# Package 'fsdaR'

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**Title** Robust Data Analysis Through Monitoring and Dynamic Visualization

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Description Provides interface to the 'MATLAB' toolbox 'Flexible Statistical Data Analysis (FSDA)' which is a comprehensive and computationally efficient software package for robust statistics in regression, multivariate and categorical data analysis. The current R version implements tools for regression: (forward search, S- and MM-estimation, least trimmed squares (LTS) and least median of squares (LMS)), for multivariate analysis (forward search, S- and MM-estimation), for cluster analysis and cluster-wise regression. The distinctive feature of our package is the possibility of monitoring the statistics of interest as function of breakdown point, efficiency or subset size, depending on the estimator. This is accompanied by a rich set of graphical features, such as dynamic brushing, linking, particularly useful for exploratory data analysis.

**Depends** R (>= 3.5.0), rrcov

**Imports** rJava, methods, stats4, ggplot2

Suggests MASS

**SystemRequirements** (license-free) MATLAB Runtime (MCR) V 9.6, Java (>=8)

LazyLoad yes

LazyData yes

License GPL (>= 2)

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### **Description**

Takes as input the output of function tclustICsol (that is a structure containing the best relevant solutions) and produces the car-bike plot. This plot provides a concise summary of the best relevant solutions. This plot shows on the horizontal axis the value of c and on the vertical axis the value of k. For each solution we draw a rectangle for the interval of values for which the solution is best and stable and a horizontal line which departs from the rectangle for the values of c in which the solution is only stable. Finally, for the best value of c associated to the solution, we show a circle with two numbers, the first number indicates the ranked solution among those which are not spurious and the second one the ranked number including the spurious solutions. This plot has been baptized 'car-bike', because the first best solutions (in general 2 or 3) are generally best and stable for a large number of values of c and therefore will have large rectangles. In addition, these solutions are likely to be stable for additional values of c and therefore are likely to have horizontal lines departing from the rectangles (from here the name 'cars'). Finally, local minor solutions (which are associated with particular values of c and k) do not generally present rectangles or lines and are shown with circles (from here the name 'bikes').

### Usage

```
carbikeplot(out, SpuriousSolutions = FALSE, trace = FALSE, ...)
```

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## Arguments

out An S3 object of class tclusticsol.object, (output of tclustICsol) contain-

ing the relevant solutions.

SpuriousSolutions

Wheather to include or not spurious solutions. By default spurios solutions are

not included into the plot.

trace Whether to print intermediate results. Default is trace=FALSE.

. . . potential further arguments passed to lower level functions.

## Author(s)

FSDA team, <valentin.todorov@chello.at>

#### References

Cerioli, A., Garcia-Escudero, L.A., Mayo-Iscar, A. and Riani M. (2017). Finding the Number of Groups in Model-Based Clustering via Constrained Likelihoods, emphJournal of Computational and Graphical Statistics, pp. 404-416, https://doi.org/10.1080/10618600.2017.1390469.

## **Examples**

```
## Not run:
data(geyser2)
out <- tclustIC(geyser2, whichIC="MIXMIX", plot=FALSE, alpha=0.1)

## Plot first two best solutions using as Information criterion MIXMIX
print("Best solutions using MIXMIX")
outMIXMIX <- tclustICsol(out, whichIC="MIXMIX", plot=TRUE, NumberOfBestSolutions=2)
print(outMIXMIX$MIXMIXDs)

carbikeplot(outMIXMIX)

## End(Not run)</pre>
```

corfwdplot

Monitoring the correlations between consecutive distances or residuals

# **Description**

Provides a method for obtaining the maximum empirical efficiency (in case of MM estimates) or maximum empirical breakdownplot (in case of S estimates) or maximum subset size (in case of forward search), using various measures of correlation between the n Mahalanobis distances or residuals at adjacent values of efficiecy, breakdown point or subset size.

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### Usage

```
corfwdplot(out, trace = FALSE, ...)
```

### **Arguments**

out

An object of S3 class returned by one of the estimation functions with the monitoring option selected (monitoring=TRUE): fsreda.object, sregeda.object, mmregeda.object fsmeda.object, smulteda.object or mmmulteda.object. This is a list containing the monitoring of minimum Mahalanobis distance in case of multivariate analysis or the monitoring of residuals in case of regression.

The needed elements of out are

- MAL: matrix containing the squared Mahalanobis distances monitored in each step of the forward search. Every row is associated with a unit (row of data matrix Y). This matrix can be created using one of the functions fsmult, smult or mmmult with the monitoring option selected, i.e. monitoring=TRUE.
- RES: matrix containing the residuals monitored in each step of the forward search. Every row is associated with a unit (row of data matrix Y). This matrix can be created using the function fsreg with the monitoring option selected, i.e. monitoring=TRUE.
- 3. bdp: a vector containing breakdown point values that have been used, in case of S estimates.
- eff: a vector containing efficiency values that have been used, in case of MM estimates.

trace

. . .

Whether to print intermediate results. Default is trace=FALSE.

potential further arguments passed to lower level functions.

### Value

A ggplot plot object which can be printed on screen or to a file.

### Author(s)

```
FSDA team, <valentin.todorov@chello.at>
```

### **Examples**

```
## Not run:

data(hbk)
(out <- fsmult(hbk[,1:3], monitoring=TRUE))
corfwdplot(out)

(out <- fsmult(hbk[,1:3], monitoring=TRUE))
corfwdplot(out)

(out1 <- smult(hbk, monitoring=TRUE, trace=TRUE))
corfwdplot(out1)</pre>
```

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```
(out2 <- mmmult(hbk[,1:3], monitoring=TRUE, trace=TRUE))
corfwdplot(out2)

(out3 <- fsreg(hbk[,1:3], hbk[,4], monitoring=TRUE, trace=TRUE, method="FS"))
corfwdplot(out3)

(out4 <- fsreg(hbk[,1:3], hbk[,4], monitoring=TRUE, trace=TRUE, method="S"))
corfwdplot(out4)

(out5 <- fsreg(hbk[,1:3], hbk[,4], monitoring=TRUE, trace=TRUE, method="MM"))
corfwdplot(out5)

## End(Not run)</pre>
```

diabetes

Diabetes data

### **Description**

The diabetes dataset, introduced by Reaven and Miller (1979), consists of 145 observations (patients). For each patient three measurements are reported: plasma glucose response to oral glucose, plasma insulin response to oral glucose, degree of insulin resistance.

# Usage

```
data("diabetes")
```

### **Format**

A data frame with the following variables:

glucose Area under plasma glucose curve after a three hour oral glucose tolerance test (OGTT).insulin Area under plasma insulin curve after a three hour oral glucose tolerance test (OGTT).sspg Steady state plasma glucose.class The type of diabete: Normal, Overt, and Chemical.

#### Source

Reaven, G. M. and Miller, R. G. (1979). An attempt to define the nature of chemical diabetes using a multidimensional analysis. *Diabetologia* 16:17-24.

# Examples

```
data(diabetes)
head(diabetes)
plot(CovMcd(diabetes[, 1:3]), which="pairs", col=diabetes$class)
```

emilia2001 7

emilia2001	Demographic data from the 341 miniciplaities in Emilia Romagna (an Italian region).

# Description

A data set containing 28 demographic variables for 341 municipalities in Emilia Romagna (an Italian region).

# Usage

```
data(emilia2001)
```

### **Format**

A data frame with 341 rows and 28 variables The variables are as follows:

- less10: population aged less than 10
- more75: population aged more than 75
- single single-member families
- · divorced": divorsed
- · widows: widows and widowers
- graduates: population aged more than 25 who are graduates
- no\_education: of those aged over 6 having no education
- · employed: activity rate
- unemployed: unemployment rate
- increase\_popul: standardised natural increase in population
- migration: standardised change in population due to migration
- birth\_92\_94: average birth rate over 1992-94
- fecundity: three-year average birth rate amongst women of child-bearing age
- houses: occupied houses built since 1982
- houses\_2WCs: occupied houses with 2 or more WCs
- · houses\_heating: occupied houses with fixed heating system
- TV: TV licence holders
- cars: number of cars for 100 inhabitants
- luxury\_cars: luxury cars
- · hotels: working in hotels and restaurants
- banking: working in banking and finance
- income: average declared income amongst those filing income tax returns
- income\_tax\_returns: inhabitants filing income tax returns

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- factories: residents employed in factories and public services
- factories\_more10: employees employed in factories withy more tha 10 employees
- factories\_more50: employees employed in factories withy more tha 50 employees
- · artisanal: artisanal enterprises
- entrepreneurs: enterpreneous and skilled self-employed among those of working age

@references Atkinson, A. C., Riani, M., and Cerioli, A. (2004). *Exploring Multivariate Data with the Forward Search*. Springer-Verlag, New York.

fsdalms.object Description of fsdalms Objects

# Description

An object of class fsdalms. object holds information about the result of a call to fsreg.

### Value

The object itself is basically a list with the following components:

rew	If rew=TRUE all subsequent output refers to reweighted else no reweighting is done.
beta	p-by-1 vector containing the estimated regression parameters.
bs	p x 1 vector containing the units forming subset associated with bLMS (bLTS).
residuals	residuals.
scale	scale estimate of the residuals.
weights	Vector like y containing weights. The elements of this vector are 0 or 1. These weights identify the h observations which are used to compute the final LTS (LMS) estimate. sum(weights)=h if there is not a perfect fit otherwise sum(weights) can be greater than h
h	The number of observations that have determined the LTS (LMS) estimator, i.e. the value of h.
outliers	vector containing the list of the units declared as outliers using confidence level specified in input scalar conflev.
conflev	confidence level which is used to declare outliers. Remark: conflev will be used to draw the horizontal lines (confidence bands) in the plots. Default value is 0.975
singsub	Number of subsets without full rank. Notice that if this number is greater than $0.1*$ (number of subsamples) a warning is produced
Χ	the data matrix X

The object has class "fsdalms".

У

the response vector y

fsdalts.object 9

### **Examples**

```
## Not run:
   (out <- fsreg(Y~., data=hbk, method="LMS"))
   class(out)
   summary(out)
## End(Not run)</pre>
```

fsdalts.object

Description of fsdalts Objects

### **Description**

An object of class fsdalts.object holds information about the result of a call to fsreg.

#### Value

The object itself is basically a list with the following components:

rew	If rew=TRUF all	subsequent ou	itput refers to	reweighted el	se no reweighting is

done.

beta p-by-1 vector containing the estimated regression parameters.

bs p x 1 vector containing the units forming subset associated with bLMS (bLTS).

residuals residuals.

scale scale estimate of the residuals.

weights Vector like y containing weights. The elements of this vector are 0 or 1. These

weights identify the h observations which are used to compute the final LTS (LMS) estimate. sum(weights)=h if there is not a perfect fit otherwise sum(weights)

can be greater than h

h The number of observations that have determined the LTS (LMS) estimator, i.e.

the value of h.

outliers vector containing the list of the units declared as outliers using confidence level

specified in input scalar conflev.

conflev confidence level which is used to declare outliers. Remark: conflev will be

used to draw the horizontal lines (confidence bands) in the plots. Default value

is 0.975

singsub Number of subsets without full rank. Notice that if this number is greater than

0.1\*(number of subsamples) a warning is produced

X the data matrix X y the response vector y

The object has class "fsdalts".

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### **Examples**

```
## Not run:
    (out <- fsreg(Y~., data=hbk, method="LTS"))</pre>
    class(out)
    summary(out)
## End(Not run)
```

fsmeda.object

Description of fsmeda.object Objects

### **Description**

An object of class fsmeda.object holds information about the result of a call to fsmult when called with parameter monitoring=TRUE.

#### Value

The object itself is basically a list with the following components:

MAL n x (n-init+1) matrix containing the monitoring of Each row represents the dis-

tance Mahalanobis distance for the corresponding unit.

BB n x (n-init+1) matrix containing the information about the units belonging to the

subset at each step of the forward search. The first column contains the indexes of the units forming subset in the initial step and each further column - the indexes of the units forming the corresponding step. The last column contains

the units forming subset in the final step (all units).

n-by-1 vector containing the estimates of the robust Mahalanobis distances (in

squared units). This vector contains the distances of each observation from the

location of the data, relative to the scatter matrix cov.

(n-init) x 3 matrix. which contains the monitoring of minimum MD or (m+1)th

ordered MD at each step of the forward search.

• 1st column = fwd search index (from init to n-1)

• 2nd column = minimum MD

• 3rd column = (m+1)th-ordered MD

(n-init+1) x 3 matrix which contains the monitoring of maximum MD or m-th ordered MD at each step of the forward search.

• 1st column = fwd search index (from init to n)

• 2nd column = maximum MD

• 3rd column = mth-ordered MD

(n-init+1) x 3 matrix which contains the monitoring of the gap (difference between minMD outside subset and max inside).

• 1st column = fwd search index (from init to n)

• 2nd column = min MD - max MD

md

mmd

msr

gap

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• 3rd column = (m+1)th-ordered MD - mth ordered distance

 $(n-init+1) \times (p+1)$  matrix which contains the monitoring of the estimated means at each step of the fwd search.

 $(n-init+1) \times (p*(p+1)/2+1)$  matrix which contains the monitoring of the of the elements of the covariance matrix in each step of the forward search.

• 1st column = fwd search index (from init to n)

• 2nd column = monitoring of S[1,1]

• 3rd column = monitoring of S[1,2]

• ..

• last column = monitoring of S[p,p]

detS (n-init+1) x 2 matrix which contains the monitoring of the determinant of the

covariance matrix in each step of the forward search.

(n-init)-by-11 matrix which contains the unit(s) included in the subset at each step of the fwd search. REMARK: in every step the new subset is compared with the old subset. Un contains the unit(s) present in the new subset but not in the old one. Un[1,2] for example contains the unit included in step init+1.

Un[end, 2] contains the units included in the final step of the search.

X the data matrix X

The object has class "fsmeda".

# **Examples**

Un

Loc

S2cov

```
## Not run:
   (out <- fsmult(hbk[,1:3], monitoring=TRUE))
   class(out)
   summary(out)
## End(Not run)</pre>
```

fsmmmdrs

Performs random start monitoring of minimum Mahalanobis distance

### **Description**

The trajectories originate from many different random initial subsets and provide information on the presence of groups in the data. Groups are investigated by monitoring the minimum Mahalanobis distance outside the forward search subset.

### Usage

```
fsmmmdrs(x, plot = FALSE, init, bsbsteps, nsimul = 200,
  nocheck = FALSE, numpool, cleanpool = FALSE, msg = FALSE,
  trace = FALSE, ...)
```

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### **Arguments**

Χ

An n x p data matrix (n observations and p variables). Rows of x represent observations, and columns represent variables.

Missing values (NA's) and infinite values (Inf's) are allowed, since observations (rows) with missing or infinite values will automatically be excluded from the computations.

plot

Plots the random starts minimum Mahalanobis distance with 1 If plot=FALSE (default) or plot=0 no plot is produced. The scale (ylim) for the y axis is defined as follows:

- ylim[2] is the maximum between the values of mmd in steps [n\*0.2 n] and the final value of the 99 per cent envelope multiplied by 1.1.
- ylim[1] is the minimum between the values of mmd in steps [n\*0.2 n] and the 1 per cent envelope multiplied by 0.9.

Remark: the plot which is produced is very simple. In order to control a series of options in this plot (including the y scale) and in order to connect it dynamically to the other forward plots it is necessary to use function mmdrsplot.

init

Point where to start monitoring required diagnostics. If init is not specified it will be set equal to (p+1).

bsbsteps

A vector which specifies for which steps of the forward search it is necessary to save the units forming subset for each random start. if bsbsteps = 0 for each random start we store the units forming subset in all steps. The default is store the units forming subset in all steps if  $n \le 500$  else to store the units forming subset at step init and steps which are multiple of 100. For example, if n = 753 and init = 6, units forming subset are stored for m=init, 100, 200, 300, 400, 500 and 600.

REMARK: The vector bsbsteps must contain numbers from init to n. if min(bsbsteps) < init a warning message will be issued.

nsimul

Number of random starts. Default value is nsimul=200.

nocheck

It controls whether to perform checks on matrix Y. If nocheck=TRUE, no check is performed.

numpool

If numpool > 1, the routine automatically checks if the Parallel Computing Toolbox is installed and distributes the random starts over numpool parallel processes. If numpool <= 1, the random starts are run sequentially. By default, numpool is set equal to the number of physical cores available in the CPU (this choice may be inconvenient if other applications are running concurrently). The same happens if the numpool value chosen by the user exceeds the available number of cores.

REMARK: up to R2013b, there was a limitation on the maximum number of cores that could be addressed by the parallel processing toolbox (8 and, more recently, 12). From R2014a, it is possible to run a local cluster of more than 12 workers.

REMARK: Unless you adjust the cluster profile, the default maximum number of workers is the same as the number of computational (physical) cores on the machine.

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REMARK: In modern computers the number of logical cores is larger than the number of physical cores. By default, MATLAB is not using all logical cores because, normally, hyper-threading is enabled and some cores are reserved to this feature.

REMARK: It is because of Remarks 3 that we have chosen as default value for numbool the number of physical cores rather than the number of logical ones. The user can increase the number of parallel pool workers allocated to the multiple start monitoring by:

- setting the NumWorkers option in the local cluster profile settings to the number of logical cores (Remark 2). To do so go on the menu *Home*|*Parallel*|*Manage Cluster Profile* and set the desired "Number of workers to start on your local machine".
- setting numpool to the desired number of workers

Therefore, \*if a parallel pool is not already open\*, UserOption numpool (if set) overwrites the number of workers set in the local/current profile. Similarly, the number of workers in the local/current profile overwrites default value of numpool obtained as feature('numCores') (i.e. the number of physical cores).

cleanpool

Set cleanpool cleanpool=TRUE if the parallel pool has to be cleaned after the execution of the random starts. Otherwise (default) cleanpool=FALSE. Clearly this option has an effect just if previous option numpool > 1.

msg

Level of output to sidplay. It controls whether to display or not messages about random start progress. More precisely, if previous option numpool > 1, then a progress bar is displayed, on the other hand a message will be displayed on the screen when 10

REMARK: in order to create the progress bar when nparpool > 1 the program writes on a temporary .txt file in the folder where the user is working. Therefore it is necessary to work in a folder where the user has write permission. If this is not the case and the user (say) is working without write permission in folder C:/Program Files/MATLAB the following message will appear on the screen:

Error using ProgressBar (line 57) Do you have write permissions for C:/Program Files/MATLAB?"

trace

. . .

Whether to print intermediate results. Default is trace=FALSE.

potential further arguments passed to lower level functions.

# Value

Returns an object of class fsmmmdrs.object.

### Author(s)

FSDA team. <valentin.todorov@chello.at>

### References

Atkinson, A.C., Riani, M., and Cerioli, A. (2006), Random Start Forward Searches with Envelopes for Detecting Clusters in Multivariate Data, in: Zani S., Cerioli A., Riani M., Vichi M., Eds., *Data Analysis, Classification and the Forward Search*, pp. 163-172, Springer Verlag.

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Atkinson, A.C. and Riani, M., (2007), Exploratory Tools for Clustering Multivariate Data, *Computational Statistics and Data Analysis*, Vol. 52, pp. 272-285, doi:10.1016/j.csda.2006.12.034

Riani, M., Cerioli, A., Atkinson, A.C., Perrotta, D. and Torti, F. (2008), Fitting Mixtures of Regression Lines with the Forward Search, in: *Mining Massive Data Sets for Security*, F. Fogelman-Soulie et al. Eds., pp. 271-286, IOS Press.

# **Examples**

```
## Not run:
data(hbk)
out <- fsmmmdrs(hbk[,1:3])
class(out)
summary(out)
## End(Not run)</pre>
```

fsmmmdrs.object

Description of fsmmmdrs.object Objects

# Description

An object of class fsmmmdrs. object holds information about the result of a call to fsmmmdrs.

### Value

The object itself is basically a list with the following components:

mmdrs

Minimum Mahalanobis distance, (n-init) by (nsimul+1) matrix which contains the monitoring of minimum Mahalanobis distance at each step of the forward search.

- 1st column = fwd search index (from init to n-1)
- 2nd column = minimum Mahalanobis distance for random start 1
- 3rd column...
- nsimul+1 columnminimum Mahalanobis distance for random start nsimul

BBrs

Units belonging to the subset at the steps specified by input option bsbsteps. If bsbsteps=0 BBrs has size n-by-(n-init+1)-by-nsimul. In this case BBrs[,,j] with j=1, 2, ..., nsimul has the following structure:

- 1st row = has number 1 in correspondence of the steps in which unit 1 is included inside subset and a missing value for the other steps
- ...
- (n-1)-th row= has number n-1 in correspondence of the steps in which unit n-1 is included inside subset and a missing value for the other steps
- n-th row= has the number n in correspondence of the steps in which unit n is included inside subset and a missing value for the other steps

If, on the other hand, bsbsteps is a vector which specifies the steps of the search in which it is necessary to store subset, BBrs has size n-by-length(bsbsteps)-by-nsimul. In other words, BBrs[,,j] with j=1,2,..., nsimul has the same structure as before, but now contains just length(bsbsteps) columns.

X the data matrix X

The object has class "fsmmmdrs".

# **Examples**

```
## Not run:
   out <- fsmmmdrs(hbk[,1:3])
   class(out)
   summary(out)
## End(Not run)</pre>
```

fsmult

Gives an automatic outlier detection procedure in multivariate analysis

### **Description**

Gives an automatic outlier detection procedure in multivariate analysis and performs forward search in multivariate analysis with exploratory data

### **Usage**

```
fsmult(x, bsb, monitoring = FALSE, crit = c("md", "biv", "uni"),
  rf = 0.95, init, plot = FALSE, bonflev, msg = TRUE,
  nocheck = FALSE, scaled = FALSE, trace = FALSE, ...)
```

### **Arguments**

Х

An n x p data matrix (n observations and p variables). Rows of x represent observations, and columns represent variables.

Missing values (NA's) and infinite values (Inf's) are allowed, since observations (rows) with missing or infinite values will automatically be excluded from the computations.

bsb

List of units forming the initial subset or size of the initial subset. If monitoring=FALSE the default is to start the search with p+1 units, containing those observations which are not outlying on any scatterplot, found as the intersection of all points lying within a robust contour containing a specified portion of the data (Riani and Zani 1997) and inside the univariate boxplot.

Remark: if bsb is a vector, the option crit is ignored.

monitoring

Wheather to perform monitoring of Mahalanobis distances and other specific quantities

crit

If specified, the criterion to be used to initialize the search.

- If crit="md" the units which form initial subset are those which have the smallest m0 pseudo Mahalanobis distances computed using procedure unibiv() (bivariate robust ellipses).
- If crit="biv" sorting is done first in terms of times units fell outside robust bivariate ellipses and then in terms of pseudoMD. In other words, the units forming initial subset are chosen first among the set of those which never fell outside robust bivariate ellipses then among those which fell only once outside bivariate ellipses ... up to reach m0.
- If crit="uni" sorting is done first in terms of times units fell outside univariate boxplots and then in terms of pseudoMD. In other words, the units forming initial subset are chosen first among the set of those which never fell outside univariate boxplots then among those which fell only once outside univariate boxplots... up to reach m0.

Remark: as the user can see the starting point of the search is not going to affect at all the results of the analysis. The user can explore this point with his own datasets.

Remark: if crit="biv" the user can also supply in scalar rf (see below) the confidence level of the bivariate ellipses.

rf

Confidence level for bivariate ellipses. The default is 0.95. This option is useful only if crit='biv'.

init

Point where to start monitoring required diagnostics. Note that if a vector m0 is supplied, init >= length(m0). If init is not specified it will be set equal to floor(n\*0.6).

plot

Plots the minimum Mahalanobis distance. If plot=FALSE (default) or plot=0 no plot is produced. If plot=TRUE the plot of minimum MD with envelopes based on n observations and the scatterplot matrix with the outliers highlighted is produced. If plot=2 the additional plots of envelope resuperimposition are produced. If plot is a list it may contain the following fields:

- ylim vector with two elements controlling minimum and maximum on the y axis. Default value is " (automatic scale)
- xlim vector with two elements controlling minimum and maximum on the x axis. Default value is " (automatic scale)
- resuper vector which specifies for which steps it is necessary to show the plots of resuperimposed envelopes if resuper is not supplied a plot of each step in which the envelope is resuperimposed is shown. Example: if resuper = c(85 87) plots of resuperimposedenvelopes are shown at steps m=85 and m=87
- ncoord If ncoord=1 plots are shown in normal coordinates else (default) plots are shown in traditional mmd coordinates
- labeladd If labeladd=1, the outliers in the spm are labelled with the unit row index. The default value is labeladd="", i.e. no label is added
- nameY character vector containing the labels of the variables. As default value, the labels which are added are Y1, ... Yp.

 lwd controls line width of the curve which contains the monitoring of minimum Mahalanobis distance. Default is lwd=2.

• lwdenv Controls linewidth of the envelopes. Default is lwdenv=2.

bonflev

Option that might be used to identify extreme outliers when the distribution of the data is strongly non normal. In these circumstances, the general signal detection rule based on consecutive exceedances cannot be used. In this case bonfley can be:

- a scalar smaller than 1, which specifies the confidence level for a signal and a stopping rule based on the comparison of the minimum deletion residual with a Bonferroni bound. For example if bonflev=0.99 the procedure stops when the trajectory exceeds for the first time the 99 per cent bonferroni bound.
- 2. a scalar value greater than 1. In this case the procedure stops when the residual trajectory exceeds for the first time this value.

Default value is empty, which means to rely on general rules based on consecutive exceedances.

msg

It controls whether to display or not messages on the screen. If msg=TRUE (default) messages about the progression of the search are displayed on the screen otherwise only error messages will be displayed.

nocheck

It controls whether to perform checks on matrix Y. If nocheck=TRUE, no check is performed.

scaled

Controls whether to monitor scaled Mahalanobis distances (only if monitoring=TRUE). If scaled=TRUE Mahalanobis distances monitored during the search are scaled using ratio of determinant. If scaled=2 Mahalanobis distances monitored during the search are scaled using asymptotic consistency factor. The default is scaled=FALSE, that is Mahalanobis distances are not scaled.

trace

Whether to print intermediate results. Default is trace=FALSE. potential further arguments passed to lower level functions.

### Value

Depending on the input parameter monitoring, one of the following objects will be returned:

- fsmult.object
- 2. fsmeda.object

## Author(s)

FSDA team, <valentin.todorov@chello.at>

#### References

Riani, M., Atkinson A.C., Cerioli A. (2009). Finding an unknown number of multivariate outliers. Journal of the Royal Statistical Society Series B, Vol. 71, pp. 201-221.

Cerioli A., Farcomeni A., Riani M., (2014). Strong consistency and robustness of the Forward Search estimator of multivariate location and scatter, Journal of Multivariate Analysis, Vol. 126, pp. 167-183, http://dx.doi.org/10.1016/j.jmva.2013.12.010.

Atkinson Riani and Cerioli (2004), *Exploring multivariate data with the forward search* Springer Verlag, New York.

# **Examples**

