# Package 'FRB'

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Description Perform robust inference based on applying Fast and Robust Bootstrap on robust estimators (Van Aelst and Willems (2013) <doi:10.18637 jss.v053.i03="">). This method constitutes an alternative to ordinary bootstrap or asymptotic inference. procedures when using robust estimators such as S-, MM- or GS-estimators. The available methods are multivariate regression, principal component analysis and one-sample and two-sample Hotelling tests. It provides both the robust point estimates and uncertainty measures based on the fast and robust bootstrap.</doi:10.18637>
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Plot Method for Objects of class 'FRBmultireg'

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# Description

Diagnostic plots for objects of class FRBmultireg, FRBpca and FRBhot. It shows robust distances and allows detection of multivariate outliers.

# Usage

```
## S3 method for class 'FRBmultireg'
diagplot(x, Xdist = TRUE, ...)

## S3 method for class 'FRBpca'
diagplot(x, EIF = TRUE, ...)

## S3 method for class 'FRBhot'
diagplot(x, ...)
```

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# Arguments

X	an R object of class FRBmultireg (typically created by FRBmultiregS, FRBmultiregMM or FRBmultiregGS or by Sest_multireg, MMest_multireg or GSest_multireg) or an R object of class FRBpca (typically created by FRBpcaS or FRBpcaMM) or an R object of class FRBhot (typically created by FRBhotellingS or FRBhotellingMM)
Xdist	logical: if TRUE, the plot shows the robust distance versus the distance in the space of the explanatory variables; if FALSE, it plots the robust distance versus the index of the observation
EIF	logical: if TRUE, the plot shows the robust distance versus an influence measure for each point; if FALSE, it plots the robust distance versus the index of the observation
	potentially more arguments to be passed

#### **Details**

The diagnostic plots are based on the robust distances of the observations. In a multivariate sample  $X_n = \{\mathbf{x}_1, ..., \mathbf{x}_n\}$ , the robust distance  $d_i$  of observation i is given by  $d_i^2 = (\mathbf{x}_i - \hat{\mu})'\hat{\Sigma}^{-1}(\mathbf{x}_i - \hat{\mu})$ . where  $\hat{\mu}$  and  $\hat{\Sigma}$  are robust estimates of location and covariance. Observations with large robust distance are considered as outlying.

The default diagnostic plot in the multivariate regresssion setting (i.e. for objects of type FRBmultireg and Xdist=TRUE), shows the residual distances (i.e. the robust distances of the multivariate residuals) based on the estimates in x, versus the distances within the space of the explanatory variables. The latter are based on robust estimates of location and scatter for the data matrix x\$X (without intercept). Computing these robust estimates may take an appreciable amount of time. The estimator used corresponds to the one which was used in obtaining Xmultireg (with the same breakdown point, for example, and the same control parameters). On the vertical axis a cutoff line is drawn at the square root of the .975 quantile of the chi-squared distribution with degrees of freedom equal to the number of response variables. On the horizontal axis the same quantile is drawn but now with degrees of freedom equal to the number of covariates (not including intercept). Those points to the right of the cutoff can be viewed as high-leverage points. These can be classified into so-called 'bad' or 'good' leverage points depending on whether they are above or below the cutoff. Points above the cutoff but to the left of the vertical cutoff are sometimes called vertical outliers. See also Van Aelst and Willems (2005) for example.

To avoid the additional computation time, one can choose Xdist=FALSE, in which case the residual distances are simply plotted versus the index of the observation.

The default plot in the context of PCA (i.e. for objects of type FRBpca and EIF=FALSE) is a plot proposed by Pison and Van Aelst (2004). It shows the robust distance versus a measure of the overall empirical influence of the observation on the (classical) principal components. The empirical influences are obtained by using the influence function of the eigenvectors of the empirical or classical shape estimator at the normal model, and by substituting therein the robust estimates for the population parameters. The overall influence value is then defined by averaging the squared influence over all coefficients in the eigenvectors. The vertical line on the plot is an indicative cutoff value, obtained through simulation. This last part takes a few moments of computation time.

Again, to avoid the additional computation time, one can choose EIF=FALSE, in which case the robust distances are simply plotted versus the index of the observation.

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For the result of the robust Hotelling test (i.e. for objects of type FRBhot), the method plots the robust distance versus the index. In case of a two-sample test, the indices are within-sample and a vertical line separates the two groups. In the two-sample case, each group has its own location estimate  $\hat{\mu}$  and a common covariance estimate  $\hat{\Sigma}$ .

#### Value

Returns invisibly the first argument.

#### Author(s)

Gert Willems and Ella Roelant

#### References

- G. Pison and S. Van Aelst (2004). Diagnostic Plots for Robust Multivariate Methods. *Journal of Computational and Graphical Statistics*, **13**, 310–329.
- S. Van Aelst and G. Willems (2005). Multivariate Regression S-Estimators for Robust Estimation and Inference. *Statistica Sinica*, **15**, 981–1001.
- S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

#### See Also

FRBmultiregS, FRBmultiregMM, FRBmultiregGS, FRBpcaS, FRBpcaMM, FRBhotellingS, FRBhotellingMM

```
## for multivariate regression:
    data(schooldata)
    MMres <- MMest_multireg(cbind(reading,mathematics,selfesteem)~., data=schooldata)
    diagplot(MMres)
    ## a large 'bad leverage' outlier should be noticeable (observation 59)

## for PCA:
    data(ForgedBankNotes)
    MMres <- FRBpcaMM(ForgedBankNotes)
    diagplot(MMres)

## a group of 15 fairly strong outliers can be seen which apparently would have
## a large general influence on a classical PCA analysis

## for Hotelling tests (two-sample)

    data(hemophilia, package="rrcov")
    MMres <- FRBhotellingMM(cbind(AHFactivity, AHFantigen) ~ gr, data=hemophilia)
    diagplot(MMres)</pre>
```

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## the data seem practically outlier-free

ForgedBankNotes

Swiss (forged) bank notes data

# **Description**

Six measurements made on 100 forged Swiss bank notes.

# Usage

data(ForgedBankNotes)

#### **Format**

The data frame contains the following columns:

Length metric length of the bill

Left height of the bill, measured on the left

Right height of the bill, measured on the right

Bottom distance of inner frame to the lower border

Top distance of inner frame to the upper border

Diagonal length of the diagonal

## **Details**

The original data set in Flury and Riedwyl (1988) additionally contained 100 genuine bank notes, but these are not included here.

### Source

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

#### References

M. Salibian-Barrera, S. Van Aelst and G. Willems (2006) PCA based on multivariate MM-estimators with fast and robust bootstrap. *Journal of the American Statistical Association*, **101**, 1198-1211.

```
data(ForgedBankNotes)
pairs(ForgedBankNotes)
```

FRBhotellingMM

EDDhotollingMM	Pobust Hotelling test using the MM estimator
FRBhotellingMM	Robust Hotelling test using the MM-estimator

# **Description**

Robust one-sample and two-sample Hotelling test using the MM-estimator and the Fast and Robust Bootstrap.

## Usage

# **Arguments**

formula	an object of class formula; a symbolic description of the model to be fit.
data	data frame from which variables specified in formula are to be taken.
X	a matrix or data-frame
Υ	an optional matrix or data-frame in case of a two-sample test
mu0	an optional vector of data values (or a single number which will be repeated $p$ times) indicating the true value of the mean (does not apply in case of the two-sample test). Default is the null vector $mu0=0$ .
R	number of bootstrap samples. Default is R=999.
conf	confidence level for the simultaneous confidence intervals. Default is conf=0.95.
method	for the two-sample Hotelling test, indicates the way the common covariance matrix is estimated: "pool"= pooled covariance matrix, "HeFung"= using the multisample method of He and Fung.
control	a list with control parameters for tuning the MM-estimate and its computing algorithm, see ${\tt MMcontrol}().$
na.action	a function which indicates what should happen when the data contain NAs. Defaults to ${\tt na.omit}$ .
	allows for specifying control parameters directly instead of via control

# **Details**

The classical Hotelling test for testing if the mean equals a certain value or if two means are equal is modified into a robust one through substitution of the empirical estimates by the MM-estimates of location and scatter. The MM-estimator, using Tukey's biweight function, is tuned by default to have a breakdown point of 50% and 95% location efficiency. This could be changed through the

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control argument if desired. The MM-estimates are obtained by first computing the S-estimates with the fast-S algorithm followed by the M-part through reweighted least squares (RWLS) iteration. See MMcontrol for some adjustable tuning parameters regarding the algorithm.

The fast and robust bootstrap is used to mimic the distribution of the test statistic under the null hypothesis. For instance, the 5% critical value for the test is given by the 95% quantile of the recalculated statistics.

Robust simultaneous confidence intervals for linear combinations of the mean (or difference in means) are developed similarly to the classical case (Johnson and Wichern, 1988, page 239). The value CI is a matrix with the confidence intervals for each element of the mean (or difference in means), with level conf. It consists of two rows, the first being the lower bound and the second the upper bound. Note that these intervals are rather conservative in the sense that the simultaneous confidence level holds for all linear combinations and here only p of these are considered (with p the dimension of the data).

For the two-sample Hotelling test we assume that the samples have an underlying distribution with the same covariance matrix. This covariance matrix can be estimated in two different ways using the pooled covariance matrix or the two-sample estimator of He and Fung (He and Fung 2000), and argument method defaults to the second option. For more details see Roelant et al. (2008).

In the two-sample version, the null hypothesis always states that the two means are equal. For the one-sample version, the default null hypothesis is that the mean equals zero, but the hypothesized value can be changed and specified through argument mu0.

