Chemical Society Reviews, 24, 309-317.

Lundstedt, T., (1991), *A QSAR Strategy for Screening of Drugs and Predicting Their Clinical Activity*, Drug News & Perspectives, 4, 468-475.

Lundstedt, T., Carlson, R., and Shabana, R., (1987), *Optimum Conditions, for the Willgerodt-Kindler Reaction. 3. Amine Variation*, Acta Chemica Scandinavica, B41, 157-163.

Lundstedt, T., Clementi, S., Cruciani, G., Pastor, M., Kettaneh, N., Andersson, P.M., Linusson, A., Sjöström, M., Wold, S., and Nordén. B., (1997), *Intelligent Combinatorial Libraries*, In: H. van de Waterbeemd, B. Testa and G. Folkers, eds., Computer-Assisted Lead Finding and Optimization, Current Tools for Medicinal Chemistry, Wiley-VCH, Weinheim.

MacFie, H., Moore, P.B., and Wakeling, I., (1999), *Changes in the Sensory Properties and Consumer Preferences for Dessert Apples*, Apples and Pears Research Council, UK.

MacGregor, J.F., and Nomikos, P., (1992), *Monitoring Batch Processes*, Proceedings NATO Advanced Study Institute for Batch Processing Systems Eng., May 29 – June 7, 1992, Antalya, Turkey.

MacGregor, J.F., and Kourti, T., (1995), *Statistical Process Control of Multivariate Processes*, Control Eng. Practice, 3, 403-414.

MacGregor, J.F., (1996), *Using On-Line Process Data to Improve Quality*, ASQC Statistics Division Newsletter, 16, 6-13.

Maitra, R., (2001), *Clustering Massive Data Sets with Applications in Software Metrics and Tomography*, Technometrics, 43, 336-346.

Mallat, S.G., (1989), *A Theory for Multiresolution Signal Decomposition: The Wavelet Representation*, IEEE Transactions on Pattern Analysis and Machine Intelligence, v.11 n.7, p.674-693, July 1989.

Mallat, S.G., (1998), *A Wavelet Tour of Signal Processing*, Academic Press.

Martens, H., and Naes, T., (1989), *Multivariate Calibration*, John Wiley, New York.

Martens, H., and Martens, M., (2000), *Modified Jack-Knife Estimation of Parameter Uncertainty in Bilinear Modeling (PLSR)*, Food Quality and Preference, 11, 5-16.

Martens, H., Pram Nielsen, J., and Engelsen, S.B., (2003), *Light Scattering and Light Absorbance Separated by Extended Multiplicative Signal Correction. Application to Near-Infrared Transmission Analysis of Powder Mixtures*, Analytical Chemistry, 75, 394-404.

Martin, E.J., Blaney, J.M., Siani, M.A., Spellmeyer, D.C., Wong, A.K., and Moos, W.H., (1995), *Measuring Diversity: Experimental Design of Combinatorial Libraries for Drug Discovery*, Journal of Medicinal Chemistry, 38, 1431-1436.

Marvanova, S., Nagata, Y., Wimmerova, M., Sykorova, J., Hynkova, K., and Damborsky, J., (2001), *Biochemical Characterization of Broad-specificity Enzymes Using Multivariate Experimental Design and a Colorimetric Microplate Assay: Characterization of the Haloalkane Dehalogenase Mutants*, Journal of Microbiological Methods, 44, 149-157.

Massart, B., (1997), *Environmental Monitoring and Forecasting by Means of Multivariate Methods*, Ph.D. Thesis, University of Bergen, Bergen, Norway.

Massart, D.L., Vandeginste, B.G.M., Deming, S.N., Michotte, Y., and Kaufman, L., (1988), *Chemometrics: A Textbook*, Elsevier.

Massart, D.L., Vandeginste, B.G.M., Buydens, L.M.C., De Jong, S., Lewi, P.J., and Smeyers-Verbeke, J., (1998), *Handbook of Chemometrics and Qualimetrics*, Elsevier.

McCloskey, J.T., Newman, M.C., and Clark, S.B., (1996), *Predicting the Relative Toxicity of Metal Ions Using Ion Characteristics: Microtox Bioluminescence Assay*, Environmental Toxicology and Chemistry, 15, 1730-1737.

McEwan, J.A., Earthy, P.J., and Ducher, C., (1998), *Preference Mapping – A Review*, Review No. 6, Campden & Chorleywood Food Research Association, Gloucestershire, UK.

McEwan, J.A., and Ducher, C., (1998), *Preference Mapping – Case Studies*, Review No. 7, Campden & Chorleywood Food Research Association, Gloucestershire, UK.

McNeese, W.H., Klein, R.A., (1991) *Statistical methods for the process industries,* Quality and Reliability/28.

Michailidis, G., and de Leeuw, J., (1998), *The GIFI System of Descriptive Multivariate Analysis*, Statistical Science, 13, 307-336.

Mittermayr, C.R., Nikolov, S.G., Hutter, H., and Grasserbauer, M., *(1996), Wavelet denoising of Gaussian peaks: a comparative study*, Chemometrics Intell. Lab. Syst., 34, 187-202.

Moberg, L., Karlberg, B., Blomqvist, S., and Larsson, U., (2000), *Comparison Between a New Application of Multivariate Regression and Current Spectroscopy Methods for the Determination of Chlorophylls and Their Corresponding Pheopigments*, Analytica Chimica Acta, 411, 137-143.

Moberg, L., and Karlberg, B., (2001), *Validation of a Multivariate Calibration Method for the Determination of Chlorophyll a, b, and c and Their Corresponding Pheopigments*, Analytica Chimica Acta, 450, 143-153.

