

# Index

## Numerics

- 2D scatter plot
  - Axes 12-6
  - Interaction 12-6
- 3D scatter plot
  - Axes 12-6
  - Preferences 10-12
  - Spinning
    - Arrow keys 12-12
    - Cylindrical vs. spherical 12-13
    - Depth cueing 12-13
    - Momentum spinning 12-12
    - Spin control buttons 12-12
    - Spinner Tool 12-11

## A

- Abort
  - Details 16-30
  - Message 18-6
- Abstract factor 5-14
- Acrobat Reader, using for on-line Help 16-44
- Activate class 12-29, 13-19, 16-15
- Activate Class button 12-37
- Active class 6-2, 6-27, 7-45
- AIA file format 4-23, 14-10, 15-6
- Alert messages 18-12
- Align
  - Discussion 4-22
  - for Chromatography 4-22
  - Options 4-24
- Alt key 16-1
- Alternating Least Squares (ALS) 8-3
- Appending data 16-5
- ARCH 5-11, 9-2
- Arrow
  - Cursor 10-6
  - in Scroll Bar 13-4
- ASCII
  - File input 14-5
  - File output 15-3
  - Models 15-9
- Asterisk (\*)
  - Class variable flag 14-8
  - Filling missing values 13-12
  - Missing value flag 16-6
- Autoscale 4-29
- Axis
  - Default label 10-17
  - Selection 10-5, 12-6

## B

- Baseline Correction 4-20
- Bidiagonalization 7-5
- Bitmap 15-2, 16-13
- Block scaling 4-18
- Buttons, Ribbon 10-3

## C

- Calibration transfer 4-33, 6-28, 7-57
- Category validation 5-21
- Centroid link 5-3, 5-9
- Centroidal clustering 5-6
- Charts
  - Creating 12-1, 12-4
  - Custom 11-8
  - Getting information 12-4
  - Graph types 12-6
  - Label preferences 10-16
  - Removing 11-6
  - Window preferences 10-16
  - Window titles 12-5
- Chemometrics, Information 1-6
- Chromatographic alignment 4-22
- Class
  - Active class cue 3-16
  - Color mapping to 12-37
  - Distances 6-21
  - Fit 6-9
  - Probabilities (SIMCA) 6-26
  - Projections 6-24
  - Variable 13-5
- Classical Least Squares (CLS)
  - Math 7-45
  - Options 7-49
  - Prediction 7-54
- Clear 13-8
- Click-drag 10-1, 13-4
- Cloaking 12-9
- Closure 4-18
- Clustering
  - Centroidal 5-6
  - Farthest neighbor 5-5
  - Nearest neighbor 5-5
- Color
  - and Dendrogram 12-25
  - Mapping from class 12-37
  - of Lines 12-17
  - of Text 10-8
  - Preferences 10-7
  - Sequence 10-18