Bootstrap samples are discarded if the fast and robust covariance estimate is not positive definite, such that the actual number of recalculations used can be lower than R. This number is returned as ROK.

## Value

An object of class FRBhot which extends class htest and contains at least the following components:

statistic the value of the robust test statistic.

pvalue p-value of the robust one or two-sample Hotelling test, determined by the fast

and robust bootstrap

estimate the estimated mean vector or vectors depending on whether it was a one-sample

test or a two-sample test.

alternative a character string describing the alternative hypothesis.

method a character string indicating what type of Hotelling test was performed.

data. name a character string giving the name(s) of the data.

teststat.boot the bootstrap recalculated values of the robust test statistic.

CI bootstrap simultaneous confidence intervals for each component of the center

conf a copy of the conf argument

Sigma covariance of one-sample or common covariance matrix in the case of two sam-

ples

w implicit weights corresponding to the MM-estimates (i.e. final weights in the

RWLS procedure)

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outFlag	outlier flags: 1 if the robust distance of the observation exceeds the .975 quantile of (the square root of) the chi-square distribution with degrees of freedom equal to the dimension of X; 0 otherwise
ROK	number of bootstrap samples actually used (i.e. not discarded due to non-positive definite covariance

## Author(s)

Ella Roelant, Stefan Van Aelst and Gert Willems

#### References

- X. He and W.K. Fung (2000) High breakdown estimation for multiple populations with applications to discriminant analysis. *Journal of Multivariate Analysis*, **72**, 151–162.
- R.A. Johnson, D.W. Wichern (1988) Applied Multivariate Statistical Analysis, 2nd Edition, Prentice-Hall.
- E. Roelant, S. Van Aelst and G. Willems, (2008) Fast Bootstrap for Robust Hotelling Tests, COMPSTAT 2008: Proceedings in Computational Statistics (P. Brito, Ed.) Heidelberg: Physika-Verlag, 709–719.
- M. Salibian-Barrera, S. Van Aelst and G. Willems (2008) Fast and robust bootstrap. *Statistical Methods and Applications*, **17**, 41–71.
- S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

#### See Also

```
plot.FRBhot, summary.FRBhot, FRBhotellingS, MMcontrol
```

```
## One sample robust Hotelling test
data(delivery, package="robustbase")
delivery.x <- delivery[, 1:2]</pre>
FRBhotellingMM(delivery.x, R=199)
## One sample robust Hotelling test
data(ForgedBankNotes)
samplemean <- apply(ForgedBankNotes, 2, mean)</pre>
res = FRBhotellingMM(ForgedBankNotes, mu0=samplemean,R=199)
res
# Note that the test rejects the hypothesis that the true mean equals the
# sample mean; this is due to outliers in the data (i.e. the robustly estimated
# mean apparently significantly differs from the non-robust sample mean.
# Graphical display of the results:
plot(res)
# It is clear from the (scaled) simultaneous confidence limits that the rejection
# of the hypothesis is due to the differences in variables Bottom and Diagonal
## Two sample robust Hotelling test
```

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```
data(hemophilia, package="rrcov")
grp <-as.factor(hemophilia[,3])
x <- hemophilia[which(grp==levels(grp)[1]),1:2]
y <- hemophilia[which(grp==levels(grp)[2]),1:2]

#using the pooled covariance matrix to estimate the common covariance matrix
    res <- FRBhotellingMM(x, y, method="pool")

#using the estimator of He and Fung to estimate the common covariance matrix
res <- FRBhotellingMM(x,y,method="HeFung",R=199)

# or using the formula interface

res <- FRBhotellingMM(as.matrix(hemophilia[,-3])~hemophilia[,3], method="HeFung")

# From the confidence limits it can be seen that the significant difference
# is mainly caused by the AHFactivity variable. The graphical display helps too:
plot(res)
# the red line on the histogram indicates the test statistic value in the original
# sample (it is omitted if the statistic exceeds 100)</pre>
```

 ${\sf FRBhotellingS}$ 

Robust Hotelling test using the S-estimator

# Description

Robust one-sample and two-sample Hotelling test using the S-estimator and the Fast and Robust Bootstrap.

# Usage

```
## S3 method for class 'formula'
FRBhotellingS(formula, data=NULL, ...)

## Default S3 method:
FRBhotellingS(X, Y=NULL, mu0 = 0, R = 999, bdp = 0.5, conf = 0.95,
method = c("HeFung", "pool"), control=Scontrol(...),
na.action=na.omit, ...)
```

# Arguments

formula an object of class formula; a symbolic description of the model to be fit.

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

X a matrix or data-frame

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Υ an optional matrix or data-frame in case of a two-sample test an optional vector of data values (or a single number which will be repeated mu0 p times) indicating the true value of the mean (does not apply in case of the two-sample test). Default is the null vector mu0=0 R number of bootstrap samples. Default is R=999. required breakdown point. Should have 0 < bdp < 0.5, the default is 0.5 bdp confidence level for the simultaneous confidence intervals. Default is conf=0.95 conf method for the two-sample Hotelling test, indicates the way the common covariance matrix is estimated: "pool"= pooled covariance matrix, "HeFung"= using the He and Fung method control a list with control parameters for tuning the computing algorithm, see Scontrol().

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

faults to na.omit.

... allows for specifying control parameters directly instead of via control

#### **Details**

The classical Hotelling test for testing if the mean equals a certain center or if two means are equal is modified into a robust one through substitution of the empirical estimates by the S-estimates of location and scatter. The S-estimator uses Tukey's biweight function where the constant is chosen to obtain the desired breakdown point as specified by bdp. One-sample S-estimates are computed by a call to the implementation of the fast-S algorithm in the **rrcov** package of Todorov and Filzmoser (2009). For two-sample S-estimates an adaptation of the fast-S algorithm is used. The tuning parameters of the algorithm can be changed via control.

The fast and robust bootstrap is used to mimic the distribution of the test statistic under the null hypothesis. For instance, the 5% critical value for the test is given by the 95% quantile of the recalculated statistics.

Robust simultaneous confidence intervals for linear combinations of the mean (or difference in means) are developed similarly to the classical case (Johnson and Wichern, 1988, page 239). The value CI is a matrix with the confidence intervals for each element of the mean (or difference in means), with level conf. It consists of two rows, the first being the lower bound and the second the upper bound. Note that these intervals are rather conservative in the sense that the simultaneous confidence level holds for all linear combinations and here only p of these are considered (with p the dimension of the data).

For the two-sample Hotelling test we assume that the samples have an underlying distribution with the same covariance matrix. This covariance matrix can be estimated in two different ways using the pooled covariance matrix or the two-sample estimator of He and Fung (He and Fung 2000), and argument method defaults to the second option. For more details see Roelant et al. (2008).

In the two-sample version, the null hypothesis always states that the two means are equal. For the one-sample version, the default null hypothesis is that the mean equals zero, but the hypothesized value can be changed and specified through argument mu0.

Bootstrap samples are discarded if the fast and robust covariance estimate is not positive definite, such that the actual number of recalculations used can be lower than R. This number is returned as ROK.

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#### Value

An object of class FRBhot which extends class htest and contains at least the following components:

statistic the value of the robust test statistic.

pvalue p-value of the robust one or two-sample Hotelling test, determined by the fast

and robust bootstrap

estimate the estimated mean vector or vectors depending on whether it was a one-sample

test or a two-sample test.

alternative a character string describing the alternative hypothesis.

method a character string indicating what type of Hotelling test was performed.

data. name a character string giving the name(s) of the data.

teststat.boot the bootstrap recalculated values of the robust test statistic.

CI bootstrap simultaneous confidence intervals for each component of the center

conf a copy of the conf argument

Sigma covariance of one-sample or common covariance matrix in the case of two sam-

ples

w implicit weights corresponding to the S-estimates (i.e. final weights in the

RWLS procedure at the end of the fast-S algorithm)

outFlag outlier flags: 1 if the robust distance of the observation exceeds the .975 quantile

of (the square root of) the chi-square distribution with degrees of freedom equal

to the dimension of X; 0 otherwise

ROK number of bootstrap samples actually used (i.e. not discarded due to non-

positive definite covariance

## Author(s)

Ella Roelant, Stefan Van Aelst and Gert Willems

#### References

- X. He and W.K. Fung (2000) High breakdown estimation for multiple populations with applications to discriminant analysis. *Journal of Multivariate Analysis*, **72**, 151–162.
- R.A. Johnson, D.W. Wichern (1988) Applied Multivariate Statistical Analysis, 2nd Edition, Prentice-Hall.
- E. Roelant, S. Van Aelst and G. Willems, (2008) Fast Bootstrap for Robust Hotelling Tests, COMPSTAT 2008: Proceedings in Computational Statistics (P. Brito, Ed.) Heidelberg: Physika-Verlag, 709–719.
- M. Salibian-Barrera, S. Van Aelst and G. Willems (2008) Fast and robust bootstrap. *Statistical Methods and Applications*, **17**, 41–71.
- V. Todorov and P. Filzmoser (2009), An Object Oriented Framework for Robust Multivariate Analysis. *Journal of Statistical Software*, **32**(3), 1–47. doi:10.18637/jss.v032.i03.
- S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

#### See Also