Mullet, G.M., (1976), *Why Regression Coefficients have the Wrong Sign*, Journal of Quality Technology, 8, 121-126.

Munck, L., Nörgaard, L., Engelsen, S.B., Bro, R., and Andersen, C., (1998), *Chemometrics in Food Science – A Demonstration of the Feasibility of a Highly Exploratory, Inductive Evaluation Strategy of Fundamental Scientific Significance*, Chemometrics and Intelligent Laboratory, 44, 31-60.

Musumarra, G., Barresi, V., Condorelli, D.F., Fortuna, C.G., and Scirè, S., (2004) *Potentialities of Multivariate Approaches in Genome-based Cancer Research: Identification of Candidate Genes for New Diagnostics by PLS Discriminant Analysis*, Journal of Chemometrics, 18, 125-132.

Naes, T., and Indahl, U., (1998), *A Unified Description of Classical Classification Methods for Multicollinear Data,* Journal of Chemometrics, 12, 205-220.

Naes, T., and Mevik, B.H., (1999), *The Flexibility of Fuzzy Clustering Illustrated by Examples*, Journal of Chemometrics, 13, 435-444.

Naes, T., Isaksson, T., Fearn, T., and Davies, T., (2002), *A User-friendly Guide to Multivariate Calibration and Classification*, NIR Publications, Chichester, UK. ISBN: 0-95286662-5.

Nelson, P.R.C., Taylor, P.A., MacGregor, J.F., *Missing Data Methods in PCA and PLS: Score Calculations with Incomplete Observation*, Chemometrics and Intelligent Laboratry Systems, 35, 45-65, 1996.

Nicholson, J.K., Lindon, J.C., Holmes, E., (1999), *Metabonomics: Understanding the Metabolic Responses of Living Systems to Pathophysiological Stimuli via Multivariate Statistical Analysis of Biological NMR Spectroscopic Data*, Xenobiotica, 29, 1181-1189.

Nicholson, J.K, Connelly, J., Lindon, J.C., and Holmes, E., (2002), *Metabonomics: a Platform for Studying Drug Toxicity and Gene Function*, Nature Reviews, 1, 153-162.

Nijhuis, A., de Jong, S., and Vandeginste, B.G.M., (1997), *Multivariate Statistical Process Control in Chromatography*, Chemometrics and Intelligent Laboratory Systems, 38, 51-62.

Nilsson, D., (2005), *Prediction of Wood Species and Pulp Brightness from Roundwood Measurements*, PhD Thesis, Umeå University, Umeå, Sweden.

Nomikos, P., and MacGregor, J.F., (1995a), *Multivariate SPC Charts for Monitoring Batch Processes,* Technometrics, 37, 41-59.

Nomikos, P., and MacGregor, J.F., (1995b), *Multiway Partial Least Squares in Monitoring of Batch Processes*, Chemometrics and Intelligent Laboratory System, 30, 97-108.

Nomizu, M., Iwaki, T., Yamashita, T., Inagaki, Y., Asano, K., Akamatsu, M., and Fujita, T., (1993), *Quantitative Structure-Activity Relationship (QSAR) Study of Elastase Substrates and Inhibitors*, International Journal of Peptide and Protein Research, 42, 216-226.

Nordahl, Å., and Carlson, R., (1993), *Exploring Organic Synthetic Procedures*, Topics in Current Chemistry, 166, 1-64.

Norinder, U., (1996), *Single and Domain Mode Variable Selection in 3D QSAR Applications*, Journal of Chemometrics, 10, 95-105.

Norinder, U., Sjöberg, P., and Österberg, T., (1998), *Theoretical Calculation and Prediction of Brain-Blood Partitioning or Organic Solutes using Molsurf Parametrization and PLS Statistics*, Journal of Pharmaceutical Sciences, 87, 952-959.

Norinder, U., (2003), *Support Vector Machine Models in Drug Design: Applications to Drug Transport Processes and QSAR Using Simplex Optimisations and Variable Selection*, Neurocomputing, 55, 337-346.

Nouwen, J., Lindgren, F., Hansen, B., Karcher, W., Verhaar, H.J.M., and Hermens, J.L.M., (1997), *Classification of Environmentally Occurring Chemicals Using Structural Fragments and PLS Discriminant Analysis,* Environmental Science and Technology, 31, 2313-2318.

Nyström, Å., Andersson, P.M., and Lundstedt, T., (2000), *Multivariate Data Analysis of Topographically Modified a-Melanotropin Analogues Using Auto- and Cross-Auto Covariances*, Quantitative Structure-Activity Relationships, 19, 264-269.

Olsson, I.M., Gottfries, J., and Wold, S., (2004a), *D-optimal Onion Design in Statistical Molecular Design*, Chemometrics and Intelligent Laboratory Systems, 73, 37-46.

Olsson, I.M., Gottfries, J, and Wold, S., (2004b), *Controlling Coverage of D-optimal Onion Designs and Selections*, Journal of Chemometrics, 18, 548-557.

Oprea, T.I., (2000), *Property Distribution of Drug-Related Chemical Data-Bases*, Journal of Computer-Aided Molecular Design, 14, 251-264.

Oprea, T.I., and Gottfries, J., (2001), *Chemography: The Art of Navigating in Chemical Space*, Journal of Combinatorial Chemistry, 3, 157-166.

Phatak, A., and DeJong, S., (1997), *The Geometry of PLS*, Journal of Chemometrics, 11, 311-338.

Press, W., Flannery, B., Teukolsky, S., and Vetterling, W., Numerical Recipes in C, Cambridge University Press.

