

# Pirouette® Specifications

Version 4.0

## Minimum System Requirements

128 MB RAM, 1 GHz PC, CD  
XGA, 100+ MB free on hard disk  
Microsoft® mouse or compatible  
Windows NT 4, 2000, XP, Vista

## 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®, EZChrome®, ChemStation®

### **Write**

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

### **Models**

Read binary; Write binary, ASCII, Galactic

### **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

### **Fill Missing Values**

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

## **Object Manager**

Data and Results tree  
Charts tree  
Drag and drop into chart windows  
Data object history  
Note writing, saves 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**

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

### **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  
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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