```
plot.FRBhot,summary.FRBhot,FRBhotellingMM,Scontrol
```

#### **Examples**

```
## One sample robust Hotelling test
data(delivery, package="robustbase")
delivery.x <- delivery[,1:2]</pre>
FRBhotellingS(delivery.x,R=199)
## One sample robust Hotelling test
data(ForgedBankNotes)
samplemean <- apply(ForgedBankNotes, 2, mean)</pre>
res = FRBhotellingS(ForgedBankNotes, mu0=samplemean,R=199)
# Note that the test rejects the hypothesis that the true mean equals the
# sample mean; this is due to outliers in the data (i.e. the robustly estimated
# mean apparently significantly differs from the non-robust sample mean.
# Graphical display of the results:
plot(res)
# It is clear from the (scaled) simultaneous confidence limits that the rejection
# of the hypothesis is due to the differences in variables Bottom and Diagonal
## Two sample robust Hotelling test
data(hemophilia, package="rrcov")
grp <-as.factor(hemophilia[,3])</pre>
x <- hemophilia[which(grp==levels(grp)[1]),1:2]</pre>
y <- hemophilia[which(grp==levels(grp)[2]),1:2]</pre>
#using the pooled covariance matrix to estimate the common covariance matrix
res = FRBhotellingS(x,y,method="pool")
#using the estimator of He and Fung to estimate the common covariance matrix
res = FRBhotellingS(x,y,method="HeFung",R=199)
# or using the formula interface
res = FRBhotellingS(as.matrix(hemophilia[,-3])~hemophilia[,3],method="HeFung",R=99)
# From the confidence limits it can be seen that the significant difference
# is mainly caused by the AHFactivity variable. The graphical display helps too:
# the red line on the histogram indicates the test statistic value in the original
# sample (it is omitted if the statistic exceeds 100)
```

FRBmultiregGS

GS-Estimates for multivariate regression with bootstrap confidence intervals

# **Description**

Computes GS-estimates for multivariate regression together with standard errors, confidence intervals and p-values based on the Fast and Robust Bootstrap.

## Usage

```
## S3 method for class 'formula'
FRBmultiregGS(formula, data=NULL, ...)
## Default S3 method:
FRBmultiregGS(X, Y, int = TRUE, R = 999, bdp = 0.5, conf = 0.95, control=GScontrol(...), na.action=na.omit, ...)
```

# **Arguments**

formula	an object of class formula; a symbolic description of the model to be fit.
data	data frame from which variables specified in formula are to be taken.
Χ	a matrix or data frame containing the explanatory variables.
Υ	a matrix or data frame containing the response variables.
int	logical: if TRUE an intercept term is added to the model (unless it is already present in X)
R	number of bootstrap samples. Default is R=999.
bdp	required breakdown point. Should have $0 < bdp \le 0.5$ , the default is 0.5.
conf	confidence level of the bootstrap confidence intervals. Default is conf=0.95.
control	a list with control parameters for tuning the computing algorithm, see ${\tt GScontrol}().$
na.action	a function which indicates what should happen when the data contain NAs. Defaults to na.omit.
	allows for specifying control parameters directly instead of via control.

# Details

Generalized S-estimators are defined by minimizing the determinant of a robust estimator of the scatter matrix of the differences of the residuals (Roelant et al. 2009). Hence, this procedure is intercept free and only gives an estimate for the slope matrix. To estimate the intercept, we use the M-type estimator of location of Lopuhaa (1992) on the residuals with the residual scatter matrix estimate of the residuals as a preliminary estimate. This computation is carried out by a call to GSest\_multireg(), which uses a fast-S-type algorithm (its tuning parameters can be changed via the control argument). The result of this call is also returned as the value est.

The Fast and Robust Bootstrap (Salibian-Barrera and Zamar 2002) is used to calculate so-called basic bootstrap confidence intervals and bias corrected and accelerated (BCa) confidence intervals (Davison and Hinkley 1997, p.194 and p.204 respectively). Apart from the intervals with the requested confidence level, the function also returns p-values for each coefficient corresponding to the hypothesis that the actual coefficient is zero. The p-values are computed as 1 minus the smallest level for which the confidence intervals would include zero. Both BCa and basic bootstrap p-values

in this sense are given. The bootstrap calculation is carried out by a call to GSboot\_multireg(), the result of which is returned as the value bootest. Bootstrap standard errors are returned as well.

Note: Bootstrap samples which contain too few distinct observations with positive weights are discarded (a warning is given if this happens). The number of samples actually used is returned via ROK.

In the formula-interface, a multivariate response is produced via cbind. For example  $cbind(x4,x5) \sim x1+x2+x3$ . All arguments from the default method can also be passed to the formula method.

The returned object inherits from class mlm such that the standard coef, residuals, fitted and predict functions can be used.

#### Value

An object of class FRBmultireg which extends class mlm and contains at least the following components:

coefficients GS-estimates of the regression coefficients
residuals the residuals, that is response minus fitted values
fitted values the fitted values.

Sigma GS-estimate of the error covariance matrix scale GS-estimate of the size of the multivariate errors

weights implicit weights corresponding to the GS-estimates (i.e. final weights in the

RWLS procedure for the intercept estimate)

outFlag outlier flags: 1 if the robust distance of the residual exceeds the .975 quantile of

(the square root of) the chi-square distribution with degrees of freedom equal to

the dimension of the responses; 0 otherwise

SE bootstrap standard errors corresponding to the regression coefficients

cov bootstrap covariance matrix corresponding to the regression coefficients (in vec-

torized form)

CI.bca.lower a matrix containing the lower bound of the bias corrected and accelerated confi-

dence intervals for the regression coefficients

CI.bca.upper a matrix containing the upper bound of the bias corrected and accelerated confi-

dence intervals for the regression coefficients

CI.basic.lower a matrix containing the lower bound of basic bootstrap intervals for the regres-

sion coefficients

CI.basic.upper a matrix containing the upper bound of basic bootstrap intervals for the regres-

sion coefficients

p.bca a matrix containing the p-values based on the BCa confidence intervals for the

regression coefficients

p.basic a matrix containing the p-values based on the basic bootstrap intervals for the

regression coefficients

est GS-estimates as returned by the call to GSest\_multireg()

bootest bootstrap results for the GS-estimates as returned by the call to GSboot\_multireg()

conf a copy of the conf argument

method	a list with following components: $est = character string indicating that GS-estimates were used, and bdp = a copy of the bdp argument$
control	a copy of the control argument
X, Y	either copies of the respective arguments or the corresponding matrices produced from formula
ROK	number of bootstrap samples actually used (i.e. not discarded due to too few distinct observations with positive weight)

## Author(s)

Ella Roelant, Stefan Van Aelst and Gert Willems

## References

- A.C. Davison and D.V. Hinkley (1997) *Bootstrap Methods and their Application*. Cambridge Series in Statistical and Probabilistic Mathematics. Cambridge: Cambridge University Press.
- H.P. Lopuhaa (1992) Highly efficient estimators of multivariate location with high breakdown point. *The Annals of Statistics*, **20**, 398-413.
- E. Roelant, S. Van Aelst and C. Croux (2009) Multivariate Generalized S-estimators. *Journal of Multivariate Analysis*, **100**, 876–887.
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- S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

## See Also

summary.FRBmultireg, plot.FRBmultireg, GSboot\_multireg, GSest\_multireg, FRBmultiregMM,
FRBmultiregS, GScontrol