Qin, S.J., and McAvoy, T.J., (1992), *Non-Linear PLS Modelling Using Neural Networks*, Computation and Chemical Engineering, 16, 379-391.

Ramos, E.U., Vaes, W.H.J., Verhaar, H.J.M., and Hermens, J.L.M., (1997), *Polar Narcosis: Designing a Suitable Training Set for QSAR Studies*, Environmental Science & Pollution Research, 4, 83-90.

Rius, A., Ruisanchez, I., Callao, M.P., Rius, F.X., (1998), *Reliability of Analytical Systems: Use of Control Charts, Time Series Models and Recurrent Neural Networks*, Chemometrics and Intelligent Laboratory Systems, 40, 1-18.

Rännar, S., MacGregor, J.F., and Wold, S., (1998), *Adaptive Batch Monitoring Using Hierarchical PCA*, Chemometrics and Intelligent Laboratory Systems, 41, 73-81.

Sandberg, M., Sjöström, M., and Jonsson, J., (1996), *A Multivariate Characterization of tRNA Nucleosides,* Journal of Chemometrics, 10, 493-508.

Sandberg, M., Eriksson, L., Jonsson, J., Sjöström, M., and Wold, S., (1998), *New Chemical Dimensions Relevant for the Design of Biologically Active Peptides. A Multivariate Characterization of 87 Amino Acids*, Journal of Medicinal Chemistry, 41, 2481-2491.

Savitzky, A., and Golay, M.J.E., (1964), *Smoothing and Differentiation by Simplified Least Squares Procedures*, Analytical Chemistry, 36, 1627-1632.

Schaper, K.J., (1991), *QSAR Analysis of Chiral Drugs Including Stereoisomer Combinations*, In: Silipo, C., and Vittoria, A, (Eds.), QSAR: Rational Approaches to the Design of Bioactive Compounds, Elsevier Science Publishers, Amsterdam, 1991, pp. 25-32.

Schüürmann, G., Rayasamuda, K., and Kristen, U., (1996), *Structure-Activity Relationships for Chloro- and Nitrophenol Toxicity in the Pollen Tube Growth Test*, Environmental Toxicology and Chemistry, 15, 1702-1708.

Sekulic, S., Seasholtz, M.B., Wang, Z., Kowalski, B., Lee, S.E., and Holt, B.R, (1993), *Non-linear Multivariate Calibration Methods in Analytical Chemistry*, Analytical Chemistry, 65, 835-845.

Seydel, J.K., Wiese, M., Cordes, H.P., Chi, H.L., Schaper, K.-J., Coats, E.A., Kunz, B., Engel, J., Kutscher, B., and Emig, H., (1991), *QSAR and Modelling of Enzyme Inhibitors, Anticonvulsants and Amphiphilic Drugs Interacting with Membranes*, In:, Silipo, C., and Vittoria, A, (Eds.), QSAR: Rational Approaches to the Design of Bioactive Compounds, Elsevier Science Publishers, Amsterdam, 1991, pp. 367-376.

Shao, J., (1993), Linear Model Selection by Cross-Validation, Journal of the American Statistical Association, 88, 486-494.

Shewhart, W., (1931), *Economic Control of Quality of Manufactured Product*, Van Nostrand, Princeton, N.J.

Singhal, A., and Seborg, D.E., (2002), *Pattern Matching in Historical Batch Data Using PCA*, IEEE Control Systems Magazine, October 2002, 53-63.

Sjöblom, J., Svensson, O., Josefson, M., Kullberg, H., and Wold, S., (1998), *An Evaluation of Orthogonal Signal Correction Applied to Calibration Transfer of Near Infrared Spectra*, Chemometrics and Intelligent Laboratory Systems, 44, 229-244.

Sjöström, M., Wold, S., Lindberg, W., Persson, J.-Å., and Martens, H., (1983), *A Multivariate Calibration Problem in Analytical Chemistry Solved by Partial Least-Squares Models in Latent Variables*, Analytica Chimica Acta, 150, 61-70.

Sjöström, M., Wold, S., and Söderström, B., (1986), *PLS Discriminant Plots,* Proceedings of PARC in Practice, Amsterdam, June 19-21, 1985. Elsevier Science Publishers B.V., North-Holland.

Sjöström, M., Eriksson, L., Hellberg, S., Jonsson, J., Skagerberg, B., and Wold, S., (1989), *Peptide QSARs: PLS Modelling and Design in Principal Properties.* In: J.L. Fauchère (ed.): QSAR - Quantitative Structure-Activity Relationships in Drug Design. Proc. 7th European Symposium on QSAR, Sept. 1988, Interlaken, Switzerland. Alan R. Liss, Inc., New York, pp. 131-134.

Sjöström, M., Rännar, S., and Rilfors, L., (1995), *Polypetide Sequence Property Relationships in Escherichica Coli Based on Auto Cross Covariances*, Chemometrics and Intelligent Laboratory Systems, 29, 295-305.

Sjöström, M., Lindgren, Å., and Uppgård, L.L., (1997), *Joint Multivariate Quantitative Structure-Property and Structure-Activity Relationships for a Series of Technical Nonionic Surfactants*, In: F. Chen & G. Schüürmann (eds.), Quantitative Structure-Activity Relationships in Environmental Sciences – VII. Proceedings of the 7th International Workshop on QSAR in Environmental Sciences, June 24-28, 1996, Elsinore, Denmark. SETAC Press, Pensacola, Florida, 1997, pp. 435-449.

Skagerberg, B., Sjöström, M., and Wold, S., (1987), *Multivariate Characterization of Amino Acids by Reversed Phase High Pressure Liquid Chromatography*, Quantitative Structure-Activity Relationships, 6, 158-164.