```
## Not run:
data(hbk)
(out <- fsmult(hbk[,1:3]))
class(out)
summary(out)
## Generate contaminated data (200,3)
n <- 200
p <- 3
set.seed(123456)
X <- matrix(rnorm(n*p), nrow=n)</pre>
Xcont <- X
Xcont[1:5, ] <- Xcont[1:5,] + 3</pre>
out1 <- fsmult(Xcont, trace=TRUE)</pre>
                                              # no plots (plot defaults to FALSE)
names(out1)
(out1 <- fsmult(Xcont, trace=TRUE, plot=TRUE))</pre>
                                                   # identical to plot=1
## plot=1 - minimum MD with envelopes based on n observations
## and the scatterplot matrix with the outliers highlighted
(out1 <- fsmult(Xcont, trace=TRUE, plot=1))</pre>
## plot=2 - additional plots of envelope resuperimposition
(out1 <- fsmult(Xcont, trace=TRUE, plot=2))</pre>
## plots is a list: plots showing envelope superimposition in normal coordinates.
(out1 <- fsmult(Xcont, trace=TRUE, plot=list(ncoord=1)))</pre>
## Choosing an initial subset formed by the three observations with
## the smallest Mahalanobis Distance.
(out1 <- fsmult(Xcont, m0=5, crit="md", trace=TRUE))</pre>
## fsmult() with monitoring
(out2 <- fsmult(Xcont, monitoring=TRUE, trace=TRUE))</pre>
names(out2)
## Monitor the exceedances from m=200 without showing plots.
n <- 1000
p <- 10
Y <- matrix(rnorm(10000), ncol=10)</pre>
(out <- fsmult(Y, init=200))</pre>
## Forgery Swiss banknotes examples.
data(swissbanknotes)
```

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```
## Monitor the exceedances of Minimum Mahalanobis Distance
(out1 <- fsmult(swissbanknotes[101:200,], plot=1))

## Control minimum and maximum on the x axis
(out1 <- fsmult(swissbanknotes[101:200,], plot=list(xlim=c(60,90))))

## Monitor the exceedances of Minimum Mahalanobis Distance using
## normal coordinates for mmd.
(out1 <- fsmult(swissbanknotes[101:200,], plot=list(ncoord=1)))

## End(Not run)</pre>
```

fsmult.object

Description of fsmult.object Objects

# Description

An object of class fsmult. object holds information about the result of a call to fsmult.

# Value

The object itself is basically a list with the following components:

outliers	kx1 vector containing the list of the k units declared as outliers or NULL if the sample is homogeneous.
loc	p-by-1 vector containing location of the data.
cov	p-by-p robust estimate of covariance matrix.
md	n-by-1 vector containing the estimates of the robust Mahalanobis distances (in squared units). This vector contains the distances of each observation from the location of the data, relative to the scatter matrix cov.
mmd	(n-init)-by-2 matrix. 1st col is the forward search index; 2nd col is the value of minimum Mahalanobis Distance in each step of the fwd search.
Un	(n-init)-by-11 matrix which contains the unit(s) included in the subset at each step of the fwd search. REMARK: in every step the new subset is compared with the old subset. Un contains the unit(s) present in the new subset but not in the old one. Un[1,2] for example contains the unit included in step init+1. Un[end, 2] contains the units included in the final step of the search.
nout	2 x 5 matrix containing the number of times mdr went out of particular quantiles. First row contains quantiles 1 99 99.9 99.99 99.999. Second row contains the frequency distribution. It is NULL if bonflev threshold is used.
constr	This output is produced only if the search found at a certain step is a non singular matrix X. In this case the search run in a constrained mode, that is including the units which produced a singular matrix in the last n-constr steps. out.constr is a vector which contains the list of units which produced a singular X matrix.
Χ	the data matrix X

The object has class "fsmult".

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### **Examples**

```
## Not run:
    (out <- fsmult(hbk[,1:3]))
   class(out)
    summary(out)
## End(Not run)
```

fsr.object

Description of fsr Objects

### **Description**

An object of class fsr. object holds information about the result of a call to fsreg.

#### Value

The object itself is basically a list with the following components:

beta p-by-1 vector containing the estimated regression parameters (in step n-k).

scale scalar containing the estimate of the scale (sigma).

residuals residuals. fittedvalues fitted values.

outliers kx1 vector containing the list of the k units declared as outliers or NULL if the

sample is homogeneous.

mdr (n-init) x 2 matrix 1st col = fwd search index, 2nd col = value of minimum

deletion residual in each step of the fwd search

Un (n-init) x 11 matrix which contains the unit(s) included in the subset at each step

> of the fwd search. REMARK: in every step the new subset is compared with the old subset. Un contains the unit(s) present in the new subset but not in the old one. Un(1,2) for example contains the unit included in step init+1. Un(end,2)

contains the units included in the final step of the search.

nout 2 x 5 matrix containing the number of times mdr went out of particular quantiles.

First row contains quantiles 1 99 99.9 99.99 99.999. Second row contains the

frequency distribution.

This output is produced only if the search found at a certain step is a non singular constr

> matrix X. In this case the search run in a constrained mode, that is including the units which produced a singular matrix in the last n-constr steps. out.constr is a

vector which contains the list of units which produced a singular X matrix.

Χ the data matrix X the response vector y y

The object has class "fsr".

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# Examples

```
## Not run:
    (out <- fsreg(Y~., data=hbk, method="FS"))
    class(out)
    summary(out)
## End(Not run)</pre>
```

fsreda.object

Description of fsreda Objects

# Description

An object of class fsreda.object holds information about the result of a call to fsreg.

# Value

The object itself is basically a list with the following components:

forward search:

RES	n x $(n-init+1)$ matrix containing the monitoring of scaled residuals: the first row is the residual for the first unit,, n-th row is the residual for the n-th unit.
LEV	(n+1) x $(n-init+1)$ matrix containing the monitoring of leverage: the first row is the leverage for the first unit,, $n-th$ row is the leverage for the $n-th$ unit.
BB	n x (n-init+1) matrix containing the information about the units belonging to the subset at each step of the forward search: first col contains indexes of the units forming subset in the initial step;; last column contains units forming subset in the final step (all units).
mdr	n-init x 3 matrix which contains the monitoring of minimum deletion residual or $(m+1)$ -ordered residual at each step of the forward search: first col is the fwd search index (from init to n-1); 2nd col = minimum deletion residual; 3rd col = $(m+1)$ -ordered residual.
	Remark: these quantities are stored with sign, that is the min deletion residual is stored with negative sign if it corresponds to a negative residual.
msr	n-init+1 x 3 matrix which contains the monitoring of maximum studentized residual or m-th ordered residual: first col is the fwd search index (from init to n); 2nd col = maximum studentized residual; 3rd col = $(m)$ -ordered studentized residual.
nor	(n-init+1) x 4 matrix containing the monitoring of normality test in each step of the forward search: first col = fwd search index (from init to n); 2nd col = Asymmetry test; 3rd col = Kurtosis test; 4th col = Normality test.
Bols	$(n-init+1) \times (p+1)$ matrix containing the monitoring of estimated beta coefficients in each step of the forward search.
S2	(n-init+1) x 4 matrix containing the monitoring of S2 or R2 in each step of the

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- 1. 1st col = fwd search index (from init to n);
- 2. 2nd col = monitoring of S2;
- 3. 3rd col = monitoring of R2;
- 4. 4th col = monitoring of rescaled S2.

In this case the estimated of s2 at step m is divided by the consistency factor (to make the estimate asymptotically unbiased).

coo

(n-init+1) x 3 matrix containing the monitoring of Cook or modified Cook distance in each step of the forward search:

- 1. 1st col = fwd search index (from init to n);
- 2. 2nd col = monitoring of Cook distance;
- 3. 3rd col = monitoring of modified Cook distance.

Tols

 $(n-init+1) \times (p+1)$  matrix containing the monitoring of estimated t-statistics (as specified in option input 'tstat') in each step of the forward search

Un

(n-init) x 11 matrix which contains the unit(s) included in the subset at each step of the fwd search.

REMARK: in every step the new subset is compared with the old subset. Un contains the unit(s) present in the new subset but not in the old one Un(1,2) for example contains the unit included in step init+1 Un(end,2) contains the units included in the final step of the search.

betaINT

Confidence intervals for the elements of  $\beta$ . betaINT is a (n-init+1)-by-2\*length(confint)-by-p 3D array. Each third dimension refers to an element of beta:

- 1. betaINT[,,1] is associated with first element of beta;
- 2. ...;
- 3. betaINT[,,p] is associated with last element of beta.

The first two columns contain the lower and upper confidence limits associated with conflev(1). Columns three and four contain the lower and upper confidence limits associated with conflev(2); ...; The last two columns contain the lower and upper confidence limits associated with conflev(end). For example betaINT[,3:4,5] contain the lower and upper confidence limits for the fifth element of beta using confidence level specified in the second element of input option conflev.

### sigma2INT

confidence interval for s2.

- 1. 1st col = fwd search index;
- 2. 2nd col = lower confidence limit based on conflev(1);
- 3. 3rd col = upper confidence limit based on conflev(1);
- 4. 4th col = lower confidence limit based on conflev(2);
- 5. 5th col = upper confidence limit based on conflev(2);
- 6. ...
- 7. penultimate col = lower confidence limit based on conflev(end);
- 8. last col = upper confidence limit based on conflev(end).

Χ

the data matrix X

У

the response vector y

The object has class "fsreda".

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# **Examples**

```
## Not run:
   (out <- fsreg(Y~., data=hbk, method="FS", monitoring=TRUE))
   class(out)
   summary(out)
## End(Not run)</pre>
```

 $FSReda\_control$ 

Creates an FSReda\_control object

# Description

Creates an object of class FSReda\_control to be used with the fsreg() function, containing various control parameters.

# Usage

# Arguments

intercept	Indicator for constant term. Scalar. If intercept=TRUE, a model with constant term will be fitted (default), else, no constant term will be included.
init	Search initialization, scalar. It specifies the initial subset size to start monitoring exceedances of minimum deletion residual, if init is not specified it set equal to: p+1, if the sample size is smaller than 40 or min(3*p+1, floor(0.5*(n+p+1))), otherwise. For example, if init=100, the procedure starts monitoring from step m=100.
nocheck	Check input arguments, scalar. If nocheck=TRUE no check is performed on matrix y and matrix X. Notice that y and X are left unchanged. In other words the additional column of ones for the intercept is not added. As default nocheck=FALSE.
tstat	The kind of t-statistics which have to be monitored. tstat="trad" implies monitoring of traditional t statistics (out\$Tols). In this case the estimate of s2 at step m is based on s2m (notice that s2m«s2 when m/n is small) tstat="scal" (default) implies monitoring of rescaled t statistics. In this case the estimate of s2 at step m is based on s2m/vartruncnorm(m/n) where vartruncnorm(m/n) is the variance of the truncated normal distribution.
conflev	Confidence level which is used to declare units as outliers. Usually conflev=0.95, 0.975, 0.99 (individual alpha) or conflev=1-0.05/n, 1-0.025/n, 1-0.01/n (simultaneous alpha). Default value is 0.975.

# **Details**

Creates an object of class FSReda\_control to be used with the fsreg() function, containing various control parameters.

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### Value

An object of class "FSReda\_control" which is basically a list with components the input arguments of the function mapped accordingly to the corresponding Matlab function.

### Author(s)

FSDA team

### See Also

See Also as FSR\_control, MMreg\_control and LXS\_control

# **Examples**

fsreg

fsreg: an automatic outlier detection procedure in linear regression

### **Description**

An automatic outlier detection procedure in linear regression

### Usage

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### **Arguments**

formula a formula of the form  $y \sim x1 + x2 + ...$ 

data frame from which variables specified in formula are to be taken.

subset an optional vector specifying a subset of observations to be used in the fitting

process.

weights an optional vector of weights to be used in the fitting process. **NOT USED** 

YET.

na.action a function which indicates what should happen when the data contain NAs. The

default is set by the na.action setting of options, and is na.fail if that is unset. The "factory-fresh" default is na.omit. Another possible value is NULL,

no action. Value na. exclude can be useful.

model, x.ret, y.ret

logicals indicating if the model frame, the model matrix and the response are

to be returned, respectively.

contrasts an optional list. See the contrasts.arg of model.matrix.default.

offset this can be used to specify an *a priori* known component to be included in the

linear predictor during fitting. An offset term can be included in the formula

instead or as well, and if both are specified their sum is used.

family family of robust regression models, can be 'homo' for homoscedastic (same

variance) regression model, 'hetero' for heteroskedastic regression model or 'bayes' Bayesian linear regression. The default is family='homo' for homoscedas-

tic regression model.

method robust regression estimation model, can be 'FS' for Forward search, 'S' for S re-

gression, 'MM' for MM regression, 'LMS' or 'LTS'. The default is method='FS'

for forward search estimation.

monitoring wheather to perform monitoring for several quantities in each step of the forward

search or for series of values of the breakdown point in case of S estimates or for series of values of the efficiency in case of MM estimates. Deafault is

monitoring=FALSE.

y Response variable. Vector. Response variable, specified as a vector of length n,

where n is the number of observations. Each entry in y is the response for the corresponding row of X. Missing values (NA's) and infinite values (Inf's) are allowed, since observations (rows) with missing or infinite values will automat-

ically be excluded from the computations.

x Predictor variables. Matrix. Matrix of explanatory variables (also called 'regres-

sors') of dimension n x (p-1) where p denotes the number of explanatory variables including the intercept. Rows of X represent observations, and columns represent variables. By default, there is a constant term in the model, unless you explicitly remove it using input option intercept=FALSE, so do not include a column of 1s in X. Missing values (NA's) and infinite values (Inf's) are allowed, since observations (rows) with missing or infinite values will automatically be

excluded from the computations.

bsb Initial subset - vector of indices. If bsb=0 (default) then the procedure starts with

p units randomly chosen. If bsb is not 0 the search will start with m0=length(bsb).

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intercept	Indicator for constant term. Scalar. If intercept=TRUE, a model with constant term will be fitted (default), else, no constant term will be included.
control	A control object (SS) containing estimation options. If the control object is supplied, the parameters from it will be used. If parameters are passed also in the invocation statement, they will override the corresponding elements of the control object.
	potential further arguments passed to lower level functions.

### Value

Depending on the input parameters family and method, one of the following objects will be returned:

```
    fsr.object
    sreg.object
    mmreg.object
    fsdalms.object
    fsdalts.object
    fsreda.object
    sregeda.object
    mmregeda.object
```

### Author(s)

FSDA team

### References

Riani, M., Atkinson A.C., Cerioli A. (2009). Finding an unknown number of multivariate outliers. Journal of the Royal Statistical Society Series B, Vol. 71, pp. 201-221.

# **Examples**

```
## Not run:

n <- 200
p <- 3

X <- matrix(data=rnorm(n*p), nrow=n, ncol=p)
y <- matrix(data=rnorm(n*1), nrow=n, ncol=1)
(out = fsreg(X, y))

## Now we use the formula interface:
(out1 = fsreg(y~X, control=FSR_control(plot=FALSE)))

## Or use the variables in a data frame
(out2 = fsreg(Y~., data=hbk, control=FSR_control(plot=FALSE)))</pre>
```

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```
## let us compare to the LTS solution
  (out3 = ltsReg(Y~., data=hbk))

## Now compute the model without intercept
  (out4 = fsreg(Y~.-1, data=hbk, control=FSR_control(plot=FALSE)))

## And compare again with the LTS solution
  (out5 = ltsReg(Y~.-1, data=hbk))

## using default (optional arguments)
  (out6 = fsreg(Y~.-1, data=hbk, control=FSR_control(plot=FALSE, nsamp=1500, h=50)))

## End(Not run)
```

FSR\_control

Creates an FSR\_control object

### **Description**

Creates an object of class FSR\_control to be used with the fsreg() function, containing various control parameters.

### Usage

```
FSR_control(intercept = TRUE, h, nsamp = 1000, lms = 1, init, nocheck = FALSE,
bonflev = "", msg = TRUE, bsbmfullrank = 1,
plot = FALSE, bivarfit = "", multivarfit = "",
labeladd = "", nameX, namey, ylim, xlim)
```

## **Arguments**

intercept

Indicator for constant term. Scalar. If intercept=TRUE, a model with constant term will be fitted (default), else, no constant term will be included.

h

The number of observations that have determined the least trimmed squares estimator, scalar. h is an integer greater or equal than p but smaller then n. Generally if the purpose is outlier detection h=[0.5\*(n+p+1)] (default value). h can be smaller than this threshold if the purpose is to find subgroups of homogeneous observations. In this function the LTS/LMS estimator is used just to initialize the search.

nsamp

Number of subsamples which will be extracted to find the robust estimator, scalar. If nsamp=0 all subsets will be extracted. They will be (n choose p). If the number of all possible subset is <1000 the default is to extract all subsets otherwise just 1000.

1ms

Criterion to use to find the initial subset to initialize the search (LMS, LTS with concentration steps, LTS without concentration steps or subset supplied directly by the user). The default value is 1 (Least Median of Squares is computed to initialize the search). On the other hand, if the user wants to initialize the search

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> with LTS with all the default options for concentration steps then lms=2. If the user wants to use LTS without concentration steps, lms can be a scalar different from 1 or 2. If lms is a list it is possible to control a series of options for concentration steps (for more details see option lms inside LXS\_control). If, on the other hand, the user wants to initialize the search with a prespecified set of units there are two possibilities:

- 1. Ims can be a vector with length greater than 1 which contains the list of units forming the initial subset. For example, if the user wants to initialize the search with units 4, 6 and 10 then lms=c(4,6,10);
- 2. Ims is a struct which contains a field named bsb which contains the list of units to initialize the search. For example, in the case of simple regression through the origin with just one explanatory variable, if the user wants to initialize the search with unit 3 then lms=list(bsb=3).

init

Search initialization, scalar. It specifies the initial subset size to start monitoring exceedances of minimum deletion residual, if init is not specified it set equal to: p+1, if the sample size is smaller than 40 or min(3\*p+1, floor(0.5\*(n+p+1))), otherwise. For example, if init=100, the procedure starts monitoring from step m = 100.

nocheck

Check input arguments, scalar. If nocheck=TRUE no check is performed on matrix y and matrix X. Notice that y and X are left unchanged. In other words the additional column of ones for the intercept is not added. As default nocheck=FALSE.

bonflev

Option to be used if the distribution of the data is strongly non normal and, thus, the general signal detection rule based on consecutive exceedances cannot be used. In this case bonflev can be:

- 1. a scalar smaller than 1 which specifies the confidence level for a signal and a stopping rule based on the comparison of the minimum MD with a Bonferroni bound. For example if bonflev=0.99 the procedure stops when the trajectory exceeds for the first time the 99% bonferroni bound.
- 2. A scalar value greater than 1. In this case the procedure stops when the residual trajectory exceeds for the first time this value.

Default value is ", which means to rely on general rules based on consecutive exceedances.

msg

Controls whether to display or not messages on the screen If msg==1 (default) messages are displayed on the screen about step in which signal took place else no message is displayed on the screen.

bsbmfullrank

How to behave in case subset at step m (say bsbm) produces a singular X. In other words, this options controls what to do when rank(X[bsbm,]) is smaller then number of explanatory variables. If bsbmfullrank=1 (default) these units (whose number is say mnofullrank) are constrained to enter the search in the final n-mnofullrank steps else the search continues using as estimate of beta at step m the estimate of beta found in the previous step.

plot

Plot on the screen. Scalar. If plots=TRUE the plot of minimum deletion residual with envelopes based on n observations and the scatterplot matrix with the outliers highlighted is produced. If plots=2 the user can also monitor the intermediate plots based on envelope superimposition. If plots=FALSE (default) no plot is produced.

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bivarfit

Wheather to superimpose bivariate least square lines on the plot (if plot=TRUE. This option adds one or more least squares lines, based on SIMPLE REGRES-SION of y on Xi, to the plots of ylXi. The default is bivarfit=FALSE: no line is fitted. If bivarfit=1, a single OLS line is fitted to all points of each bivariate plot in the scatter matrix ylX. If bivarfit=2, two OLS lines are fitted: one to all points and another to the group of the genuine observations. The group of the potential outliers is not fitted. If bivarfit=0 one OLS line is fitted to each group. This is useful for the purpose of fitting mixtures of regression lines. If bivarfit='i1' or bivarfit='i2', etc. an OLS line is fitted to a specific group, the one with index 'i' equal to 1, 2, 3 etc. Again, useful in case of mixtures.

multivarfit

Wheather to superimpose multivariate least square lines. This option adds one or more least square lines, based on MULTIVARIATE REGRESSION of y on X, to the plots of y|Xi. The default is multivarfit=FALSE: no line is fitted. If bivarfit=1, a single OLS line is fitted to all points of each bivariate plot in the scatter matrix y|X. The line added to the scatter plot y|Xi is avconst + Ci\*Xi, where Ci is the coefficient of Xi in the multivariate regression and avconst is the effect of all the other explanatory variables different from Xi evaluated at their centroid (that is overline(y)'C)). If multivarfit=2, same action as with multivarfit=1 but this time we also add the line based on the group of unselected observations (i.e. the normal units).

labeladd

Add outlier labels in plot. If labeladd=TRUE, we label the outliers with the unit row index in matrices X and y. The default value is labeladd=FALSE, i.e. no label is added.

nameX

Add variable labels in plot. A vector of strings of length p containing the labels of the variables of the regression dataset. If it is empty (default) the sequence  $X1, \ldots, Xp$  will be created automatically

namey

Add response label. A string containing the label of the response

ylim

Control y scale in plot. Vector with two elements controlling minimum and maximum on the y axis. Default is to use automatic scale.

xlim

Control x scale in plot. Vector with two elements controlling minimum and maximum on the x axis. Default is to use automatic scale.

### **Details**

Creates an object of class FSR\_control to be used with the fsreg() function, containing various control parameters.

### Value

An object of class "FSR\_control" which is basically a list with components the input arguments of the function mapped accordingly to the corresponding Matlab function.

### Author(s)

FSDA team

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### See Also

See Also Sreg\_control, MMreg\_control, LXS\_control, FSReda\_control, Sregeda\_control and MMregeda\_control.

### **Examples**

```
## Not run:

(out <- fsreg(Y~., data=hbk, method="FS", control=FSR_control(h=56, nsamp=500, lms=2)))
summary(out)

## End(Not run)</pre>
```

geyser2

Old Faithful Geyser Data.

# **Description**

A bivariate data set obtained from the Old Faithful Geyser, containing the eruption length and the length of the previous eruption for 271 eruptions of this geyser in minutes.

# Usage