```
#("BCA" method by default)
summary(GSres)
summary(GSres, confmethod="basic")
#ask explicitely for the coefficient matrix:
GSres$coefficients
# or equivalently,
coef(GSres)
#For the error covariance matrix:
GSres$Sigma
#plot some bootstrap histograms for the coefficient estimates
#(with "BCA" intervals by default)
plot(GSres, expl=c("education", "occupation"), resp=c("selfesteem","reading"))
#plot bootstrap histograms for all coefficient estimates
plot(GSres)
#possibly the plot-function has made a selection of coefficients to plot here,
#since 'all' may have been too many to fit on one page, see help(plot.FRBmultireg);
#this is platform-dependent
```

FRBmultiregMM

MM-Estimates for Multivariate Regression with Bootstrap Inference

# Description

Computes MM-estimates for multivariate regression together with standard errors, confidence intervals and p-values based on the Fast and Robust Bootstrap.

# Usage

#### **Arguments**

formula	an object of class formula; a symbolic description of the model to be fit.
data	data frame from which variables specified in formula are to be taken.
X	a matrix or data frame containing the explanatory variables.
Υ	a matrix or data frame containing the response variables.
int	logical: if TRUE an intercept term is added to the model (unless it is already present in $X$ )

R number of bootstrap samples. Default is R=999.

conf level of the bootstrap confidence intervals. Default is conf=0.95

control a list with control parameters for tuning the MM-estimate and its computing

algorithm, see MMcontrol().

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

faults to na.omit.

... allows for specifying control parameters directly instead of via control

#### **Details**

Multivariate MM-estimates combine high breakdown point and high Gaussian efficiency. They are defined by first computing an S-estimate of regression, then fixing the scale component of the error covariance estimate, and finally re-estimating the regression coefficients and the shape part of the error covariance by a more efficient M-estimate (see Tatsuoka and Tyler (2000) for MM-estimates in the special case of location/scatter estimation, and Van Aelst and Willems (2005) for S-estimates of multivariate regression).

Tukey's biweight is used for the loss functions. By default, the first loss function (in the S-estimate) is tuned in order to obtain 50% breakdown point. The default tuning of the second loss function (M-estimate) ensures 95% efficiency at the normal model for the coefficient estimates. The desired efficiency can be changed through argument control.

The computation is carried out by a call to MMest\_multireg(), which first performs the fast-S algorithm (see Sest\_multireg) and does the M-part by reweighted least squares (RWLS) iteration. See MMcontrol for some adjustable tuning parameters regarding the algorithm. The result of this call is also returned as the value est.

The Fast and Robust Bootstrap (Salibian-Barrera and Zamar 2002) is used to calculate so-called basic bootstrap confidence intervals and bias corrected and accelerated (BCa) confidence intervals (Davison and Hinkley 1997, p.194 and p.204 respectively). Apart from the intervals with the requested confidence level, the function also returns p-values for each coefficient corresponding to the hypothesis that the actual coefficient is zero. The p-values are computed as 1 minus the smallest level for which the confidence intervals would include zero. Both BCa and basic bootstrap p-values in this sense are given. The bootstrap calculation is carried out by a call to MMboot\_multireg(), the result of which is returned as the value bootest. Bootstrap standard errors are returned as well.

Note: Bootstrap samples which contain too few distinct observations with positive weights are discarded (a warning is given if this happens). The number of samples actually used is returned via

In the formula-interface, a multivariate response is produced via cbind. For example  $cbind(x4,x5) \sim x1+x2+x3$ . All arguments from the default method can also be passed to the formula method except for int (passing int explicitly will produce an error; the inclusion of an intercept term is determined by formula).

The returned object inherits from class mlm such that the standard coef, residuals, fitted and predict functions can be used.

#### Value

An object of class FRBmultireg which extends class mlm and contains at least the following components:

MM-estimates of the regression coefficients coefficients residuals the residuals, that is response minus fitted values fitted.values the fitted values. Sigma MM-estimate of the error covariance matrix MM-estimate of the size of the multivariate errors scale weights implicit weights corresponding to the MM-estimates (i.e. final weights in the RWLS procedure) outFlag outlier flags: 1 if the robust distance of the residual exceeds the .975 quantile of (the square root of) the chi-square distribution with degrees of freedom equal to the dimension of the responses; 0 otherwise SE bootstrap standard errors corresponding the regression coefficients cov bootstrap covariance matrix corresponding to the regression coefficients (in vectorized form) CI.bca.lower a matrix containing the lower bounds of the bias corrected and accelerated confidence intervals for the regression coefficients. a matrix containing the upper bounds of the bias corrected and accelerated con-CI.bca.upper fidence intervals for the regression coefficients. CI.basic.lower a matrix containing the lower bounds of basic bootstrap intervals for the regression coefficients. CI.basic.upper a matrix containing the upper bounds of basic bootstrap intervals for the regression coefficients. a matrix containing the p-values based on the BCa confidence intervals for the p.bca regression coefficients. p.basic a matrix containing the p-values based on the basic bootstrap intervals for the regression coefficients. MM-estimates as returned by the call to MMest\_multireg() est bootstrap results for the MM-estimates as returned by the call to MMboot\_multireg() bootest conf a copy of the conf argument method a list with following components: est = character string indicating that MMestimates were used, bdp = a copy of bdp from the control argument, and eff = a copy of eff from the control argument control a copy of the control argument either copies of the respective arguments or the corresponding matrices pro-X, Y duced from formula

number of bootstrap samples actually used (i.e. not discarded due to too few

#### Author(s)

ROK

Gert Willems, stefan Van Aelst and Ella Roelant

distinct observations with positive weight)

#### References

 A.C. Davison and D.V. Hinkley (1997) Bootstrap Methods and their Application. Cambridge Series in Statistical and Probabilistic Mathematics. Cambridge: Cambridge University Press.

- M. Salibian-Barrera, S. Van Aelst and G. Willems (2008) Fast and robust bootstrap. *Statistical Methods and Applications*, **17**, 41-71.
- M. Salibian-Barrera, R.H. Zamar (2002) Bootstrapping robust estimates of regression. *The Annals of Statistics*, **30**, 556-582.
- K.S. Tatsuoka and D.E. Tyler (2000) The uniqueness of S and M-functionals under non-elliptical distributions. *The Annals of Statistics*, **28**, 1219-1243.
- S. Van Aelst and G. Willems (2005) Multivariate regression S-estimators for robust estimation and inference. *Statistica Sinica*, **15**, 981-1001.
- S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

#### See Also

summary.FRBmultireg,plot.FRBmultireg,MMboot\_multireg,MMest\_multireg,FRBmultiregS,FRBmultiregGS,MMcontrol

```
data(schooldata)
school.x <- data.matrix(schooldata[,1:5])</pre>
school.y <- data.matrix(schooldata[,6:8])</pre>
#computes MM-estimate and 95% confidence intervals
#based on 999 bootstrap samples:
MMres <- FRBmultiregMM(school.x, school.y, R=999, conf = 0.95)
#or, equivalently using the formula interface
MMres <- FRBmultiregMM(cbind(reading, mathematics, selfesteem)~., data=schooldata,
             R=999, conf = 0.95)
#the print method displays the coefficient estimates
MMres
#the summary function additionally displays the bootstrap standard errors and p-values
#("BCA" method by default)
summary(MMres)
summary(MMres, confmethod="basic")
#ask explicitely for the coefficient matrix:
MMres$coefficients
# or equivalently,
coef(MMres)
#For the error covariance matrix:
MMres$Sigma
```

```
#plot some bootstrap histograms for the coefficient estimates
#(with "BCA" intervals by default)
plot(MMres, expl=c("education", "occupation"), resp=c("selfesteem","reading"))
#plot bootstrap histograms for all coefficient estimates
plot(MMres)
#probably the plot-function has made a selection of coefficients to plot here,
#since 'all' was too many to fit on one page, see help(plot.FRBmultireg);
#this is platform-dependent
```

FRBmultiregS

S-Estimates for Multivariate Regression with Bootstrap Inference

# **Description**

Computes S-estimates for multivariate regression together with standard errors, confidence intervals and p-values based on the Fast and Robust Bootstrap.

# Usage

# **Arguments**

formula	an object of class formula; a symbolic description of the model to be fit.
data	data frame from which variables specified in formula are to be taken.
Χ	a matrix or data frame containing the explanatory variables.
Υ	a matrix or data frame containing the response variables.
int	logical: if TRUE an intercept term is added to the model (unless it is already present in X)
R	number of bootstrap samples. Default is R=999.
bdp	required breakdown point for the S-estimates. Should have $0 < \mathrm{bdp} \leq 0.5,$ the default is $0.5$
conf	level of the bootstrap confidence intervals. Default is conf=0.95
control	a list with control parameters for tuning the computing algorithm, see $Scontrol()$ .
na.action	a function which indicates what should happen when the data contain NAs. Defaults to na.omit.
	allows for specifying control parameters directly instead of via control

#### **Details**

Multivariate S-estimates were introduced by Davies (1987) and can be highly robust while enjoying a reasonable Gaussian efficiency. Their use in the multivariate regression setting was discussed in Van Aelst and Willems (2005). The loss function used here is Tukey's biweight. It is tuned in order to achieve the required breakdown point bdp (any value between 0 and 0.5).

The computation is carried out by a call to Sest\_multireg(), which performs the fast-S algorithm (Salibian-Barrera and Yohai 2006), see Scontrol for its tuning parameters. The result of this call is also returned as the value est.

The Fast and Robust Bootstrap (Salibian-Barrera and Zamar 2002) is used to calculate so-called basic bootstrap confidence intervals and bias corrected and accelerated (BCa) confidence intervals (Davison and Hinkley 1997, p.194 and p.204 respectively). Apart from the intervals with the requested confidence level, the function also returns p-values for each coefficient corresponding to the hypothesis that the actual coefficient is zero. The p-values are computed as 1 minus the smallest level for which the confidence intervals would include zero. Both BCa and basic bootstrap p-values in this sense are given. The bootstrap calculation is carried out by a call to Sboot\_multireg(), the result of which is returned as the value bootest. Bootstrap standard errors are returned as well.

Note: Bootstrap samples which contain too few distinct observations with positive weights are discarded (a warning is given if this happens). The number of samples actually used is returned via ROK.

In the formula-interface, a multivariate response is produced via cbind. For example  $cbind(x4,x5) \sim x1+x2+x3$ . All arguments from the default method can also be passed to the formula method except for int (passing int explicitly will produce an error; the inclusion of an intercept term is determined by formula).

The returned object inherits from class mlm such that the standard coef, residuals, fitted and predict functions can be used.

#### Value

An object of class FRBmultireg which extends class mlm and contains at least the following components:

ponents:

coefficients MM-estimates of the regression coefficients

residuals the residuals, that is response minus fitted values

fitted.values the fitted values.

Sigma S-estimate of the error covariance matrix

scale MM-estimate of the size of the multivariate errors

weights implicit weights corresponding to the S-estimates (i.e. final weights in the

RWLS procedure at the end of the fast-S algorithm)

outFlag outlier flags: 1 if the robust distance of the residual exceeds the .975 quantile of

(the square root of) the chi-square distribution with degrees of freedom equal to

the dimension of the responses; 0 otherwise

SE bootstrap standard errors corresponding to the regression coefficients.

cov bootstrap covariance matrix corresponding to the regression coefficients (in vec-

torized form)

CI.bca.lower	a matrix containing the lower bounds of the bias corrected and accelerated confidence intervals for the regression coefficients.
CI.bca.upper	a matrix containing the upper bounds of the bias corrected and accelerated confidence intervals for the regression coefficients.
CI.basic.lower	a matrix containing the lower bounds of basic bootstrap intervals for the regression coefficients.
CI.basic.upper	a matrix containing the upper bounds of basic bootstrap intervals for the regression coefficients.
p.bca	a matrix containing the p-values based on the BCa confidence intervals for the regression coefficients.
p.basic	a matrix containing the p-values based on the basic bootstrap intervals for the regression coefficients.
est	S-estimates as returned by the call to Sest_multireg()
bootest	bootstrap results for the S-estimates as returned by the call to Sboot_multireg()
conf	a copy of the conf argument
method	a list with following components: $est = character string indicating that S-estimates were used, and bdp = a copy of the bdp argument$
control	a copy of the control argument
X, Y	either copies of the respective arguments or the corresponding matrices produced from formula
ROK	number of bootstrap samples actually used (i.e. not discarded due to too few distinct observations with positive weight)

# Author(s)

Gert Willems, Stefan Van Aelst and Ella Roelant

#### References

- P.L. Davies (1987) Asymptotic behavior of S-estimates of multivariate location parameters and dispersion matrices. *The Annals of Statistics*, **15**, 1269-1292.
- A.C. Davison and D.V. Hinkley (1997) *Bootstrap Methods and their Application*. Cambridge Series in Statistical and Probabilistic Mathematics. Cambridge: Cambridge University Press.
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- S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

#### See Also

summary.FRBmultireg, plot.FRBmultireg, Sboot\_multireg, Sest\_multireg, FRBmultiregMM,
FRBmultiregGS, Scontrol

