

# 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**

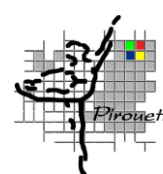
2D Scatter, 3D Rotatable Scatter  
Line  
Multiple 2D Scatter  
Plot arrays  
Point labels, Cloaking

#### **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



**InfoMetrix®**

19119 North Creek Pkwy  
Suite 100  
Bothell, WA 98011  
425/402-1450 7:00 - 5:00 PST  
<https://www.infometrix.com/>  
info@infometrix.com