LIBRA: a MATLAB Library for Robust Analysis

List of Functions

22 December, 2006

This document contains the list of functions that are currently available in the 'MATLAB Library for Robust Analysis'. This toolbox is developed at the research groups on robust statistics at the Katholieke Universiteit Leuven and the University of Antwerp and can be downloaded from the website

http://wis.kuleuven.be/stat/robust/Libra.html

It contains user-friendly implementations of several robust procedures, most of them being developed at both research groups. These methods are resistant to outliers in the data. Many graphical tools are provided for model checking and outlier detection.

Most of the functions can be used with MATLAB 5.2, 6.1, 6.5. All of them should work with MATLAB 7.0. Many functions require the MATLAB Statistics Toolbox.

Contributions to this toolbox have been made by (in alphabetical order): Guy Brys, Sanne Engelen, Mia Hubert, Nele Smets, Karlien Vanden Branden, Ellen Vandervieren, Katrien Van Driessen, Sabine Verboven en Wai Yan Kong.

The toolbox can be freely used for non-commercial use only. Please make appropriate references to the corresponding paper(s) if you use any of our programs. The correct references can be found in the help-files, or at the web pages:

> http://wis.kuleuven.be/stat/robust http://www.agoras.ua.ac.be/

Bugs or comments on the programs can be reported to Mia Hubert:

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| Name | Description | Available since | | |
|----------------------------|---|-----------------|--|--|
| Robust estimator | rs of location, scale, skewness. | | | |
| mlochuber | M-estimator of location with Huber psi-function | 22-04-2004 | | |
| mloclogist | M-estimator of location with logistic psi-function | 22-04-2004 | | |
| hl | Hodge-Lehmann location estimator | 22-04-2004 | | |
| unimcd | MCD estimator of location and scale | 30-06-2003 | | |
| mad | Median absolute deviation | 30-06-2003 | | |
| mscalelogist | M-estimator of scale with logistic psi-function | 22-04-2004 | | |
| qn | Qn-estimator of scale. | 30-06-2003 | | |
| adm | Scale estimator given by the Average Distance to the Median | 22-04-2004 | | |
| mc | Medcouple: robust estimator of skewness | 22-04-2004 | | |
| robstd | Columnwise robust standardization | 22-04-2004 | | |
| adjusted boxplot | Computes and plots skewness adjusted boxplot | 22-12-2006 | | |
| Robust multivari | ate analysis. | | | |
| l1median | L1-median of multivariate location | 30-06-2003 | | |
| mcdcov | Minimum Covariance Determinant estimator | 22-04-2003 | | |
| | of multivariate location and covariance | | | |
| rapca | Robust principal component analysis | 30-06-2003 | | |
| | (based on projection pursuit) | | | |
| robpca | Robust principal component analysis | 30-06-2003 | | |
| | (based on projection pursuit and MCD estimation) | | | |
| rda | Robust linear and quadratic discriminant analysis | 22-04-2004 | | |
| | (classification of low-dimensional data) | | | |
| rsimca | Robust soft independent modelling of class analogies | 20-09-2004 | | |
| | (classification of high-dimensional data) | | | |
| Robust regression methods. | | | | |
| ltsregres | Least Trimmed Squares regression | 30-06-2003 | | |
| mcdregres | Multivariate MCD regression | 30-06-2003 | | |
| rpcr | Robust principal component regression | 30-06-2003 | | |
| rsimpls | Robust partial least squares regression | 30-06-2003 | | |

| Name | Description | Available since | | |
|---|--|-----------------|--|--|
| Plot functions. | | | | |
| makeplot | PlotGUI which includes the following plot functions: | 30-06-2003 | | |
| chiqqplot | Quantile-Quantile-plot of a vector | 22-04-2004 | | |
| | against the square root of the χ^2 -quantiles | | | |
| ddplot | Robust distances versus Mahalanobis distances | 22-04-2004 | | |
| distplot | Plots a vector of distances | 22-04-2004 | | |
| ellipsplot | Scatter plot of bivariate data with 97.5% tolerance ellipse | 22-04-2004 | | |
| lsscatter | Scatter plot of bivariate data with regression line | 22-04-2004 | | |
| normqqplot | Quantile-Quantile plot of a vector against | 22-04-2004 | | |
| | the quantiles of a standard normal distribution | | | |
| daplot | Scatter plot of grouped bivariate data with their | 22-04-2004 | | |
| | 97.5% tolerances ellipses (estimated from a discr. analysis) | | | |
| regressing plot | Regression diagnostic plot | 30-06-2003 | | |
| | (residual distance versus score distance) | | | |
| regresdiagplot3D | 3D diagnostic plot | 30-06-2003 | | |
| | (residual distance versus score distance and orth. distance) | | | |
| residualplot | Plots the residuals from a regression analysis | 22-04-2004 | | |
| screeplot | Plots eigenvalues or their logarithm | 30-06-2003 | | |
| scorediagplot | Score diagnostic plot | 30-06-2003 | | |
| | (orthogonal distance versus score distance) | | | |
| simcaplot | Scatter plot with boundaries defined by | 20-09-2004 | | |
| | the number of principal components (estimated from simca) | | | |
| Classical multivariate analysis and regression. | | | | |
| ols | Ordinary (multiple) linear least squares regression | 22-04-2004 | | |
| mlr | Multivariate (multiple) linear regression | 22-04-2004 | | |
| classSVD | Singular value decomposition if more cases than variables | 30-06-2003 | | |
| kernelEVD | Singular value decomposition if less cases than variables | 30-06-2003 | | |
| cda | Classical linear and quadratic discriminant analysis | 22-04-2004 | | |
| cpca | Classical principal component analysis | 30-06-2003 | | |
| cpcr | Classical principal component regression | 30-06-2003 | | |
| csimca | Classical soft independent modelling of class analogies | 20-09-2004 | | |
| csimpls | Partial least squares regression (SIMPLS) | 30-06-2003 | | |