```
data(schooldata)
school.x <- data.matrix(schooldata[,1:5])</pre>
school.y <- data.matrix(schooldata[,6:8])</pre>
## computes 25% breakdown point S-estimate and 99% confidence intervals
## based on 999 bootstrap samples:
Sres <- FRBmultiregS(school.x, school.y, R=999, bdp = 0.25, conf = 0.99)</pre>
## or, equivalently using the formula interface
   Sres <- FRBmultiregS(cbind(reading,mathematics,selfesteem)~., data=schooldata,</pre>
            R=999, bdp = 0.25, conf = 0.99)
## the print method displays the coefficient estimates
Sres
## the summary function additionally displays the bootstrap standard errors and p-values
## ("BCA" method by default)
summary(Sres)
summary(Sres, confmethod="basic")
## ask explicitely for the coefficient matrix:
Sres$coefficients
## or equivalently,
coef(Sres)
## For the error covariance matrix:
Sres$Sigma
## plot some bootstrap histograms for the coefficient estimates
## (with "BCA" intervals by default)
plot(Sres, expl=c("education", "occupation"), resp=c("selfesteem","reading"))
## plot bootstrap histograms for all coefficient estimates
plot(Sres)
## probably the plot-function has made a selection of coefficients to plot here,
## since 'all' was too many to fit on one page, see help(plot.FRBmultireg);
## this is platform-dependent
```

FRBpcaMM	PCA based on Multivariate MM-estimators with Fast and Robust Bootstrap
	Βοσιστιάρ

# **Description**

Performs principal components analysis based on the robust MM-estimate of the shape matrix. Additionally uses the Fast and Robust Bootstrap method to compute inference measures such as standard errors and confidence intervals.

# Usage

```
## S3 method for class 'formula'
FRBpcaMM(formula, data=NULL, ...)

## Default S3 method:
FRBpcaMM(Y, R = 999, conf = 0.95, control=MMcontrol(...),
na.action=na.omit, ...)
```

# **Arguments**

formula	an object of class formula; a symbolic description of the model to be fit.
data	data frame from which variables specified in formula are to be taken.
Υ	matrix or data frame.
R	number of bootstrap samples. Default is R=999.
conf	level of the bootstrap confidence intervals. Default is conf=0.95.
control	a list with control parameters for tuning the MM-estimate and its computing algorithm, see MMcontrol().
na.action	a function which indicates what should happen when the data contain NAs. Defaults to na.omit.
	allows for specifying control parameters directly instead of via control.

# **Details**

Multivariate MM-estimates are defined by first computing an S-estimate of location and covariance, then fixing its scale component and re-estimating the location and the shape by a more efficient M-estimate, see Tatsuoka and Tyler (2000). Tukey's biweight is used for the loss functions. By default, the first loss function (in the S-estimate) is tuned in order to obtain 50% breakdown point. The default tuning of the second loss function (M-estimate) ensures 95% efficiency for the shape matrix estimate at the normal model. The desired efficiency can be changed through argument control. (However, control parameter shapeEff will always be considered as TRUE by this function, whichever value is specified.) The MM-estimates are computed by a call to the implementation in the **rrcov** package of Todorov and Filzmoser (2009). The result of this call is also returned as the value est.

PCA is performed by computing the eigenvalues (eigval) and eigenvectors (eigvec) of the MM-estimate of shape, which is a rescaled version of the MM-estimate of covariance (rescaled to have determinant equal to 1). With pvar the function also provides the estimates for the percentage of variance explained by the first k principal components, which are simply the cumulative proportions of the eigenvalues sum. Here, k ranges from 1 to p-1 (with p the number of variables in Y). The eigenvectors are always given in the order of descending eigenvalues.

The Fast and Robust Bootstrap (Salibian-Barrera and Zamar 2002) is used to calculate standard errors, and also so-called basic bootstrap confidence intervals and bias corrected and accelerated (BCa) confidence intervals (Davison and Hinkley 1997, p.194 and p.204 respectively) corresponding to the estimates eigval, eigvec and pvar. The bootstrap is also used to estimate the average angles between true and estimated eigenvectors, returned as avgangle. See Salibian-Barrera, Van Aelst and Willems (2006). The fast and robust bootstrap computations for the MM-estimates are performed by MMboot\_loccov() and its raw result can be found in bootest. The actual bootstrap recalculations for the PCA-related quantities can be found in eigval.boot, eigvec.boot and pvar.boot, where each column represents a bootstrap sample. For eigvec.boot, the eigenvectors are stacked on top of each other and the same goes for eigvec.CI.bca and eigvec.CI.basic which hold the confidence limits.

The two columns in the confidence limits always respectively represent the lower and upper limits. For the percentage of variance the function also provides one-sided confidence intervals ([-infty upper]), which can be used to test the hypothesis that the true percentage at least equals a certain value.

Bootstrap samples are discarded if the fast and robust shape estimate is not positive definite, such that the actual number of recalculations used can be lower than R. This actual number equals R - failedsamples. However, if more than 0.75R of the bootstrap shape estimates is non-positive definite, all bootstrap samples will be used anyway, and the negative eigenvalues are simply set to zero (which may impact the confidence limits and standard errors for the smallest eigenvalues in eigval and pvar).

#### Value

An object of class FRBpca, which contains the following components:

shape	(p x p) MM-estimate of the shape matrix of Y
eigval	(p x 1) eigenvalues of MM shape
eigvec	(p x p) eigenvectors of MM-shape
pvar	(p-1 x 1) percentages of variance for MM eigenvalues
eigval.boot	(p x R) eigenvalues of MM shape
eigvec.boot	(p*p x R) eigenvectors of MM-shape (vectorized)
pvar.boot	(p-1 x R) percentages of variance for MM eigenvalues
eigval.SE	(p x 1) bootstrap standard error for MM eigenvalues
eigvec.SE	(p x p) bootstrap standard error for MM eigenvectors
pvar.SE	(p-1 x 1) bootstrap standard error for percentage of variance for MM-eigenvalues
angles	(p x R) angles between bootstrap eigenvectors and original MM eigenvectors (in radians; in [0 pi/2])

avgangle (p x 1) average angles between bootstrap eigenvectors and original MM eigenvectors (in radians; in [0 pi/2]) eigval.CI.bca (p x 2) BCa intervals for MM eigenvalues eigvec.CI.bca (p\*p x 2) BCa intervals for MM eigenvectors (vectorized) (p-1 x 2) BCa intervals for percentage of variance for MM-eigenvalues pvar.CI.bca pvar. CIone. bca (p-1 x 1) one-sided BCa intervals for percentage of variance for MM-eigenvalues ([-infty upper]) eigval.CI.basic (p x 2) basic bootstrap intervals for MM eigenvalues eigvec.CI.basic (p\*p x 2) basic bootstrap intervals for MM eigenvectors (vectorized) (p-1 x 2) basic bootstrap intervals for percentage of variance for MM-eigenvalues pvar.CI.basic pvar.CIone.basic (p-1 x 1) one-sided basic bootstrap intervals for percentage of variance for MMeigenvalues ([-infty upper]) est list containing the MM-estimates of location and scatter (list) result of MMboot\_loccov() bootest failedsamples number of bootstrap samples with non-positive definiteness of shape a copy of the conf argument conf method a character string giving the robust PCA method that was used implicit weights corresponding to the MM-estimates (i.e. final weights in the RWLS procedure) outlier flags: 1 if the robust distance of the observation exceeds the .975 quantile outFlag of (the square root of) the chi-square distribution with degrees of freedom equal to the dimension of Y; 0 otherwise Υ copy of the data argument as a matrix

#### Author(s)

Gert Willems, Stefan Van Aelst and Ella Roelant

#### References

- A.C. Davison and D.V. Hinkley (1997) *Bootstrap Methods and their Application*. Cambridge Series in Statistical and Probabilistic Mathematics. Cambridge: Cambridge University Press.
- M. Salibian-Barrera, S. Van Aelst and G. Willems (2006) PCA based on multivariate MM-estimators with fast and robust bootstrap. *Journal of the American Statistical Association*, **101**, 1198-1211.
- M. Salibian-Barrera, S. Van Aelst and G. Willems (2008) Fast and robust bootstrap. *Statistical Methods and Applications*, **17**, 41-71.
- M. Salibian-Barrera, R.H. Zamar (2002) Bootstrapping robust estimates of regression. *The Annals of Statistics*, **30**, 556-582.

• K.S. Tatsuoka and D.E. Tyler (2000) The uniqueness of S and M-functionals under non-elliptical distributions. *The Annals of Statistics*, **28**, 1219-1243

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- S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

#### See Also