```
data(geyser2)
```

### **Format**

A data frame with 271 rows and 2 variables The variables are as follows:

- Eruption length: The eruption length in minutes.
- Previous eruption length: The length of the previous eruption in minutes.

### References

Garcia-Escudero, L.A., Gordaliza, A. (1999). Robustness properties of k-means and trimmed k-means, *Journal of the American Statistical Assoc.*, Vol.**94**, No.447, 956-969.

Haerdle, W. (1991). Smoothing Techniques with Implementation in S, New York: Springer.

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Plots the trajectories of the monitored scaled (squared) residuals

### **Description**

Plots the trajectories of the monitored scaled (squared) residuals

# Usage

```
levfwdplot(out,
   xlim, ylim, xlab, ylab, main, lwd, lty, col, cex.lab, cex.axis,
   xvalues,
    fg.thresh, fg.unit, fg.labstep, fg.lwd, fg.lty, fg.col, fg.mark, fg.cex,
   bg.thresh, bg.style,
  xground=c("lev", "res"), tag, datatooltip, label, nameX, namey, msg, databrush,
    standard, fground, bground, ...)
```

# **Arguments**

out

An object containing monitoring of leverage, fsreda.object.

The needed elements of out are

- 1. LEV: matrix containing the leverage monitored in each step of the forward search. Every row is associated with a unit. This matrix can be created using function fsreg() with method="FS", monitoring=TRUE.
- 2. Un: (for FSR only) matrix containing the order of entry in the subset of each unit (required only when datatooltip is true or databrush is not empty).
- 3. y: a vector containing the response (required only when option databrush is requested).
- 4. X: a matrix containing the explanatory variables (required only when option databrush is requested).
- 5. Bols: (n-init+1) x (p+1) matrix containing the estimated beta coefficients monitored in each step of the robust procedure (required only when option databrush is requested and suboption multivarfit is requested).

ylim	Control y scale in plot. Vector with two elements controlling minimum and
	maximum on the y axis. Default is to use automatic scale.

Control x scale in plot. Vector with two elements controlling minimum and maximum on the x axis. Default is to use automatic scale.

xlab a title for the x axis vlab a title for the y axis an overall title for the plot main

The line width, a positive number, defaulting to 1

The line type. Line types can either be specified as an integer (1=solid (default), 2=dashed, 3=dotted, 4=dotdash, 5=longdash, 6=twodash) or as one of the character strings "solid", "dashed", "dotted", "dotdash", "longdash", or "twodash". The latter two are not supported by Matlab.

xlim

lwd

lty

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col colors to be used for the highlighted units cex.lab The magnification to be used for x and y labels relative to the current setting of cex The magnification to be used for axis annotation relative to the current setting cex.axis xvalues values for the x axis. Numeric vector of ncol (RES) controlling the x axis coordinates. The default value of xvalues is (nrow(RES) -ncol(RES) + 1):nrow(RES) fg.thresh (alternative to fg.unit) numeric vector of length 1 or 2 which specifies the highlighted trajectories. If length(fthresh) == 1 the highlighted trajectories are those of units that throughtout the search had at leat once a residual greater (in absolute value) than thresh. The default value is fg. thresh=2.5. If length(fthresh) == 2 the highlighted trajectories are those of units that throughtout the search had a residual at leat once bigger than fg. thresh[2] or smaller than fg. thresh[1]. fg.unit (alternative to fg.thresh), vector containing the list of the units to be highlighted. If fg. unit is supplied, fg. thresh is ignored. fg.labstep numeric vector which specifies the steps of the search where to put labels for the highlighted trajectories (units). The default is to put the labels at the initial and final steps of the search. flabstep=' ' means no label. fg.lwd The line width for the highlighted trajectories (units). Default is 1. fg.lty The line type for the highlighted trajectories (units). Line types can either be specified as an integer (1=solid (default), 2=dashed, 3=dotted, 4=dotdash, 5=longdash, 6=twodash) or as one of the character strings "solid", "dashed", "dotted", "dotdash", "longdash", or "twodash". The latter two are not supported by Matlab. fg.col colors to be used for the highlighted units. fg.mark Controlls whether to plot highlighted trajectories as symbols. if fg.mark==TRUE each line is plotted using a different symbol else no marker is used (default). fg.cex controls the font size of the labels of the trajectories in foreground. bg.thresh numeric vector of length 1 or 2 which specifies how to define the unimmportant trajectories. Unimmportant trajectories will be plotted using a colormap, in greysh or will be hidden. If length(thresh) == 1 the irrelevant units are those which always had a residual smaller (in absolute value) than thresh. If length(bthresh) == 2 the irrelevant units are those which always had a residual greater than bthresh(1) and smaller than bthresh(2). The default is: bg.thresh=2.5 if n > 100 and bg. thresh=-Inf if n <= 100 i.e. to treat all trajectories as important if  $n \le 100$  and, if n > 100, to reduce emphasis only to trajectories having in all steps of the search a value of scaled residual smaller than 2.5. bg.style specifies how to plot the unimportant trajectories as defined in option bthresh. 1. bg.style="faint": unimportant trajectories are plotted using a colormap. 2. bg.style="hide": unimportant trajectories are hidden. 3. bg.style="greyish": unimportant trajectories are displayed in a faint

When n>100 the default option is bg.style='faint'. When  $n \le 100$  and bg.thresh == -Inf option bstyle is ignored. Remark: bground=" is equivalent to -Inf that is all trajectories are considered relevant.

grey.

tag

Plot handle. String which identifies the handle of the plot which is about to be created. The default is to use tag 'pl\_resfwd'. Notice that if the program finds a plot which has a tag equal to the one specified by the user, then the output of the new plot overwrites the existing one in the same window else a new window is created.

xground

trajectories to highlight in connection with resfwdplot. If xground="lev" (default), the levfwdplot trajectories are put in foreground or in background depending on the leverage values. If xground="res", the levfwdplot trajectories are put in foreground or in background depending on the residual values. See options bg. thresh and fg. thresh.

datatooltip

Interactive clicking. It is inactive if this parameter is missing or empty. The default is datatooltip=TRUE, i.e. the user can select with the mouse an individual residual trajectory in order to have information about the corresponding unit. The information displayed depends on the estimator in use.

For example for class fsreda.object the information concerns the label and the step of the search in which the unit enters the subset. If datatooltip is a list it may contain the following fields:

- DisplayStyle determines how the data cursor displays. Possible values are 'datatip' and 'window' (default). 'datatip' displays data cursor information in a small yellow text box attached to a black square marker at a data point you interactively select. 'window' displays data cursor information for the data point you interactively select in a floating window within the figure.
- 2. SnapToDataVertex: specifies whether the data cursor snaps to the nearest data value or is located at the actual pointer position. Possible values are SnapToDataVertex='on' (default) and SnapToDataVertex='off'.
- 3. LineColor: controls the color of the trajectory selected with the mouse. It can be an RGB triplet of values between 0 and 1, or character vector indicating a color name. Note that a RGB vector can be conveniently chosen with our MATLAB class FSColor, see documentation.
- 4. SubsetLinesColor: enables to control the color of the trajectories of the units that are in the subset at a given step of the search (if levfwdplot() is applied to an object of class fsreda.object) or have a weight greater than 0.9 (if levfwdplot() is applied to an object of class sregeda.object or mmregeda.object). This can be done (repeatedly) with a left mouse click in proximity of the step of interest. A right mouse click will terminate the selection by marking with a up-arrow the step corresponding to the highlighted lines. The highlighted lines by default are in red, but a different color can be specified as RGB triplet or character of color name. Note that a RGB vector can be conveniently chosen with our MATLAB class FSColor, see documentation. By default SubsetLinesColor="", i.e. the modality is not active. Any initialization for SubsetLinesColor which cannot be interpreted as RGB vector will be converted to blue, i.e. SubsetLinesColor will be forced to be [0 0 1]. If SubsetLinesColor is not empty the previous option LineColor is ignored.

label

Character vector containing the labels of the units (optional argument used when datatooltip=TRUE. If this field is not present labels row1, ..., rown will be

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automatically created and included in the pop up datatooltip window).

nameX

Add variable labels in plot. A vector of strings of length p containing the labels of the variables of the regression dataset. If it is empty (default) the sequence X1,..., Xp will be created automatically

namey

Add response label. A string containing the label of the response

msg

Controls whether to display or not messages on the screen If msg==1 (default) messages are displayed on the screen about step in which signal took place else no message is displayed on the screen.

databrush

interactive mouse brushing. If databrush is missing or empty (default), no brushing is done. The activation of this option (databrush is a scalar or a list) enables the user to select a set of trajectories in the current plot and to see them highlighted in the yIX plot, i.e. a matrix of scatter plots of y against each column of X, grouped according to the selection(s) done by brushing. If the plot y|X does not exist it is automatically created. In addition, brushed units are automatically highlighted in the minimum deletion residual plot if it is already open. The extension to the following plots will be available in future versions of the toolbox:

- 1. monitoring leverage plot;
- 2. maximum studentized residual:
- 3. s^2 and R^2;
- 4. Cook distance and modified Cook distance;
- 5. deletion t statistics.

Note that the window style of the other figures is set equal to that which contains the monitoring residual plot. In other words, if the monitoring residual plot is docked all the other figures will be docked too

If databrush=TRUE the default selection tool is a rectangular brush and it is possible to brush only once (that is persist=").

If databrush=list(...), it is possible to use all optional arguments of function selectdataFS() and the following optional argument:

- 1. persist. Persist is an empty value or a character containing 'on' or 'off'. The default value is persist="", that is brushing is allowed only once. If persist="on" or persis="off" brushing can be done as many time as the user requires. If persist='on' then the unit(s) currently brushed are added to those previously brushed. It is possible, every time a new brushing is done, to use a different color for the brushed units. If persist='off' every time a new brush is performed units previously brushed are removed.
- 2. bivarfit. This option adds one or more least square lines based on SIMPLE REGRESSION to the plots of yIX, depending on the selected groups.
- 3. bivarfitWheather to superimpose bivariate least square lines on the plot (if plot=TRUE. This option adds one or more least squares lines, based on SIMPLE REGRESSION of y on Xi, to the plots of ylXi. The default is bivarfit=FALSE: no line is fitted. If bivarfit=1, a single OLS line is fitted to all points of each bivariate plot in the scatter matrix ylX. If bivarfit=2, two OLS lines are fitted: one to all points and another to the group of the genuine observations. The group of the potential outliers is not

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fitted. If bivarfit=0 one OLS line is fitted to each group. This is useful for the purpose of fitting mixtures of regression lines. If bivarfit='i1' or bivarfit='i2', etc. an OLS line is fitted to a specific group, the one with index 'i' equal to 1, 2, 3 etc. Again, useful in case of mixtures.

- 4. multivarfitWheather to superimpose multivariate least square lines. This option adds one or more least square lines, based on MULTIVARIATE REGRESSION of y on X, to the plots of y|Xi. The default is multivarfit=FALSE: no line is fitted. If bivarfit=1, a single OLS line is fitted to all points of each bivariate plot in the scatter matrix y|X. The line added to the scatter plot y|Xi is avconst + Ci\*Xi, where Ci is the coefficient of Xi in the multivariate regression and avconst is the effect of all the other explanatory variables different from Xi evaluated at their centroid (that is overline(y)'C)). If multivarfit=2, same action as with multivarfit=1 but this time we also add the line based on the group of unselected observations (i.e. the normal units).
- 5. labeladdAdd outlier labels in plot. If labeladd=TRUE, we label the outliers with the unit row index in matrices X and y. The default value is labeladd=FALSE, i.e. no label is added.

standard

(MATLAB-style arguments) appearance of the plot in terms of xlim, ylim, axes labels and their font size style, color of the lines, etc.

fground

MATLAB-style arguments for the fground trajectories in foregroud.

bground

MATLAB-style arguments for the fground trajectories in backgroud.

... potential further arguments passed to lower level functions.

### **Details**

No details

### Value

No value returned

### Author(s)

FSDA team

# **Examples**

```
## Not run:

n <- 100
y <- rnorm(n)
X <- matrix(rnorm(n*4), nrow=n)

out <- fsreg(y~X, method="LTS")
out <- fsreg(y~X, method="FS", bsb=out$bs, monitoring=TRUE)
levfwdplot(out)</pre>
```

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```
## End(Not run)
```

loyalty

Loyalty data

# **Description**

The loyalty data consist of 509 observations on the behaviour of customers with loyalty cards from a supermarket chain in Northern Italy. The response y is the amount in euros spent at the shop over six months and the explanatory variables are: X1, the number of visits to the supermarket in the six month period; X2, the age of the customer; X3, the number of members of the customers' family. To find out more about this data set please see Atkinson and Riani (2006), JCGS

### Usage

```
data("loyalty")
```

#### **Format**

A data frame with 509 observations on the following 4 variables.

visits the number of visits to the supermarket in the six month period age the age of the customer

family the number of members of the customers' family amount\_spent the amount in euros spent at the shop over six months

### **Details**

To find out more about this data set please see Atkinson and Riani (2006), JCGS

# Source

The data are themselves a random sample from a larger database. The sample of 509 observations is available at http://www.riani.it/trimmed.

## References

Atkinson, A. and Riani, M (2006) Distribution Theory and Simulations for Tests of Outliers in Regression, *Journal of Computational and Graphical Statistics*, **15** 2, pp 460–476.

# **Examples**

```
data(loyalty)
```

LXS\_control 37

LXS\_control

Creates an LSX\_control object

## Description

Creates an object of class LXS\_control to be used with the fsreg() function, containing various control parameters.

## Usage

```
LXS_control(intercept = TRUE, lms, h, bdp, nsamp, rew = FALSE, conflev = 0, msg = TRUE, nocheck = FALSE, nomes = FALSE, plot = FALSE)
```

# **Arguments**

intercept

Indicator for constant term. Scalar. If intercept=TRUE, a model with constant term will be fitted (default), else, no constant term will be included.

1ms

Criterion to use to find the initial subset to initialize the search (LMS, LTS with concentration steps, LTS without concentration steps or subset supplied directly by the user). The default value is 1 (Least Median of Squares is computed to initialize the search). On the other hand, if the user wants to initialize the search with LTS with all the default options for concentration steps then lms=2. If the user wants to use LTS without concentration steps, lms can be a scalar different from 1 or 2. If lms is a list it is possible to control a series of options for concentration steps (for more details see option lms inside LXS\_control). If, on the other hand, the user wants to initialize the search with a prespecified set of units there are two possibilities:

- 1. Ims can be a vector with length greater than 1 which contains the list of units forming the initial subset. For example, if the user wants to initialize the search with units 4, 6 and 10 then lms=c(4,6,10);
- 2. Ims is a struct which contains a field named bsb which contains the list of units to initialize the search. For example, in the case of simple regression through the origin with just one explanatory variable, if the user wants to initialize the search with unit 3 then lms=list(bsb=3).

h

The number of observations that have determined the least trimmed squares estimator, scalar. h is an integer greater or equal than p but smaller then n. Generally if the purpose is outlier detection h=[0.5\*(n+p+1)] (default value). h can be smaller than this threshold if the purpose is to find subgroups of homogeneous observations. In this function the LTS/LMS estimator is used just to initialize the search.

bdp

Breakdown point. It measures the fraction of outliers the algorithm should resist. In this case any value greater than 0 but smaller or equal than 0.5 will do fine. If on the other hand the purpose is subgroups detection then bdp can be greater than 0.5. In any case however n\*(1-bdp) must be greater than p. If this condition is not fulfilled an error will be given. Please specify h or bdp not both.

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nsamp Number of subsamples which will be extracted to find the robust estimator,

scalar. If nsamp=0 all subsets will be extracted. They will be (n choose p). If the number of all possible subset is <1000 the default is to extract all subsets

otherwise just 1000.

rew LXS reweighted - if rew=1 the reweighted version of LTS (LMS) is used and

the output quantities refer to the reweighted version else no reweighting is per-

formed (default).

conflev Confidence level which is used to declare units as outliers, usually conflev=0.95,0.975,0.99

(individual alpha) or 1-0.05/n, 1-0.025/n, 1-0.01/n (simultaneous alpha). Default

value is 0.975.

msg Controls whether to display or not messages on the screen If msg==1 (default)

messages are displayed on the screen about step in which signal took place else

no message is displayed on the screen.

nocheck Check input arguments, scalar. If nocheck=TRUE no check is performed on ma-

trix y and matrix X. Notice that y and X are left unchanged. In other words the additional column of ones for the intercept is not added. As default nocheck=FALSE.

nomes It controls whether to display or not on the screen messages about estimated

time to compute LMS (LTS). If nomes is equal to 1 no message about estimated time to compute LMS (LTS) is displayed, else if nomes is equal to 0 (default), a

message about estimated time is displayed.

plot Plot on the screen. Scalar. If plots=TRUE the plot of minimum deletion resid-

ual with envelopes based on n observations and the scatterplot matrix with the outliers highlighted is produced. If plots=2 the user can also monitor the intermediate plots based on envelope superimposition. If plots=FALSE (default) no

plot is produced.

### Details

Creates an object of class FSR\_control to be used with the fsreg() function, containing various control parameters.

#### Value

An object of class "LXS\_control" which is basically a list with components the input arguments of the function mapped accordingly to the corresponding Matlab function.

#### Author(s)

FSDA team

## See Also

See Also as Sreg\_control, MMreg\_control and FSR\_control

M5data 39

### **Examples**

```
## Not run:
(out <- fsreg(Y~., data=hbk, method="LMS", control=LXS_control(h=56, nsamp=500, lms=2)))
## End(Not run)</pre>
```

M5data

Mixture M5 Data.

# **Description**

A bivariate data set obtained from three normal bivariate distributions with different scales and proportions 1:2:2. One of the components is strongly overlapping with another one. A 10 noise is added uniformly distributed in a rectangle containing the three normal components and not strongly overlapping with the three mixture components. A precise description of the M5 data set can be found in Garcia-Escudero et al. (2008).

### Usage

data(M5data)

#### **Format**

A data frame with 2000 rows and 3 variables The first two columns are the two variables. The last column is the true classification vector where symbol "0" stands for the contaminating data points.

#### Source

Garcia-Escudero, L.A., Gordaliza, A., Matran, C. and Mayo-Iscar, A. (2008). A General Trimming Approach to Robust Cluster Analysis, *Annals of Statistics*, Vol.**36**, 1324-1345. Technical report available at http://www.eio.uva.es/inves/grupos/representaciones/trTCLUST.pdf

malfwdplot Plots the trajectories of scaled Mahalanobis distances along the search

# **Description**

Plots the trajectories of scaled Mahalanobis distances along the forward search

# Usage

```
malfwdplot(out, xlim, ylim, xlab, ylab, main, lwd, lty, col, cex.lab,
  cex.axis, subsize, fg.thresh, fg.unit, fg.labstep, fg.lwd, fg.lty,
  fg.col, fg.mark, fg.cex, bg.thresh, bg.style, standard, fground, bground,
  tag, datatooltip, label, nameX, databrush, conflev, trace = FALSE, ...)
```

#### **Arguments**

out

An object of S3 class fsmeda.object returned by fsmult with monitoring=TRUE - a list containing the monitoring of minimum Mahalanobis distance.

The needed elements of out are

- 1. MAL: matrix containing the squared Mahalanobis distances monitored in each step of the forward search. Every row is associated with a unit (row of data matrix Y). This matrix can be created using function FSMeda (mandatory argument)
- 2. Un: matrix containing the order of entry of each unit (necessary if datatooltip or databrush is selected).
- 3. X: The data matrix.

xlim Controls the x scale in the plot. xlim is a vector with two elements controlling minimum and maximum on the x-axis. Default is to use automatic scale.

Controls the y scale in the plot. ylim is a vector with two elements controlling minimum and maximum on the y-axis. Default is to use automatic scale.

xlab A title for the x axis ylab A title for the y axis

main An overall title for the plot

lwd The line width, a positive number, defaulting to 1

> The line type. Line types can either be specified as an integer (1=solid (default), 2=dashed, 3=dotted, 4=dotdash, 5=longdash, 6=twodash) or as one of the character strings "solid", "dashed", "dotted", "dotdash", "longdash", or "twodash". The latter two are not supported by Matlab.

col Colors to be used for the highlighted units

cex.lab The magnification to be used for x and y labels relative to the current setting of

The magnification to be used for axis annotation relative to the current setting cex.axis

> Numeric vector containing the subset size with length equal to the number of columns of matrix of mahalanobis distances. The default value of subsize is (nrow(MAL) -ncol(MAL) + 1):nrow(MAL)

> (alternative to fg.unit) numeric vector of length 1 or 2 which specifies the highlighted trajectories. If length(fg.thresh) == 1 the highlighted trajectories are those of units that throughtout the search had at leat once a mahalanobis distance greater than fg.thresh. The default value is fg.thresh=2.5. If length(fg.thresh) == 2 the highlighted trajectories are those of units that throughtout the search had a mahalanobis distance at least once bigger than fg. thresh[2] or smaller than fg. thresh[1].

> (alternative to fg.thresh), vector containing the list of the units to be highlighted. If fg. unit is supplied, fg. thresh is ignored.

> numeric vector which specifies the steps of the search where to put labels for the highlighted trajectories (units). The default is to put the labels at the initial and final steps of the search. fg.labstep='' means no label.

ylim

lty

subsize

fg.thresh

fg.unit

fg.labstep

fg.lwd The line width for the highlighted trajectories (units). Default is 1.

fg.lty The line type for the highlighted trajectories (units). Line types can either be specified as an integer (1=solid (default), 2=dashed, 3=dotted, 4=dotdash, 5=longdash, 6=twodash) or as one of the character strings "solid", "dashed", "dotted", "dotdash", "longdash", or "twodash". The latter two are not supported

by Matlab.

fg.col colors to be used for the highlighted units.

fg.mark Controlls whether to plot highlighted trajectories as symbols. if fg.mark==TRUE each line is plotted using a different symbol else no marker is used (default).

fg.cex Controls the font size of the labels of the trajectories in foreground. If fg.cex=0 no labels will be shown - equivalent to fg.labstop="".

bg.thresh Numeric vector of length 1 or 2 which specifies how to define the unimmpor-

tant trajectories. Unimmportant trajectories will be plotted using a colormap, in greysh or will be hidden. If length(bg.thresh) == 1 the irrelevant units are those which always had a mahalanobis distance smaller than bg. thresh. If length(bg.thresh) == 2 the irrelevant units are those which always had a mahalanobis distance greater than bg. thresh[1] and smaller than bg. thresh[2]. The default is bg. thresh=2.5 if n > 100 and bg. thresh=-Inf if n <= 100 i.e. to treat all trajectories as important if n <= 100 and, if n > 100, to reduce emphasis only to trajectories having in all steps of the search a value of mahalanobis distance smaller than 2.5.

Specifies how to plot the unimportant trajectories as defined in option bg.thresh.

- 1. bg.style="faint": unimportant trajectories are plotted using a colormap.
- 2. bg.style="hide": unimportant trajectories are hidden.
- 3. bg.style="greyish": unimportant trajectories are displayed in a faint grey.

When n > 100 the default option is bg.style='faint'. When n <= 100 and bg.thresh == -Inf option bg.style is ignored. Remark: bground=" is equivalent to -Inf that is all trajectories are considered relevant.

MATLAB-style arguments - appearance of the plot in terms of xlim, ylim, axes labels and their font size style, color of the lines, etc.

MATLAB-style arguments - for the trajectories in foregroud.

MATLAB-style arguments - for the trajectories in backgroud.

Plot handle. String which identifies the handle of the plot which is about to be created. The default is to use tag 'pl\_resfwd'. Notice that if the program finds a plot which has a tag equal to the one specified by the user, then the output of the new plot overwrites the existing one in the same window else a new window is created.

Interactive clicking. It is inactive if this parameter is set to FALSE. The default is datatooltip=TRUE, the user can select with the mouse an individual mahalanobis distance trajectory in order to have information about the corresponding unit, the associated label and the step of the search in which the unit enters the subset. If datatooltip is a list it may contain the following fields:

bg.style

standard

fground bground

tag

datatooltip

 DisplayStyle determines how the data cursor displays. Possible values are 'datatip' and 'window' (default). 'datatip' displays data cursor information in a small yellow text box attached to a black square marker at a data point you interactively select. 'window' displays data cursor information for the data point you interactively select in a floating window within the figure.

