PLS_Toolbox 7.0

Quick-Reference Card

Help and Information

helppls - Context related help on the PLS_Toolbox.
readme - Release notes for Version 4.1 of PLS_Toolbox.
demos - Demo list for the PLS_Toolbox.
evricompatibility - Tests for inter-product compatibility of Eigenvector toolboxes.
evridebug - Checks the PLS_Toolbox installation for problems.
evridir - Locate and or create EVRI home directory.
evriinstall - Install Eigenvector Research Product.
evriuninstall - Uninstall an Eigenvector Research toolbox.
evriupdate - Check Eigenvector.com for available PLS_Toolbox updates.
plsver - Displays version information.

Plotting Analysis Aids and I/O Functions

abline - Draws a line on the current axes with a given slope and intercept.
analysis - Graphical user interface for data analysis.
areadr - Reads ascii data and strips header.
autoexport - Exports a DataSet object to a file of the specified format.
autoimport - Automatically reads specified file. Handles all standard filetypes.
b3spline - Univariate spline fit and prediction.
boxplot - Box plot of a data matrix.
builddbstr - Builds a database connection string.
dp - Draws a diagonal line on an existing figure.
ellps - Plots an ellipse on an existing figure.
explode - Extracts variables from a structure array
exportfigure - Automatically export figures to an external program.
figuretheme - Resets a figure background and axes color.
getpidata - Uses the current PI connection to construct a DSO.
gselect - Selects objects in a figure (various selection styles).
hjyreadr - Reads HORIBA Jobin Yvon files (Windows Only).
hline - Adds horizontal lines to figure at specified locations.
infobox - Display a string in an information box.
loopfilereadr - An example function for reading files in a loop.
mplot - Automatic creation of subplots and plotting.
mtfreadr - Read AdventaCT Multi-Trace Format (MTF) files.
parsemixed - Parse numerical and text data into a DataSet Object.
pcolormap - Pseudocolor plot with labels and colorbar.
ploteigen - Builds dataset object of eigenvalues/RMSECV information.
plotgui - Interactive data viewer.
plttern - Plots a 2D ternary diagram.
plternf - Plots a 3D ternary diagram with frequency of occurrence.
querydb - Executes a query on a database defined by connection string.
reportwriter - Write a summary of the analysis including associated figures to html/word/powerpoint.
rwb - Red white and blue color map.
setpath - Modifies and saves current directory to the MATLAB search path.
snabsreadr - Reads Stellarnet ABS XY files.
spcreadr - Reads a Galactic SPC file.
trendtool - Univariate trend analysis tool.
vline - Adds vertical lines to figure at specified locations.
writeasf - Writes AIT ASF files from a dataset object.
writecsv - Export a DataSet object to a comma-separated values (CSV) file.
xclgetdata - Extracts matrix from an Excel spreadsheet.
xclputdata - Write matrix to an Excel spreadsheet.
xclreadr - Reads an ASCII or .XLS file in as a DataSet Object.
xlsreadr - Reads .XLS files from MS Excel and other spreadsheets.
xyreadr - Reads one or more ASCII XY or XY... files into a DataSet object.
yscale - Rescales the y-axis limits on each subplot in a figure.
zline - Adds vertical lines to 3D figure at specified locations.

Data Editing Scaling and Preprocessing

alignmat - Alignment of matrices and N-way arrays.
alignpeaks - Calibrates wavelength scale using standard peaks.
alignspectra - Calibrates wavelength scale using standard spectrum.
auto - Autoscales matrix to mean zero unit variance.
baseline - Subtracts a polynomial baseline offset from spectra.
baselinew - Baseline using windowed polynomial filter.
batchdigester - Parse wafer or batch data into MPCA or Summary PCA form.
classcenter - Centers classes in data to the mean of each class.
coadd - Reduce resolution through combination of adjacent variables or samples.
delsamps - Deletes samples (rows) or variables (columns) from data matrices.
deresolv - Changes high resolution spectra to low resolution.
editds - Editor for DataSet Objects.
excludemissing - Automatically exclude too-much missing data in a matrix.
glsw - Generalized least-squares weighting/preprocessing.
gscale - Group/block scaling for a single or multiple blocks.
gscaler - Applies group/block scaling to submatrices of a single matrix.
lamsel - Determines indices of wavelength axes in specified ranges.
logdecay - Mean centers and variance scales a matrix using the log decay of the variable axis.
lsq2top - Fits a polynomial to the top/(bottom) of data.
mdcheck - Missing Data Checker and infiller.
med2top - Fits a constant to top/(bottom) of data.
medcn - Median center scales matrix to median zero.
mncn - Scale matrix to mean zero.
mscorr - Multiplicative scatter/signal correction (MSC).
normaliz - Normalize rows of matrix.
npreprocess - Preprocessing of multi-way arrays.
oscapp - Applies OSC model to new data.
osccalc - Calculates orthogonal signal correction (OSC).
poissonscale - Perform Poisson scaling with scaling offset.
polyinterp - Polynomial interpolation, smoothing, and differentiation.
preprocess - Selection and application of standard preprocessing structures.
preprouser - User-defined preprocessing methods.
registerspec - Shift spectra based on expected peak locations.
rescale - Scales data back to original scaling.
savgol - Savitzky-Golay smoothing and differentiation.
savgolcv - Cross-validation for Savitzky-Golay smoothing and differentiation.
scale - Scales data using specified means and std. devs.
shuffle - Randomly re-orders matrix and multiple blocks rows.
snv - Standard normal variate scaling.
specedit - GUI for selecting spectral regions on a plot.
super_reduce - Eliminates highly correlated variables.
unfoldm - Rearranges (unfolds) an augmented matrix to row vectors.
unfoldmw - Unfolds multiway arrays along specified order.
windowfilter - Spectral filtering.
wlsbaseline - Weighted least squares baseline function.