Skagerberg, B., Bonelli, D., Clementi, S., Cruciani, G., and Ebert, C., (1989), *Principal Properties for Aromatic Substituents. A Multivariate Approach for Design in QSAR*, Quantitative Structure-Activity Relationships, 8, 32-38.

Skoglund, A., Brundin, A., and Mandenius C.F., (2004), *Monitoring a Paperboard Machine Using Multivariate Statistical Process Control*, Chemometrics and Intelligent Laboratory Systems, 73, 3-6.

Spellman, P.T., Sherlock, G., Zhang, M.Q., Iyer, V.R., Anders, K., Eisen, M.B., Brown, P.O., Botstein, D., and Futcher, B., (1998), *Comprehensive Identification of Cell Cycle-Regulated Genes of the Yeast Saccharomyces Cerevisiae by Microarray Hybridization*, Molecular Biology of the Cell, 9, 3273-3297.

Stefanov, Z.I., and Hoo, K.A., (2003), *Hierarchical Multivariate Analysis of Cockle Phenomena*, Journal of Chemometrics, 17, 550-568.

Stork, C.L., and Kowalski, B.R., (1999), *Distinguishing Between Process Upsets and Sensor Malfunctions Using Sensor Redundancy*, Chemometrics and Intelligent Laboratory Systems, 46, 117-131.

Strouf, O., (1986), *Chemical Pattern Recognition*, John Wiley, New York.

Ståhle, L., and Wold, S., (1987), *Partial Least Squares Analysis with Cross-Validation for the Two-Class Problem: A Monte Carlo Study*, Journal of Chemometrics, 1, 185-196.

Ståhle, L., and Wold, S., (1989), *Analysis of variance (ANOVA)*, Chemometrics and Intelligent Laboratory Systems, 6, , 259-272.

Ståhle, L., and Wold, S., (1990), *Multivariate analysis of variance (MANOVA)*, Chemometrics and Intelligent Laboratory Systems, 9, 127-141.

Svensson, O., Josefsson, M., and Langkilde, F.W., (1997), *Classification of Chemically Modified Celluloses Using a Near-Infrared Spectrometer and Soft Independent Modelling of Class Analogy*, Applied Spectroscopy, 51, 1826-1835.

Svensson, O., Josefsson, M., and Langkilde, F.W., (1999), *Reaction Monitoring Using Raman Spectroscopy and Chemometrics*, Chemometrics and Intelligent Laboratory Systems, 49, 49-66.

Svensson, O., Kourti, T., and MacGregor, J.F., (2002), *An Investigation of Orthogonal Signal Correction Algorithms and their Characteristics*, Journal of Chemometrics, 16, 176-188.

Taft, R.W., (1956), In: Newman, M.S., (ed.), *Steric Effects in Organic Chemistry*, Wiley, New York.

Tano, K., (1996), *Multivariate Modelling and Monitoring of Mineral Processes using Partial Least Squares Regression*, Licentiate Thesis, Luleå University of Technology, Sweden.

Tano, K., (2005), *Continuous Monitoring of Mineral Processes with Special Focus on Tumbling Mills*, PhD Thesis, Luleå University of Technology, Sweden.

Teague, S.J., Davis, A.M., Leeson, P.D., and Oprea, T., (1999), *The Design of Leadlike Combinatorial Libraries*, Angewandte Chemie International Edition, 38, 3743-3748.

Tenenhaus, M., Esposito Vinzi, V., Chatelin, Y.M., and Lauro, C., (2005), *PLS Path Modelling*, Computational Statistics & Data Analysis, 48, 159-205.

Teppola, P., Mujunen, S.P., Minkkinen, P., Puijola, T., and Pursiheimo, P., (1998), *Principal Component Analysis, Contribution Plots and Feature Weights of Sequential Process Data from a Paper Machine's Wet End*, Chemometrics and Intelligent Laboratory Systems, 44, 307-317.

Teppola, P., and Minkkinen, P., (2000), *Wavelet-PLS Regression Models for Both Exploratory Data Analysis and Process Monitoring*, Journal of Chemometrics, 14, 383-400.

Teppola, P., and Minkkinen, P., (2001), *Wavelets for Scrutinizing Multivariate Exploratory Models Through Multiresolution Analysis*, Journal of Chemometrics, 15, 1-18.

Tompson, C.J.S., (1990), *The Lure and Romance of Alchemy - a History of the Secret Link Between Magic and Science*, Bell Publishing Company, New York.

Topliss, J.G., and Edwards, R.P., (1979), *Chance Factors in Studies of Quantitative Structure-Activity Relationships*, Journal of Medicinal Chemistry, 22, 1238-1244.

Trygg, J., and Wold, S., (1998), *PLS Regression on Wavelet Compressed NIR Spectra*, Chemometrics and Intelligent Laboratory Systems, 42, 209-220.

Trygg, J., Kettaneh-Wold, N., and Wallbäcks, L., (2001), *2-D Wavelet Analysis and Compression of On-line Industrial Process Data*, Journal of Chemometrics, 15, 299-319.

Trygg, J., and Wold, S., (2002), *Orthogonal Projections to Latent Structures (OPLS)*, Journal of Chemometrics, 16, 119-128.

Trygg, J., (2002), *O2-PLS for Qualitative and Quantitative Analysis in Multivariate Calibration*, Journal of Chemometrics, 16, 283-293.

Trygg, J., and Wold, S., (2003), *O2-PLS, a Two-Block (X-Y) Latent Variable Regression (LVR) Method With an Integral OSC Filter*, Journal of Chemometrics, 17, 53-64.