- Column
  - Index 13-19
  - Types 13-5
- Communality 5-28
- Complete link 5-3, 5-8
- Confidence ellipse 5-35
- Confidence limits 6-24, 7-12, 7-36
- Confusion matrix 7-40
- Contributions 5-26, 5-40, 5-46
- Control-click 10-2
- Copy
  - Data values 13-8
  - Graphics 15-2
  - Results 16-13
- Correlation spectrum 7-26
- Cross validation 5-20, 7-47
- Crossover 5-9
- Ctrl-click 16-5
- Current cell 13-15
- Cursor descriptions 10-6
- Curve resolution 8-1, 8-12
- Cut, Copy, Paste 16-13
- D**
- DAT file 1-2, 14-5
- Data point, Size 10-11
- Data scaling 12-13
- Data sets
  - ALCOHOL 9-2
  - ARCH 5-11, 9-2
  - DAIRY 9-2
  - DIESEL 9-3
  - FUEL 9-3
  - HYDROCRB 9-3
  - MNAPS 9-4
  - MYCALIGN 9-4
  - MYCOSING 9-4
  - OCT\_TEST 3-33
  - OCTANE20 3-4, 5-11, 9-4
  - PALMCHRO 14-3
  - RANDOM 5-4, 9-5
  - SEVEN 9-5
  - TERNARY 9-5
  - XRF 9-5
- Decision diagram 6-10, 6-22
- Defaults
  - Preferences 10-20
  - Subset name 11-6
- Delete
  - Charts 11-6
  - Data values 13-9
  - Objects 11-6
  - Samples, variables 16-14
- Demonstration version 18-8
- Dendrogram
  - Activating a class 12-29
  - Arrow keys in 12-26
  - Description 5-1, 12-24
  - Navigation 12-26
  - Similarity 12-24, 12-27
- Dependent variable 4-5, 7-1, 7-3, 13-5
- Derivative 4-13
- Determinant (of a matrix) 17-6
- Diagonal matrix 17-2
- Diamond marker 7-16
- DIESEL 9-3
- Dimensionality 5-14, 14-6
- Direct Standardization 4-35
- Discriminant Analysis 6-1
- Discrimination Power 6-20
- Disk icon 11-9
- Display Menu 16-33
- Displaying results 10-17
- Distance
  - Between classes (SIMCA) 6-20
  - Euclidean 6-3
  - Leverage 7-11
  - Metric 5-2
  - Prediction (SIMCA) 6-21
  - Similarity 5-2
- Divide by
  - Options 4-16
  - Vector range 4-17
- Dollar sign (\$) 14-8
- Drag and drop
  - Charts 12-2, 12-4
  - Data files 14-5
- Drop button 12-4
- E**
- Edit
  - Menu 16-11
  - Tools 10-4
- Eigenvalues 5-18, 5-22, 7-15, 17-7
- Eigenvector 5-14, 17-6
- Elevator box 13-4
- Email address 18-14
- Enhanced Meta File (EMF) 15-2, 16-14
- Error Analysis 7-32
- Error contribution 5-26
- Error messages 18-4
- Euclidean distance 5-2, 6-3
- Excel file 14-5
- Exclude 13-20, 16-15
- Exclusion sets 11-9, 12-34
- Exploratory Data Analysis
  - Example 2-7
  - Preparation 4-2
- F**
- F test 5-22
- Factor Selection 5-32
- FAQ 18-2
- Farthest neighbor clustering 5-5
- Feasible Region 8-21
- Feature selection 11-11
- File
  - Drag and drop 14-4
  - Format
    - Agilent ChemStation 14-10
    - AIA chromatography standard 4-23, 14-10, 15-6
    - Analect 14-11
    - ASCII 1-2, 14-5
    - ASD Indico Pro 14-10

- Brimrose AOTF 14-11
- Bruker OPUS 14-13
- Excel 1-2, 14-5
- Guided Wave 14-11
- Hamilton Sundstram PIONIR 14-13
- Hewlett Packard 8452 14-10, 14-12
- JCAMP-DX 14-12
- LT Industries 14-12
- Perkin-Elmer spectroscopy 14-12
- Pirouette 1-2, 14-5
- Menu 16-3
- Merging 16-5
- Fill
  - by PCA 13-18
  - for Mask 13-17
  - Options 13-13, 16-19
- Find 11-5
- Fisher weight 11-12
- Flexible link 5-3, 5-9
- French 10-22
- Frequently asked questions 18-2
- FUEL 9-3
- G**
- German 10-22
- Global scope (SIMCA) 16-24
- Go to 13-3, 13-13
- Graphics
  - Capture of 15-2
  - Color 12-36
  - Creating subsets 12-34
  - Labeling 12-18, 16-33
  - Linking 12-30
  - Magnifying 12-10
  - Plot types
    - Line plots 12-15
    - Scatter plots 12-6 to 12-15
  - Scaling 12-13
  - Types 12-6
- Grid lines 10-9
- Group average link 5-3, 5-9
- H**
- Help
  - Menu 16-44
  - System description 1-6
- Hierarchical classification 6-25
- Hierarchical Cluster Analysis (HCA)
  - Activate class 12-29
  - Definition 5-1
  - Options 16-21
- Highlighting 10-1, 13-5
- Hotelling's T2 5-25
- HYDROCRB 9-3
- Hyperbox (for PCA and SIMCA) 5-30
- I**
- ID Tool 16-35
- Identity matrix 17-2
- Ill-conditioned matrix 18-7
- Incremental link 5-3, 5-9, 5-12
- Independent variable 4-4, 7-3, 13-5
- Indicator function 5-22
- Inner bound 8-23
- Insert 13-9
- Insertion cursor 10-6
- InStep 6-25, 9-6
- Interaction tools 16-34
- Interpolated fill 16-19
- Inverse (of a matrix) 17-6
- Inverse least squares 7-3
- Italian 10-22
- J**
- Jaggedness 7-9
- Japanese 10-22
- JCAMP file format 14-12
- K**
- Kennard-Stone 11-10
- K-Nearest Neighbors (KNN)
  - Definition 6-2
  - Misclassification 6-8
  - Model 6-5
  - Optimization 6-10
  - Options 16-23
- Kovats retention index 4-22
- L**
- Labels
  - Attributes of 10-17
  - Line plot axis 10-13
- Lack of Fit (in ALS) 8-5
- Language 10-21
- Latent variable 5-14
- Leverage 7-11, 7-12
- Limits 12-18
- Linear Learning Machine 6-1
- Linking
  - Complete link 5-8
  - HCA methods 5-3
  - in HCA 16-21
  - Single link 5-6, 5-11
  - Views 12-30, 13-6
- Loading data 14-3
- Loadings 5-18, 5-36, 7-18
- Local scope (SIMCA) 16-24
- Locally Weighted Regression 7-59
- Logarithm 4-15
- M**
- Magnify tool 12-10, 16-35
- Mahalanobis distance 5-25, 6-14, 7-49
- Marker, for alignment 4-22
- Mask
  - Preparing via Fill 13-17
  - to Indicate transfer samples 6-28, 7-57
  - Using 4-13
- Matrix 4-36, 17-2
- MCR
  - Discussion 8-12
  - Math 8-15
  - Options 8-4, 8-19
- Mean center 4-26

