Pirouette® Specifications

Version 5.0

Minimum System Requirements

3 GHz PC, 12 GB RAM
100+ MB free on hard disk
Pointing device
Windows Vista, 7, 8, 10, 11

Help

Full documentation as cross-referenced PDF
Link to Adobe® Acrobat® Reader

Data

Files

No size limitations

Read

Binary, ASCII, Lotus®, Excel®
Common Instrument Formats, AIA, JCAMP, Galactic®, ChemStation®

Write

Files, Subsets, Calculated objects in Binary, ASCII, Excel, SPC and AIA formats

Models

Read binary; Write binary, ASCII, Galactic, Guided Wave

Merge

Single or Multiple files, drag and drop, by Sample, by Variable

Subsets

Unlimited number
By exclusion or inclusion
Saved with file, Separate results maintained

Sample selection

Kennard & Stone, PCA Hypergrid, Leverage

Variable selection

Fisher or Variance weights, StDev rank

Output

Printers, via Print Manager
Clipboard, of graphics, data or results

Edit functions

Cell contents and ranges
Columns and/or Rows
Cut, Copy, Paste, & Clear; Insert & Delete

Spreadsheet

X-block, Y-block, & Category-block
Go To; Sort, by value or by name
Find missing values

Fill Missing Values

Zero, By value, Mean, Median, Interpolation, PCA fill

Object Manager

Data and Results tree
Drag and drop into chart windows
Data object history
Note writing, saved with file

Pretreatments

Transforms

1st & 2nd Derivative (5 - 95 points)
Smoothing (5 - 95 points)
Log10, Multiply, Normalize
Subtract (value or variable)
Divide by (2-norm, 1-norm, max, range, value)
Baseline correction (linear, quadratic, cubic fit, selected sample)
Multiplicative Scatter Correction
Standard Normal Variate

Preprocessing Options

Mean-centering, Variance scale
Autoscale, Pareto, Range scale

Multivariate Analysis

Hierarchical Cluster Analysis

Linking Methods

Single, Centroid, Complete, Incremental, Median, Group Average, Flexible

Orientation

by Sample or by Variable

Results

Sample or Variable Dendrogram

Principal Components Analysis

Model Probability Control
Projection Model

Validation

Cross, Step
Any number of left out samples

Varimax Rotation

Raw, Normal, & Weighted

Results

Scores, Rotated Scores
Loadings, Rotated Loadings
Eigenvalues, Rotated Eigenvalues
Errors (PRESS)
Outlier Diagnostics, Contributions
Modeling Power
X Residuals, X Reconstructed

Prediction

Dynamic factor selector
Projected Scores
X Residuals, X Reconstructed
Outlier Diagnostics, Contributions

K Nearest Neighbors

Unlimited number of neighbors or classes
Classification Model

Results

Votes Matrix
Misses Vector
Misclassification Matrix

Prediction

Predicted Class
Class fit

Soft Independent Modeling of Class Analogy

Model Probability control
Prediction Probability control
Unlimited number of classes
Classification Model

Results

Scores
Loadings
Eigenvalues
X Residuals
Modeling Power
Outlier Diagnostics
Interclass Residual
Interclass Distance
Discrimination Power
Misclassification Matrix
Class Projections

Prediction

Projected Scores
X Residuals
Class Distances
Class Probabilities
Best & Next Best Predicted Class
Misclassification Matrix
Class Projections

Classical Least Squares

Prediction Model

Validation

Cross, Step, by Category
Any number of left out samples

Results

Pures and uncertainty bounds
Errors (PRESS, SEC, r)
Y Fit
Outlier Diagnostics
X Residuals
Regression Vector

Prediction

Predicted properties
Errors, slope, intercept
X Residuals
Probabilities
Y Fit

Principal Components Regression, Partial Least Squares Regression, and Partial Least Squares-Discriminant Analysis, Locally Weighted Regression

Unlimited number of dependent variables
Prediction Model

Validation

Cross, Step, by Category
Any number of left out samples

Orthogonal Signal Correction

Results

Scores
Loadings
Eigenvalues
Errors (PRESS, SEC, SEV)
Y Fit
Outlier Diagnostics, Contributions
X Residuals, X Reconstructed
Correlation spectrum
Regression Vector
Class Predicted, Misclassifications (PLS-DA)

Prediction

Dynamic factor selector
Predicted properties
Errors
Prediction scores
Outlier diagnostics, Contributions
Y Fit
X Residuals, X Reconstructed
Class Predicted, Misclassifications (PLS-DA)

Mixture Analysis

Multivariate Curve Resolution, Alternating Least Squares
Prediction Model

Results

Eigenvalues, Scores, Loadings
Solution Select, Feasible Region, Source Amounts & Profiles, X Residuals

Prediction

Feasible Regions
Source Amounts

Calibration Transfer

Algorithms supported

KNN, SIMCA, PLS, PCR

Transfer Functions

Direct standardization, Piecewise direct, Additive, Multiplicative

Graphics

Plots

2D Scatter, 3D Rotatable Scatter
Line
Multiple 2D Scatter
Plot arrays
Point labels, Cloaking

Interaction

Point Selection
Range Selection
Magnify
Point Labeling
3D Spinning
Linking selections across views
Color by category

Preferences

Custom interface colors, graphics, fonts
Custom plot symbol size, window size
User defined preference sets
English, Spanish, German, Japanese, Portuguese, French, Italian

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