Trygg, J., (2004), *Prediction and Spectral Profile Estimation in Multivariate Calibration*, Journal of Chemometrics, 18, 166-172.

Tysklind, M., Andersson, P., Haglund, P., van Bavel, B., and Rappe, C., (1995), *Selection of Polychlorinated Biphenyls for use in Quantitative Structure-Activity Modelling*, SAR and QSAR in Environmental Research, 4, 11-19.

Umetrics, SIMCA user guide, Sartorius Stedim Data Analytics AB.

Undey, C., and Cinar, A., (2002), *Statistical Monitoring of Multistage, Multiphase Batch Processes*, IEEE Control Systems Magazine, October 2002, 40-52.

Uppgård, L., Sjöström, M., and Wold, S., (2000). *Multivariate Quantitative Structure-Activity Relationships for the Aquatic Toxicity of Alkyl Polyglucosides*, Tenside Surfactants Detergents, 37, 131-138.

Walczak, B., Bogaert, B., and Massart, D.L., (1996), *Application of Wavelet Packet Transform in Pattern Recognition of Near-IR Data*, Anal. Chem., 68, 1742-1747.

Walczak, B. and Massart, D.L., (1997), *Noise Suppression and Signal Compression using the Wavelet Packet Transform*, Chemometrics Intell. Lab. Syst., 36, 81-94.

Van der Voet, H., (1994), *Comparing the Predictive Accuracy of Models Using a Simple Randomization Test*, Chemometrics and Intelligent Laboratory Systems, 25, 313-323.

Van de Waterbeemd, H., (1995), *Chemometric Methods in Molecular Design,* In: Mannhold, R., Krogsgaard-Larsen, P., and Timmerman, H., (Eds.), Methods and Principles in Medicinal Chemistry, Vol 2, VCH, Weinheim, Germany.

Van Espen, P., Janssens, G., Vanhoolst, W., and Geladi, P., (1992), *Imaging and Image Processing in Analytical Chemistry*, Analusis, 20, 81-90.

Verron, T., Sabatier, R., and Joffre, R., (2004), *Some Theoretical Properties of the OPLS Method*, Journal of Chemometrics, 18, 62-68.

Wakeling, I.N., Morris, J.J., (1993), *A Test of Significance for Partial Least Squares Regression*, Journal of Chemometrics, 7, 291-304.

Ward, J. H. *Hierarchical grouping to optimize an objective function*, J. Am. Stat. Assoc. 1963, 58, 236-244.

Westerhuis, J., Kourti, T., and MacGregor, J.F., (1998), *Analysis of Multiblock and Hierarchical PCA and PLS Models*, Journal of Chemometrics, 12, 301-321.

Westerhuis, J.A., de Jong, S., and Smilde, A.K., (2001), *Direct Orthogonal Signal Correction*, Chemometrics and Intelligent Laboratory Systems, 56, 13-25.

Whelehan, O.P.W., Eriksson, L., Earll, M.E., Johansson, E., and Dyrby, M., (2005), *Detection of Ovarian Cancer using Chemometric Analysis of Proteomic Profiles*, In manuscript.

Wickerhauser, M.V., (1994), *Adapted Wavelet Analysis from Theory to Software*, AK Peters.

Wiklund, S., Johansson, E., Sjöström, L., Mellerowicz, E.J., Edlund, U., Shockcor, J.P., Gottfries, J., Moritz, T., and Trygg, J., (2008), *Visualization of GC/TOF-MS-Based Metabolomics Data for Identification of Biochemically Interesting Compounds Using OPLS Class Models,* Anal. Chem. 80, 115-122.

Wikström, C., Albano, C., Eriksson, L., Fridén, H., Johansson, E., Nordahl, Å., Rännar, S., Sandberg, M., Kettaneh-Wold, N., and Wold, S., (1998a), *Multivariate Process and Quality Monitoring Applied to an Electrolysis Process – Part I. Process Supervision with Multivariate Control Charts*, Chemometrics and Intelligent Laboratory Systems, 42, 221-231.

Wikström, C., Albano, C., Eriksson, L., Fridén, H., Johansson, E., Nordahl, Å., Rännar, S., Sandberg, M., Kettaneh-Wold, N., and Wold, S., (1998b), *Multivariate Process and Quality Monitoring Applied to an Electrolysis Process – Part II. Multivariate Time-series Analysis of Lagged Latent Variables*, Chemometrics and Intelligent Laboratory Systems, 42, 233-240.

Wikström, P.B., Andersson, A.C., Forsman, M., (1999), *Biomonitoring Complex Microbial Communities Using Random Amplified Polymorphic DNA and PCA*, FEMS – Microbiology, Ecology, 28, 131-139.

Wikström, P.B., (2001), *Biomonitoring of Complex Microbial Communities that Biodegrade Aromatics*, Ph.D. Thesis, Umeå University, Umeå, Sweden.

Wikström, M., and Sjöström, M., (2004), *Identifying Cause of Quality Defect in Cheese Using Qualitative Variables in a Statistical Experimental Design*, Journal of Chemometrics, 18, 139-145.

Winiwarter, S., Bonham, N.M., Ax, F., Hallberg, A., Lennernäs, H., and Karlén, A., (1998), *Correlation of Human Jejunal Permeability (in Vivo) of Drugs with Experimentally and Theoretically Derived Parameters – A Multivariate Data Analysis Approach*, Journal of Medicinal Chemistry, 41, 4939-4949.