- Mean fill 16-19
  - Median link 5-3, 5-9
  - Menu
    - Display 16-33
    - Edit 16-11
    - File 16-3
    - Help 16-44
    - Objects 16-36
    - Process 16-19
    - Windows 16-38
  - Merge
    - Description 16-5
    - Drag and drop 14-4
  - Messages 18-3
  - Metafile, EMF 15-2, 16-14
  - Misclassification matrix 6-8, 6-23, 6-27
  - Missing value
    - Finding 13-12
    - symbol in file (M) 14-8
    - symbol in table (\*) 13-7, 13-12, 16-6
  - Mixture analysis 8-1
  - MNAPS 8-22, 9-4
  - MOD 16-7
  - Model
    - ASCII 15-9
    - Galactic CAL file 15-9
    - Guided Wave calibration file 15-9
    - KNN 6-5
    - PCA 5-43
    - Regression 7-14, 7-50
    - Save 15-6
    - SIMCA 6-18
  - Model files
    - MOD 16-7
    - PMF 16-7
  - Model optimization
    - PLS 7-16
    - PLS-DA 7-39
    - SIMCA 6-24
  - Modeling Power 5-27
  - Momentum spinning 12-12
  - Most recent files 16-11
  - Mouse actions
    - Click-drag 10-1, 13-4
    - Control-click 10-2
    - Right mouse button 11-4, 12-4, 12-10
    - Shift-click 10-1
  - MSC 4-21
  - Multiple Linear Regression 7-3
  - Multiplication 4-15
  - Multiplicative Scatter Correction 4-21
  - Multiplot 10-15, 12-21
  - Multivariate Curve Resolution 8-12
  - MYCALIGN 4-24, 9-4
  - MYCOSING 9-4
- N**
- Names
    - in Plots 16-33, 16-34
    - in Spreadsheet 13-1
    - of Objects 11-3
    - of Sets 11-6
    - of Windows 12-5
  - Near infrared spectroscopy (NIR) 3-2
  - Nearest neighbor 6-3
  - Nearest neighbor clustering 5-5
  - New 16-3
  - NIPALS 5-28, 7-5
  - Node of dendrogram 12-24
  - Non-negativity 8-16
  - Normalization
    - Examples 4-18
    - Maximum value 4-17
    - using a Mask 4-17
    - Vector area 4-16
    - Vector length 4-16
    - Vector range 4-17
  - Notes 10-15, 11-4, 16-14
  - Number of factors 5-19 to 5-27, 6-24, 7-6 to 7-9
- O**
- Object Manager
    - Creating charts from 11-7
    - Description 11-1
    - Finding text 11-5
    - Icons 11-1
    - Information 11-4
    - Naming subsets 11-6
  - Objects
    - Deleting 11-6
    - Menu 16-36
    - Names 11-3
  - OCT\_TEST 3-33
  - OCTANE20 3-4, 5-11, 9-4
  - Optimization
    - F test 5-22
    - IND function 5-22
    - KNN 6-10
    - Number of factors 5-19 to 5-27, 6-24, 7-6 to 7-9
    - Number of neighbors 6-7
    - PRESS 7-7, 7-48
    - Regression models 3-22
    - SIMCA 6-24
  - Options (setting of) 4-32
  - Orthogonal Leverage 11-10
  - Orthogonal signal correction (OSC) 7-12
  - Outlier detection
    - Importance 5-23
    - in CLS 7-48
    - in Scatter plots 4-9
    - using Leverage 3-22, 7-11
    - using Mahalanobis distance 5-38, 6-14
    - using Q statistic 5-25
    - using Sample Residual 7-49
    - using Studentized residuals 7-24
  - Overview region (of dendrogram) 12-25
- P**
- PALMCHRO 14-3
  - Pareto scale 4-31
  - Parsimonious model 5-27, 7-9
  - Partial Least Squares (PLS)
    - Example 3-17