- SnapToDataVertex: specifies whether the data cursor snaps to the nearest data value or is located at the actual pointer position. Possible values are SnapToDataVertex='on' (default) and SnapToDataVertex='off'.
- 3. LineColor: controls the color of the trajectory selected with the mouse. It can be an RGB triplet of values between 0 and 1, or character vector indicating a color name. Note that a RGB vector can be conveniently chosen with our MATLAB class FSColor, see documentation.
- 4. SubsetLinesColor: enables to control the color of the trajectories of the units that are in the subset at a given step of the search (if resfwdplot() is applied to an object of class fsreda.object) or have a weight greater than 0.9 (if resfwdplot() is applied to an object of class sregeda.object or mmregeda.object). This can be done (repeatedly) with a left mouse click in proximity of the step of interest. A right mouse click will terminate the selection by marking with a up-arrow the step corresponding to the highlighted lines. The highlighted lines by default are in red, but a different color can be specified as RGB triplet or character of color name. Note that a RGB vector can be conveniently chosen with our MATLAB class FSColor, see documentation. By default SubsetLinesColor="", i.e. the modality is not active. Any initialization for SubsetLinesColor which cannot be interpreted as RGB vector will be converted to blue, i.e. SubsetLinesColor will be forced to be [0 0 1]. If SubsetLinesColor is not empty the previous option LineColor is ignored.

label

Character vector containing the labels of the units (optional argument used when datatooltip=TRUE. If this field is not present labels row1, ..., rown will be automatically created and included in the pop up datatooltip window).

nameX

Add variable labels in plot. A vector of strings of length p containing the labels of the variables in the dataset. If it is empty (default) the sequence X1,...,Xp will be created automatically

databrush

Interactive mouse brushing. If databrush is missing or empty (default), no brushing is done. The activation of this option (databrush is TRUE or a list) enables the user to select a set of trajectories in the current plot and to see them highlighted in the scatterplot matrix. If the scatterplot matrix does not exist it is automatically created. In addition, brushed units can be highlighted in the monitoring mahalanobis distance plot. Note that the window style of the other figures is set equal to that which contains the monitoring mahalanobis distance plot. In other words, if the monitoring mahalanobis distance plot is docked all the other figures will be docked too.

If databrush=TRUE the default selection tool is a rectangular brush and it is possible to brush only once (that is persist=").

If databrush=list(...), it is possible to use all optional arguments of the MATLAB function selectdataFS() and the following optional arguments:

- persist. Persist is an empty value or a character containing 'on' or 'off'. The default value is persist="", that is brushing is allowed only once. If persist="on" or persis="off" brushing can be done as many time as the user requires. If persist='on' then the unit(s) currently brushed are added to those previously brushed. It is possible, every time a new brushing is done, to use a different color for the brushed units. If persist='off' every time a new brush is performed units previously brushed are removed.
- label: add labels of brushed units in the monitoring plot.
- labeladd: add labels of brushed units in the scatterplot matrix. If this option is '1', we label the units of the last selected group with the unit row index in the matrix X. The default value is labeladd=", i.e. no label is added.

conflev

confidence interval for the horizontal bands. It can be a vector of different confidence level values, e.g. c(0.95, 0.99, 0.999). The confidence interval is based on the \$chi^2\$ distribution.

trace

Whether to print intermediate results. Default is trace=FALSE.

. . .

potential further arguments passed to lower level functions.

#### Value

none

#### Author(s)

FSDA team, <valentin.todorov@chello.at>

#### References

Atkinson A.C., Riani M. and Cerioli A. (2004), Exploring Multivariate Data with the Forward Search, Springer Verlag, New York.

```
## Not run:
## Produce monitoring MD plot with all the default options.
## Generate input structure for malfwdplot
n <- 100
p <- 4
Y <- matrix(rnorm(n*p), ncol=p)
Y[1:10,] <- Y[1:10,] + 4

out <- fsmult(Y, monitoring=TRUE, init=30)

## Produce monitoring MD plot with all the default options
malfwdplot(out)
## End(Not run)</pre>
```

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malindexplot	Plots the trajectory of minimum Mahalanobis distance (mmd)

# Description

Plots the trajectory of minimum Mahalanobis distance (mmd)

# Usage

```
malindexplot(out, p, xlab, ylab, main, nameX, conflev, trace = FALSE,
    ...)
```

# Arguments

out	a numeric vector or an object of S3 class (one of fsmult.object, smult.object or mmmult.object) returned by one of the functions fsmult or smult or mmmult - a list containing the monitoring of minimum Mahalanobis distance
р	If out is a vector, p is its length (i.e. number of variables).
xlab	A title for the x axis
ylab	A title for the y axis
main	An overall title for the plot
nameX	Add variable labels in the plot. A vector of strings of length p containing the labels of the variables of the original data matrix X. If it is empty (default) the sequence X1,,Xp will be created automatically
conflev	confidence interval for the horizontal bands. It can be a vector of different confidence level values, e.g. c(0.95, 0.99, 0.999). The confidence interval is based on the chi^2 distribution.
trace	Whether to print intermediate results. Default is trace=FALSE.
	potential further arguments passed to lower level functions.

# Value

none

# Author(s)

FSDA team, <valentin.todorov@chello.at>

# References

Atkinson and Riani (2000), Robust Diagnostic Regression Analysis, Springer Verlag, New York.

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## **Examples**

```
## Not run:
## Mahalanobis distance plot of 100 random numbers.
## Numbers are from from the chisq with 5 degrees of freedom
malindexplot(rchisq(100, 5), 5)
## End(Not run)
```

mdrplot

Plots the trajectory of minimum deletion residual (mdr)

# Description

Plots the trajectory of minimum deletion residual (mdr).

# Usage

```
mdrplot(out, quant = c(0.01, 0.5, 0.99), sign = TRUE,
    mplus1 = FALSE, envm,
    xlim, ylim, xlab, ylab, main,
    lwdenv, lwd, cex.lab, cex.axis,
    tag, datatooltip, label, nameX, namey, databrush,
    ...)
```

#### **Arguments**

out

An object returned by FSReda() (see FSReda\_control).

The needed elements of out are

- mdr: Minimum deletion residual. A matrix containing the monitoring of minimum deletion residual in each step of the forward search. The first column of mdr must contain the fwd search index.
- 2. Un: (for FSR only) matrix containing the order of entry in the subset of each unit (required only when datatooltip is true or databrush is not empty).
- 3. y: a vector containing the response (required only when option databrush is requested).
- 4. X: a matrix containing the explanatory variables (required only when option databrush is requested).
- 5. Bols: (n-init+1) x (p+1) matrix containing the estimated beta coefficients monitored in each step of the robust procedure (required only when option databrush is requested and suboption multivarfit is requested).

quant

Quantiles for which envelopes have to be computed. The default is to produce 1%, 50% and 99% envelopes. In other words the default is quant=c(0.01,0.5,0.99).

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sign Wheather to use MDR with sign: if sign=TRUE (default) we distinguish steps for which minimum deletion residual was associated with positive or negative value of the residual. Steps associated with positive values of mdr are plotted in black, while other steps are plotted in red. Wheather to plot the (m+1)-th order statistic. Specifies if it is necessary to plot mplus1 the curve associated with (m+1)-th order statistic. Sample size for drawing enevlopes. Specifies the size of the sample which is envm used to superimpose the envelope. The default is to add an envelope based on all the observations (size n envelope). ylim Control y scale in plot. Vector with two elements controlling minimum and maximum on the y axis. Default is to use automatic scale. xlim Control x scale in plot. Vector with two elements controlling minimum and maximum on the x axis. Default is to use automatic scale. xlab a title for the x axis a title for the y axis ylab main an overall title for the plot lwdenv Controls the width of the lines associated with the envelopes, default is lvdenv=1. lwd Controls the linewidth of the curve which contains the monitoring of minimum deletion residual. cex.lab The magnification to be used for x and y labels relative to the current setting of cex.axis The magnification to be used for axis annotation relative to the current setting Plot handle. String which identifies the handle of the plot which is about to be tag created. The default is to use tag 'pl\_mdr'. Notice that if the program finds a plot which has a tag equal to the one specified by the user, then the output of the new plot overwrites the existing one in the same window else a new window is created. datatooltip If datatooltip is not empty the user can use the mouse in order to have information about the unit selected, the step in which the unit enters the search and the associated label. If datatooltip is a list, it is possible to control the aspect of the data cursor (see MATLAB function datacursormode() for more details or see the examples below). The default options are DisplayStyle="Window" and SnapToDataVertex="on". label Character vector containing the labels of the units (optional argument used when datatooltip=TRUE. If this field is not present labels row1, ..., rown will be automatically created and included in the pop up datatooltip window). nameX Add variable labels in plot. A vector of strings of length p containing the labels of the variables of the regression dataset. If it is empty (default) the sequence X1,..., Xp will be created automatically namey Add response label. A string containing the label of the response databrush interactive mouse brushing. If databrush is missing or empty (default), no brushing is done. The activation of this option (databrush is a scalar or a list) enables

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the user to select a set of trajectories in the current plot and to see them highlighted in the y|X plot, i.e. a matrix of scatter plots of y against each column of X, grouped according to the selection(s) done by brushing. If the plot y|X does not exist it is automatically created. In addition, brushed units are automatically highlighted in the minimum deletion residual plot if it is already open. The extension to the following plots will be available in future versions of the toolbox:

- 1. monitoring leverage plot;
- 2. maximum studentized residual;
- 3. s<sup>2</sup> and R<sup>2</sup>;
- 4. Cook distance and modified Cook distance;
- 5. deletion t statistics.

Note that the window style of the other figures is set equal to that which contains the monitoring residual plot. In other words, if the monitoring residual plot is docked all the other figures will be docked too

If databrush=TRUE the default selection tool is a rectangular brush and it is possible to brush only once (that is persist=").

If databrush=list(...), it is possible to use all optional arguments of function selectdataFS() and the following optional argument:

- 1. persist. Persist is an empty value or a character containing 'on' or 'off'. The default value is persist="", that is brushing is allowed only once. If persist="on" or persis="off" brushing can be done as many time as the user requires. If persist='on' then the unit(s) currently brushed are added to those previously brushed. It is possible, every time a new brushing is done, to use a different color for the brushed units. If persist='off' every time a new brush is performed units previously brushed are removed.
- 2. bivarfitWheather to superimpose bivariate least square lines on the plot (if plot=TRUE. This option adds one or more least squares lines, based on SIMPLE REGRESSION of y on Xi, to the plots of ylXi. The default is bivarfit=FALSE: no line is fitted. If bivarfit=1, a single OLS line is fitted to all points of each bivariate plot in the scatter matrix ylX. If bivarfit=2, two OLS lines are fitted: one to all points and another to the group of the genuine observations. The group of the potential outliers is not fitted. If bivarfit=0 one OLS line is fitted to each group. This is useful for the purpose of fitting mixtures of regression lines. If bivarfit='i1' or bivarfit='i2', etc. an OLS line is fitted to a specific group, the one with index 'i' equal to 1, 2, 3 etc. Again, useful in case of mixtures.
- 3. multivarfitWheather to superimpose multivariate least square lines. This option adds one or more least square lines, based on MULTIVARIATE RE-GRESSION of y on X, to the plots of y|Xi. The default is multivarfit=FALSE: no line is fitted. If bivarfit=1, a single OLS line is fitted to all points of each bivariate plot in the scatter matrix y|X. The line added to the scatter plot y|Xi is avconst + Ci\*Xi, where Ci is the coefficient of Xi in the multivariate regression and avconst is the effect of all the other explanatory variables different from Xi evaluated at their centroid (that is overline(y)'C)). If multivarfit=2, same action as with multivarfit=1 but this time we also

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- add the line based on the group of unselected observations (i.e. the normal units).
- 4. labeladdAdd outlier labels in plot. If labeladd=TRUE, we label the outliers with the unit row index in matrices X and y. The default value is labeladd=FALSE, i.e. no label is added.

potential further arguments passed to lower level functions.

### **Details**

No details

### Value

No value returned

# Author(s)

FSDA team

# **Examples**

```
## Not run:

n <- 100
y <- rnorm(n)
X <- matrix(rnorm(n*4), nrow=n)

out <- fsreg(y~X, method="LTS")
out <- fsreg(y~X, method="FS", bsb=out$bs, monitoring=TRUE)
mdrplot(out)

## End(Not run)</pre>
```

mmdplot

Plots the trajectory of minimum Mahalanobis distance (mmd)

# **Description**

Plots the trajectory of minimum Mahalanobis distance (mmd)

## Usage

```
mmdplot(out, quant = c(0.01, 0.5, 0.99), mplus1 = FALSE, envm, lwd,
  lwdenv, xlim, ylim, tag, datatooltip, label, xlab, ylab, main, nameX,
  cex.lab, cex.axis, databrush, trace = FALSE, ...)
```

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#### **Arguments**

An object of S3 class fsmeda.object returned by fsmult with monitoring=TRUE out

- a list containing the monitoring of minimum Mahalanobis distance

Quantiles for which envelopes have to be computed. The default is to produce quant

1%, 50% and 99% envelopes. In other words the default is quant=c(0.01,0.5,0.99).

mplus1 Wheather to plot the (m+1)-th order statistic.

Sample size for drawing enevlopes. Specifies the size of the sample which is envm

used to superimpose the envelope. The default is to add an envelope based on

all the observations (size n envelope).

lwd Controls the line width of the curve which contains the monitoring of minimum

deletion residual.

lwdenv Controls the width of the lines associated with the envelopes. Default is lwdenv=1

Control the x scale in plot. Vector with two elements controlling minimum and xlim

maximum on the x axis. Default is to use automatic scale.

ylim Control the y scale in plot. Vector with two elements controlling minimum and

maximum on the y axis. Default is to use automatic scale.

tag Plot handle. String which identifies the handle of the plot which is about to be

> created. The default is tag='pl\_mmd'. Notice that if the program finds a plot which has a tag equal to the one specified by the user, then the output of the new plot overwrites the existing one in the same window else a new window is

created.

datatooltip If datatooltip is not empty the user can use the mouse in order to have infor-

> mation about the unit selected, the step in which the unit enters the search and the associated label. If datatooltip is a list, it is possible to control the aspect of the data cursor (see MATLAB function datacursormode() for more details or see the examples below). The default options are DisplayStyle="Window" and

SnapToDataVertex="on".

label Row labels. Character vector containing the labels of the units (optional ar-

> gument used when datatooltip=TRUE. If this field is not present labels row1, ..., rown will be automatically created and included in the pop up datatooltip

window).

xlab A title for the x axis

ylab A title for the y axis

main An overall title for the plot

Add variable labels in the plot. A vector of strings of length p containing the nameX

labels of the variables of the original data matrix X. If it is empty (default) the

sequence X1, ..., Xp will be created automatically

cex.lab The magnification to be used for x and y labels relative to the current setting of

cex.axis The magnification to be used for axis annotation relative to the current setting

of cex

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databrush

Interactive mouse brushing. If databrush is missing or empty (default), no brushing is done. The activation of this option (databrush is TRUE or a list) enables the user to select a set of trajectories in the current plot and to see them highlighted in the scatterplot matrix. If the scatterplot matrix does not exist it is automatically created. In addition, brushed units can be highlighted in the monitoring MD plot. Note that the window style of the other figures is set equal to that which contains the monitoring residual plot. In other words, if the monitoring residual plot is docked all the other figures will be docked too.

If databrush=TRUE the default selection tool is a rectangular brush and it is possible to brush only once (that is persist=").

Note that the window style of the other figures is set equal to that which contains the monitoring residual plot. In other words, if the monitoring residual plot is docked all the other figures will be docked too

If databrush=TRUE the default selection tool is a rectangular brush and it is possible to brush only once (that is persist=").

If databrush=list(...), it is possible to use all optional arguments of the MATLAB function selectdataFS() and the following optional arguments:

- persist: This option can be an empty value or a character containing 'on' or 'off'. The default value is persist="", that is brushing is allowed only once. If persist="on" or persis="off" brushing can be done as many time as the user requires. If persist='on' then the unit(s) currently brushed are added to those previously brushed. It is possible, every time a new brushing is done, to use a different color for the brushed units. If persist='off' every time a new brush is performed units previously brushed are removed.
- labeladd: add labels of brushed units in the scatterplot matrix. If this option is '1', we label the units of the last selected group with the unit row index in the matrix X. The default value is labeladd=", i.e. no label is added.

trace

Whether to print intermediate results. Default is trace=FALSE.

potential further arguments passed to lower level functions.

# Value

none

#### Author(s)

FSDA team, <valentin.todorov@chello.at>

#### References

Atkinson and Riani (2000), Robust Diagnostic Regression Analysis, Springer Verlag, New York.

## **Examples**

## Not run:
data(hbk)

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```
(out <- fsmult(hbk[,1:3], monitoring=TRUE))
mmdplot(out)
## End(Not run)</pre>
```

mmdrsplot

Plots the trajectories of minimum Mahalanobis distances from different starting points

## Description

Plots the trajectories of minimum Mahalanobis distances from different starting points

## Usage

```
mmdrsplot(out, quant = c(0.01, 0.5, 0.99), envm, lwd, lwdenv, xlim, ylim,
  tag, datatooltip, label, xlab, ylab, envlab = TRUE, main, nameX,
  cex.lab, cex.axis, databrush, scaled = FALSE, trace = FALSE, ...)
```

#### **Arguments**

out

An object of S3 class fsmmmdrs.object returned by fsmmmdrs - a list containing the following elements:

- mmdrs = a matrix of size (n-ninit)-by-(nsimul+1) containing the monitoring of minimum Mahalanobis distance in each step of the forward search for each of the nsimul random starts. The first column of mmdrs must contain the forward search index. This matrix can be created using function fsmmmdrs.
- BBrs = 3D array of size n-by-n-(init)-by-nsimul containing units forming subset for rach random start. This field is necessary if datatooltip is true or databrush is not empty.
- X = n-by-v matrix containing the original data matrix. This field is necessary if datatooltip is true or databrush is not empty.

quant

Quantiles for which envelopes have to be computed. The default is to produce 1%, 50% and 99% envelopes. In other words the default is quant=c(0.01, 0.5, 0.99).

envm

Sample size for drawing enevlopes. Specifies the size of the sample which is used to superimpose the envelope. The default is to add an envelope based on all the observations (size n envelope).

lwd

Controls the linewidth of the curve which contains the monitoring of minimum deletion residual.

lwdenv

line width: a scalar which controls the width of the lines associated with the envelopes. Default is lwdenv=1

xlim

Control the x scale in plot. Vector with two elements controlling minimum and maximum on the x axis. Default is to use automatic scale.

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ylim Control the y scale in plot. Vector with two elements controlling minimum and

maximum on the y axis. Default is to use automatic scale.

Plot handle. String which identifies the handle of the plot which is about to be tag

created. The default is tag='pl\_mmd'. Notice that if the program finds a plot which has a tag equal to the one specified by the user, then the output of the new plot overwrites the existing one in the same window else a new window is

created.

datatooltip If datatooltip is not empty the user can use the mouse in order to have infor-

> mation about the unit selected, the step in which the unit enters the search and the associated label. If datatooltip is a list, it is possible to control the aspect of the data cursor (see MATLAB function datacursormode() for more details or see the examples below). The default options are DisplayStyle="Window" and

SnapToDataVertex="on".

label Row labels. Character vector containing the labels of the units (optional ar-

> gument used when datatooltip=TRUE. If this field is not present labels row1, ..., rown will be automatically created and included in the pop up datatooltip

window).

xlab A title for the x axis ylab A title for the y axis

envlab wheather to label the envelopes. If envlab is true (default) labels of the confi-

dence envelopes which are used are added on the y axis.

main An overall title for the plot

nameX Add variable labels in the plot. A vector of strings of length p containing the

labels of the variables of the original data matrix X. If it is empty (default) the

sequence X1, ..., Xp will be created automatically

cex.lab The magnification to be used for x and y labels relative to the current setting of

cex

The magnification to be used for axis annotation relative to the current setting cex.axis

of cex

databrush Interactive mouse brushing. If databrush is missing or empty (default), no brushing is done. The activation of this option (databrush is TRUE or a list) enables

the user to select a set of trajectories in the current plot and to see them highlighted in the scatterplot matrix. If the scatterplot matrix does not exist it is automatically created. In addition, brushed units can be highlighted in the monitoring MD plot. Note that the window style of the other figures is set equal to that which contains the monitoring residual plot. In other words, if the monitor-

ing residual plot is docked all the other figures will be docked too.

If databrush=TRUE the default selection tool is a rectangular brush and it is

possible to brush only once (that is persist=").

Note that the window style of the other figures is set equal to that which contains the monitoring residual plot. In other words, if the monitoring residual plot is

docked all the other figures will be docked too

If databrush=TRUE the default selection tool is a rectangular brush and it is

possible to brush only once (that is persist=").

If databrush=list(...), it is possible to use all optional arguments of the MATLAB function selectdataFS() and the following optional arguments:

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1. persist. Persist is an empty value or a character containing 'on' or 'off'. The default value is persist="", that is brushing is allowed only once. If persist="on" or persis="off" brushing can be done as many time as the user requires. If persist='on' then the unit(s) currently brushed are added to those previously brushed. It is possible, every time a new brushing is done, to use a different color for the brushed units. If persist='off' every time a new brush is performed units previously brushed are removed.

scaled

Wheather to use scaled or unscaled envelopes. If scaled=TRUE the envelopes are produced for scaled Mahalanobis distances (no consistency factor is applied) else the traditional consistency factor is applied. Default is scaled=FALSE

trace

Whether to print intermediate results. Default is trace=FALSE.

. . .

potential further arguments passed to lower level functions.

### Value

none

#### Author(s)

FSDA team, <valentin.todorov@chello.at>

# References

Atkinson, A.C., Riani, M. and Cerioli, A. (2004), 'Exploring multivariate data with the forward search, Springer Verlag, New York.

# **Examples**

```
## Not run:
data(hbk)
out <- fsmmmdrs(hbk[,1:3])
mmdrsplot(out)
## End(Not run)</pre>
```

mmmult

Computes MM estimators in multivariate analysis with auxiliary S-scale

### **Description**

Computes MM estimators in multivariate analysis with auxiliary S-scale

#### Usage

```
mmmult(x, monitoring = FALSE, plot = FALSE, eff, conflev = 0.975,
  nocheck = FALSE, trace = FALSE, ...)
```

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### **Arguments**

plot

x An n x p data matrix (n observations and p variables). Rows of x represent observations, and columns represent variables.

Missing values (NA's) and infinite values (Inf's) are allowed, since observations (rows) with missing or infinite values will automatically be excluded from the computations.

monitoring Wheather to perform monitoring of Mahalanobis distances and other specific

quantities

Plots the Mahalanobis distances against index number. If plot=FALSE (default) or plot=0 no plot is produced. The confidence level used to draw the confidence bands for the MD is given by the input option conflev. If conflev is not specified a nominal 0.975 confidence interval will be used. If plot=2 a scatter plot matrix with the outliers highlighted is produced. If plot is a list it may contain the following fields:

- labeladd If labeladd=1, the outliers in the spm are labelled with the unit row index. The default value is labeladd="", i.e. no label is added
- nameY character vector containing the labels of the variables. As default value, the labels which are added are Y1, ... Yp.

eff Defining the nominal efficiency (i.e. a number between 0.5 and 0.99). The

default value is eff=0.95.

confilev confidence interval for the horizontal bands. It can be a vector of different con-

fidence level values, e.g.  $c(0.95,\,0.99,\,0.999)$ . The confidence interval is based

on the chi^2 distribution.

nocheck It controls whether to perform checks on matrix Y. If nocheck=TRUE, no check

is performed.

trace Whether to print intermediate results. Default is trace=FALSE.

... potential further arguments passed to lower level functions.

#### **Details**

This function follows the lines of MATLAB/R code developed during the years by many authors. For more details see http://www.econ.kuleuven.be/public/NDBAE06/programs/ and the R package CovMMest The core of these routines, e.g. the resampling approach, however, has been completely redesigned, with considerable increase of the computational performance.

# Value

Depending on the input parameter monitoring, one of the following objects will be returned:

- mmmult.object
- 2. mmmulteda.object

## Author(s)

FSDA team, <valentin.todorov@chello.at>

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#### References

Maronna, R.A., Martin D. and Yohai V.J. (2006), Robust Statistics, Theory and Methods, Wiley, New York.