```
plot.FRBpca, summary.FRBpca, print.FRBpca, FRBpcaS, MMboot_loccov, MMcontrol
```

```
data(ForgedBankNotes)
MMpcares <- FRBpcaMM(ForgedBankNotes, R=999, conf=0.95)</pre>
# or using the formula interface
MMpcares <- FRBpcaMM(~.,data=ForgedBankNotes, R=999, conf=0.95)</pre>
# the simple print method shows the standard deviations with confidence limits:
MMpcares
# the summary functions shows a lot more (see help(summary.FRBpca)):
summary(MMpcares)
# ask for the eigenvalues:
MMpcares$eigval
# or, in more pretty format, with confidence limits:
summary(MMpcares)$eigvals
# note that the standard deviations of the print-output can also be asked for by:
sqrt( summary(MMpcares)$eigvals )
# the eigenvectors and their standard errors:
MMpcares$eigvec # or prettier: summary(MMpcares)$eigvecs
MMpcares$eigvec.SE
    # take a look at the bootstrap distribution of the first eigenvalue
   hist(MMpcares$eigval.boot[1,])
    # that bootstrap distribution is used to compute confidence limits as depicted
    # by the screeplot function:
   plotFRBvars(MMpcares, cumul=0)
    # all plots for the FRB-PCA result:
   plot(MMpcares)
```

28 FRBpcaS

FRBpcaS	PCA based on Multivariate S-estimators with Fast and Robust Boot-
	strap

## **Description**

Performs principal components analysis based on the robust S-estimate of the shape matrix. Additionally uses the Fast and Robust Bootstrap method to compute inference measures such as standard errors and confidence intervals.

## Usage

```
## S3 method for class 'formula'
FRBpcaS(formula, data=NULL, ...)
## Default S3 method:
FRBpcaS(Y, R = 999, bdp = 0.5, conf = 0.95, control=Scontrol(...),
na.action=na.omit, ...)
```

#### **Arguments**

formula	an object of class formula; a symbolic description of the model to be fit.
data	data frame from which variables specified in formula are to be taken.
Υ	matrix or data frame.
R	number of bootstrap samples. Default is R=999.
bdp	required breakdown point for the S-estimates. Should have $0 < \mathrm{bdp} \leq 0.5,$ the default is 0.5.
conf	level of the bootstrap confidence intervals. Default is conf=0.95.
control	a list with control parameters for tuning the computing algorithm, see Scontrol().
na.action	a function which indicates what should happen when the data contain NAs. Defaults to na.omit.
	allows for specifying control parameters directly instead of via control.

# **Details**

Multivariate S-estimates were introduced by Davies (1987) and can be highly robust while enjoying a reasonable Gaussian efficiency. The loss function used here is Tukey's biweight. It will be tuned in order to achieve the required breakdown point bdp (any value between 0 and 0.5). The MM-estimates are computed by a call to the implementation of the fast-S algorithm (Salibian-Barrera and Yohai 2006) in the **rrcov** package of Todorov and Filzmoser (2009). Scontrol provides some adjustable tuning parameters regarding the algorithm. The result of this call is also returned as the value est.

PCA is performed by computing the eigenvalues (eigval) and eigenvectors (eigvec) of the S-estimate of shape, which is a rescaled version of the S-estimate of covariance (rescaled to have

FRBpcaS 29

determinant equal to 1). With pvar the function also provides the estimates for the percentage of variance explained by the first k principal components, which are simply the cumulative proportions of the eigenvalues sum. Here, k ranges from 1 to p-1 (with p the number of variables in Y). The eigenvectors are always given in the order of descending eigenvalues.

The Fast and Robust Bootstrap (Salibian-Barrera and Zamar 2002) is used to calculate standard errors, and also so-called basic bootstrap confidence intervals and bias corrected and accelerated (BCa) confidence intervals (Davison and Hinkley 1997, p.194 and p.204 respectively) corresponding to the estimates eigval, eigvec and pvar. The bootstrap is also used to estimate the average angles between true and estimated eigenvectors, returned as avgangle. See Salibian-Barrera, Van Aelst and Willems (2006). The fast and robust bootstrap computations for the S-estimates are performed by Sboot\_loccov() and its raw result can be found in bootest. The actual bootstrap values of the PCA-related quantities can be found in eigval.boot, eigvec.boot and pvar.boot, where each column represents a bootstrap sample. For eigvec.boot, the eigenvectors are stacked on top of each other and the same goes for eigvec.CI.bca and eigvec.CI.basic which hold the confidence limits.

The two columns in the confidence limits always respectively represent the lower and upper limits. For the percentage of variance the function also provides one-sided confidence intervals ([-infty upper]), which can be used to test the hypothesis that the true percentage at least equals a certain value.

Bootstrap samples are discarded if the fast and robust covariance estimate is not positive definite, such that the actual number of recalculations used can be lower than R. This actual number equals R - failedsamples. However, if more than 0.75R of the bootstrap shape estimates is non-positive definite, the failed bootstrap samples are recovered by applying the make.positive.definite function (from package corpcor). If this also fails, the corresponding bootstrap sample is discarded after all, but such situation should be rare. This recovery may have an impact on the confidence limits and standard errors of especially the smallest eigenvalues in eigval and pvar.

# Value

An object of class FRBpca, which contains the following components:

shape	(p x p) S-estimate of the shape matrix of Y
eigval	(p x 1) eigenvalues of S shape
eigvec	(p x p) eigenvectors of S-shape
pvar	(p-1 x 1) percentages of variance for S eigenvalues
eigval.boot	(p x R) eigenvalues of S shape
eigvec.boot	(p*p x R) eigenvectors of S-shape (vectorized)
pvar.boot	(p-1 x R) percentages of variance for S eigenvalues
eigval.SE	(p x 1) bootstrap standard error for S eigenvalues
eigvec.SE	(p x p) bootstrap standard error for S eigenvectors
pvar.SE	(p-1 x 1) bootstrap standard error for percentage of variance for S eigenvalues
angles	(p x R) angles between bootstrap eigenvectors and original S eigenvectors (in radians; in $[0 \ pi/2])$
avgangle	(p x 1) average angles between bootstrap eigenvectors and original S eigenvectors (in radians; in [0 pi/2])

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eigval.CI.bca (p x 2) BCa intervals for S eigenvalues eigvec.CI.bca (p\*p x 2) BCa intervals for S eigenvectors (vectorized) pvar.CI.bca (p-1 x 2) BCa intervals for percentage of variance for S-eigenvalues pvar.CIone.bca (p-1 x 1) one-sided BCa intervals for percentage of variance for S-eigenvalues ([-infty upper]) eigval.CI.basic (p x 2) basic bootstrap intervals for S eigenvalues eigvec.CI.basic (p\*p x 2) basic bootstrap intervals for S eigenvectors (vectorized) (p-1 x 2) basic bootstrap intervals for percentage of variance for S-eigenvalues pvar.CI.basic pvar.CIone.basic (p-1 x 1) one-sided basic bootstrap intervals for percentage of variance for Seigenvalues ([-infty upper]) list containing the S-estimates of location and scatter est bootest (list) result of Sboot\_loccov() failedsamples number of bootstrap samples with non-positive definiteness of shape conf a copy of the conf argument method a character string giving the robust PCA method that was used implicit weights corresponding to the S-estimates (i.e. final weights in the RWLS procedure at the end of the fast-S algorithm) outFlag outlier flags: 1 if the robust distance of the observation exceeds the .975 quantile of (the square root of) the chi-square distribution with degrees of freedom equal to the dimension of Y; 0 otherwise Υ copy of the data argument as a matrix

## Author(s)

Gert Willems, Stefan Van Aelst and Ella Roelant

#### References

- P.L. Davies (1987) Asymptotic behavior of S-estimates of multivariate location parameters and dispersion matrices. *The Annals of Statistics*, **15**, 1269-1292.
- A.C. Davison and D.V. Hinkley (1997) *Bootstrap Methods and their Application*. Cambridge Series in Statistical and Probabilistic Mathematics. Cambridge: Cambridge University Press.
- M. Salibian-Barrera, S. Van Aelst and G. Willems (2006) PCA based on multivariate MM-estimators with fast and robust bootstrap. *Journal of the American Statistical Association*, **101**, 1198-1211.
- M. Salibian-Barrera, S. Van Aelst and G. Willems (2008) Fast and robust bootstrap. *Statistical Methods and Applications*, **17**, 41-71.
- M. Salibian-Barrera, R.H. Zamar (2002) Bootstrapping robust estimates of regression. *The Annals of Statistics*, **30**, 556-582.
- V. Todorov and P. Filzmoser (2009), An Object Oriented Framework for Robust Multivariate Analysis. *Journal of Statistical Software*, **32**(3), 1–47. doi:10.18637/jss.v032.i03.
- S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

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# See Also

```
plot.FRBpca, summary.FRBpca, print.FRBpca, FRBpcaMM, Sboot_loccov, Scontrol
```