- for Classification 7-39
  - Math 7-5
  - Model 7-14, 7-49
  - Optimization 7-16
  - Options 16-24
  - Prediction 3-33, 7-31
  - PCA (see Principal Components Analysis)
  - PCA Fill 13-18
  - PCA Hypergrid 11-10
  - PCR (see Principal Components Regression)
  - Piecewise Direct Standardization 4-35
  - PIONIR 14-13
  - PIR file 1-2, 14-5
  - Pirouette, Lite versions 18-3
  - Plot
    - Labels 10-17
    - Preferences 10-16
    - Scaling 12-13
    - Symbols 10-11
  - PLS (see Partial Least Squares)
  - PLS-DA 7-39
  - Plus sign cursor 10-6
  - PMF 16-7
  - Point
    - Default label 10-16
    - Labels 16-33
    - Size 10-11
  - Pointer Tool 16-34
  - Pointer tool 10-2
  - Portuguese 10-22
  - Pound sign (#)
    - ASCII file specifier 14-6
    - Examples 14-6 to 14-9
  - Prediction
    - KNN 6-12
    - Options 10-19
    - PCA 5-43
    - PLS/PCR 7-31
    - Preferences 10-19
    - SIMCA 6-25
  - Preferences
    - Color
      - Color sequence 10-18
      - General settings 10-7
    - Info Box Font 10-20
    - Language 10-21
    - Prediction 10-19
    - Sets of 10-21
    - Text 10-8
    - Views 10-7
  - Preprocessing, Options 16-21
  - PRESS 7-7, 7-48
  - Principal Component Analysis (PCA)
    - Definition 5-13
    - Math 5-16
    - Options 16-22, 16-23
    - Prediction 5-43
    - Terminology 5-14
  - Principal Component Regression (PCR)
    - Math 7-4
    - Model 7-14, 7-49
  - Optimization 7-16
  - Options 16-24
  - Prediction 7-31
  - Print setup 15-1, 16-10
  - Printing 16-9
  - Probability 5-23, 5-24, 7-22, 10-19
  - Process Menu 16-19
  - Projections, in SIMCA 6-24
  - Pseudo-eigenvalue 7-5
  - Pure Component Spectra 7-47
- Q**
- Q statistic 5-24
  - Qualify
    - in KNN 6-9
    - in SIMCA 6-23
- R**
- RANDOM 5-4, 9-5
  - Random sample selection 11-11
  - Range scale 4-30
  - Range tool 12-20, 16-35
  - Rank 4-35, 5-16, 18-7
  - Recent files 16-11
  - Redraw 10-13
  - Regression
    - Example 3-19
    - Linear 7-3
    - Model 7-14, 7-50
    - Multivariate 7-3
    - Prediction 7-31
    - Validation 7-7
    - Vector 7-24, 15-10
  - Rename 11-6
  - Residuals
    - Between classes (SIMCA) 6-19
    - Sample, in CLS 7-48
    - Sample, in PCA 5-23
    - Studentized 7-11
    - X-block, in PCA 5-38
  - Results, Display 10-17
  - Retention index 4-22
  - Ribbon
    - Description 10-3
    - Edit tools 10-4
    - File and window tools 10-3
    - Navigation aids 10-5
    - Spin control 10-5
    - View buttons 10-4
  - Rotation
    - Spinning 3D views 12-11
    - Varimax 5-41
  - Run status 18-6
- S**
- Sample residual 5-23, 7-48
  - Sample selection 11-9
  - Save
    - Data 16-5
    - Model 15-6
    - Objects 15-5
  - Savitzky-Golay 4-13