```
## Not run:
data(hbk)
(out <- mmmult(hbk[,1:3]))</pre>
class(out)
summary(out)
## Generate contaminated data (200,3)
n <- 200
p <- 3
set.seed(123456)
X <- matrix(rnorm(n*p), nrow=n)</pre>
Xcont <- X
Xcont[1:5, ] \leftarrow Xcont[1:5,] + 3
out1 <- mmmult(Xcont, trace=TRUE)</pre>
                                              # no plots (plot defaults to FALSE)
names(out1)
## plot=TRUE - generates: (1) a plot of Mahalanobis distances against
       index number. The confidence level used to draw the confidence bands for
##
       the MD is given by the input option conflev. If conflev is
##
       not specified a nominal 0.975 confidence interval will be used and
       (2) a scatter plot matrix with the outliers highlighted.
(out1 <- mmmult(Xcont, trace=TRUE, plot=TRUE))</pre>
## plots is a list: the spm shows the labels of the outliers.
(out1 <- mmmult(Xcont, trace=TRUE, plot=list(labeladd="1")))</pre>
## plots is a list: the spm uses the variable names provided by 'nameY'.
(out1 <- mmmult(Xcont, trace=TRUE, plot=list(nameY=c("A", "B", "C"))))</pre>
## mmmult() with monitoring
(out2 <- mmmult(Xcont, monitoring=TRUE, trace=TRUE))</pre>
names(out2)
## Forgery Swiss banknotes examples.
data(swissbanknotes)
(out1 <- mmmult(swissbanknotes[101:200,], plot=TRUE))</pre>
(out1 <- mmmult(swissbanknotes[101:200,], plot=list(labeladd="1")))</pre>
## End(Not run)
```

56 mmmult.object

mmmult.object	Description of mmmult.object Objects

# **Description**

An object of class mmmult.object holds information about the result of a call to mmmult.

#### Value

The object itself is basically a list with the following components:

loc p-by-1 vector containing MM estimate of location.
shape p-by-p matrix with MM estimate of the shape matrix.

cov matrix with MM estimate of the covariance matrix. Remark: covariance =

auxscale^2 \* shape.

weights A vector containing the estimates of the weights.

outliers A vector containing the list of the units declared as outliers using confidence

level specified in input scalar conflev.

Sloc A vector with S estimate of location.

Sshape A matrix with S estimate of the shape matrix.

Scov A matrix with S estimate of the covariance matrix.

auxscale S estimate of the scale.

md n-by-1 vector containing the estimates of the robust Mahalanobis distances (in

squared units).

conflev Confidence level that was used to declare outliers.

X the data matrix X

The object has class "mmmult".

```
## Not run:
  data(hbk)
  (out <- mmmult(hbk[,1:3]))
  class(out)
  summary(out)

## End(Not run)</pre>
```

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# Description

An object of class mmmulteda.object holds information about the result of a call to mmmult with monitoring=TRUE.

# Value

The object itself is basically a list with the following components:

Loc	length(eff)-by-p matrix containing MM estimate of location for each value of eff.
Shape	p-by-p-by-length(eff) 3D array containing robust estimate of the shape for each value of eff. Remark: detlshapel=1.
Scale	length(eff) vector containing robust estimate of the scale for each value of eff.
Cov	p-by-p-by-length(eff) 3D array containing robust estimate of covariance matrix for each value of eff. Note that $scale(i)^2 * shape[,,i] = robust estimate of covariance matrix.$
Bs	(p+1)-by-length(eff) matrix containing the units forming best subset for each value of eff.
MAL	n-by-length(eff) matrix containing the estimates of the robust Mahalanobis distances (in squared units) for each value of eff.
Outliers	n-by-length(eff) matrix containing flags for the outliers. Boolean matrix containing the list of the units declared as outliers for each value of eff using confidence level specified in input scalar conflev
Weights	n x length(eff) matrix containing the weights for each value of eff.
conflev	Confidence level that was used to declare outliers.
singsub	Number of subsets without full rank. Notice that $singsub > 0.1*(number of subsamples)$ produces a warning.
eff	vector which contains the values of eff which have been used.
Χ	the data matrix X.

The object has class "mmmulteda".

```
## Not run:
    data(hbk)
    (out <- mmmult(hbk[,1:3], monitoring=TRUE))
    class(out)
    summary(out)

## End(Not run)</pre>
```

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mmreg.object	Description of mmreg Objects	
--------------	------------------------------	--

#### **Description**

An object of class mmreg. object holds information about the result of a call to fsreg with method="MM".

#### Value

The object itself is basically a list with the following components:

beta p-by-1 vector containing the MM estimate of regression coefficients.

auxscale scalar, S estimate of the scale (or supplied external estimate of scale, if option

InitialEst is not empty).

residuals residuals.
fittedvalues fitted values.

weights n x 1 vector. Weights assigned to each observation.

Sbeta p x 1 vector containing S estimate of regression coefficients (or supplied initial

external estimate of regression coefficients, if option InitialEst is not empty)

Ssingsub Number of subsets without full rank in the S preliminary part. Notice that

out.singsub > 0.1\*(number of subsamples) produces a warning.

outliers kx1 vector containing the list of the k units declared as outliers or NULL if the

sample is homogeneous.

conflev Confidence level which is used to declare units as outliers. Usually conflev=0.95,0.975,0.99

(individual alpha) or conflev=1-0.05/n,1-0.025/n,1-0.01/n (simultaneous

alpha). Default value is 0.975

rhofunc Specifies the rho function which has been used to weight the residuals. If a

different rho function is specified for S and MM loop then insted of rhofunc we

will have rhofuncS and rhofuncMM.

rhofuncparam Vector which contains the additional parameters for the specified rho function

which has been used. For hyperbolic rho function the value of k =sup CVC. For Hampel rho function the parameters a, b and c. If a different rho function is specified for S and MM loop then insted of rhofuncparam we will have

rhofuncparamS and rhofuncparamMM.

X the data matrix X

y the response vector y

The object has class "mmreg".

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# **Examples**

```
## Not run:
    (out <- fsreg(Y~., data=hbk, method="MM"))</pre>
   class(out)
   summary(out)
## End(Not run)
```

mmregeda.object

Description of mmregeda Objects

# Description

An object of class mmregeda.object holds information about the result of a call to fsreg when method="MM" and monitoring=TRUE.

### Value

The object itself is basically a list with the following components:

auxscale	scalar, S estimate of the scale (or supplied external estimate of scale, if option InitialEst is not empty).
Beta	p x length(eff) matrix containing MM estimate of regression coefficients for each value of eff.
RES	n x length(eff) matrix containing the monitoring of scaled residuals for each value of eff.
Weights	n x length(eff) matrix containing the estimates of the weights for each value of eff
Outliers	Boolean matrix containing the list of the units declared as outliers for each value of eff using confidence level specified in input scalar conflev.
conflev	Confidence level which is used to declare units as outliers. Remark: conflev will be used to draw the horizontal line (confidence band) in the plot.
Ssingsub	Number of subsets without full rank. Notice that Notice that singsub $> 0.1*$ (number of subsamples) produces a warning
rhofunc	string identifying the rho function which has been used.
rhofuncparam	vector which contains the additional parameters for the specified rho function which have been used. For hyperbolic rho function the value of $k$ =sup CVC. For Hampel rho function the parameters $a, b$ and $c$ .

vector containing the value of eff which have been used.

the data matrix X Χ

the response vector y У

The object has class "mmregeda".

eff

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# **Examples**

```
## Not run:
   (out <- fsreg(Y~., data=hbk, method="MM", monitoring=TRUE))
   class(out)
   summary(out)

## End(Not run)</pre>
```

MMregeda\_control

Creates an MMregeda\_control object

# Description

Creates an object of class MMregeda\_control to be used with the fsreg() function, containing various control parameters.

# Usage

```
MMregeda_control(intercept = TRUE, InitialEst, Soptions, eff, effshape,
refsteps = 3, tol = 1e-07, conflev, nocheck = FALSE, plot = FALSE)
```

# **Arguments**

tol

intercept	Indicator for constant term. Scalar. If intercept=TRUE, a model with constant term will be fitted (default), else, no constant term will be included.
InitialEst	Starting values of the MM-estimator, a list with the fiollowing elements: loc, a \$p x 1\$ vector, location vector estimate and scale, a scaler, estimate of the scale. If empty (default) the program will use S estimators. In this last case it is possible to specify the options given in function Sreg.
Soptions	Options to pass to Sreg, an Sreg_control object.
	The options are: Srhofunc, Snsamp, Srefsteps, Sreftol, Srefstepsbestr, Sreftolbestr, Sminsctol, Sbestr. See function Sreg_control for more details on these options.
	It is necessary to add to the S options the letter S at the beginning. For example, if you want to use the optimal rho function the supplied option is 'Srhofunc','optimal'. For example, if you want to use 3000 subsets, the supplied option is 'Snsamp',3000
eff	Vector defining nominal efficiency (i.e. a series of numbers between 0.5 and 0.99). The default value is the sequence seq(0.5,0.99,0.01)
effshape	Location or scale efficiency. If effshape=1 efficiency refers to shape efficiency else (default) efficiency refers to location efficiency.
refsteps	Number of refining iterations in each subsample (default is refsteps=3). refsteps

= 0 means "raw-subsampling" without iterations.

Scalar controlling tolerance in the MM loop. The default value is tol=1e-6.

MMreg\_control 61

conflev Confidence level which is used to declare units as outliers. Usually conflev=0.95,

0.975, 0.99 (individual alpha) or conflev=1-0.05/n, 1-0.025/n, 1-0.01/n (simul-

taneous alpha). Default value is 0.975

nocheck Check input arguments, scalar. If nocheck=TRUE no check is performed on ma-

trix y and matrix X. Notice that y and X are left unchanged. In other words the additional column of ones for the intercept is not added. As default nocheck=FALSE.

plot Plot on the screen. Scalar. If plots=TRUE the plot of minimum deletion resid-

ual with envelopes based on n observations and the scatterplot matrix with the outliers highlighted is produced. If plots=2 the user can also monitor the intermediate plots based on envelope superimposition. If plots=FALSE (default) no

plot is produced.

### **Details**

Creates an object of class MMregeda\_control to be used with the fsreg() function, containing various control parameters.

### Value

An object of class "MMregeda\_control" which is basically a list with components the input arguments of the function mapped accordingly to the corresponding Matlab function.

## Author(s)

FSDA team

#### See Also

```
See Also as FSR_control, Sreg_control, MMreg_control and LXS_control
```

#### **Examples**

MMreg\_control

Creates an MMreg\_control object

# Description

Creates an object of class MMreg\_control to be used with the fsreg() function, containing various control parameters for calling the MATLAB function MMreg().

MMreg\_control

### Usage

```
MMreg_control(intercept = TRUE, InitialEst, Soptions, eff, effshape,
   rhofunc = c("bisquare", "optimal", "hyperbolic", "hampel"), rhofuncparam,
   refsteps = 3, tol = 1e-07, conflev,
   msg = TRUE, nocheck = FALSE, plot = FALSE)
```

## **Arguments**

intercept Indicator for constant term. Scalar. If intercept=TRUE, a model with constant

term will be fitted (default), else, no constant term will be included.

InitialEst Starting values of the MM-estimator, a list with the fiollowing elements: loc,

> a \$p x 1\$ vector, location vector estimate and scale, a scaler, estimate of the scale. If empty (default) the program will use S estimators. In this last case it is

possible to specify the options given in function Sreg.

Soptions Options to pass to Sreg, an Sreg\_control object.

> The options are: Srhofunc, Snsamp, Srefsteps, Sreftol, Srefstepsbestr, Sreftolbestr, Sminsctol, Sbestr. See function Sreg\_control for more details on these

options.

It is necessary to add to the S options the letter S at the beginning. For example, if you want to use the optimal rho function the supplied option is 'Srhofunc','optimal'. For example, if you want to use 3000 subsets, the supplied

option is 'Snsamp',3000

Scalar defining nominal efficiency (i.e. a number between 0.5 and 0.99). The eff

default value is 0.95.

Location or scale efficiency. If effshape=1 efficiency refers to shape efficiency

else (default) efficiency refers to location efficiency.

Specifies the rho function which must be used to weight the residuals. Possible rhofunc

values are 'bisquare' 'optimal' 'hyperbolic' 'hampel'.

1. 'bisquare' uses Tukey's rho and psi functions. See TBrho and TBpsi.

- 2. 'optimal' uses optimal rho and psi functions. See OPTrho and OPTpsi.
- 3. 'hyperbolic' uses hyperbolic rho and psi functions. See HYPrho and HYPpsi.
- 4. 'hampel' uses Hampel rho and psi functions. See HArho and HApsi.

The default is 'bisquare'.

rhofuncparam Additional parameters for the specified rho function. For hyperbolic rho func-

tion it is possible to set up the value of  $k = \sup CVC$  (the default value of k is

4.5).

For Hampel rho function it is possible to define parameters a, b and c (the default

values are a=2, b=4, c=8)

refsteps Number of refining iterations in each subsample (default is refsteps=3). refsteps

= 0 means "raw-subsampling" without iterations.

tol Scalar controlling tolerance in the MM loop. The default value is tol=1e-6

conflev Confidence level which is used to declare units as outliers. Usually conflev=0.95,

0.975, 0.99 (individual alpha) or conflev=1-0.05/n, 1-0.025/n, 1-0.01/n (simul-

taneous alpha). Default value is 0.975

effshape

msg	Controls whether to display or not messages on the screen If msg==1 (default)
	1. 1 1 1 1 1 1 1 1 1 1 1 1 1

messages are displayed on the screen about step in which signal took place else

no message is displayed on the screen.

nocheck Check input arguments, scalar. If nocheck=TRUE no check is performed on ma-

trix y and matrix X. Notice that y and X are left unchanged. In other words the additional column of ones for the intercept is not added. As default nocheck=FALSE.

plot Plot on the screen. Scalar. If plots=TRUE the plot of minimum deletion resid-

ual with envelopes based on n observations and the scatterplot matrix with the outliers highlighted is produced. If plots=2 the user can also monitor the intermediate plots based on envelope superimposition. If plots=FALSE (default) no

plot is produced.

### **Details**

Creates an object of class MMreg\_control to be used with the fsreg() function, containing various control parameters.

## Value

An object of class "MMreg\_control" which is basically a list with components the input arguments of the function mapped accordingly to the corresponding Matlab function.

#### Author(s)

FSDA team

#### See Also

See Also as FSR\_control, MMreg\_control and LXS\_control

### **Examples**

```
## Not run:
## (out <- fsreg(Y~., data=hbk, method="MM", control=MMreg_control(eff=0.99, rhofunc="optimal")))
(out <- fsreg(Y~., data=hbk, method="MM", control=MMreg_control(eff=0.99)))
## End(Not run)</pre>
```

resfwdplot

Plots the trajectories of the monitored scaled (squared) residuals

# **Description**

Plots the trajectories of the monitored scaled (squared) residuals

### Usage

```
resfwdplot(out,
    xlim, ylim, xlab, ylab, main, lwd, lty, col, cex.lab, cex.axis,
    xvalues,
    fg.thresh, fg.unit, fg.labstep, fg.lwd, fg.lty, fg.col, fg.mark, fg.cex,
   bg.thresh, bg.style,
    tag, datatooltip, label, nameX, namey, msg, databrush,
    standard, fground, bground, ...)
```

#### **Arguments**

out

An object returned by one of the monitoring functions (see FSReda\_control, Sregeda\_control and MMregeda\_control). The object is one of fsreda.object, sregeda.object or mmregeda.object.

The needed elements of out are

- 1. RES: matrix containing the residuals monitored in each step of the forward search or any other robust procedure. Every row is associated with a residual (unit). This matrix can be created using function FSReda, Sregeda, MMregeda.
- 2. Un: (for FSR only) matrix containing the order of entry in the subset of each unit (required only when datatooltip is true or databrush is not empty).
- 3. bdp: (for Sreg only) vector containing a sequence of breakdown point values to monitor on.
- 4. eff: (for MMreg only) vector containing a sequence of efficiency values to monitor on.
- 5. y: a vector containing the response (required only when option databrush is requested).
- 6. X: a matrix containing the explanatory variables (required only when option databrush is requested).
- 7. Bols: (n-init+1) x (p+1) matrix containing the estimated beta coefficients monitored in each step of the robust procedure (required only when option databrush is requested and suboption multivarfit is requested).

ylim Control y scale in plot. Vector with two elements controlling minimum and maximum on the y axis. Default is to use automatic scale.

> Control x scale in plot. Vector with two elements controlling minimum and maximum on the x axis. Default is to use automatic scale.

xlab a title for the x axis

ylab a title for the y axis

main an overall title for the plot

lwd The line width, a positive number, defaulting to 1

> The line type. Line types can either be specified as an integer (1=solid (default), 2=dashed, 3=dotted, 4=dotdash, 5=longdash, 6=twodash) or as one of the character strings "solid", "dashed", "dotted", "dotdash", "longdash", or "twodash". The latter two are not supported by Matlab.

xlim

lty

col colors to be used for the highlighted units cex.lab The magnification to be used for x and y labels relative to the current setting of cex The magnification to be used for axis annotation relative to the current setting cex.axis xvalues values for the x axis. Numeric vector of ncol (RES) controlling the x axis coordinates. The default value of xvalues is (nrow(RES) -ncol(RES) + 1):nrow(RES) fg.thresh (alternative to fg.unit) numeric vector of length 1 or 2 which specifies the highlighted trajectories. If length(fthresh) == 1 the highlighted trajectories are those of units that throughtout the search had at leat once a residual greater (in absolute value) than thresh. The default value is fg. thresh=2.5. If length(fthresh) == 2 the highlighted trajectories are those of units that throughtout the search had a residual at leat once bigger than fg. thresh[2] or smaller than fg. thresh[1]. fg.unit (alternative to fg.thresh), vector containing the list of the units to be highlighted. If fg. unit is supplied, fg. thresh is ignored. fg.labstep numeric vector which specifies the steps of the search where to put labels for the highlighted trajectories (units). The default is to put the labels at the initial and final steps of the search. fg.labstep=' ' means no label. fg.lwd The line width for the highlighted trajectories (units). Default is 1. fg.lty The line type for the highlighted trajectories (units). Line types can either be specified as an integer (1=solid (default), 2=dashed, 3=dotted, 4=dotdash, 5=longdash, 6=twodash) or as one of the character strings "solid", "dashed", "dotted", "dotdash", "longdash", or "twodash". The latter two are not supported by Matlab. fg.col colors to be used for the highlighted units. fg.mark Controlls whether to plot highlighted trajectories as symbols. if fg.mark==TRUE each line is plotted using a different symbol else no marker is used (default). fg.cex controls the font size of the labels of the trajectories in foreground. bg.thresh numeric vector of length 1 or 2 which specifies how to define the unimmportant trajectories. Unimmportant trajectories will be plotted using a colormap, in greysh or will be hidden. If length(thresh) == 1 the irrelevant units are those which always had a residual smaller (in absolute value) than thresh. If length(bthresh) == 2 the irrelevant units are those which always had a residual greater than bthresh(1) and smaller than bthresh(2). The default is: bg.thresh=2.5 if n > 100 and bg. thresh=-Inf if n <= 100 i.e. to treat all trajectories as important if  $n \le 100$  and, if n > 100, to reduce emphasis only to trajectories having in all steps of the search a value of scaled residual smaller than 2.5. bg.style specifies how to plot the unimportant trajectories as defined in option bthresh. 1. bg.style="faint": unimportant trajectories are plotted using a colormap. 2. bg.style="hide": unimportant trajectories are hidden. 3. bg.style="greyish": unimportant trajectories are displayed in a faint grey.

When n>100 the default option is bg.style='faint'. When n <= 100 and bg.thresh == -Inf option bstyle is ignored. Remark: bground=" is equivalent

to -Inf that is all trajectories are considered relevant.

tag

Plot handle. String which identifies the handle of the plot which is about to be created. The default is to use tag 'pl\_resfwd'. Notice that if the program finds a plot which has a tag equal to the one specified by the user, then the output of the new plot overwrites the existing one in the same window else a new window is created.

datatooltip

Interactive clicking. It is inactive if this parameter is missing or empty. The default is datatooltip=TRUE, i.e. the user can select with the mouse an individual residual trajectory in order to have information about the corresponding unit. The information displayed depends on the estimator in use.

For example for class fsreda.object the information concerns the label and the step of the search in which the unit enters the subset. If datatooltip is a list it may contain the following fields:

- DisplayStyle determines how the data cursor displays. Possible values are 'datatip' and 'window' (default). 'datatip' displays data cursor information in a small yellow text box attached to a black square marker at a data point you interactively select. 'window' displays data cursor information for the data point you interactively select in a floating window within the figure.
- 2. SnapToDataVertex: specifies whether the data cursor snaps to the nearest data value or is located at the actual pointer position. Possible values are SnapToDataVertex='on' (default) and SnapToDataVertex='off'.
- 3. LineColor: controls the color of the trajectory selected with the mouse. It can be an RGB triplet of values between 0 and 1, or character vector indicating a color name. Note that a RGB vector can be conveniently chosen with our MATLAB class FSColor, see documentation.
- 4. SubsetLinesColor: enables to control the color of the trajectories of the units that are in the subset at a given step of the search (if resfwdplot() is applied to an object of class fsreda.object) or have a weight greater than 0.9 (if resfwdplot() is applied to an object of class sregeda.object or mmregeda.object). This can be done (repeatedly) with a left mouse click in proximity of the step of interest. A right mouse click will terminate the selection by marking with a up-arrow the step corresponding to the highlighted lines. The highlighted lines by default are in red, but a different color can be specified as RGB triplet or character of color name. Note that a RGB vector can be conveniently chosen with our MATLAB class FSColor, see documentation. By default SubsetLinesColor="", i.e. the modality is not active. Any initialization for SubsetLinesColor which cannot be interpreted as RGB vector will be converted to blue, i.e. SubsetLinesColor will be forced to be [0 0 1]. If SubsetLinesColor is not empty the previous option LineColor is ignored.

label

Character vector containing the labels of the units (optional argument used when datatooltip=TRUE. If this field is not present labels row1, ..., rown will be automatically created and included in the pop up datatooltip window).

nameX

Add variable labels in plot. A vector of strings of length p containing the labels of the variables of the regression dataset. If it is empty (default) the sequence X1,...,Xp will be created automatically

namey

Add response label. A string containing the label of the response

msg

Controls whether to display or not messages on the screen If msg==1 (default) messages are displayed on the screen about step in which signal took place else no message is displayed on the screen.

databrush

interactive mouse brushing. If databrush is missing or empty (default), no brushing is done. The activation of this option (databrush is a scalar or a list) enables the user to select a set of trajectories in the current plot and to see them highlighted in the ylX plot, i.e. a matrix of scatter plots of y against each column of X, grouped according to the selection(s) done by brushing. If the plot ylX does not exist it is automatically created. In addition, brushed units are automatically highlighted in the minimum deletion residual plot if it is already open. The extension to the following plots will be available in future versions of the toolbox:

- 1. monitoring leverage plot;
- 2. maximum studentized residual;
- 3. s^2 and R^2;
- 4. Cook distance and modified Cook distance;
- 5. deletion t statistics.

Note that the window style of the other figures is set equal to that which contains the monitoring residual plot. In other words, if the monitoring residual plot is docked all the other figures will be docked too

If databrush=TRUE the default selection tool is a rectangular brush and it is possible to brush only once (that is persist=").

If databrush=list(...), it is possible to use all optional arguments of function selectdataFS() and the following optional argument:

- 1. persist. Persist is an empty value or a character containing 'on' or 'off'. The default value is persist="", that is brushing is allowed only once. If persist="on" or persis="off" brushing can be done as many time as the user requires. If persist='on' then the unit(s) currently brushed are added to those previously brushed. It is possible, every time a new brushing is done, to use a different color for the brushed units. If persist='off' every time a new brush is performed units previously brushed are removed.
- 2. bivarfitWheather to superimpose bivariate least square lines on the plot (if plot=TRUE. This option adds one or more least squares lines, based on SIMPLE REGRESSION of y on Xi, to the plots of ylXi. The default is bivarfit=FALSE: no line is fitted. If bivarfit=1, a single OLS line is fitted to all points of each bivariate plot in the scatter matrix ylX. If bivarfit=2, two OLS lines are fitted: one to all points and another to the group of the genuine observations. The group of the potential outliers is not fitted. If bivarfit=0 one OLS line is fitted to each group. This is useful for the purpose of fitting mixtures of regression lines. If bivarfit='i1' or bivarfit='i2', etc. an OLS line is fitted to a specific group, the one with index 'i' equal to 1, 2, 3 etc. Again, useful in case of mixtures.
- 3. multivarfitWheather to superimpose multivariate least square lines. This option adds one or more least square lines, based on MULTIVARIATE REGRESSION of y on X, to the plots of ylXi. The default is multivarfit=FALSE: no line is fitted. If bivarfit=1, a single OLS line is fitted to all points of

each bivariate plot in the scatter matrix y|X. The line added to the scatter plot y|Xi is avconst + Ci\*Xi, where Ci is the coefficient of Xi in the multivariate regression and avconst is the effect of all the other explanatory variables different from Xi evaluated at their centroid (that is overline(y)'C)). If multivarfit=2, same action as with multivarfit=1 but this time we also add the line based on the group of unselected observations (i.e. the normal units).

4. labeladdAdd outlier labels in plot. If labeladd=TRUE, we label the outliers with the unit row index in matrices X and y. The default value is labeladd=FALSE, i.e. no label is added.

standard

(MATLAB-style arguments) appearance of the plot in terms of xlim, ylim, axes labels and their font size style, color of the lines, etc.

fground

MATLAB-style arguments for the fground trajectories in foregroud.

bground

MATLAB-style arguments for the fground trajectories in backgroud.

. . . potential further arguments passed to lower level functions.

## **Details**

No details

### Value

No value returned

## Author(s)

FSDA team