Winiwarter, S., Ax, F., Lennernäs, H., Hallberg, A., Pettersson, Cu., and Karlén, A., (2003), *Hydrogen Bonding Descriptors in the Prediction of Human In Vivo Intestinal Permeability*, Journal of Molecular Graphics and Modelling, 21, 273-287.

Wise, B.M., Gallagher, N.B, and Martin, E.B., (2001), *Application of PARAFAC2 to Fault Detection and Diagnosis in Semiconductor Etch*, Journal of Chemometrics, 15, 285-298.

Wold, S., (1978), *Cross-Validatory Estimation of the Number of Components in Factor and Principal Components Models*, Technometrics, 20, 397-405.

Wold, H., (1982), *Soft Modelling. The Basic Design and Some Extensions*. In: Jöreskog, K.G., and Wold, H., (eds.), Systems Under Indirect Observation, Vol. I and II, North-Holland, Amsterdam, The Netherlands.

Wold, S., and Dunn, III, W.J., (1983), *Multivariate Quantitative Structure-Activity Relationships (QSAR): Conditions for their Applicability*, Journal Chemical Information & Computer Science, 23, 6-13.

Wold, S., Albano, C., Dunn, W.J., Edlund, U., Esbensen, K., Geladi, P., Hellberg, S., Johansson, E., Lindberg, W., and Sjöström, M., (1984), Multivariate Data Analysis in Chemistry, In: B.R. Kowalski (ed.) *Chemometrics: Mathematics and Statistics in Chemistry*, D. Reidel Publishing Company, Dordrecht, Holland.

Wold, S., Geladi, P., Esbensen, K., and Öhman, J., (1987a), *Multiway Principal Components and PLS-Analysis*, Journal of Chemometrics, 1, 41-56.

Wold, S., Hellberg, S., Lundstedt, T., Sjöström, M. and Wold, H., (1987b), *PLS Modeling with Latent Variables in Two or More Dimensions*, Proceedings Frankfurt PLS-meeting, September, 1987.

Wold, S., Carlson, R., and Skagerberg, B., (1989a), *Statistical Optimization as a Means to Reduce Risks in Industrial Processes*, The Environmental Professional, 11, 127-131.

Wold, S., Kettaneh-Wold, N., and Skagerberg, B. (1989b), *Nonlinear PLS Modelling*, Chemometrics and Intelligent Laboratory Systems, 7, 53-65.

Wold, S., (1992), *Non-linear Partial Least Squares Modelling. II. Spline Inner Relation*, Chemometrics and Intelligent Laboratory Systems, 14, 71-84.

Wold, S., Johansson, E., and Cocchi, M., (1993a), *PLS*, In: Kubinyi, H., (ed.), 3D-QSAR in Drug Design, Theory, Methods, and Applications, ESCOM Science, Ledien, pp. 523-550.

Wold, S., Jonsson, J., Sjöström, M., Sandberg, M., and Rännar, S., (1993b), *DNA and Peptide Sequences and Chemical Processes Multivariately Modelled by Principal Components Analysis and Partial Least Squares Projections to Latent Structures*, Analytica Chimica Acta, 277, 239-253.

Wold, S., (1994), *Exponentially Weighted Moving Principal Components Analysis and Projections to Latent Structures*, Chemometrics and Intelligent Laboratory Systems, 23, 149-161.

Wold, S., Kettaneh, N., and Tjessem, K., (1996), *Hierarchical Multiblock PLS and PC Models for Easier Model Interpretation and as an Alternative to Variable Selection*, Journal of Chemometrics, 10, 463-482.

Wold, S., Antti, H., Lindgren, F., and Öhman, J., (1998a), *Orthogonal Signal Correction of Near-Infrared Spectra*, Chemometrics and Intelligent Laboratory Systems, 44, 175-185.

Wold, S., Kettaneh, N., Fridén, H., and Holmberg, A., (1998b), *Modelling and Diagnostics of Batch Processes and Analogous Kinetic Experiments*, Chemometrics and Intelligent Laboratory Systems, 44, 331-340.

Wold, S., Sjöström, M., Eriksson, L., (1999), *PLS in Chemistry*, In: The Encyclopedia of Computational Chemistry, Schleyer, P. v. R.; Allinger, N. L.; Clark, T.; Gasteiger, J.; Kollman, P. A.; Schaefer III, H. F.; Schreiner, P. R., Eds., John Wiley & Sons, Chichester, 1999, pp 2006-2020.

Wold, S. and Josefson, M., (2000), Multivariate Calibration of Analytical Data, in: Meyers, R., Encyclopedia of Analytical Chemistry, John Wiley & Sons, Ltd., pp 9710-9736.

Wold, S., Trygg, J., Berglund, A., and Antti, H., (2001a), *Some Recent Developments in PLS Modeling*, Chemometrics and Intelligent Laboratory Systems, 58, 131-150.

Wold, S., Sjöström, M., and Eriksson, L., (2001b), *PLS-Regression: A Basic Tool of Chemometrics*, Journal of Chemometrics, 58, 109-130.

Wold, S., Berglund, A., and Kettaneh, N., (2002), *New and Old Trends in Chemometrics. How to Deal With the Increasing Data Volumes in RDP – With Examples From Pharmaceutical Research and Process Modelling*, Journal of Chemometrics, 16, 377-386.

Wold, S., Josefson, M., Gottfries, J., and Linusson, A., (2004), *The Utility of Multivariate Design in PLS Modeling*, Journal of Chemometrics, 18, 156-165.

Wold, S., and Kettaneh, N., (2005), *PLS and Data Mining*, Computational Statistics, In press.