- Scaling, in Plots 12-13
  - Scatter plots 12-6 to 12-15
  - Scores
    - contributions to 5-26
    - Graphical description 5-17
    - in PCA 5-36
    - in Regression 7-17
  - Screen capture to printer 15-1
  - Scroll tools 13-4
  - SEC 7-12
  - Selecting data
    - Cloaking 12-9
    - in Charts 12-7
    - in Tables 13-5
  - Selectivity 6-28
  - Selector button 10-5, 12-16, 12-21
  - Sensitivity 6-28
  - SEVEN 9-5
  - Shift-click 10-1, 16-5
  - SIMCA (see Soft Independent Modeling of Class Analogy)
  - Similarity 5-2, 12-24, 12-27
  - Simplicity 5-28
  - Single link 5-3, 5-6, 5-11
  - Singular Value Decomposition (SVD) 7-4
  - SMCR 8-12
  - Smoothing 4-13
  - SNV 4-22
  - Soft Independent Modeling of Class Analogy (SIMCA)
    - Definition 6-14
    - Model 6-18
    - Optimization 6-24
    - Options 16-23
    - Prediction 6-25
  - Sort 13-10
  - Source
    - Amounts 8-20
    - Apportionment 8-1, 8-24
    - Profiles 8-20
  - Spanish 10-22
  - SPE 5-24
  - Spin control buttons 12-12
  - Spinner Tool 12-11, 16-35
  - Spreadsheet
    - Cursors 10-6
    - Entering data 14-1
    - Labels
      - in ASCII file 14-6
      - in spreadsheet file 14-9
    - Navigation 13-2
    - Variable types 13-9
  - Squared prediction error (SPE) 5-24
  - Standard deviation 5-13
  - Standard Error
    - of Calibration (SEC) 7-7, 7-12, 7-48, 7-50
    - of Prediction (SEP) 7-7, 7-48
    - of Validation (SEV) 7-8
  - Standard Normal Variate 4-22
  - Statistical Prediction Error (SPE) 7-47
  - Studentized residual 7-11
  - Submenu 16-1
  - Subset selection 4-34
  - Subsets
    - by Variable selection 11-11
    - from Plots 12-34
    - from Sample selection 11-9
    - from Spreadsheets 13-20
    - making a Full Data set 11-9, 18-2
    - Naming 11-6
    - Removing 11-6
  - Subtraction 4-19
  - Support 18-14
  - Symmetric matrix 17-2
- T**
- Technical assistance 1-6, 18-14
  - TERNARY 9-5
  - Test set 3-33
  - TIFF 15-2
  - Total contribution 5-26
  - Total Modeling Power 6-21
  - Training set 4-5
  - Transfer of calibration 4-33, 4-34, 6-28, 7-57
  - Transfer samples 6-28, 7-57
  - Transforms 4-11, 16-28
  - Transmittance spectra 4-15
  - Transpose
    - function 13-12, 16-7
    - of a matrix 17-3
    - of data 14-7
  - Troubleshooting 18-1
- U**
- Uncertainty 7-12
  - Undo 16-13
  - Unmagnify 12-10
  - Unzoom 10-4
  - User charts 12-1
  - User permissions 1-6, 18-1
- V**
- Validation
    - Regression 7-7
    - Standard Error of 7-8
  - Variable
    - Dependent vs. independent 4-5
    - Selection 11-11
    - Types 13-9
  - Variance 5-13, 5-23, 7-48
  - Variance scale 4-27
  - Variance weight 11-12
  - Varimax 5-28 to 5-29, 5-41
  - Vector
    - Area normalization 4-16
    - Definition 17-1
    - Length normalization 4-16
  - Version of software 16-45
  - View
    - Preferences 10-7
    - Types 10-4, 12-6
  - Votes matrix 6-5

**W**

Warning messages 18-8

Web site 18-14

Weight loadings 7-6

Window

Preferences 10-16

Titles 12-5

Window size

Align transform 4-24

PDS 4-35

Windows Explorer, load data from 14-4

Windows Menu 16-38

**X**

X Limits 12-18

X Preprocessed 5-32

X Residuals

in PCA 5-38

in PLS 7-26

Prediction 7-34

X variable 4-4, 13-5

XLS file 1-2

XRF 9-5

**Y**

Y variable 4-5, 13-5

**Z**

Zero fill 13-13, 16-19

Zoom button 10-4, 12-22

A

B

C

D

E

F

G

H

I

J

K

L

M

N

O

P

Q

R

S

T

U

V

W

X

Y

Z