```
## Not run:

n <- 100
y <- rnorm(n)
X <- matrix(rnorm(n*4), nrow=n)

out <- fsreg(y~X, method="LTS")
out <- fsreg(y~X, method="FS", bsb=out$bs, monitoring=TRUE)
resfwdplot(out)

## End(Not run)</pre>
```

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resindexplot	Plots the residuals from a regression analysis versus index number or any other variable

# Description

The function resindexplot() plots the residuals from a regression analysis versus index number or any other variable. The residuals come from an output object of any of the regression functions or a simply a vector of values. In order to use the databrush option, the residuals must come from one of the fsdaR regression functions.

# Usage

```
resindexplot(out, x, xlim, ylim, xlab, ylab, main, numlab, indlab, conflev, cex.axis,
      cex.lab, lwd, nameX, namey, tag, col, cex, databrush, ...)
```

# **Arguments**

out	A vector containing the residuals from a regression analysis or an object returned by one of the regression functions (see FSR_control, LXS_control, Sreg_control and MMreg_control). The object is one of fsr.object, fsdalts.object, fsdalms.object, sreg.object or mmreg.object. The needed elements of out are at least residuals, but if the option databrush is used, also X amd y will be needed.
x	The vector to be plotted on the x-axis. As default the sequence 1:length(residuals) will be used
xlim	Control x scale in plot. Vector with two elements controlling minimum and maximum on the x axis. Default is to use automatic scale.
ylim	Control y scale in plot. Vector with two elements controlling minimum and maximum on the y axis. Default is to use automatic scale.
xlab	a title for the x axis
ylab	a title for the y axis
main	an overall title for the plot
numlab	Number of points to be identified in plots (see also indlab). By default the five points with largest values will be identified. If numlab is a single number containing scalar k, the units with the k largest residuals are labelled in the plots. If numlab is a vector, the units inside vector numlab are labelled in the plots. The default value of numlab=5 and the units with the 5 largest residuals will be labelled. If numlib=0 or numlib=NULL no labelling will be done.
indlab	Which points to be identified in plots (see also numlab) - the units with indexes in the vector indlab are labelled in the plots.
conflev	Confidence interval for the horizontal bands (a numeric vector). It can be a vector of different confidence level values.
	Remark: confidence interval is based on the chi^2 distribution

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cex.axis The magnification to be used for axis annotation relative to the current setting of cex

cex.lab The magnification to be used for x and y labels relative to the current setting of

1wd The line width, a positive number, defaulting to 1

Figure tag (character). Tag of the figure which will host the resindexplot. The default tag iscodepl\_resindex.

Fill color for markers that are closed shapes (circle, square, diamond, pentagram, hexagram, and the four triangles). Can be 'none' or 'auto' or color name(string) or RGB triplet.

Size of the point symbols. The magnification to be used relative to the current setting of cex.

Add variable labels in plot. A vector of strings of length p containing the labels of the variables of the regression dataset. If it is empty (default) the sequence X1,...,Xp will be created automatically

Add response label. A string containing the label of the response

Interactive mouse brushing. If databrush is missing or empty (default) or databrush=FALSE, no brushing is done. The activation of this option (databrush is a scalar or a list) enables the user to select a set of trajectories in the current plot and to see them highlighted in the ylX plot, i.e. a matrix of scatter plots of y against each column of X, grouped according to the selection(s) done by brushing. If the plot ylX does not exist it is automatically created. In addition, brushed units are automatically highlighted in the minimum deletion residual plot if it is already open. The extension to the following plots will be available in future versions of the package:

- 1. monitoring leverage plot;
- 2. maximum studentized residual;
- 3. s^2 and R^2:
- 4. Cook distance and modified Cook distance;
- 5. deletion t statistics.

Note that the window style of the other figures is set equal to that which contains the monitoring residual plot. In other words, if the monitoring residual plot is docked all the other figures will be docked too

If databrush=TRUE the default selection tool is a rectangular brush and it is possible to brush only once (that is persist=").

If databrush=list(...), it is possible to use all optional arguments of function selectdataFS() and the following optional argument:

1. persist: Persist is an empty value or a character containing 'on' or 'off'. The default value is persist="", that is brushing is allowed only once. If persist="on" or persis="off" brushing can be done as many time as the user requires. If persist='on' then the unit(s) currently brushed are added to those previously brushed. It is possible, every time a new brushing is done, to use a different color for the brushed units. If persist='off' every time a new brush is performed units previously brushed are removed.

cex

col

nameX

namey

databrush

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2. bivarfit: This option adds one or more least square lines based on SIMPLE REGRESSION to the plots of ylX, depending on the selected groups. The default is bivarfit=FALSE: no line is fitted. If bivarfit=1, a single OLS line is fitted to all points of each bivariate plot in the scatter matrix ylX. If bivarfit=2, two OLS lines are fitted: one to all points and another to the group of the genuine observations. The group of the potential outliers is not fitted. If bivarfit=0 one OLS line is fitted to each group. This is useful for the purpose of fitting mixtures of regression lines. If bivarfit='i1' or bivarfit='i2', etc. an OLS line is fitted to a specific group, the one with index 'i' equal to 1, 2, 3 etc. Again, useful in case of mixtures.

- 3. multivarfit: Wheather to superimpose multivariate least square lines. This option adds one or more least square lines, based on MULTIVARIATE REGRESSION of y on X, to the plots of y|Xi. The default is multivarfit=FALSE: no line is fitted. If bivarfit=1, a single OLS line is fitted to all points of each bivariate plot in the scatter matrix y|X. The line added to the scatter plot y|Xi is avconst + Ci\*Xi, where Ci is the coefficient of Xi in the multivariate regression and avconst is the effect of all the other explanatory variables different from Xi evaluated at their centroid (that is overline(y)'C)). If multivarfit=2, same action as with multivarfit=1 but this time we also add the line based on the group of unselected observations (i.e. the normal units).
- 4. labeladd: Add outlier labels in plot. If labeladd=TRUE, we label the outliers with the unit row index in matrices X and y. The default value is labeladd=FALSE, i.e. no label is added.

potential further arguments passed to lower level functions.

#### **Details**

No details

## Value

No value returned

#### Author(s)

FSDA team

```
## Not run:
out <- fsreg(stack.loss~., data=stackloss)
resindexplot(out, conflev=c(0.95,0.99), col="green")
## End(Not run)</pre>
```

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smult

Computes S estimators in multivariate analysis

#### **Description**

Computes S estimators in multivariate analysis

#### Usage

```
smult(x, monitoring = FALSE, plot = FALSE, bdp, nsamp,
 conflev = 0.975, nocheck = FALSE, trace = FALSE, ...)
```

### **Arguments**

An n x p data matrix (n observations and p variables). Rows of x represent observations, and columns represent variables.

Missing values (NA's) and infinite values (Inf's) are allowed, since observations (rows) with missing or infinite values will automatically be excluded from the computations.

monitoring

Wheather to perform monitoring of Mahalanobis distances and other specific quantities

plot

Plots the Mahalanobis distances against index number. If plot=FALSE (default) or plot=0 no plot is produced. The confidence level used to draw the confidence bands for the MD is given by the input option confley. If confley is not specified a nominal 0.975 confidence interval will be used. If plot=2 a scatter plot matrix with the outliers highlighted is produced. If plot is a list it may contain the following fields:

- labeladd If labeladd=1, the outliers in the spm are labelled with the unit row index. The default value is labeladd="", i.e. no label is added
- nameY character vector containing the labels of the variables. As default value, the labels which are added are Y1, ... Yp.

bdp

Measures the fraction of outliers the algorithm should resist. In this case any value greater than 0 but smaller or equal than 0.5 will do fine (default is bdp=0.5). Note that given bdp nominal efficiency is automatically determined.

nsamp

Number of subsamples which will be extracted to find the robust estimator. If nsamp=0 all subsets will be extracted. They will be (n choose p). If the number of all possible subset is <1000 the default is to extract all subsets otherwise just

conflev

confidence interval for the horizontal bands. It can be a vector of different confidence level values, e.g. c(0.95, 0.99, 0.999). The confidence interval is based on the chi^2 distribution.

nocheck

It controls whether to perform checks on matrix Y. If nocheck=TRUE, no check is performed.

trace

Whether to print intermediate results. Default is trace=FALSE.

potential further arguments passed to lower level functions.

Х

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#### **Details**

This function follows the lines of MATLAB/R code developed during the years by many authors. For more details see http://www.econ.kuleuven.be/public/NDBAE06/programs/ and the R package CovSest The core of these routines, e.g. the resampling approach, however, has been completely redesigned, with considerable increase of the computational performance.

#### Value

Depending on the input parameter monitoring, one of the following objects will be returned:

```
    smult.object
    smulteda.object
```

#### Author(s)

FSDA team, <valentin.todorov@chello.at>

#### References

Maronna, R.A., Martin D. and Yohai V.J. (2006), Robust Statistics, Theory and Methods, Wiley, New York.

## **Examples**

```
## Not run:
data(hbk)
(out <- smult(hbk[,1:3]))</pre>
class(out)
summary(out)
## Generate contaminated data (200,3)
n <- 200
p <- 3
set.seed(123456)
X <- matrix(rnorm(n*p), nrow=n)</pre>
Xcont <- X
Xcont[1:5, ] \leftarrow Xcont[1:5,] + 3
out1 <- smult(Xcont, trace=TRUE)</pre>
                                             # no plots (plot defaults to FALSE)
names(out1)
## plot=TRUE - generates: (1) a plot of Mahalanobis distances against
      index number. The confidence level used to draw the confidence bands for
##
      the MD is given by the input option conflev. If conflev is
##
      not specified a nominal 0.975 confidence interval will be used and
      (2) a scatter plot matrix with the outliers highlighted.
(out1 <- smult(Xcont, trace=TRUE, plot=TRUE))</pre>
## plots is a list: the spm shows the labels of the outliers.
```

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```
(out1 <- smult(Xcont, trace=TRUE, plot=list(labeladd="1")))</pre>
 ## plots is a list: the spm uses the variable names provided by 'nameY'.
 (out1 <- smult(Xcont, trace=TRUE, plot=list(nameY=c("A", "B", "C"))))</pre>
 ## smult() with monitoring
 (out2 <- smult(Xcont, monitoring=TRUE, trace=TRUE))</pre>
names(out2)
## Forgery Swiss banknotes examples.
data(swissbanknotes)
 (out1 <- smult(swissbanknotes[101:200,], plot=TRUE))</pre>
(out1 <- smult(swissbanknotes[101:200,], plot=list(labeladd="1")))</pre>
## End(Not run)
```

smult.object

Description of smult.object Objects

# Description

An object of class smult. object holds information about the result of a call to smult.

## Value

The object itself is basically a list with the following components:

loc	p-by-1 vector containing S estimate of location.
shape	p-by-p matrix containing robust estimate of the shape matrix. Remark: detlshapel=1.
scale	robust estimate of the scale.
cov	scale^2 * shape: robust estimate of covariance matrix.
bs	a (p+1) vector containing the units forming best subset associated with S estimate of location.
md	n-by-1 vector containing the estimates of the robust Mahalanobis distances (in squared units). This vector contains the distances of each observation from the location of the data, relative to the scatter matrix cov.
outliers	A vector containing the list of the units declared as outliers using confidence level specified in input scalar conflev.
conflev	Confidence level that was used to declare outliers.
singsub	Number of subsets without full rank. Notice that singsub > 0.1*(number of subsamples) produces a warning.
weights	n x 1 vector containing the estimates of the weights.
Χ	the data matrix X

The object has class "smult".

smulteda.object 75

# **Examples**

```
## Not run:
data(hbk)
(out <- smult(hbk[,1:3]))
class(out)
summary(out)

## End(Not run)</pre>
```

smulteda.object

Description of smulteda.object Objects

# Description

An object of class smulteda.object holds information about the result of a call to smult with monitoring=TRUE.

## Value

The object itself is basically a list with the following components:

Loc	length(bdp)-by-p matrix containing S estimate of location for each value of bdp.
Shape	p-by-p-by-length(bdp) 3D array containing robust estimate of the shape for each value of bdp. Remark: det shape =1.
Scale	length(bdp) vector containing robust estimate of the scale for each value of bdp.
Cov	p-by-p-by-length(bdp) 3D array containing robust estimate of covariance matrix for each value of bdp. Note that $scale(i)^2 * shape[,,i] = robust$ estimate of covariance matrix.
Bs	(p+1)-by-length(bdp) matrix containing the units forming best subset for each value of bdp.
MAL	n-by-length(bdp) matrix containing the estimates of the robust Mahalanobis distances (in squared units) for each value of bdp.
Outliers	n-by-length(bdp) matrix containing flags for the outliers. Boolean matrix containing the list of the units declared as outliers for each value of bdp using confidence level specified in input scalar conflev
Weights	n x length(bdp) matrix containing the weights for each value of bdp.
conflev	Confidence level that was used to declare outliers.
singsub	Number of subsets without full rank. Notice that singsub > 0.1*(number of subsamples) produces a warning.
bdp	vector which contains the values of bdp which have been used.
Χ	the data matrix X.

The object has class "smulteda".

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## **Examples**

```
## Not run:
    data(hbk)
    (out <- smult(hbk[,1:3], monitoring=TRUE))
    class(out)
    summary(out)
## End(Not run)</pre>
```

sreg.object

Description of sreg Objects

## **Description**

An object of class sreg. object holds information about the result of a call to fsreg.

#### Value

The object itself is basically a list with the following components:

p-by-1 vector containing the estimated regression parameters (in step n-k).

scale scalar containing the estimate of the scale (sigma).

bs p x 1 vector containing the units forming best subset associated with S estimate

of regression coefficient.

residuals residuals.
fittedvalues fitted values.

outliers kx1 vector containing the list of the k units declared as outliers or NULL if the

sample is homogeneous.

conflev Confidence level which is used to declare units as outliers. Usually conflev=0.95,0.975,0.99

(individual alpha) or conflev=1-0.05/n,1-0.025/n,1-0.01/n (simultaneous

alpha). Default value is 0.975

singsub Number of subsets without full rank. Notice that singsub > 0.1\*(number of

subsamples) produces a warning

weights n x 1 vector containing the estimates of the weights

rhofunc Specifies the rho function which has been used to weight the residuals.

rhofuncparam Vector which contains the additional parameters for the specified rho function

which has been used. For hyperbolic rho function the value of k =sup CVC. For

Hampel rho function the parameters a, b and c.

X the data matrix X y the response vector y

The object has class "sreg".

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## **Examples**

```
## Not run:
    (out <- fsreg(Y~., data=hbk, method="S"))
    class(out)
    summary(out)

## End(Not run)</pre>
```

sregeda.object

Description of sregeda Objects

# Description

An object of class sregeda.object holds information about the result of a call to fsreg when method="S" and monitoring=TRUE.

## Value

The object itself is basically a list with the following components:

Beta	matrix containing the S estimator of regression coefficients for each value of bdp.
Scale	vector containing the estimate of the scale (sigma) for each value of bdp. This is the value of the objective function.
BS	p x 1 vector containing the units forming best subset associated with S estimate of regression coefficient.
RES	n x length(bdp) matrix containing the monitoring of scaled residuals for each value of bdp.
Weights	n x length(bdp) matrix containing the estimates of the weights for each value of bdp
Outliers	Boolean matrix containing the list of the units declared as outliers for each value of bdp using confidence level specified in input scalar conflev.
conflev	Confidence level which is used to declare units as outliers. Remark: conflev will be used to draw the horizontal line (confidence band) in the plot.
Singsub	Number of subsets without full rank. Notice that singsub[bdp[jj]] $> 0.1*$ (number of subsamples) produces a warning
rhofunc	Specifies the rho function which has been used to weight the residuals.
rhofuncparam	Vector which contains the additional parameters for the specified rho function which has been used. For hyperbolic rho function the value of k =sup CVC. For Hampel rho function the parameters a, b and c.
Χ	the data matrix X
У	the response vector y

The object has class "sregeda".

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## **Examples**

```
## Not run:
    (out <- fsreg(Y~., data=hbk, method="S", monitoring=TRUE))
    class(out)
    summary(out)
## End(Not run)</pre>
```

Sregeda\_control

Creates an Sregeda\_control object

## **Description**

Creates an object of class Sregeda\_control to be used with the fsreg() function, containing various control parameters.

## Usage

```
Sregeda_control(intercept = TRUE, bdp = seq(0.5, 0.01, -0.01),
    rhofunc = c("bisquare", "optimal", "hyperbolic", "hampel"), rhofuncparam,
    nsamp = 1000, refsteps = 3, reftol = 1e-06, refstepsbestr = 50, reftolbestr = 1e-08,
    minsctol = 1e-07, bestr = 5,
    conflev, msg = TRUE, nocheck = FALSE, plot = FALSE)
```

## **Arguments**

intercept

 $Indicator\ for\ constant\ term.\ Scalar.\ If\ intercept=TRUE,\ a\ model\ with\ constant$ 

term will be fitted (default), else, no constant term will be included.

bdp

Breakdown point. It measures the fraction of outliers the algorithm should resist. In this case any value greater than 0 but smaller or equal than 0.5 will do fine.

The default value of bdp is a sequence from 0.5 to 0.01 with step 0.01

rhofunc

Specifies the rho function which must be used to weight the residuals. Possible values are 'bisquare' 'optimal' 'hyperbolic' 'hampel'.

- 1. 'bisquare' uses Tukey's rho and psi functions. See TBrho and TBpsi.
- 2. 'optimal' uses optimal rho and psi functions. See OPTrho and OPTpsi.
- 3. 'hyperbolic' uses hyperbolic rho and psi functions. See HYPrho and HYPpsi.
- 4. 'hampel' uses Hampel rho and psi functions. See HArho and HApsi.

The default is 'bisquare'.

rhofuncparam

Additional parameters for the specified rho function. For hyperbolic rho function it is possible to set up the value of  $k = \sup CVC$  (the default value of k is 4.5).

For Hampel rho function it is possible to define parameters a, b and c (the default values are a=2, b=4, c=8)

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nsamp Number of subsamples which will be extracted to find the robust estimator,

scalar. If nsamp=0 all subsets will be extracted. They will be (n choose p). If the number of all possible subset is <1000 the default is to extract all subsets

otherwise just 1000.

refsteps Number of refining iterations in each subsample (default is refsteps=3). refsteps

= 0 means "raw-subsampling" without iterations.

reftol Tolerance for the refining steps. The default value is 1e-6

refstepsbestr Scalar defining number of refining iterations for each best subset (default = 50).

Tolerance for the refining steps for each of the best subsets. The default value is

reftolbestr=1e-8.

minsctol Value of tolerance for the iterative procedure for finding the minimum value of

the scale for each subset and each of the best subsets (It is used by subroutine

minscale.m). The default value is minsctol=1e-7.

bestr Defins the number of "best betas" to remember from the subsamples. These will

be later iterated until convergence (default is bestr=5).

conflev Confidence level which is used to declare units as outliers. Usually conflev=0.95,

0.975, 0.99 (individual alpha) or conflev=1-0.05/n, 1-0.025/n, 1-0.01/n (simul-

taneous alpha). Default value is 0.975

msg Controls whether to display or not messages on the screen If msg==1 (default)

messages are displayed on the screen about step in which signal took place else

no message is displayed on the screen.

nocheck Check input arguments, scalar. If nocheck=TRUE no check is performed on ma-

trix y and matrix X. Notice that y and X are left unchanged. In other words the additional column of ones for the intercept is not added. As default nocheck=FALSE.

plot Plot on the screen. Scalar. If plots=TRUE the plot of minimum deletion resid-

ual with envelopes based on n observations and the scatterplot matrix with the outliers highlighted is produced. If plots=2 the user can also monitor the intermediate plots based on envelope superimposition. If plots=FALSE (default) no

plot is produced.

#### **Details**

Creates an object of class Sregeda\_control to be used with the fsreg() function, containing various control parameters.

# Value

An object of class "Sregeda\_control" which is basically a list with components the input arguments of the function mapped accordingly to the corresponding Matlab function.

## Author(s)

FSDA team

## See Also

See Also as FSR\_control, MMreg\_control and LXS\_control

Sreg\_control

## **Examples**

Sreg\_control

Creates an Sreg\_control object

# Description

Creates an object of class Sreg\_control to be used with the fsreg() function, containing various control parameters for calling the MATLAB function Sreg().

## Usage

```
Sreg_control(intercept = TRUE, bdp = 0.5,
    rhofunc = c("bisquare", "optimal", "hyperbolic", "hampel"), rhofuncparam,
    nsamp = 1000, refsteps = 3, reftol = 1e-06, refstepsbestr = 50, reftolbestr = 1e-08,
    minsctol = 1e-07, bestr = 5,
    conflev, msg = TRUE, nocheck = FALSE, plot = FALSE)
```

## **Arguments**

intercept Indicator for constant term. Scalar. If intercept=TRUE, a model with constant

term will be fitted (default), else, no constant term will be included.

bdp Breakdown point. It measures the fraction of outliers the algorithm should resist.

In this case any value greater than 0 but smaller or equal than 0.5 will do fine.

Note that given bdp nominal efficiency is automatically determined.

rhofunc Specifies the rho function which must be used to weight the residuals. Possible

values are 'bisquare' 'optimal' 'hyperbolic' 'hampel'.

1. 'bisquare' uses Tukey's rho and psi functions. See TBrho and TBpsi.

- 2. 'optimal' uses optimal rho and psi functions. See OPTrho and OPTpsi.
- 3. 'hyperbolic' uses hyperbolic rho and psi functions. See HYPrho and HYPpsi.
- 4. 'hampel' uses Hampel rho and psi functions. See HArho and HApsi.

The default is 'bisquare'.

rhofuncparam

Additional parameters for the specified rho function. For hyperbolic rho function it is possible to set up the value of  $k = \sup CVC$  (the default value of k is 4.5).

For Hampel rho function it is possible to define parameters a, b and c (the default values are a=2, b=4, c=8)

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nsamp Number of subsamples which will be extracted to find the robust estimator,

scalar. If nsamp=0 all subsets will be extracted. They will be (n choose p). If the number of all possible subset is <1000 the default is to extract all subsets

otherwise just 1000.

refsteps Number of refining iterations in each subsample (default is refsteps=3). refsteps

= 0 means "raw-subsampling" without iterations.

reftol Tolerance for the refining steps. The default value is 1e-6

refstepsbestr Scalar defining number of refining iterations for each best subset (default = 50).

Tolerance for the refining steps for each of the best subsets. The default value is

reftolbestr=1e-8.

minsctol Value of tolerance for the iterative procedure for finding the minimum value of

the scale for each subset and each of the best subsets (It is used by subroutine

minscale.m). The default value is minsctol=1e-7.

bestr Defins the number of "best betas" to remember from the subsamples. These will

be later iterated until convergence (default is bestr=5).

conflev Confidence level which is used to declare units as outliers. Usually conflev=0.95,

0.975, 0.99 (individual alpha) or conflev=1-0.05/n, 1-0.025/n, 1-0.01/n (simul-

taneous alpha). Default value is 0.975

msg Controls whether to display or not messages on the screen If msg==1 (default)

messages are displayed on the screen about step in which signal took place else

no message is displayed on the screen.

nocheck Check input arguments, scalar. If nocheck=TRUE no check is performed on ma-

trix y and matrix X. Notice that y and X are left unchanged. In other words the additional column of ones for the intercept is not added. As default nocheck=FALSE.

plot Plot on the screen. Scalar. If plots=TRUE the plot of minimum deletion resid-

ual with envelopes based on n observations and the scatterplot matrix with the outliers highlighted is produced. If plots=2 the user can also monitor the intermediate plots based on envelope superimposition. If plots=FALSE (default) no

plot is produced.

#### **Details**

Creates an object of class Sreg\_control to be used with the fsreg() function, containing various control parameters.

# Value

An object of class "Sreg\_control" which is basically a list with components the input arguments of the function mapped accordingly to the corresponding Matlab function.

## Author(s)

FSDA team

## See Also

See Also as FSR\_control, MMreg\_control and LXS\_control

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## **Examples**

```
## Not run:
(out <- fsreg(Y~., data=hbk, method="S", control=Sreg_control(bdp=0.25, nsamp=500)))
## End(Not run)</pre>
```

summary.fsdalms

Summary Method for fsdalms objects

## **Description**

summary method for class "fsdalms".