| Name | Description | Available since | | |
|---------------------|--|-----------------|--|--|
| Clustering Methods. | | | | |
| agnes | Agglomerative Nesting | 20-10-2006 | | |
| clara | Clustering method for Large Applications | 20-10-2006 | | |
| clusplot | Bivariate clustering plot of output from pam, fanny or clara | 20-10-2006 | | |
| daisy | Computing pairwise dissimilarities | 20-10-2006 | | |
| diana | Divisive Analysis | 20-10-2006 | | |
| fanny | Fuzzy Analysis | 20-10-2006 | | |
| mona | Monothetic Analysis | 20-10-2006 | | |
| pam | Partitioning Around Medoids | 20-10-2006 | | |

20-10-2006

Tree plot for the output of agnes or diana

 tree

| Name | Description | Available since | | |
|---|---|-----------------|--|--|
| Functions used as subroutines and which can make life easy. | | | | |
| greatsort | Sorts a vector in descending order | 30-06-2003 | | |
| mahalanobis | Computes the distance of an observation | 22-04-2004 | | |
| | with respect to the location and the shape of the data | | | |
| mcenter | Mean-centers a data matrix | 30-06-2003 | | |
| plotnumbers | Puts index of observations on a plot | 30-06-2003 | | |
| putlabel | Puts labels of observations on a plot | 30-06-2003 | | |
| removal | Deletes rows/columns from a matrix | 30-06-2003 | | |
| robstd | Columnwise robust standardization | 22-04-2004 | | |
| uniran | Random uniform generator | 30-06-2003 | | |
| weightmecov | Weighted mean and covariance matrix | 17-12-2004 | | |
| Functions used only | as subroutines. | | | |
| cvMcd | Cross-validated PRESS value for the MCD method | 20-09-2004 | | |
| $\operatorname{cvRobpca}$ | Cross-validated PRESS value for the ROBPCA method | 20-09-2004 | | |
| cvRpcr | Cross-validated RMSE value for the RPCR method | 17-12-2004 | | |
| cvRsimpls | Cross-validated RMSE value for the RSIMPLS method | 17-12-2004 | | |
| extractmcdregress | Auxiliary function for cross-valid. with RPCR and RSIMPLS | 17-12-2004 | | |
| removeObsMcd | Removal of observations for calculation of PRESS | 20-09-2004 | | |
| | (used in cvMcd) | | | |
| ${ m removeObsRobpca}$ | Removal of observations for calculation of PRESS | 20-09-2004 | | |
| | (used in cvRobpca, cvRpcr, cvRsimpls) | | | |
| robpcaregres | Robust regression based on results from ROBPCA | 17-12-2004 | | |
| | (used in rsimpls and cvRsimpls) | | | |
| rrmse | Robust RMSECV and RMSEP values | 30-06-2003 | | |
| | (used in rpcr and rsimpls) | | | |
| rsquared | Robust and classical \mathbb{R}^2 values | 30-06-2003 | | |
| rstep | Reflection step (used in rapca) | 30-06-2003 | | |

Datasets

Datasets from the book *Finding groups in data: An introduction to cluster analysis*, Kaufman L. and Rousseeuw P.J., Wiley-Interscience: New York, ISBN:0-471-87876-6.

- agricul.mat
- $\bullet\,$ animal.mat
- country.mat
- $\bullet~{\rm flower.mat}$
- obj200.mat
- ruspini.mat

History and major updates

Release June 30, 2003

The toolbox is made available with main functions: mcdcov, rapca, robpca, ltsregres, mcdregres, rpcr, rsimpls.

Release April 22, 2004

Several robust and classical procedures have been added:

- robust estimators of location and scale (M-estimators, Hodges-Lehmann, ...)
- the medcouple: a robust estimator of skewness
- robstd: robust standardization of multivariate data
- rda/cda: robust and classical discriminant analysis (classification)
- ols, mlr: classical least squares regression

Moreover several of the main functions are updated:

- mcdcov,rapca,ltsregres: the input and output structure is made conform to that of robpca, rpcr,...
- ltsregres: the intercept adjustment is now made optional. In the default setting, no adjustment is performed to save computation time. Also in mcdcov, some improvements have been made to speed up the computations.

Release September 20, 2004

Several robust and classical procedures have been added:

- csimca/rsimca: classical and robust SIMCA
- pressmcd/pressrobpca/removeobsmcd/removeobsrobpca/updatecov: subroutines to use in fast cross-validation methods for MCD en ROBPCA.

Updates of some of the main functions were performed:

• makeplot: accompanying plots for csimca, rsimca, were added Classical plots will now automatically be plotted if classical output is provided.

Release December 17, 2004

- Cross-validation for robust calibration methods (RPCR, RSIMPLS) has been added. The 'pressmcd' and 'pressrobpca' auxiliary functions are renamed into 'cvMcd' and 'cvRobpca'. To select the appropriate number of latent variables, several graphical displays are added, among which the Robust Component Selection (RCS) curve.
- The classification functions (cda, rda, csimca, rsimca) allow an extra argument: a prediction set, different from the training set, on which the classification rules are applied.

Release March 23, 2005

LIBRA now also works with MATLAB version 7.0. Reported bugs have been fixed (especially in the function makeplot.m) and some minor updates were performed on the functions: robpca, rsimpls, rrmse, cvMcd.

Release October 20, 2006

LIBRA includes the clustering algorithms described in the book *Finding groups in data: An introduction to cluster analysis* of Kaufman and Rousseeuw (Wiley, 1990).

Release December 22, 2006

The function to compute and plot a skewness adjusted boxplot has been added.