Statistics, ANOVA, Experimental Design +

anova1w - One-way analysis of variance.
anova2w - Two-way analysis of variance.
anovadoe - Function to perform ANOVA for 2^k factorial model X, Y data.
boxbehnken - Create a Box-Behnken Design of Experiments.
ccdface - Create a Face-Centered Central Composite Design of Experiments.
ccdsphere - Create a Spherical Central Composite Design of Experiments.
corrmap - Correlation map with variable grouping.
cov_cv - Estimation of a regularized inverse covariance matrix.
distslct - Selects samples on outside of data space.
doeeffectsplot - Create main effect or interaction plot, incl LSD bars.
doegen - Generate a Design of Experiments (DOE) DataSet object.
doegui - Design of Experiments tool.

Statistics, ANOVA, Experimental Design + cont...

doeinteractions - Calculates interaction terms of a raw DOE matrix.
doerunsheet - Create a doe run sheet.
doescale - Convert coded DOE to scaled DOE or scaled back to coded.
doptimal - Selects samples based on D-Optimal criteria.
durbin_watson - Criterion for measure of continuity.
exteriorpts - Selects samples on outside of data space after normalizing data.
factdes - Full factorial design of experiments.
ffacconfusion - Generates confusion table for a fractional factorial DOE.
ffacdes1 - Fractional factorial design of experiments.
ftest - F test and inverse F test statistic.
halfnormplot - Produce Half-Normal or Normal plot from DOE dataset object.
percentile - Finds percentile point (similar to MEDIAN).
reducennsamples - Selects a subset of samples by removing nearest neighbors.
stdsslct - Selects data subsets (often for use in standardization).
ttestp - Evaluates t-distribution and its inverse.

Principal Components Analysis

chilimit - Chi-squared confidence limits from sum-of-squares residuals.
datahat - Calculates the model estimate and residuals of the data.
estimatefactors - Estimate number of significant factors in multivariate data.
jmlimit - Confidence limits for Q residuals via Jackson-Mudholkar.
knnscoredistance - Calculate the average distance to the k-Nearest Neighbors in score space.
manrotate - Graphical interface to manually rotate model loadings.
mlpca - Maximum likelihood principal components analysis.
pca - Principal components analysis.
pcaengine - Principal Components Analysis computational engine.
pcapro - Projects new data on old principal components model.
plotloads - Extract and display loadings information from a model structure.
plotscores - Extract and display score information from a model.
residuallimit - Estimates confidence limits for sum squared residuals.
ssqtable - Displays variance captured table for model.
subgroupcl - Displays a confidence ellipse for points in a two-dimensional plot.
tsqlim - Confidence limits for Hotelling's T^2.
tsqmtx - Calculates matrix for T^2 contributions for PCA.
varcap - Variance captured for each variable in PCA model.
varimax - Orthogonal rotation of loadings.

Curve Resolution and Factor Analysis

als - Alternating Least Squares computational engine.
comparelcms_simengine - Calculational Engine for comparelcms.
comparelcms_sim_interactive - Interactive interface for COMPARELCMS.
coda_dw_interactive - Interactive version of CODA_DW.
coda_dw - Calculates values for the Durbin_Watson criterion of columns of data set.
corrspec - Resolves correlation spectroscopy maps.
dispmat - Calculates the dispersion matrix of two spectral sets.
evolvfa - Evolving factor analysis (forward and reverse).
ewfa - Evolving window factor analysis.
mcr - Multivariate curve resolution with constraints.
purity - Self-modeling mixture analysis method based on purity of variables or spectra.
purityengine - calculates purity values of columns of data set.
wtfa - Window target factor analysis.