# Usage

## **Arguments**

```
object, x an object of class "fsdalms" (or "summary.fsdalms"); usually, a result of a call to fsreg.

correlation logical; if TRUE, the correlation matrix of the estimated parameters is returned and printed.

digits the number of significant digits to use when printing.

signif.stars logical indicating if "significance stars" should be printer, see printCoefmat.

further arguments passed to or from other methods.
```

#### **Details**

summary.fsdalms(), the S3 method, simply returns an (S3) object of class "summary.fsdalms" for which there's a print method:

print.summary.fsdalms prints summary statistics for the forward search (FS) regression estimates. While the function print.fsdalms prints only the robust estimates of the coefficients, print.summary.fsdalms will print also the regression table.

#### Value

summary.fsdalms returns an summary.fsdalms object, whereas the print methods returns its first argument via invisible, as all print methods do.

## See Also

```
fsreg, summary
```

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## **Examples**

```
## Not run:

data(Animals, package = "MASS")
brain <- Animals[c(1:24, 26:25, 27:28),]
lbrain <- log(brain)
  (fs <- fsreg(brain~body, data=lbrain, method="LTS"))
  summary(fs)

## compare to the result of ltsReg() from 'robustbase'
  (lts <- ltsReg(brain~body, data=lbrain))
  summary(lts)

## End(Not run)</pre>
```

summary.fsdalts

Summary Method for fsdalts objects

# **Description**

summary method for class "fsdalts".

## Usage

#### **Arguments**

object, x an object of class "fsdalts" (or "summary.fsdalts"); usually, a result of a call to fsreg.

correlation logical; if TRUE, the correlation matrix of the estimated parameters is returned and printed.

digits the number of significant digits to use when printing.

signif.stars logical indicating if "significance stars" should be printer, see printCoefmat.

further arguments passed to or from other methods.

#### **Details**

summary.fsdalts(), the S3 method, simply returns an (S3) object of class "summary.fsdalts" for which there's a print method:

print.summary.fsdalts prints summary statistics for the forward search (FS) regression estimates. While the function print.fsdalts prints only the robust estimates of the coefficients, print.summary.fsdalts will print also the regression table.

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## Value

summary.fsdalts returns an summary.fsdalts object, whereas the print methods returns its first argument via invisible, as all print methods do.

## See Also

```
fsreg, summary
```

## **Examples**

```
## Not run:

data(Animals, package = "MASS")
brain <- Animals[c(1:24, 26:25, 27:28),]
lbrain <- log(brain)
  (fs <- fsreg(brain~body, data=lbrain, method="LTS"))
  summary(fs)

## compare to the result of ltsReg() from 'robustbase'
  (lts <- ltsReg(brain~body, data=lbrain))
  summary(lts)

## End(Not run)</pre>
```

summary.fsr

Summary Method for FSR objects

# Description

```
summary method for class "fsr".
```

# Usage

# **Arguments**

```
object, x an object of class "fsr" (or "summary.fsr"); usually, a result of a call to fsreg.
correlation logical; if TRUE, the correlation matrix of the estimated parameters is returned and printed.

digits the number of significant digits to use when printing.
signif.stars logical indicating if "significance stars" should be printer, see printCoefmat.
... further arguments passed to or from other methods.
```

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#### **Details**

summary.fsr(), the S3 method, simply returns an (S3) object of class "summary.fsr" for which there's a print method:

print.summary.fsr prints summary statistics for the forward search (FS) regression estimates. While the function print.fsr prints only the robust estimates of the coefficients, print.summary.fsr will print also the regression table.

## Value

summary.fsr returns an summary.fsr object, whereas the print methods returns its first argument via invisible, as all print methods do.

#### See Also

```
fsreg, summary
```

## **Examples**

```
## Not run:

data(Animals, package = "MASS")
brain <- Animals[c(1:24, 26:25, 27:28),]
lbrain <- log(brain)
  (fs <- fsreg(brain~body, data=lbrain, method="FS"))
  summary(fs)

## End(Not run)</pre>
```

swissbanknotes

Swiss banknote data

## **Description**

Six variables measured on 100 genuine and 100 counterfeit old (printed before the second world war) Swiss 1000-franc bank notes (Flury and Riedwyl, 1988).

## Usage

```
data(swissbanknotes)
```

# Format

A data frame with 200 observations on the following 7 variables.

```
length Length of bill, mm
left Width of left edge, mm
right Width of right edge, mm
```

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```
bottom Bottom margin width, mm
top Top margin width, mm
diagonal Length of image diagonal, mm
class 1 = genuine, 2 = counterfeit
```

#### **Source**

Flury, B. and Riedwyl, H. (1988). *Multivariate Statistics: A practical approach*. London: Chapman & Hall.

#### References

Weisberg, S. (2005). Applied Linear Regression, 3rd edition. New York: Wiley, Problem 12.5.

## **Examples**

```
data(swissbanknotes)
head(swissbanknotes)
plot(CovMcd(swissbanknotes[, 1:6]), which="pairs", col=swissbanknotes$class)
```

swissheads

Swiss banknote data

## **Description**

Six dimensions in millimetres of the heads of 200 twenty year old Swiss soldiers (Flury and Riedwyl, 1988, p. 218 and also Flury, 1997, p. 6).

The data were collected to determine the variability in size and shape of heads of young men in order to help in the design of a new protection mask for the Swiss army.

## Usage

```
data(swissheads)
```

## **Format**

A data frame with 200 observations on the following 6 variables.

```
minimal_frontal_breadth Minimal frontal breadth, mm
breadth_angulus_mandibulae Breadth of angulus mandibulae, mm
true_facial_height True facial height, mm
length_glabella_nasi Length from glabella to apex nasi, mm
length_tragion_nasion Length from tragion to nasion, mm
length_tragion_gnathion Length from tragion to gnathion, mm
```

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## **Source**

Flury, B. and Riedwyl, H. (1988). *Multivariate Statistics: A practical approach*. London: Chapman & Hall.

## References

Atkinson, A. C., Riani, M. and Cerioli, A. (2004) *Exploring multivariate data with the forward search*, New York: Springer-Verlag.

# **Examples**

```
data(swissheads)
head(swissheads)
plot(CovMcd(swissheads), which="pairs")
```

tclusteda.object

Objects returned by the function tclustfsda with the option monitoring=TRUE

# **Description**

An object of class tclusteda.object holds information about the result of a call to tclustfsda with the option monitoring=TRUE.

## Value

The functions print() and summary() are used to obtain and print a summary of the results. An object of class tclusteda is a list containing at least the following components:

call	the matched call
k	number of groups
alpha	trimming level
restrfactor	restriction factor
IDX	an n-by-length(alpha) vector containing assignment of each unit to each of the k groups. Cluster names are integer numbers from 1 to k. 0 indicates trimmed observations. The first column refers to alpha[1], the second column refers to alpha[2],, the last column refers to alpha[length(alpha)].
MU	a 3 dimensional array of size k-by-p-by-length(alpha) containing the monitoring of the centroid for each value of alpha. MU[,,1], refers to alpha[1], MU(,,length(alpha)] refers to alpha[length(alpha)]. The first row in each slice refers to group 1, second row refers to group 2, etc.
SIGMA	A list of length length(alpha) containing in element j, with j=1,2,,length(alpha), the 3D array of size p-by-p-by-k containing the k (constrained) estimated covari-

ance matrices associated with alpha[j].

Amon

Amon stands for alpha monitoring. Matrix of size (length(alpha)-1)-by-4 which contains for two consecutive values of alpha the monitoring of three quantities (change in classification, change in centroid location, change in covariance location).

- 1st col = value of alpha.
- 2nd col = ARI index.
- 3rd col = squared Euclidean distance between centroids.
- 4th col = squared Euclidean distance between covariance matrices.

## **Examples**

```
## Not run:
data(hbk)
  (out <- tclustfsda(hbk[, 1:3], k=2, monitoring=TRUE))
class(out)
summary(out)
## End(Not run)</pre>
```

tclustfsda

Computes trimmed clustering with scatter restrictions

# Description

Partitions the points in the n-by-v data matrix Y into k clusters. This partition minimizes the trimmed sum, over all clusters, of the within-cluster sums of point-to-cluster-centroid distances. Rows of Y correspond to points, columns correspond to variables. Returns in the output object of class tclustfsda.object an n-by-1 vector idx containing the cluster indices of each point. By default, tclustfsda() uses (squared), possibly constrained, Mahalanobis distances.

# Usage

```
tclustfsda(x, k, alpha, restrfactor = 12, monitoring = FALSE,
  plot = FALSE, nsamp, refsteps = 15, reftol = 1e-13,
  equalweights = FALSE, mixt = 0, msg = TRUE, nocheck = FALSE,
  startv1 = 1, restrtype = c("eigen", "deter"), UnitsSameGroup,
  numpool, cleanpool, trace = FALSE, ...)
```

# **Arguments**

Χ

An n x p data matrix (n observations and p variables). Rows of x represent observations, and columns represent variables.

Missing values (NA's) and infinite values (Inf's) are allowed, since observations (rows) with missing or infinite values will automatically be excluded from the computations.

k

Number of groups.

alpha

A scalar between 0 and 0.5 or an integer specifying the number of observations which have to be trimmed. If alpha=0, tclust reduces to traditional model based or mixture clustering (mclust): see for example the Matlab function gmdistribution.

More in detail, if 0 < alpha < 1 clustering is based on h = fix(n \* (1-alpha)) observations, else if alpha is an integer greater than 1 clustering is based on h = n - floor(alpha). If monitoring=TRUE, alpha is a vector which specifies the values of trimming levels which have to be considered - contains decresing elements which lie in the interval 0 and 0.5. For example if alpha = c(0.1, 0.05, 0), tclust() considers these 3 values of trimming level. The default for alpha is vector alpha = c(0.1, 0.05, 0). The sequence is forced to be monotonically decreasing.

restrfactor

Positive scalar which constrains the allowed differences among group scatters. Larger values imply larger differences of group scatters. On the other hand a value of 1 specifies the strongest restriction forcing all eigenvalues/determinants to be equal and so the method looks for similarly scattered (respectively spherical) clusters. The default is to apply restrfactor to eigenvalues. In order to apply restrfactor to determinants it is is necessary to use optional input argument restrtype.

monitoring

If monitoring=TRUE TCLUST is performed for a series of values of the trimming factor alpha given k (number of groups) and given c (restriction factor). In order to increase the speed of the computations, *parfor* is used.

plot

If plot=FALSE (default) or plot=0 no plot is produced. If plot=TRUE and monitoring=FALSE a plot with the classification is shown (using the spmplot function). The plot can be:

- for p = 1, a histogram of the univariate data,
- for p = 2, a bivariate scatterplot,
- for p > 2, a scatterplot matrix generated by the MATLAB function spmplot().

When  $p \ge 2$  the following additional features are offered (for p = 1 the behaviour is forced to be as for plots=TRUE):

- plot = 'contourf' adds in the background of the bivariate scatterplots a filled contour plot. The colormap of the filled contour is based on grey levels as default. This argument may also be inserted in a field named 'type' of a list. In the latter case it is possible to specify the additional field 'cmap', which changes the default colors of the color map used. The field 'cmap' may be a three-column matrix of values in the range [0,1] where each row is an RGB triplet that defines one color. Check the colormap function for additional informations.
- plot = 'contour' adds in the background of the bivariate scatterplots a contour plot. The colormap of the contour is based on grey levels as default. This argument may also be inserted in a field named type of a list. In the latter case it is possible to specify the additional field cmap, which changes the default colors of the color map used. The field cmap may be a three-column matrix of values in the range [0,1] where each row is an RGB triplet that defines one color. Check the colormap() (MATLAB) function for additional information.

• plot = 'ellipse' superimposes confidence ellipses to each group in the bivariate scatterplots. The size of the ellipse is qchisq(0.95,2), i.e. the confidence level used by default is 95 percent. This argument may also be inserted in a field named type of a list. In the latter case it is possible to specify the additional field conflev, which specifies the confidence level to use and it is a value between 0 and 1.

• plot = 'boxplotb' superimposes on the bivariate scatterplots the bivariate boxplots for each group, using the boxplotb function. This argument may also be inserted in a field named type of a list.

The parameter plot can be also a list and in this case its elements are:

- type specifies the type of plot as when plot option is a character. Therefore, plots\$type can be one of 'contourf', 'contour', 'ellipse' or 'boxplotb'.
- cmap used to set a colormap for the plot type (MATLAB style). For example, plot\$cmap = 'autumn'. See the MATLAB help of colormap for a list of colormap possiblilites.
- conflev this is the confidence level for the confidence ellipses. It must me a scalar between 0 and 1.

If plot=TRUE and monitoring=TRUE two plots are shown. The first plot (*monitor plot*) shows three panels with the monitoring between two consecutive values of alpha: (i) the change in classification using ARI index (top panel), (ii) the change in centroids using squared euclidean distances (central panel) and (iii) the change in covariance matrices using squared euclidean distance (bottom panel).

The second plot (*gscatter plot*) shows a series of subplots which monitor the classification for each value of alpha. In order to make sure that consistent labels are used for the groups, between two consecutive values of alpha, we assign label r to a group if this group shows the smallest distance with group r for the previous value of alpha. The type of plot which is used to monitor the stability of the classification depends on the data dimensionality p.

- for p = 1, a histogram of the univariate data (the MATLAB function histFS() is called),
- for p = 2, a bivariate scatterplot (the MATLAB function gscatter() is called),
- for p > 2, a scatterplot of the first two principal components (function gscatter() is called and we show on the axes titles the percentage of variance explained by the first two principal components).

Also in the case of monitoring=TRUE the parameter plot can be a list and its elements are:

• name: character vector which enables to specify which plot to display. name = "gscatter" produces a figure with a series of subplots which show the classification for each value of alpha. name = "monitor" shows a figure with three panels which monitor between two consecutive values of alpha the change in classification using ARI index (top panel), the change in centroids using squared euclidean distances (central panel), the change in covariance matrices using squared euclidean distance (bottom panel). If this field is not specified, by default name=c("gscatter", "monitor") and both figures will be shown.

• alphasel: a numeric vector which specifies for which values of alpha it is possible to see the classification. For example if alphasel = c(0.05,0.02), the classification will be shown just for alpha=0.05 and alpha=0.02. If this field is not specified alphasel=alpha and therefore the classification is shown for each value of alpha.

nsamp

If a scalar, it contains the number of subsamples which will be extracted. If nsamp = 0 all subsets will be extracted. Remark - if the number of all possible subset is greater than 300 the default is to extract all subsets, otherwise just 300. If nsamp is a matrix it contains in the rows the indexes of the subsets which have to be extracted. nsamp in this case can be conveniently generated by function subsets(). nsamp can have k columns or k \* (p + 1) columns. If nsamp has k columns the k initial centroids each iteration i are given by X[nsamp[i,],] and the covariance matrices are equal to the identity.

If nsamp has k \* (p + 1) columns, the initial centroids and covariance matrices in iteration i are computed as follows:

- X1 <- X[nsamp[i,],]
- mean(X1[1:p+1, ]) contains the initial centroid for group 1
- cov(X1[1:p + 1, ]) contains the initial cov matrix for group 1
- mean(X1[(p + 2):(2\*p + 2), ]) contains the initial centroid for group 2
- cov(X1[(p+2):(2\*p+2),]) contains the initial cov matrix for group 2
- .
- mean(X1[(k-1)\*p+1):(k\*(p+1), ]) contains the initial centroids for group k
- cov(X1[(k-1)\*p+1):(k\*(p+1), ]) contains the initial cov matrix for group k.

REMARK: If nsamp is not a scalar, the option startv1 given below is ignored. More precisely, if nsamp has k columns startv1 =  $\emptyset$  else if nsamp has k\*(p+1) columns option startv1=1.

refsteps

Number of refining iterations in each subsample. Default is refsteps=15. refsteps = 0 means "raw-subsampling" without iterations.

reftol

Tolerance of the refining steps. The default value is 1e-14

equalweights

A logical specifying wheather cluster weights in the concentration and assignment steps shall be considered. If equalweights=TRUE we are (ideally) assuming equally sized groups, else if equalweights = false (default) we allow for different group weights. Please, check in the given references which functions are maximized in both cases.

mixt

Specifies whether mixture modelling or crisp assignment approach to model based clustering must be used. In the case of mixture modelling parameter mixt also controls which is the criterion to find the untrimmed units in each step of the maximization. If mixt >= 1 mixture modelling is assumed else crisp assignment. The default value is mixt=0, i.e. crisp assignment. Please see for details the provided references. The parameter mixt also controls the criterion to select the units to trim. If mixt=2 the h units are those which give the largest contribution to the likelihood, else if mixt=1 the criterion to select the h units is exactly the same as the one which is used in crisp assignment.

msg

Controls whether to display or not messages on the screen If msg==TRUE (default) messages are displayed on the screen. If msg=2, detailed messages are displayed, for example the information at iteration level.

nocheck Check input arguments. If nocheck=TRUE no check is performed on matrix X.

The default nocheck=FALSE.

startv1 How to initialize centroids and covariance matrices. Scalar. If startv1=1 then

initial centroids and covariance matrices are based on (p+1) observations randomly chosen, else each centroid is initialized taking a random row of input data matrix and covariance matrices are initialized with identity matrices. The

default value isstartv1=1.

Remark 1: in order to start with a routine which is in the required parameter

space, eigenvalue restrictions are immediately applied.

Remark 2 - option startv1 is used just if nsamp is a scalar (see for more details

the help associated with nsamp).

restrtype Type of restriction to be applied on the cluster scatter matrices. Valid values are

'eigen' (default), or 'deter'. "eigen" implies restriction on the eigenvalues

while "deter" implies restriction on the determinants.

UnitsSameGroup List of the units which must (whenever possible) have a particular label. For

example UnitsSameGroup=c(20,26), means that group which contains unit 20 is always labelled with number 1. Similarly, the group which contains unit 26 is always labelled with number 2, (unless it is found that unit 26 already belongs to group 1). In general, group which contains unit UnitsSameGroup(r) where  $r=2,\ldots$ length(kk)-1 is labelled with number r (unless it is found that unit

UnitsSameGroup(r) has already been assigned to groups 1, 2, ..., r-1.

numpool The number of parallel sessions to open. If numpool is not defined, then it is set

equal to the number of physical cores in the computer.

cleanpool Logical, indicating if the open pool must be closed or not. It is useful to leave it

open if there are subsequent parallel sessions to execute, so that to save the time

required to open a new pool.

trace Whether to print intermediate results. Default is trace=FALSE.

... potential further arguments passed to lower level functions.

#### **Details**

This iterative algorithm initializes k clusters randomly and performs concentration steps in order to improve the current cluster assignment. The number of maximum concentration steps to be performed is given by input parameter refsteps. For approximately obtaining the global optimum, the system is initialized nsamp times and concentration steps are performed until convergence or refsteps is reached. When processing more complex data sets higher values of nsamp and refsteps have to be specified (obviously implying extra computation time). However, if more then 10 per cent of the iterations do not converge, a warning message is issued, indicating that nsamp has to be increased.

#### Value

Depending on the input parameter monitoring, one of the following objects will be returned:

- 1. tclustfsda.object
- 2. tclusteda.object

#### Author(s)

FSDA team, <valentin.todorov@chello.at>

#### References

Garcia-Escudero, L.A., Gordaliza, A., Matran, C. and Mayo-Iscar, A. (2008). A General Trimming Approach to Robust Cluster Analysis. Annals of Statistics, Vol. 36, 1324-1345. [Technical Report available at: http://www.eio.uva.es/inves/grupos/representaciones/trTCLUST.pdf]

## **Examples**

```
## Not run:
data(hbk)
(out <- tclustfsda(hbk[, 1:3], k=2))</pre>
class(out)
summary(out)
## TCLUST of Gayser data with three groups (k=3), 10%% trimming (alpha=0.1)
        and restriction factor (c=10000)
data(geyser2)
(out <- tclustfsda(geyser2, k=3, alpha=0.1, restrfactor=10000))</pre>
## Use the plot options to produce more complex plots -----
## Plot with all default options
out <- tclustfsda(geyser2, k=3, alpha=0.1, restrfactor=10000, plot=TRUE)
## Default confidence ellipses.
out <- tclustfsda(geyser2, k=3, alpha=0.1, restrfactor=10000, plot="ellipse")
## Confidence ellipses specified by the user: confidence ellipses set to 0.5
plots <- list(type="ellipse", conflev=0.5)</pre>
out <- tclustfsda(geyser2, k=3, alpha=0.1, restrfactor=10000, plot=plots)
## Confidence ellipses set to 0.9
plots <- list(type="ellipse", conflev=0.9)</pre>
out <- tclustfsda(geyser2, k=3, alpha=0.1, restrfactor=10000, plot=plots)
## Contour plots
out <- tclustfsda(geyser2, k=3, alpha=0.1, restrfactor=10000, plot="contour")
## Filled contour plots with additional options: contourf plot with autumn colormap
plots <- list(type="contourf", cmap="autumn")</pre>
out <- tclustfsda(geyser2, k=3, alpha=0.1, restrfactor=10000, plot=plots)</pre>
## We compare the output using three different values of restriction factor
        nsamp is the number of subsamples which will be extracted
data(geyser2)
out <- tclustfsda(geyser2, k=3, alpha=0.1, restrfactor=10000, nsamp=500, plot="ellipse")
out <- tclustfsda(geyser2, k=3, alpha=0.1, restrfactor=10, nsamp=500, refsteps=10, plot="ellipse")
out <- tclustfsda(geyser2, k=3, alpha=0.1, restrfactor=1, nsamp=500, refsteps=10, plot="ellipse")</pre>
```

```
## TCLUST applied to M5 data: A bivariate data set obtained from three normal
## bivariate distributions with different scales and proportions 1:2:2. One of the
## components is very overlapped with another one. A 10 per cent background noise is
## added uniformly distributed in a rectangle containing the three normal components
## and not very overlapped with the three mixture components. A precise description
## of the M5 data set can be found in Garcia-Escudero et al. (2008).
##
data(M5data)
plot(M5data[, 1:2])
## Scatter plot matrix
plot(CovClassic(M5data[,1:2]), which="pairs")
out <- tclustfsda(M5data[,1:2], k=3, alpha=0, restrfactor=1000, nsamp=100, plot=TRUE)
out <- tclustfsda(M5data[,1:2], k=3, alpha=0, restrfactor=10, nsamp=100, plot=TRUE)
out <- tclustfsda(M5data[,1:2], k=3, alpha=0.1, restrfactor=1, nsamp=1000,
        plot=TRUE, equalweights=TRUE)
out <- tclustfsda(M5data[,1:2], k=3, alpha=0.1, restrfactor=1000, nsamp=100, plot=TRUE)
## TCLUST with simulated data: 5 groups and 5 variables
##
n1 <- 100
n2 <- 80
n3 <- 50
n4 <- 80
n5 <- 70
p <- 5
Y1 <- matrix(rnorm(n1 * p) + 5, ncol=p)
Y2 <- matrix(rnorm(n2 * p) + 3, ncol=p)
Y3 \leftarrow matrix(rnorm(n3 * p) - 2, ncol=p)
Y4 \leftarrow matrix(rnorm(n4 * p) + 2, ncol=p)
Y5 <- matrix(rnorm(n5 * p), ncol=p)
group <- c(rep(1, n1), rep(2, n2), rep(3, n3), rep(4, n4), rep(5, n5))
Y <- Y1
Y \leftarrow rbind(Y, Y2)
Y \leftarrow rbind(Y, Y3)
Y \leftarrow rbind(Y, Y4)
Y \leftarrow rbind(Y, Y5)
dim(Y)
table(group)
out <- tclustfsda(Y, k=5, alpha=0.05, restrfactor=1.3, refsteps=20, plot=TRUE)
## Automatic choice of best number of groups for Geyser data -------------
##
data(geyser2)
maxk < -6
CLACLA <- matrix(0, nrow=maxk, ncol=2)
CLACLA[,1] <- 1:maxk
MIXCLA <- MIXMIX <- CLACLA
```

```
for(j in 1:maxk) {
    out <- tclustfsda(geyser2, k=j, alpha=0.1, restrfactor=5, msg=FALSE)</pre>
    CLACLA[j, 2] <- out$CLACLA</pre>
}
for(j in 1:maxk) {
    out <- tclustfsda(geyser2, k=j, alpha=0.1, restrfactor=5, mixt=2, msg=FALSE)
    MIXMIX[j ,2] <- out$MIXMIX</pre>
    MIXCLA[j, 2] <- out$MIXCLA
}
oldpar <- par(mfrow=c(1,3))
plot(CLACLA[,1:2], type="l", xlim=c(1, maxk), xlab="Number of groups", ylab="CLACLA")
plot(MIXMIX[,1:2], type="l", xlim=c(1, maxk), xlab="Number of groups", ylab="MIXMIX")
plot(MIXCLA[,1:2], type="1", xlim=c(1, maxk), xlab="Number of groups", ylab="MIXCLA")
par(oldpar)
## Monitoring examples ------
## Monitoring using Geyser data
## Monitoring using Geyser data (all default options)
## alpha and restriction factor are not specified therefore alpha=c(0.10, 0.05, 0)
\#\# is used while the restriction factor is set to c=12
out <- tclustfsda(geyser2, k=3, monitoring=TRUE)</pre>
## Monitoring using Geyser data with alpha and c specified.
out <- tclustfsda(geyser2, k=3, restrfac=100, alpha=seq(0.10, 0, by=-0.01), monitoring=TRUE)
## Monitoring using Geyser data with plot argument specified as a list.
##
        The trimming levels to consider in this case are 31 values of alpha
##
out <- tclustfsda(geyser2, k=3, restrfac=100, alpha=seq(0.30, 0, by=-0.01), monitoring=TRUE,
        plot=list(alphasel=c(0.2, 0.10, 0.05, 0.01)), trace=TRUE)
##
   Monitoring using Geyser data with argument UnitsSameGroup
##
##
       Make sure that group containing unit 10 is in a group which is labelled "group 1"
##
        and group containing unit 12 is in group which is labelled "group 2"
##
##
        Mixture model is used (mixt=2)
out <- tclustfsda(geyser2, k=3, restrfac=100, alpha=seq(0.30, 0, by=-0.01), monitoring=TRUE,
        mixt=2, UnitsSameGroup=c(10, 12), trace=TRUE)
## Monitoring using M5 data
data(M5data)
## alphavec=vector which contains the trimming levels to consider
## in this case 31 values of alpha are considered
alphavec <- seq(0.10, 0, by=-0.02)
out <- tclustfsda(M5data[, 1:2], 3, alpha=alphavec, restrfac=1000, monitoring=TRUE,
```

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```
nsamp=1000, plots=TRUE)
## End(Not run)
```

tclustfsda.object

Objects returned by the function tclustfsda

# Description

An object of class tclustfsda. object holds information about the result of a call to tclustfsda.