Wormbs, G., Larsson, A., Alm, J., Tunklint-Aspelin, C., Strinning, O., Danielsson, E., and Larsson, H., (2004), *The use of Design of Experiments and Sensory Analysis as Tools for the Evaluation of Production Methods for Milk*, Chemometrics and Intelligent Laboratory Systems, 73, 67-71.

Wu, J., Hammarström, L.G., Claesson, O., and Fängmark, I.E., (2003), *Modeling the Influence of Physico-Chemical Properties of Volatile Organic Compounds on Activated Carbon Adsorption Capacity*, Carbon, 41, 1309-1328.

Zuegge, J., Fechner, U., Roche, O., Parrott, N.J., Engkvist, O., and Schneider, G., (2002), *A Fast Virtual Screening Filter of Cytochrome P450 3A4 Inhibition Liability of Compound Libraries*, QSAR, 21, 249-256, 2002.

Öberg, T., (2003), *Optimization of an Industrial Afterburner*, Journal of Chemometrics, 17, 5-8.

Österberg, T., and Norinder, U., (2000), *Theoretical Calculation and Prediction of P-Glycoprotein-Interacting Drugs Using Molsurf Parametrization and PLS Statistics*, European Journal of Pharmaceutical Sciences,10, 295-303.

19Glossary

A

AR model: Auto regressive model.

ARL: Average Run Length.

ARMA model: Auto Regressive Moving Average model.

B

Batch conditions: Batch conditions pertain to the whole batch and are therefore used in the batch level model. Also named Initial condition, Final condition.

Batch process: A finite duration process.

Best basis: Best basis is an option used in wavelet transformation for high frequency signals. See also DWT.

Bilinear modeling: Matrices modeled as a product of two low rank matrices, e.g. X=T*P'.

Block-wise variable scaling: Making the total variance equal for each block of similar variables in a dataset.

C

Calibration dataset: See: Reference dataset.

Characteristic vector analysis: See: Principal component analysis.

Class: A subset of similar observations from a dataset.

Closed form: The calculation of a closed form can be completed without iterations.

Cluster analysis: Techniques for dividing a set of observations into subgroups or clusters.

Column space: Space spanned by the column vectors of a matrix.

Contingency table: A table which contains counts or frequencies of different events.

Contribution: A measure of the differences in variable values between two observations. The differences might optionally be weighted by model loadings or modeled variability.

Correspondence analysis: A special double scaled variant of PCA, suitable for some applications, e.g. analysis of contingency tables.

Cross validation: Parameters are estimated on one part of a matrix and the goodness of the parameters tested in terms of its success in the prediction of another part of the matrix.

CUSUM: CUmulative SUM.

D

Dataset: A dataset is the base of all multivariate data analysis, often also called a data matrix. It is made up of values of several different variables for a number of observations.The data are collected in a data matrix (data table) of N rows and K columns, often denoted X. The N rows in the table are termed observations. The K columns are termed variables.

Dependent variables: Variables (often denoted y or Y) that are modeled as dependent on other variables.The later variables (often denoted x or X) are often in this context misleadingly called independent, rather than predictor variables.

Discriminant analysis: A method for allocating observations to one class of a given set of classes by means of a decision rule based on a function of the data. The function is derived from data for a reference set of individuals where it is known which class each individual belongs to.

Duration: The number of points in the batch.

DWT: Discrete wavelet transform option used in wavelet transformation when the signal is fairly smooth, that is, the information is mainly contained in the low frequencies. See also Best basis.

E

Eigenvalue: The length change when an eigenvector is projected onto itself. This is equivalent to the length of a principal diameter of the data.

Eigenvector: Eigenvectors exists only for square matrices. An eigenvector to a square matrix has the property of being projected onto itself when projected by the matrix. The degree of elongation or diminution is expressed by the eigenvalue.

Eigenvector analysis: See: Principal component analysis.

Endpoint: The last maturity value for the batch.

Euclidean distance: Geometric distance in a Euclidean space (isomorphic with orthogonal basis vectors).

EWMA model: Exponentially Weighted Moving Average model.

Explanatory variables: Variables (x) used to 'explain' the variation in the dependent variables (y). Also often called predictor variables.

F

Factor: A term often used in experimental design. It signifies controlled and varied variable. See: Predictor. Also a term for one model dimension in factor and bilinear models.

Factor analysis: Has an aim similar to PCA, but assumes an underlying model with a specified number of factors which are linear combinations of the original variables. The analysis is more concerned with 'explaining' the covariance structure of the variables rather than with 'explaining' the variances.

I

Identifiers: Variable and observation identifiers are displayed in plots and lists. The Find function searches the identifiers in the Workset dialog. In the Observations page of the Workset dialog the identifiers can be used to set classes.

Independent variable: Often misleading connotation. See: Predictor variable.

Inner vector product: The product of two vectors that produces a scalar.

J

Jack-knifing: A method for finding the precision of an estimate, by iteratively keeping out parts of the underlying data, making estimates from the subsets and comparing these estimates.

K

K-space: A space, spanned by K orthogonal variable axes. See: Variable space.

Karhunen-Loève transformation: See: Principal component analysis.

L

Least squares estimate: A method to estimate model parameters by minimizing the sum of squares of the differences between the actual response value and the value predicted by the model. (SASSTAT).

Leverage: Observations in the periphery of a dataset might have great influence on the modeling of the dataset. That influence is termed leverage, based on the Archimedian idea that anything can be lifted out of balance if the lifter has a long enough lever.

Loading vector: Direction coefficients of a PC or PLS component axis.

M

M-space: Measurement space, or: multivariate space. Synonym: K-space. See: K-space

MA model: Moving Average model.

