



# What's New in 6.5

## Classification Methods (SIMCA, KNN, PLSDA, SVMDA)

- Total flexibility in choosing class sets to model (through class groups interfaces or Edit > Options > Method Options menu)
- Confusion table and matrix tools added
- Unified reporting of classification results including: all class probabilities, most probable, strict in-class, and strict multi-class assignments
- KNN Cross-validation fully supported

## Design Of Experiments (DOE) Tools

- Significant addition of tools for DOE generation and testing
- Experiment Designer tool added to create, examine, and print run sheets for designed experiments [doegui]
- DOE Anova tool added to calculate significance of factors and interactions
- Added support tools to: scale factors, calculate interactions, identify confused factors and interactions
- Design generation tools included for:
  - Mixed-level Full Factorial Designs (factdes)
  - Fractional Factorial Designs (ffacdes1)
  - Face and Spherical Central Composite Designs (ccdface, ccdsphere)
  - Box-Behnken Designs (boxbehnken)
- Command-line tools added include:
  - anovadoe - Function to perform ANOVA for 2<sup>k</sup> factorial model X, Y data
  - boxbehnken - Create a Box-Behnken Design of Experiments.
  - ccdface - Create a Face-Centered Central Composite Design of Experiments.
  - ccdsphere - Create a Spherical Central Composite Design of Experiments.
  - doegen - Generate a Design of Experiments (DOE) DataSet object.
  - doegui - Design of Experiments tool.
  - doeffectsplot - Main & Interaction Effects plots.
  - doeinteractions - Calculates interaction terms of a raw DOE matrix.
  - doescale - Convert coded DOE to scaled DOE or scaled back to coded.
  - factdes - Full factorial design of experiments.
  - ffacconfusion - DOECONFUSION Generates confusion table for a fractional factorial DOE.
  - ffacdes1 - FACTDES Fractional factorial 2-level design of experiments.

## Other Method Improvements

- Permutation testing of regression and classification models greatly improved with probabilities of model significance and plots
- Support Vector Machine One-Class support added (svmoc; command-line only)
- MCR/ALS contrast algorithm improved providing better handling of low signal cases.
- MLR support for studentized residuals, T<sup>2</sup> and limits added
- MODELSELECTOR trigger can now use of any classification model or a simple logical test on predictions from a regression or PCA model.

## Preprocessing

- Spectral Alignment method added (using either peak alignment using [registerspec]) or Correlation Optimized Warping (COW))
- Correlation Optimized Warping (COW) and Dynamic Time Warping (DTW) added (from [http://www.models.kvl.dk/DTW\\_COW](http://www.models.kvl.dk/DTW_COW))
- Poisson scaling offset support added
- Class centering method added for Multilevel PLS models and other clutter-correction methods
- "Transform" options for data blocks in Analysis window. Context menu gives quick access to:
  - \* Batch Digestion (MPCA, Summary PCA)
  - \* Calibration Transfer
  - \* Polynomial Augmentation (Non-linear modeling)
  - \* Coadd Data Reduction (Down-sampling)
  - \* Calibration Sample Selection (redundant sample exclusion, re Westerhuis method)
- Baseline removal improved with manual entry of baseline points and easier graphical selection.
- GLSW improved to work with multi-class PLSDA classification models (multivariate logical y-blocks)
- Help and technical details easy-access links added to Preprocessing Window
- Descriptions automatically update to show current settings for adjustable methods

## Import / Export

- Omnic SPA file importer added
- Galactic DHB file importer added (support in SPC reader)
- 3-way data importing from multiple files or multiple Excel spreadsheets added
- Excel multi-sheet document importing improved (better labeling and concatenation options)
- XML format, improved importing of objects and image DataSets
- System clipboard importing improved
- Importer list easier to navigate
- Autoexport tool added for easy saving of data to external formats

## DataSet Editor

- Summary statistics for all or part of the given data (View > Summary Statistics, context menu access) added
- Access to all classes, labels, and axis scales on data table view (pull-down menus on Data tab)
- Date stamps as axis scales improved. Dates are displayed as text dates and not timestamp values
- Selection of data improved with easier selection full integration with plots of data
- Data exchange between interfaces improved (File > Send To menu)
- Quick access to commonly used operations (via toolbar buttons)

## Plot Controls

- "Stacked" plots (automatic y-scale toolbar button cycles through scaled data, stacked data, normal view)
- "Color by" any related data or user-selected data
- "Invert selection" toolbar button added
- Improved access to data in table format
- Persistent selection capability. Selection mode stays activated after a selection. (Optional - disable through settings)
- Customizable line widths (context menu on the plot)
- Customizable figure toolbar to choose which toolbar buttons are shown.
- Time-based axes have improved automatic update after a zoom or pan

## Analysis Window

- Automatic data augmentation by simply importing / loading new data
- Easier to read format for main table with improved information
- Model Cache speed improvements

## Workspace Browser

- DOE Experiment Designer and easy Calibration Transfer model application added
- Drag/drop of multiple items improved

## Command-line Tool Changes

### Full Support for Matlab R2011b

- |                |  |
|----------------|--|
| crossval       | - improved display of classification results   |
|                | - improved integration with model input  |
| fasternnl      | - improved performance for large numbers of factors and for low signal problems      |
| flucut         | - new function to remove scatter from fluorescence EEM data                          |
| parafac2       | - improved memory efficiency and missing data support                                |
| residuallimit  | - add support for calculating confidence level from given Q value and a model        |
| stdgen         | - tuned performance  |
| summary        | - improved output and display options. Now outputs DSO or displays more useful data. |
| svmda          | - improved parameter selection for special cases                                     |
| svmoc          | - Add support for one-class SVM.   |
| wlsbaseline    | - added variable weights as output (weighting used on each variable in spectrum)     |
| excludemissing | - improved handling of unusual missing data patterns                                 |