## Value

The functions print() and summary() are used to obtain and print a summary of the results. An object of class tclustfsda is a list containing at least the following components:

call	the matched call
muopt	a k-by-p matrix containing cluster centroid locations. Robust estimate of final centroids of the groups
sigmaopt	a p-by-p-by-k array rray containing estimated constrained covariance for the k groups
idx	a vector of length n containing assignment of each unit to each of the k groups. Cluster names are integer numbers from 1 to k. 0 indicates trimmed observations.
size	a matrix of size (k+1)-by-3. The 1st col is sequence from 0 to k (cluster name); the 2nd col is the number of observations in each cluster; the 3rd col is the percentage of observations in each cluster.
	Remark: 0 denotes unassigned units.
postprob	n-by-k matrix containing posterior probabilities. postprob[i,j] contains posterior probabilities of unit i from component (cluster) j. For the trimmed units posterior probabilities are 0.
emp	"Empirical" statistics computed on final classification. When convergence is reached, emp=0. When convergence is not obtained, this field is a list which contains the statistics of interest: idxemp (ordered from 0 to k*, k* being the number of groups with at least one observation and 0 representing the possible group of outliers), muemp, sigmaemp and sizemp, which are the empirical counterparts of idx, muopt, sigmaopt and \codesize.
MIXMIX	BIC which uses parameters estimated using the mixture loglikelihood and the maximized mixture likelihood as goodness of fit measure.
	Remark: this output is present just if $mixt > 0$ .
MIXCLA	BIC which uses parameters estimated using the mixture loglikelihood and the maximized mixture likelihood as goodness of fit measure.

Remark: this output is present just if mixt > 0.

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CLACLA BIC which uses the classification likelihood based on parameters estimated using the classification likelihood. Remark: this output is present just if mixt > 0. number of subsets without convergence notconver a vector of length k containing the units forming initial subset associated with bs muopt. obj value of the objective function which is minimized (value of the best returned solution). equalweights if equalweights=TRUE means that in the clustering procedure we (ideally) assumed equal cluster weights else (codeequalweitghts=FALSE means that we allowed for different cluster sizes. h number of observations that have determined the centroids (number of untrimmed units). fullsol a vector of size nsamp which contains the value of the objective function at the

end of the iterative process for each extracted subsample.

X the original data matrix X.

## **Examples**

```
## Not run:
data(hbk)
(out <- tclustfsda(hbk[, 1:3], k=2))
class(out)
summary(out)
## End(Not run)</pre>
```

tclustIC

Performs cluster analysis by calling tclustfsda for different number of groups k and restriction factors c

# **Description**

Computes the values of BIC (MIXMIX), ICL (MIXCLA) or CLA (CLACLA), for different values of k (number of groups) and different values of c (restriction factor), for a prespecified level of trimming (the last two letters in the name stand for 'Information Criterion'). If Parallel Computing toolbox is installed, parfor is used to compute tclust for different values of c. In order to minimize randomness, given k, the same subsets are used for each value of c.

# Usage

```
tclustIC(x, kk = 1:5, cc = c(1, 2, 4, 8, 16, 32, 64, 128), alpha = 0,
  whichIC = c("ALL", "MIXMIX", "MIXCLA", "CLACLA"), nsamp,
  refsteps = 15, reftol = 1e-14, equalweights = FALSE, msg = TRUE,
  nocheck = FALSE, plot = FALSE, startv1 = 1,
  restrtype = c("eigen", "deter"), UnitsSameGroup, numpool, cleanpool,
  trace = FALSE, ...)
```

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#### **Arguments**

Х

An n x p data matrix (n observations and p variables). Rows of x represent observations, and columns represent variables.

Missing values (NA's) and infinite values (Inf's) are allowed, since observations (rows) with missing or infinite values will automatically be excluded from the computations.

kk

an integer vector specifying the number of mixture components (clusters) for which the BIC is to be calculated. By default kk=1:5.

CC

an vector specifying the values of the restriction factor which have to be considered. By default cc=c(1,2,4,8,16,32,64,128).

alpha

Global trimming level. A scalar between 0 and 0.5 or an integer specifying the number of observations which have to be trimmed. If alpha=0 all observations are considered. By default alpha=0.

More in detail, if  $\emptyset$  < alpha < 1 clustering is based on h = fix(n \* (1-alpha)) observations, else if alpha is an integer greater than 1 clustering is based on h = n-floor(alpha).

whichIC

A character value which specifies which information criteria must be computed for each k (number of groups) and each value of the restriction factor c. Possible values for whichIC are:

- "MIXMIX": a mixture model is fitted and for computing the information criterion the mixture likelihood is used. This option corresponds to the use of the Bayesian Information criterion (BIC). In output just the matrix MIXMIX is given.
- "MIXCLA": a mixture model is fitted but to compute the information criterion the classification likelihood is used. This option corresponds to the use of the Integrated Complete Likelihood (ICL). In the output just the matrix MIXCLA is given.
- "CLACLA": everything is based on the classification likelihood. This information criterion will be called CLA. In the output just the matrix CLACLA is given.
- "ALL": both classification and mixture likelihood are used. In this case all three information criteria CLA, ICL and BIC are computed. In the output all three matrices MIXMIX, MIXCLA and CLACLA are given.

nsamp

If a scalar, it contains the number of subsamples which will be extracted. If nsamp = 0 all subsets will be extracted. Remark - if the number of all possible subset is greater than 300 the default is to extract all subsets, otherwise just 300. If nsamp is a matrix it contains in the rows the indexes of the subsets which have to be extracted. nsamp in this case can be conveniently generated by function subsets(). nsamp can have k columns or k \* (p + 1) columns. If nsamp has k columns the k initial centroids each iteration i are given by X[nsamp[i,],] and the covariance matrices are equal to the identity.

If nsamp has k \* (p + 1) columns, the initial centroids and covariance matrices in iteration i are computed as follows:

- X1 <- X[nsamp[i,],]
- mean(X1[1:p + 1, ]) contains the initial centroid for group 1

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- cov(X1[1:p + 1, ]) contains the initial cov matrix for group 1
- mean(X1[(p + 2):(2\*p + 2), ]) contains the initial centroid for group 2
- cov(X1[(p+2):(2\*p+2),]) contains the initial cov matrix for group 2

• .

- mean(X1[(k-1)\*p+1):(k\*(p+1), ]) contains the initial centroids for group k
- cov(X1[(k-1)\*p+1):(k\*(p+1), ]) contains the initial cov matrix for group k.

REMARK: If nsamp is not a scalar, the option startv1 given below is ignored. More precisely, if nsamp has k columns startv1 = 0 else if nsamp has k\*(p+1) columns option startv1=1.

refsteps

Number of refining iterations in each subsample. Default is refsteps=15. refsteps = 0 means "raw-subsampling" without iterations.

reftol

Tolerance of the refining steps. The default value is 1e-14

equalweights

A logical specifying wheather cluster weights in the concentration and assignment steps shall be considered. If equalweights=TRUE we are (ideally) assuming equally sized groups, else if equalweights = false (default) we allow for different group weights. Please, check in the given references which functions are maximized in both cases.

msg

Controls whether to display or not messages on the screen If msg==TRUE (default) messages are displayed on the screen. If msg=2, detailed messages are displayed, for example the information at iteration level.

nocheck

Check input arguments. If nocheck=TRUE no check is performed on matrix X. The default nocheck=FALSE.

plot

If plot=TRUE, a plot of the BIC (MIXMIX), ICL (MIXCLA) curve and CLA-CLA is shown on the screen. The plots which are shown depend on the input option whichIC.

startv1

How to initialize centroids and covariance matrices. Scalar. If startv1=1 then initial centroids and covariance matrices are based on (p+1) observations randomly chosen, else each centroid is initialized taking a random row of input data matrix and covariance matrices are initialized with identity matrices. The default value isstartv1=1.

Remark 1: in order to start with a routine which is in the required parameter space, eigenvalue restrictions are immediately applied.

Remark 2 - option startv1 is used just if nsamp is a scalar (see for more details the help associated with nsamp).

restrtype

Type of restriction to be applied on the cluster scatter matrices. Valid values are 'eigen' (default), or 'deter'. "eigen" implies restriction on the eigenvalues while "deter" implies restriction on the determinants.

UnitsSameGroup

List of the units which must (whenever possible) have a particular label. For example UnitsSameGroup=c(20,26), means that group which contains unit 20 is always labelled with number 1. Similarly, the group which contains unit 26 is always labelled with number 2, (unless it is found that unit 26 already belongs to group 1). In general, group which contains unit UnitsSameGroup(r) where r=2,...length(kk)-1 is labelled with number r (unless it is found that unit UnitsSameGroup(r) has already been assigned to groups 1,2,...,r-1.

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numpool	The number of parallel sessions to open. If numpool is not defined, then it is set equal to the number of physical cores in the computer.
cleanpool	Logical, indicating if the open pool must be closed or not. It is useful to leave it open if there are subsequent parallel sessions to execute, so that to save the time required to open a new pool.
trace	Whether to print intermediate results. Default is trace=EALSE

whether to print intermediate results. Default is trace=FALSE.

potential further arguments passed to lower level functions.

## Value

```
An S3 object of class tclustic.object
```

## Author(s)

```
FSDA team, <valentin.todorov@chello.at>
```

## References

Cerioli, A., Garcia-Escudero, L.A., Mayo-Iscar, A. and Riani M. (2017). Finding the Number of Groups in Model-Based Clustering via Constrained Likelihoods, emphJournal of Computational and Graphical Statistics, pp. 404-416, https://doi.org/10.1080/10618600.2017.1390469.

## See Also

```
tclustfsda, tclustICplot, tclustICsol, carbikeplot
```

## **Examples**

```
## Not run:
data(geyser2)
out <- tclustIC(geyser2, whichIC="MIXMIX", plot=FALSE, alpha=0.1)
out
summary(out)
## End(Not run)</pre>
```

tclustic.object

Objects returned by the function tclustIC

## **Description**

An object of class tclustic.object holds information about the result of a call to tclustIC.

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# Value

The functions print() and summary() are used to obtain and print a summary of the results. An object of class tclustic is a list containing at least the following components:

call	the matched call
kk	a vector containing the values of $k$ (number of components) which have been considered. This vector is identical to the optional argument $kk$ (default is $kk=1:5$ .
сс	a vector containing the values of c (values of the restriction factor) which have been considered. This vector is identical to the optional argument cc (defalt is $cc=c(1,2,4,8,16,32,64,128)$ .
alpha	trimming level
whichIC	Information criteria used
CLACLA	a matrix of size length(kk)-times-length(cc) containing the value of the penalized classification likelihood. This output is present only if whichIC="CLACLA" or whichIC="ALL".
IDXCLA	a matrix of lists of size length(kk)-times-length(cc) containing the assignment of each unit using the classification model. This output is present only if whichIC="CLACLA" or whichIC="ALL".
MIXMIX	a matrix of size length(kk)-times-length(cc) containing the value of the penalized mixtrue likelihood. This output is present only if whichIC="MIXMIX" or whichIC="ALL".
IDXMIX	a matrix of lists of size length(kk)-times-length(cc) containing the assignment of each unit using the classification model. This output is present only if whichIC="MIXMIX" or whichIC="ALL".
MIXCLA	a matrix of size length(kk)-times-length(cc) containing the value of the ICL criterion. This output is present only if whichIC="MIXCLA" or whichIC="ALL".

# **Examples**

```
## Not run:
data(hbk)
(out <- tclustIC(hbk[, 1:3]))
class(out)
summary(out)
## End(Not run)</pre>
```

tclustICplot

Plots information criterion as a function of c and k, based on the

solutions obtained by tclustIC

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# **Description**

The function tclustICplot() takes as input an object of class tclustic.object, the output of function tclustIC (that is a series of matrices which contain the values of the information criteria BIC/ICL/CLA for different values of k and c) and plots them as function of c or of k. The plot enables interaction in the sense that, if option databrush has been activated, it is possible to click on a point in the plot and to see the associated classification in the scatter plot matrix.

## Usage

```
tclustICplot(out, whichIC = c("ALL", "MIXMIX", "MIXCLA", "CLACLA"), tag,
  datatooltip, databrush, nameY, trace = FALSE, ...)
```

#### **Arguments**

out

An S3 object of class tclustic.object (output of tclustIC) containing the values of the information criteria BIC (MIXMIX), ICL (MIXCLA) or CLA (CLACLA), for different values of k (number of groups) and different values of c (restriction factor), for a prespecified level of trimming.

whichIC

Specifies the information criterion to use for the plot. See codetclustIC() for the possible values of whichIC.

tag

plot handle. String which identifies the handle of the plot which is about to be created. The default is to use tag 'pl\_IC'. Notice that if the program finds a plot which has a tag equal to the one specified by the user, then the output of the new plot overwrites the existing one in the same window else a new window is created.

datatooltip

Interactive clicking. It is inactive if this parameter is set to FALSE. The default is datatooltip=TRUE, the user can select with the mouse a solution in order to have the following information:

- 1) value of k which has been selected
- 2) value of c which has been selected
- 3) values of the information criterion
- 4) frequency distribution of the associated classification.

If datatooltip is a list it may contain the following fields:

- DisplayStyle determines how the data cursor displays. Possible values are 'datatip' and 'window' (default). 'datatip' displays data cursor information in a small yellow text box attached to a black square marker at a data point you interactively select. 'window' displays data cursor information for the data point you interactively select in a floating window within the figure.
- 2. SnapToDataVertex: specifies whether the data cursor snaps to the nearest data value or is located at the actual pointer position. Possible values are SnapToDataVertex='on' (default) and SnapToDataVertex='off'.

databrush

Interactive mouse brushing. If databrush is missing or empty (default), no brushing is done. The activation of this option (databrush is TRUE or a list) enables the user to select a set of values of IC in the current plot and to see the corresponding classification highlighted in the scatterplot matrix. If the scatterplot matrix does

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not exist it is automatically created. Note that the window style of the other figures is set equal to that which contains the IC plot. In other words, if the IC plot is docked all the other figures will be docked too.

If databrush=TRUE the default selection tool is a rectangular brush and it is possible to brush only once (that is persist=").

If databrush=list(...), it is possible to use all optional arguments of the MATLAB function selectdataFS() and the following optional arguments:

- persist: Persist is an empty value or a character containing 'on' or 'off'. The default value is persist="", that is brushing is allowed only once. If persist="on" or persis="off" brushing can be done as many time as the user requires. If persist='on' then the unit(s) currently brushed are added to those previously brushed. It is possible, every time a new brushing is done, to use a different color for the brushed units. If persist='off' every time a new brush is performed units previously brushed are removed.
- label: add labels of brushed units in the monitoring plot.
- dispopt: controls how to fill the diagonals in the scatterplot matrix of the brushed solutions. Set dispopt="hist" (default) to plot histograms, or dispopt="box" to plot boxplots.

nameY

Add variable labels in plot. A vector of strings of length p containing the labels of the variables in the dataset. If it is empty (default) the sequence X1,...,Xp will be created automatically

trace

Whether to print intermediate results. Default is trace=FALSE.

. . .

potential further arguments passed to lower level functions.

#### Author(s)

FSDA team, <valentin.todorov@chello.at>

#### References

Cerioli, A., Garcia-Escudero, L.A., Mayo-Iscar, A. and Riani M. (2017). Finding the Number of Groups in Model-Based Clustering via Constrained Likelihoods, emphJournal of Computational and Graphical Statistics, pp. 404-416, https://doi.org/10.1080/10618600.2017.1390469.

Hubert L. and Arabie P. (1985), Comparing Partitions, *Journal of Classification*, Vol. 2, pp. 193-218.

# See Also

```
tclustIC, tclustfsda
```

## **Examples**

```
## Not run:
data(geyser2)
out <- tclustIC(geyser2, whichIC="MIXMIX", plot=FALSE, alpha=0.1)
tclustICplot(out)</pre>
```

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```
## End(Not run)
```

tclustICsol

Extracts a set of best relevant solutions obtained by tclustIC

## **Description**

The function tclustICsol() takes as input an object of class tclustic.object, the output of function tclustIC (that is a series of matrices which contain the values of the information criteria BIC/ICL/CLA for different values of k and c) and extracts the first best solutions. Two solutions are considered equivalent if the value of the adjusted Rand index (or the adjusted Fowlkes and Mallows index) is above a certain threshold. For each tentative solution the program checks the adjacent values of c for which the solution is stable. A matrix with adjusted Rand indexes is given for the extracted solutions.

## Usage

```
tclustICsol(out, NumberOfBestSolutions = 5, ThreshRandIndex = 0.7,
  whichIC = c("ALL", "CLACLA", "MIXMIX", "MIXCLA"), Rand = TRUE,
  msg = TRUE, plot = FALSE, trace = FALSE, ...)
```

#### **Arguments**

out

An S3 object of class tclustic.object (output of tclustIC) containing the values of the information criteria BIC (MIXMIX), ICL (MIXCLA) or CLA (CLACLA), for different values of k (number of groups) and different values of c (restriction factor), for a prespecified level of trimming.

#### NumberOfBestSolutions

Number of best solutions to extract from BIC/ICL matrix. The default value of NumberOfBestSolutions is 5

## ThreshRandIndex

Threshold to identify spurious solutions - the threshold of the adjusted Rand index to use to consider two solutions as equivalent. The default value of ThreshRandIndex is 0.7

whichIC

Specifies the information criterion to use to extract best solutions. Possible values for whichIC are:

- CLACLA = in this case best solutions are referred to the classification likelihood
- MIXMIX = in this case in this case best solutions are referred to the mixture likelihood (BIC).
- MIXCLA = in this case in this case best solutions are referred to ICL.
- ALL = in this case best solutions both three solutions using classification and mixture likelihood are produced. In the output class out all the three matrices MIXMIXbs, CLACLAbs and MIXCLAbs are given.

The default value is whichIC="ALL".

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Rand	Index to use to compare partitions. If Rand=TRUE (default) the adjusted Rand index is used, else the adjusted Fowlkes and Mallows index is used.
msg	It controls whether to display or not messages (from MATLAB) on the screen. If msg=TRUE (default) messages about the progression of the search are displayed on the screen otherwise only error messages will be displayed.
plot	If $plot=TRUE$ , the best solutions which have been found are shown on the screen.
trace	Whether to print intermediate results. Default is trace=FALSE.
	potential further arguments passed to lower level functions.

## Value

An S3 object of class tclusticsol.object

## Author(s)

FSDA team, <valentin.todorov@chello.at>

#### References

Cerioli, A., Garcia-Escudero, L.A., Mayo-Iscar, A. and Riani M. (2017). Finding the Number of Groups in Model-Based Clustering via Constrained Likelihoods, emphJournal of Computational and Graphical Statistics, pp. 404-416, https://doi.org/10.1080/10618600.2017.1390469.

Hubert L. and Arabie P. (1985), Comparing Partitions, *Journal of Classification*, Vol. 2, pp. 193-218.

#### See Also

```
tclustIC, tclustfsda, carbikeplot
```

## **Examples**

```
## Not run:
data(geyser2)
out <- tclustIC(geyser2, whichIC="MIXMIX", plot=FALSE, alpha=0.1)

## Plot first two best solutions using as Information criterion MIXMIX
print("Best solutions using MIXMIX")
outMIXMIX <- tclustICsol(out, whichIC="MIXMIX", plot=TRUE, NumberOfBestSolutions=2)
print(outMIXMIX$MIXMIXDs)

## End(Not run)</pre>
```

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tclusticsol.object

Objects returned by the function tclustICsol

# Description

An object of class tclusticsol. object holds information about the result of a call to tclustICsol.

#### Value

The functions print() and summary() are used to obtain and print a summary of the results. An object of class tclusticsol is a list containing at least the following components:

the matched call

kk a vector containing the values of k (number of components) which have been considered. This vector is identical to the optional argument kk (default is kk=1:5.

cc a vector containing the values of c (values of the restriction factor) which have been considered. This vector is identical to the optional argument cc (defalt is cc=c(1,2,4,8,16,32,64,128).

alpha trimming level

whichIC Information criteria used

MIXMIXbs a matrix of lists of size NumberOfBestSolutions-times-5 which contains the details of the best solutions for MIXMIX (BIC). Each row refers to a solution.

The information which is stored in the columns is as follows.

- 1st col = value of k for which solution takes place
- 2nd col = value of c for which solution takes place;
- 3rd col = a vector of length d which contains the values of c for which the solution is uniformly better.
- 4th col = a vector of length d + r which contains the values of c for which
  the solution is considered stable (i.e. for which the value of the adjusted
  Rand index (or the adjusted Fowlkes and Mallows index) does not go below
  the threshold defined in input option ThreshRandIndex).
- 5th col = string which contains 'true' or 'spurious'. The solution is labelled spurious if the value of the adjusted Rand index with the previous solutions is greater than ThreshRandIndex.

Remark: the field MIXMIXbs is present only if whichIC=ALL or whichIC="MIXMIX".

MIXMIXbsari

a matrix of adjusted Rand indexes (or Fowlkes and Mallows indexes) associated with the best solutions for MIXMIX. A matrix of size NumberOfBestSolutions-times-NumberOfBestSolutions i, j-th entry contains the adjusted Rand index between classification produced by solution i and solution j, i, j=1,2,..., NumberOfBestSolutions.

Remark: the field MIXMIXbsari is present only if whichIC=ALL or whichIC="MIXMIX".

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ARIMIX a matrix of adjusted Rand indexes between two consecutive value of c. Matrix of

size k-by-length(cc)-1. The first column contains the ARI indexes between cc[2] and cc[1] given k. The second column contains the the ARI indexes

between cc[3] and cc[2] given k.

Remark: the field ARIMIX is present only if whichIC=ALL or whichIC="MIXMIX"

or whichIC="MIXCLA".

MIXCLAbs has the same structure as MIXMIXbs but referres to MIXCLA.

Remark: the field MIXCLAbs is present only if whichIC=ALL or whichIC="MIXCLA".

MIXCLAbsari has the same structure as MIXMIXbsari but referres to MIXCLA.

Remark: the field MIXMIXbsari is present only if whichIC=ALL or whichIC="MIXCLA".

CLACLAbs has the same structure as MIXMIXbs but referres to CLACLA.

Remark: the field CLACLAbs is present only if whichIC=ALL or whichIC="CLACLA".

CLACLAbsari has the same structure as MIXMIXbsari but referres to CLACLA.

Remark: the field CLACLAbsari is present only if whichIC=ALL or whichIC="CLACLA".

ARICLA a matrix of adjusted Rand indexes between two consecutive value of c. Matrix of

size k-by-length(cc)-1. The first column contains the ARI indexes between cc[2] and cc[1] given k. The second column contains the the ARI indexes

between cc[3] and cc[2] given k.

Remark: the field ARICLA is present only if whichIC=ALL or whichIC="CLACLA".

#### See Also

tclustICsol, carbikeplot

## **Examples**

```
## Not run:
data(hbk)
(out <- tclustIC(hbk[, 1:3]))
class(out)
summary(out)
## End(Not run)</pre>
```

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