Cluster Analysis and Classification

class2logical - Create a PLSDA logical block from class assignments.
cluster - KNN and K-means cluster analysis with dendrograms.
discrimprob - Discriminate probabilities for continuous predicted values.
knn - K-nearest neighbor classifier.
plsda - Partial least squares discriminant analysis.
plsdaroc - Calculate and display ROC curves for PLSDA model.
plsdthres - Bayesian threshold determination for PLS Discriminate Analysis.
simca - Soft Independent Method of Class Analogy.
svmda - SVM Support Vector Machine for classification.

Multi way Functions

alignmat - Alignment of matrices and N-way arrays.
corcondia - Evaluates consistency of PARAFAC model.
coreanal - Analysis of the core array of a Tucker model.
corecalc - Calculate the Tucker3 core given the data array and loadings.
gram - Generalized rank annihilation method.
modelviewer - Visualization tool for multi-way models.
mpca - Multi-way (unfold) principal components analysis.
nassign - Generic subscript assignment indexing for n-way arrays.
nindex - Generic subscript indexing for n-way arrays.
npls - Multilinear-PLS (N-PLS) for true multi-way regression.
npreprocess - Preprocessing of multi-way arrays.
outerm - Computes outer product of any number of vectors.
parafac - Parallel factor analysis for n-way arrays.
parafac2 - Parallel factor analysis for unevenly sized n-way arrays.
tld - Trilinear decomposition.
tucker - Analysis for n-way arrays.

Linear and Non Linear Regression

cls - Classical Least Squares regression for multivariate Y.
cr - Continuum Regression for multivariate y.
crcvrnd - Cross-validation for continuum regression.
crossval - Cross-validation for decomposition and linear regression.
fastnnls - Fast non-negative least squares.
figmerit - Analytical figures of merit for multivariate calibration.
frpcr - Full-ratio PCR calibration and prediction.
frpcrengine - Engine for full-ratio PCR regression.
leverag - Calculate sample leverages.
lwr - Locally weighted regression for univariate Y.
lwrpred - Engine for locally weighted regression models.
mlr - Multiple Linear Regression for multivariate Y.
mlrengine - Multiple Linear Regression computational engine.
modlpred - Predictions using standard model structures.
modlrder - Displays model info for standard model structures.
nippls - NIPALS Partial Least Squares computational engine.
pcr - Principal components regression for multivariate Y.
pcrengine - Principal Component Regression computational engine.
pls - Partial least squares regression for multivariate Y.
plsnipal - NIPALS algorithm for one PLS latent variable.
polypls - PLS regression with polynomial inner-relation.
regcon - Converts regression model to y = ax + b form.
ridge - Ridge regression by Hoerl-Kennard-Baldwin.
ridgecv - Ridge regression by cross validation.
rinverse - Calculate pseudo inverse for PLS, PCR and RR models.
rmse - Calculate Root Mean Square Error.
simpls - Partial Least Squares computational engine using SIMPLS algorithm.
svm - SVM Support Vector Machine for regression.
svmda - SVM Support Vector Machine for classification.
varcapy - Calculate percent y-block variance captured by a PLS regression model.
vip - Calculate Variable Importance in Projection from regression model.

Variable Selection

calibsel - Statistical procedure for variable selection.
fullsearch - Exhaustive Search Algorithm for small problems.
gaselctr - Genetic algorithm for variable selection with PLS.
genalg - Genetic Algorithm for Variable Selection.
genalgplot - Plot GA results using selected variable plot, color-coded by RMSECV.
ipls - Interval PLS variable selection.

Quick-reference card for PLS_Toolbox 7.0

Multivariate Instrument Standardization

caltransfer - Create or apply calibration and instrument transfer models.
deresolv - Changes high resolution spectra to low resolution.
stdfir - Standardization based on FIR modelling.
stdgen - Piecewise and direct standardization transform generator.
stdize - Applies transform from STDGEN to new spectra.

MSPC and Identification of Finite Impulse Response Models

autocor - Auto-correlation function for time series data.
crosscor - Cross-correlation function for time series data.
fir2ss - Transform FIR model into equivalent state space model.
plspulsm - Identifies FIR dynamics models for MISO systems.
plsrsgcv - Generate PLS models for MSPC with cross-validation.
plsrsgn - Generates a matrix of PLS models for MSPC.
replace - Replaces variables based on PCA or PLS models.
wrtpulse - Create input/output matrices for dynamic model identification.