```
data(ForgedBankNotes)
Spcares <- FRBpcaS(ForgedBankNotes, R=999, bdp=0.25, conf=0.95)</pre>
## or using the formula interface
   Spcares <- FRBpcaMM(~.,data=ForgedBankNotes, R=999, conf=0.95)</pre>
## the simple print method shows the standard deviations with confidence limits:
Spcares
## the summary functions shows a lot more (see help(summary.FRBpca)):
summary(Spcares)
## ask for the eigenvalues:
Spcares$eigval
## or, in more pretty format, with confidence limits:
summary(Spcares)$eigvals
## note that the standard deviations of the print-output can also be asked for by:
sqrt(summary(Spcares)$eigvals)
## the eigenvectors and their standard errors:
Spcares$eigvec # or prettier: summary(MMpcares)$eigvecs
Spcares$eigvec.SE
   ## take a look at the bootstrap distribution of the first eigenvalue
   hist(Spcares$eigval.boot[1,])
    ## that bootstrap distribution is used to compute confidence limits as depicted
    ## by the screeplot function:
   plotFRBvars(Spcares, cumul=0)
    ## all plots for the FRB-PCA result:
   plot(Spcares)
```

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#### **Description**

Calculates bootstrapped GS-estimates and bootstrap confidence intervals using the Fast and Robust Bootstrap method.

# Usage

```
GSboot_multireg(X, Y, R = 999, conf=0.95, ests = GSest_multireg(X, Y))
```

# Arguments

X a matrix or data frame containing the explanatory variables (possibly including intercept).

Y a matrix or data frame containing the response variables.

R number of bootstrap samples. Default is R=999.

confidence level of the bootstrap confidence intervals. Default is conf=0.95.

ests GS-estimates as returned by GSest\_multireg().

#### **Details**

Called by FRBmultiregGS and typically not to be used on its own. If no original GS-estimates are provided the function calls GSest\_multireg with its default settings.

The fast and robust bootstrap was first introduced by Salibian-Barrera and Zamar (2002) for univariate regression MM-estimators and developed for GS-estimates by Roelant et al. (2009).

The value centered gives a matrix with R columns and p\*q+q\*q rows (p is the number of explanatory variables and q is the number of response variables), containing the recalculated GS-estimates. Each column represents a different bootstrap sample. The first p\*q rows are the recalculated coefficient estimates and the next q\*q rows are the covariance estimates (the estimates are vectorized, i.e. columns stacked on top of each other). These bootstrap estimates are centered by the original estimates, which are also returned through vecest in vectorized form.

The output list further contains bootstrap standard errors, as well as so-called basic bootstrap confidence intervals and bias corrected and accelerated confidence intervals (Davison and Hinkley, 1997, p.194 and p.204 respectively). Also in the output are p-values defined as 1 minus the smallest confidence level for which the confidence intervals would include the (hypothesised) value of zero. Both BCa and basic bootstrap p-values are given. These are only useful for the regression coefficient estimates (not really for the covariance estimates).

Bootstrap samples which contain too few distinct observations with positive weights are discarded (a warning is given if this happens). The number of samples actually used is returned via ROK.

#### Value

A list containing the following components:

centered a matrix of all fast and robust bootstrap recalculations where the recalculations

are centered by the original estimates (see Details)

vecest a vector containing the original estimates stacked on top of each other

SE bootstrap standard errors for the estimates in vecest

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COV	bootstrap covariance matrix for the estimates in vecest
CI.bca	a matrix containing bias corrected and accelerated confidence intervals, corresponding to the estimates in vecest (first column are lower limits, second column are upper limits)
CI.basic	a matrix containing basic bootstrap intervals, corresponding to the estimates in vecest (first column are lower limits, second column are upper limits)
p.bca	a vector containing p-values based on the bias corrected and accelerated confidence intervals (corresponding to the estimates in vecest)
p.basic	a vector containing p-values based on the basic bootstrap intervals (corresponding to the estimates in vecest)
ROK	number of bootstrap samples actually used (i.e. not discarded due to too few distinct observations with positive weight)

#### Author(s)

Ella Roelant, Stefan Van Aelst and Gert Willems

#### References

- A.C. Davison, D.V. Hinkley (1997) Bootstrap methods and their application. Cambridge University Press.
- E. Roelant, S. Van Aelst and C. Croux (2009) Multivariate Generalized S-estimators. *Journal of Multivariate Analysis*, **100**, 876–887.
- M. Salibian-Barrera, S. Van Aelst and G. Willems (2008) Fast and robust bootstrap. *Statistical Methods and Applications*, **17**, 41–71.
- M. Salibian-Barrera, R.H. Zamar (2002) Bootstrapping robust estimates of regression. *The Annals of Statistics*, **30**, 556–582.
- S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

# See Also

```
FRBmultiregGS, GSest_multireg
```

```
data(schooldata)
school.x1 <- data.matrix(schooldata[,1:2])
school.y <- data.matrix(schooldata[,6:8])

## computes 10 bootstrap recalculations starting from the GS-estimator
## obtained from GSest_multireg

bootres <- GSboot_multireg(school.x1,school.y,R=5)</pre>
```

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	GSest_multireg	GS Estimates for Multivariate Regression	
--	----------------	--	--

# **Description**

Computes GS-Estimates of multivariate regression based on Tukey's biweight function.

# Usage

```
## S3 method for class 'formula'
GSest_multireg(formula, data=NULL, ...)
## Default S3 method:
GSest_multireg(X, Y, int = TRUE, bdp = 0.5, control=GScontrol(...),
na.action=na.omit, ...)
```

## **Arguments**

formula	an object of class formula; a symbolic description of the model to be fit.
data	data frame from which variables specified in formula are to be taken.
X	a matrix or data frame containing the explanatory variables.
Υ	a matrix or data frame containing the response variables.
int	logical: if TRUE an intercept term is added to the model (unless it is already present in $X$ )
bdp	required breakdown point. Should have $0 < bdp \le 0.5$ , the default is 0.5.
control	a list with control parameters for tuning the computing algorithm, see ${\tt GScontrol}().$
na.action	a function which indicates what should happen when the data contain NAs. Defaults to na.omit.
	allows for specifying control parameters directly instead of via control.

# **Details**

Generalized S-estimators are defined by minimizing the determinant of a robust estimator of the scatter matrix of the differences of the residuals. Hence, this procedure is intercept free and only gives an estimate for the slope matrix. To estimate the intercept, we use the M-type estimator of location of Lopuhaa (1992) on the residuals with the residual scatter matrix estimate of the residuals as a preliminary estimate. We use a fast algorithm similar to the one proposed by Salibian-Barrera and Yohai (2006) for the regression case. See GScontrol for the adjustable tuning parameters of this algorithm.

The returned object inherits from class mlm such that the standard coef, residuals, fitted and predict functions can be used.

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#### Value

An object of class FRBmultireg which extends class mlm and contains at least the following components:

coefficients GS-estimates of the regression coefficients residuals the residuals, that is response minus fitted values

fitted.values the fitted values.

Sigma GS-estimate of the error covariance matrix
Gamma GS-estimate of the error shape matrix

scale GS-estimate of the size of the multivariate errors

weights implicit weights corresponding to the GS-estimates (i.e. final weights in the

RWLS procedure for the intercept estimate)

outFlag outlier flags: 1 if the robust distance of the residual exceeds the .975 quantile of

(the square root of) the chi-square distribution with degrees of freedom equal to

the dimension of the responses; 0 otherwise

b, c tuning parameters used in Tukey biweight loss function, as determined by bdp method a list with following components: est = character string indicating that GS-

estimates were used, and bdp = a copy of the bdp argument

control a copy of the control argument

## Author(s)

Ella Roelant, Gert Willems and Stefan Van Aelst

#### References

- H.P. Lopuhaa (1992) Highly efficient estimators of multivariate location with high breakdown point. *The Annals of Statistics*, **20**, 398-413.
- E. Roelant, S. Van Aelst and C. Croux (2009) Multivariate Generalized S-estimators. *Journal of Multivariate Analysis*, **100**, 876–887.
- M. Salibian-Barrera and V. Yohai (2006) A fast algorithm for S-regression estimates. *Journal of Computational and Graphical Statistics*, **15**, 414-427.
- S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

#### See Also

```
{\tt FRB multiregGS, GS boot\_multireg, Sest\_multireg, GS control}
```

```
data(schooldata)
school.x <- data.matrix(schooldata[,1:5])
school.y <- data.matrix(schooldata[,6:8])
GSest <- GSest_multireg(school.x,school.y,nsamp=50)</pre>
```

MMboot\_loccov

```
## or using the formula interface
GSests <- GSest_multireg(cbind(reading,mathematics,selfesteem)~., data=schooldata)</pre>
```

MMboot\_loccov

Fast and Robust Bootstrap for MM-estimates of Location and Covariance

# **Description**

Calculates bootstrapped MM-estimates of multivariate location and scatter using the Fast and Robust Bootstrap method.

# Usage

```
MMboot_loccov(Y, R = 999, ests = MMest_loccov(Y))
```

# **Arguments**

Y matrix or data frame.

R number of bootstrap samples. Default is R=999.

ests original MM-estimates as returned by MMest\_loccov().

#### **Details**

This function is called by FRBpcaMM and FRBhotellingMM, it is typically not to be used on its own. It requires the MM-estimates of multivariate location and scatter/shape (the result of MMest\_loccov applied on Y), supplied through the argument ests. If ests is not provided, MMest\_loccov calls the implementation of the multivariate MM-estimates in package **rrcov** of Todorov and Filzmoser (2009) with default arguments.

For multivariate data the fast and robust bootstrap was developed by Salibian-Barrera, Van Aelst and Willems (2006).

The value centered gives a matrix with R columns and 2\*(p+p\*p) rows (p is the number of variables in Y), containing the recalculated estimates of the MM-location, MM-shape, S-covariance and S-location. Each column represents a different bootstrap sample. The first p rows are the MM-location estimates, the next p\*p rows are the MM-shape estimates (vectorized). Then the next p\*p rows are the S-covariance estimates (vectorized) and the final p rows are the S-location estimates. The estimates are centered by the original estimates, which are also returned through MMest in vectorized form.

#### Value

# A list containing:

centered recalculated MM- and S-estimates of location and scatter (centered by original

estimates), see Details

MMest original MM- and S-estimates of location and scatter, see Details

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#### Author(s)

Gert Willems, Ella Roelant and Stefan Van Aelst

#### References

- M. Salibian-Barrera, S. Van Aelst and G. Willems (2006) PCA based on multivariate MM-estimators with fast and robust bootstrap. *Journal of the American Statistical Association*, **101**, 1198–1211.
- M. Salibian-Barrera, S. Van Aelst and G. Willems (2008) Fast and robust bootstrap. *Statistical Methods and Applications*, **17**, 41–71.
- V. Todorov and P. Filzmoser (2009), An Object Oriented Framework for Robust Multivariate Analysis. *Journal of Statistical Software*, **32**(3), 1–47. doi:10.18637/jss.v032.i03.
- S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

#### See Also