Mahalanobis distance: In short: Eigenvalue-weighed distance.

Matrix: A rectangular array of elements, with certain rules of computations.

Missing value: Element in a data matrix without a defined value. As a rule of thumb, each observation and variable should have more than five defined values per PC. Observations (or variables) with missing values that show up as outliers should be treated with suspicion.

Model: 1) An approximation of reality. A good model preserves all properties of interest. 2) Hyperplane, with limited extension, that approximates the variable space spanned by a class of observations.

MSPC: Multivariate Statistical Process Control - The use of multivariate methods to characterize the state of a process with respect to known states. The state is determined from model score plots and distance to model plots. See also: SPC.

Multidimensional scaling: Roughly corresponding to a principal component analysis of a matrix of 'distances' between observations.

Multiple linear regression: The linear regression of one variable, Y, in many Xs. See also: Regression.

Multivariate analysis: A group of statistical methods, which are appropriate when measurements are made on several variables for each of a large number of individuals or observations.

Multivariate data: Multivariate data consist of observations on several different variables for a number of individuals or observations. Indeed, the vast majority of data is multivariate, although introductory statistics courses naturally concentrate on the simpler problems raised by observations on a single variable.

N

NIPALS: Non-linear Iterative Partial Least Squares

Non-linear: Two uses:1) Curved relationship between X and Y. 2) A model, which parameters cannot be estimated by a closed form.

O

Observation space: The space spanned by the observation vectors of a data matrix. Each variable vector is represented as a point in that space. See also: Row space.

Ordinal data: A discrete variable is called ordinal if its possible data can be arranged in some numerical order.

Ordinal number: Showing order or position in a series, e.g. first, second, third.

Outer vector product: Product of two vectors that produces a matrix: M = t * p' where mij = ti * pj

P

Pareto's principle: 20% of the variables account for 80% of the effect.

Partial Least Squares: See: Projection to Latent Structures.

PC: See: Principal component.

PC modeling: See: Principal component modeling.

PCA: See: Principal component analysis.

Phase conditions: Phase conditions pertain to the whole phase and are therefore used in the batch level model. Also named Initial condition, Final condition.

Phase iteration conditions: Phase iteration conditions pertain to the whole phase iteration and are therefore used in the batch level model. Also named Initial condition, Final condition.

PLS: Partial Least Squares Projection to Latent Structures. See: Projection to Latent Structures.

Power method: An iterative projection method for finding eigenvectors.

Predictionset: A dataset used together with an established model in order to obtain model predictions for each of the observations in the set.

Predictor variable: See: Explanatory variables.

Principal component: One model dimension of a PC model. Often also used as a term for the scores t.

Principal component analysis: Principal Component Analysis is the technique for finding a transformation that transforms an original set of correlated variables to a new set of uncorrelated variables, called principal components. The components are obtained in order of decreasing importance, the aim being to reduce the dimensionally of the data. The analysis can also be seen as an attempt to uncover approximate linear dependencies among variables (SASSTAT).

Principal component modeling: 1) The use of PCs to define a model. 2) The approximation of a matrix by a model, defined by averages and a relatively small number of outer vector products. The components can often be used in place of the original variables for plotting, regression, clustering and so on (SASSTAT).

Principal coordinate analysis: The aim is an algebraic reconstruction of the positions of the observations assuming that the distances are approximately Euclidean. See also: Multidimensional scaling.

Principal factor analysis: See: Principal component analysis.

Projection: 1) The act of projecting. 2) Something that has been projected, i.e. the 'picture' of orthogonally projected points on a line, plane or hyperplane.

Projection methods: A group of methods that can efficiently extract the information inherent in MVD. They give results that are easy to interpret because they can be presented as pictures. Such methods are efficient for pattern recognition, classification, and predictions. The most commonly used methods are PC and PLS modeling.

Projection point: The point, along a line or in a plane or hyperplane (created by approximating data in k-space as a low dimensional hyperplane), which is closest to the original point.

Projection to Latent Structures: A generalization of PCA where a projection model is developed predicting Y from X via scores of X. Can also be seen as a generalized multiple regression method that can cope with multiple collinear X and Y variables.

R

Reference dataset: This term is used for datasets with known properties and origin, often used to define models. Synonyms: Calibration dataset, training dataset, workset.

Regression: In mathematics Y is called a function of X, but in statistics the term regression of Y on X is generally used to describe the (sound, approximate) relationship.

Regression analysis: The fitting of an equation to a set of values. The equation predicts a response variable from a function of regressor variables and parameters, adjusting the parameters such that a measure of fit is optimized. (SASSTAT)

Regressor variable: See: dependent variable

Residual: Left-over; un-modeled part. The mismatch between the observed and modeled values.

Response variable: See: dependent variable

Row space: The space spanned by the row vectors of a matrix.

S

Score: Distance from the origin, along a loading vector, to the projection point of an observation in K- or M-space. Or: the coordinates of a point when it is projected on a model hyperplane.

Score vector: Observation coordinates along a PC or PLS component axis. Scores for all observations for one model dimension (component).

Singular value decomposition: See: Principal component analysis

SPC: Statistical Process Control - The behavior of a process is characterized using data when the process is operating well and is in a state of control. In the monitoring phase the new incoming, measured, data are used to detect whether the process is in control or not. See also: MSPC.

Subspace methods: See: Projection methods.

T

Test dataset: A dataset with unknown properties, often subjected to projections to models.

Training dataset: See: Reference dataset.

V

Variable space: The space spanned by the variable vectors of a data matrix. Each observation vector is represented as a point in that space. See also: K space, and M space.

VSI: Variable Sampling Interval.