Model Utilities

browse - PLS_Toolbox Toolbar and Workspace browser.
choosecomp - Automatic selection of components for various model types.
choosencomp - GUI to select number of components from SSQ table.
compressmodel - Remove references to unused variables from a model.
copydsfields - Copies informational fields between datasets and/or models.
correctbias - Adjusts a regression model for bias and slope errors.
matchvars - Align variables of a dataset to allow prediction with a model.
modelcache - Stores and retrieves models in the model cache.
modelselector - Create or apply a model selector model.
modelstruct - Constructs an empty model structure.
reviewmodel - Examines a standard model structure for typical problems.
updatemod - Update model structure to be compatible with the current version.

Non Linear Optimization Tools

lmoptimize - Levenberg-Marquardt non-linear optimization.
lmoptimizebnd - Bounded Levenberg-Marquardt non-linear optimization.

Peak Fitting Tools

fitpeaks - Peak fitting routine.
peakfind - Automated identification of peaks.
peakstruct - Makes an empty peak definition structure.
peakfunction - Outputs the estimated peaks from parameters in PEAKDEF.
localmax - Automated identification of local maxima.
peakidtext - Writes peak ID information on present graph.

Distribution Fitting Tools

Graphical Interfaces

ktool - GUI tool for investigating the density of a sample.
qtool - GUI tool for investigating the QQ-plot.
cqtool - GUI tool for investigating the conditional QQ-plot.

Distribution Goodness of fit tests

chitest - Chi-squared goodness-of-fit distribution test.
kstest - Kolmogorov-Smirnov goodness-of-fit distribution test.
distfit - Perform chitest for all distributions.

kdensity - Kernel density estimation.

Distribution Functions

Density, Probability, Quantile, Random Numbers

betadf - Beta
chidf - Chi-squared
gammadf - Gamma
laplacedf - Laplace (double exp.)
logisdf - Logistic
normdf - Normal (gaussian)
raydf - Rayleigh
triangledf - Triangle
weibulldf – Weibull
cauchydf - Cauchy (Lorentzian)
expdf - Exponential
gumbeldf - Gumbel
lognormdf - Lognormal
newtondf - Newton's root
paretodf - Pareto
tdf - Student's t
unifdf - Continuous uniform

Distribution Plot functions

plotedf - Empirical distribution plot.
plotkd - Kernel density plot with overlay.
plotpct - Percentile plot.
plotcqq - Conditional quantile plot.
plotqq - Quantile plot.
plotsym - Symmetry plot.

Basic Statistical Tests + Utility Functions

means - Arithmethic, geometric, and harmonic means.
parammle - Maximum likelihood parameter estimates for DF_Toolbox.
pctile1 - Percentile function (used by summary).
pctile2 - Alternative definition percentile function.
randomttest - Randomization t-test for evaluating residuals from two models.
resize - Resizes arguments to same length.
signtest - Pairwise sign test for evaluating residuals from two models.
summary - Summary statistics for a data vector.
ttest1 - 1 sample t-test.
ttest2e - 2 sample t-test assuming equal variances.
ttest2u - 2 sample t-test assuming unequal variances.
ttest2p - 2 sample paired t-test.
wilcoxon - Pairwise Wilcoxon signed rank test for evaluating residuals from two models.

Programming Utilities

besttime - Returns a string describing the time interval provided (in seconds).
cellne - Compares two cells for inequality in size and/or values.
classsummary - List class and axisscale distributions for a DataSet.
comparevars - Compares two variables of any type and returns differences.
contents - Mfile of functions to enable Matlab helpwin.
encode - Translates a variable into matlab-executable code.
erdlgpls - Error dialog.
evrirelease - Returns Eigenvector product release number.
evriscript - Create a chain of steps where each step applies a single pls_toolbox function.
exportfigure - Automatically export figures to an external program.
figbrowser - Browser with icons of all Matlab figures.
figuretheme - Resets a figure background and axes to a specified color.
findindx - Finds the index of the array element closest to value r.
getdatasource - Extract summary dataset info.
getmlversion - Returns current Matlab version as an integer.
getplspref - Get overriding options (preferences) for PLS_Toolbox functions.
lddlgpls - Dialog to load variable from workspace or MAT file.
moveobj - Interactively reposition graphics objects.
helppls - Context related help on the PLS_Toolbox.
readme - Release notes for PLS_Toolbox.
reversebytes - Flips order of bytes in a word.
setplspref - Set overriding options (preferences) for PLS_Toolbox functions.
string_x - Add backslash before troublesome TeX characters.
svdlgpls - Dialog to save variable to workspace or MAT file.

Frequently Asked Questions: http://www.eigenvector.com/faq/
Request Help at: helpdesk@eigenvector.com
Send the output of the commands: evridebug, ver, path

Quick-reference card for PLS_Toolbox 7.0

www.Eigenvector.com