

Pirouette® Specifications

MINIMUM SYSTEM REQUIREMENTS

64 MB RAM
90 MHz Pentium PC
SVGA
30+ MB free on hard disk
Microsoft® mouse or compatible
Windows 95/98 or NT 4.0/2000

DATA

Files

No size limitations

Read

Binary, ASCII, Lotus®, Excel®
Common instrument formats, AIA, JCAMP,
Galactic®

Write

Files, Subsets, Calculated objects in Binary,
ASCII, Lotus and Excel formats

Models

Read binary
Write binary, ASCII, Galactic

Merge

Single or Multiple files
by Sample, by Variable

Subsets

Unlimited number
Create by exclusion or inclusion
Saved with file
Separate results

Output

Printers

via Print Manager

Clipboard

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

Fill Missing Values

Zero
by Value
Mean, Median
Interpolation

Object Manager

Data and Results tree
Charts tree
Drag and drop into chart windows
Data object history
Note writing capability

MULTIVARIATE ANALYSIS

Transforms

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

Preprocessing Options

Mean-centering
Variance scale
Autoscale
Range scale

Hierarchical Cluster Analysis

Linking Methods

Single
Centroid
Complete
Incremental
Median
Group Average
Flexible

Orientation

by Sample
by Variable

Results

Sample Dendrogram
Variable Dendrogram

Principal Components Analysis

Model Probability Control
Projection Model

Varimax Rotation

Raw, Normal, & Weighted

Results

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

Prediction

Dynamic factor selector
Projected Scores
X Residuals
X Reconstructed
Outlier Diagnostics

K Nearest Neighbors

Unlimited number of neighbors or classes
Classification Model

Results

Votes Matrix
Misses Vector
Misclassification Matrix

Prediction

Predicted Class

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 and Partial Least Squares Regression

Unlimited number of dependent variables
Prediction Model

Validation

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

Results

Scores
Loadings
Eigenvalues
Errors (PRESS, SEC, SEV)
Y Fit

Outlier Diagnostics

X Residuals

X Reconstructed

Correlation spectrum

Regression Vector

Prediction

Dynamic factor selector
Predicted properties
Errors
Prediction scores
Outlier diagnostics
Y Fit
X Residuals
X Reconstructed

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
Magnify
Point Labeling
3D Spinning
Linking
Color by category

Preferences

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

HELP

Full documentation as cross-referenced PDF
Adobe® Acrobat® Reader provided



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