SIMCA
Feature List

Technical Features of SIMCA 14

March 13, 2015

Highlights

- **Scripting your own workflows using Python**
- **Workspace including open plots – with customizations - and lists are saved in SIMCA usp-file.**
- **What-If analysis – simulate disturbances in the data**
- **Backstage view**

Import

- Supported file formats: Excel up to 2013, DIF, CSV, Text files, Galactic SPC, Bruker OPUS, JCAMP-DX, Matlab 5, Lotus1-2-3, NSAS, Brimrose version 1, Unscrambler ASCII, Net-CDF, HPLC ChemStation, Thermo SIEVE files, SIMCA and MODDE files
- Direct import from databases
- Import by pasting entire dataset
- Plug-in support for custom file formats
- Edit data sets: Transpose, merge cut, copy, paste and insert
- Specification of identifiers, variable roles and data types
  - Primary, secondary, class, phase and batch identifiers
  - X or Y variables
  - Quantitative, qualitative or date/time data type
- Missing value map
- Downsizing number of observations
- Flexible Find and replace feature
- Issues view – identification of problems in the dataset that must be resolved before importing
- Dataset properties overview in panes
- Import multiple datasets with different properties and content to the same SIMCA project

Data viewing

- Missing values map
- Quick info connected to all lists and plots
  - Data overview with Frequency histogram, Spectrum/Time series, Auto- or cross-correlation, Power spectrum
  - Trimming/Winsorizing of selected variables or the whole dataset
- Spectra plot
- Plots can be created directly from dataset or any open spreadsheet or list

Data preprocessing

- First, second and third derivatives
- Multiplicative Signal Correction (MSC)
- Standard Normal Variate (SNV)
- Row Center
- Wavelet denoising and decimation of spectral data
- Wavelet transform and compression, row wise or column wise
- EWMA
- Savitzky-Golay
- Chaining of filters
- Filter summary
- Automatic filtering of predictionsets
- Spectral filter plug-in
- Local centering of data

Generate new variables

- Variables as functions of existing ones or as functions of result variables from existing models
- Possibility to establish user specific functions

Workset

- Workset spreadsheet with Quick info and Trimming/Winsorizing variables
- Exclude variables and specify X and Y-block
- Qualitative Y-variables supported
- Different X and Y-block for different classes and blocks
- Transformations: Linear, Log, Neglog, Logit, Exponential, Power
- Lag time series data
- Expand with square, cross, and cubic terms
- User defined default scaling of X and Y-block
- Variable and block scaling
- Flexible scaling from file, secondary IDs or manually entered
- Exclude/Include observations
- Group observations by classes
- Autogenerate classes from ID, variable or score values

Model

- Unlimited number of models in a project
- All methods handle missing data
- Model types: PCA
  PLS, OPLS and O2PLS
  PCA, PLS, OPLS and O2PLS
  PLS-DA, OPLS-DA and O2PLS-DA
- Hierarchical Cluster Analysis (HCA)
- Cluster analysis with PLS-Tree
- Hierarchical models

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Model review and interpretation

- Summary of the model fit Q2,R2
- Multivariate model parameters
- Coefficients and Variable influence (VIP) for PLS and **OPLS**
- Calibration diagnostics: RMSEE and RMSECV
- Contribution plots
- Confidence intervals from jack-knifing on column plots
- S-plots
- **ROC plot for interpretation of discriminating power of model**

Model validation

- Cross validation
- Permutation test for PLS and **OPLS** models
- CV-ANOVA table
- CV Scores

Prediction

- Prediction results presented as lists, plots, and diagnostics
- Classification list and misclassification table
- RMSEP for predictions
- Predictionset automatically preprocessed as workset
- Option to trim predictionset as workset

Plots and Lists

- Mini-toolbars for direct plot editing
- Plot formatting templates to save, load and share preferred layout
- Interactive tool to remove or include a group of observations from observation plots
- Interactive tool to remove model terms directly from loading, coefficient and VIP plots
- Color by values of variables, scores, model vectors, IDs, classes, batches
- Size by variable, DModX or any model vector
- Highlight series; grays all but the hovered series
- Sorting of column plots
- Use any observation or variable ID as labels on points or axes
- Trend plot of a variable by double clicking it in a plot
- Full screen mode

Plot types

- 2D and 3D Scatter, Line, Column, Histogram, **Dot**, Time series, Response contour, Response surfaces, Normal probability Dendrogram
- Control charts both of scores and individual variables: Shewhart, EWMA, CUSUM, EWMA/Shewhart
- Wavelet structure and power spectrum plots
- Auto- and cross correlation, power spectrum, wavelet, coefficients and EWMA transformations

Multivariate batch analysis

- Batch Evolution Models (BEM) and Batch Level Model (BLM) handled in same project
- Batch tab with all batch evolution plots and features collected
- Batch conditions imported with batch evolution dataset or separately
- Contribution plots in batch level can be resolved regular or combined for batch evolution
- Option to automatically generate batch evolution level datasets after removal of outliers in batch level

Batch evolution models

- **OPLS for Batch Evolution Modeling**
- Support for multiple phases, i.e. process steps
- Phases can have different variables
- Local centering per batch and phase
- Different maturity variables for different phases
- Batch control chart including several phases in one plot

Batch level models

- Flexible creation of batch level datasets
- Hierarchical batch level models
- Automatic Partial models for modeling e.g. 10, 20, 30 % of phase length
- Batch VIP plot available for all types of models
- Source of variation plot displaying all phases

Additional features

- Flexible report generator in html
- Plug-in for display of chemical structures from SMILES codes
- Sort of datasets, lists and column plots
- Automation object; SIMCA can be started from external programs and data, and results exchanged with SIMCA
- Command to save reduced project files
- Favorites with Export and Import
- Audit trail 21 CFR Part 11 compliant
- Analysis Advisor to help interpret plots and guide you through the analysis

System recommendations

- 1.5 GHz Processor
- 1 GB RAM
- 1 GB free hard disk space
- Color graphics display with at least 1366x768 resolution
- Windows 7 or Windows 8.1