```
FRBpcaMM, FRBhotellingMM, Sboot_loccov
```

## **Examples**

```
Y <- matrix(rnorm(50*5), ncol=5)
MMests <- MMest_loccov(Y)
bootresult <- MMboot_loccov(Y, R = 1000, ests = MMests)</pre>
```

MMboot\_multireg

Fast and Robust Bootstrap for MM-Estimates of Multivariate Regression

## **Description**

Calculates bootstrapped MM-estimates of multivariate regression and corresponding bootstrap confidence intervals using the Fast and Robust Bootstrap method.

#### Usage

```
MMboot_multireg(X, Y, R = 999, conf=0.95, ests = MMest_multireg(X, Y))
```

# **Arguments**

X	a matrix or data frame containing the explanatory variables (possibly including intercept).
Υ	a matrix or data frame containing the response variables.
R	number of bootstrap samples. Default is R=999.
conf	level of the bootstrap confidence intervals. Default is conf=0.95.
ests	MM-estimates as returned by MMest_multireg().

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#### **Details**

Called by FRBmultiregMM and typically not to be used on its own. It requires the result of MMest\_multireg applied on X and Y, supplied through the argument ests. If ests is not provided, MMest\_multireg will be called with default arguments.

The fast and robust bootstrap was first developed by Salibian-Barrera and Zamar (2002) for univariate regression MM-estimators and extended to multivariate regression by Van Aelst and Willems (2005).

The value centered gives a matrix with R columns and 2\*(p\*q+q\*q) rows (p is the number of explanatory variables and q the number of response variables), containing the recalculated MMestimates and initial S-estimates. Each column represents a different bootstrap sample.

The first p\*q rows are the MM-coefficient estimates, the next q\*q rows represent the MM-estimate of the error shape matrix (having determinant 1). Then the next q\*q rows are the S-estimate of error covariance and the final p\*q rows are the S-estimates of the regression coefficients (all estimates are vectorized, i.e. columns stacked on top of each other). These estimates are centered by the original estimates, which are also returned through vecest in vectorized form.

The output list further contains bootstrap standard errors, as well as so-called basic bootstrap confidence intervals and bias corrected and accelerated confidence intervals (Davison and Hinkley, 1997, p.194 and p.204 respectively). Also in the output are p-values defined as 1 minus the smallest confidence level for which the confidence intervals would include the (hypothesised) value of zero. Both BCa and basic bootstrap p-values are given. These are only useful for the regression coefficient estimates (not really for the covariance estimates).

Bootstrap samples which contain less than p distinct observations with positive weights are discarded (a warning is given if this happens). The number of samples actually used is returned via ROK.

## Value

A list containing the following components:

centered	a matrix of all fast/robust bootstrap recalculations where the recalculations are centered by original estimates (see Details)
vecest	a vector containing the original estimates (see Details)
SE	bootstrap standard errors for the estimates in vecest
cov	bootstrap covariance matrix for the estimates in vecest
CI.bca	a matrix containing 95% bias corrected and accelerated confidence intervals corresponding to the estimates in vecest (first column are lower limits, second column are upper limits)
CI.basic	a matrix containing 95% basic bootstrap intervals corresponding to the estimates in vecest (first column are lower limits, second column are upper limits)
p.bca	a vector containing p-values based on the bias corrected and accelerated confidence intervals (corresponding to the estimates in vecest)
p.basic	a vector containing p-values based on the basic bootstrap intervals (corresponding to the estimates in vecest)
ROK	number of bootstrap samples actually used (i.e. not discarded due to too few distinct observations with positive weight)

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## Author(s)

Gert Willems, Ella Roelant and Stefan Van Aelst

#### References

- A.C. Davison, D.V. Hinkley (1997) Bootstrap methods and their application. Cambridge University Press.
- M. Salibian-Barrera, S. Van Aelst and G. Willems (2008) Fast and robust bootstrap. *Statistical Methods and Applications*, **17**, 41–71.
- M. Salibian-Barrera, R.H. Zamar (2002) Bootstrapping robust estimates of regression. *The Annals of Statistics*, **30**, 556–582.
- S. Van Aelst and G. Willems (2005) Multivariate regression S-estimators for robust estimation and inference. *Statistica Sinica*, **15**, 981–1001.
- S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

#### See Also

```
FRBmultiregMM, MMest_multireg, Sboot_multireg
```

# **Examples**

```
data(schooldata)
school.x <- data.matrix(schooldata[,1:5])
school.y <- data.matrix(schooldata[,6:8])

## computes 1000 bootstrap recalculations starting from the MM-estimator
## obtained from MMest_multireg()
bootres <- MMboot_multireg(school.x,school.y,R=1000)</pre>
```

MMboot\_twosample

Fast and Robust Bootstrap for Two-Sample MM-estimates of Location and Covariance

# Description

Calculates bootstrapped two sample MM-estimates using the Fast and Robust Bootstrap method.

#### Usage

```
MMboot_twosample(X, groups, R = 999, ests = MMest_twosample(X, groups))
```

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#### **Arguments**

X matrix of data frame.

groups vector of 1's and 2's, indicating group numbers.

R number of bootstrap samples. Default is R=999.

ests original MM-estimates as returned by MMest\_twosample().

#### **Details**

This function is called by FRBhotellingMM, it is typically not to be used on its own. It requires the result of MMest\_twosample applied on X, supplied through the argument ests. If ests is not provided, MMest\_twosample will be called with default arguments.

The fast and robust bootstrap was first developed by Salibian-Barrera and Zamar (2002) for univariate regression MM-estimators and extended to the two sample setting by Roelant et al. (2008).

The value centered gives a matrix with R columns and 2\*(2\*p+p\*p) rows (p) is the number of variables in X), containing the recalculated estimates of the MM-locations, MM-shape, S-covariance and S-locations. Each column represents a different bootstrap sample. The first p rows are the MM-location estimates of the first sample, the next p rows are the MM-location estimates of the second sample, the next p\*p rows are the common MM-shape estimates (vectorized). Then the next p\*p rows are the common S-covariance estimates (vectorized), the next p are the S-location estimates of the first sample, the final p rows are the S-location estimates of the second sample. The estimates are centered by the original estimates, which are also returned through MMest in vectorized form.

#### Value

# A list containing:

centered recalculated two sample MM- and S-estimates of location and scatter (centered

by original estimates), see Details

MMest original two sample MM- and S-estimates of location and scatter, see Details

# Author(s)

Ella Roelant, Gert Willems and Stefan Van Aelst

#### References

- E. Roelant, S. Van Aelst and G. Willems, (2008) Fast Bootstrap for Robust Hotelling Tests, COMPSTAT 2008: Proceedings in Computational Statistics (P. Brito, Ed.) Heidelberg: Physika-Verlag, 709–719.
- M. Salibian-Barrera, S. Van Aelst and G. Willems (2008) Fast and robust bootstrap. *Statistical Methods and Applications*, **17**, 41–71.
- M. Salibian-Barrera, R.H. Zamar (2002) Bootstrapping robust estimates of regression. *The Annals of Statistics*, **30**, 556–582.
- S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

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## See Also

See Also FRBhotellingMM, Sboot\_twosample

## **Examples**

```
Y1 <- matrix(rnorm(50*5), ncol=5)
Y2 <- matrix(rnorm(50*5), ncol=5)
Ybig <- rbind(Y1,Y2)
grp <- c(rep(1,50),rep(2,50))
MMests <- MMest_twosample(Ybig, grp)
bootresult <- MMboot_twosample(Ybig, grp, R=500, ests=MMests)
```

MMest\_loccov

S- and MM-Estimates of multivariate location and covariance matrix

## **Description**

Compute S- and MM-Estimates of multivariate location and covariance matrix

# Usage

```
MMest_loccov(Y, control=MMcontrol(...), ...)
Sest_loccov(Y, bdp=.5, control=Scontrol(...), ...)
MMest_twosample(X, groups, control=MMcontrol(...), ...)
Sest_twosample(X, groups, bdp=0.5, control=Scontrol(...), ...)
```

## **Arguments**

Υ	input matrix or data frame
Χ	input matrix or data frame
bdp	breakdown point, defaults to 0.5
groups	grouping variable
control	a list with control parameters for tuning the S- or MM-estimate and its computing algorithm, see Scontrol and MMcontrol.
	further arguments to be passed to CovMMest()

## **Details**

This functions are internal, wrappers around the functions Sest() CovMMest().

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# Value

Return lists with the following components:

Mu	location
Gamma	shape
scale	$scale=det^{(1/(2*m))}$
Sigma	covariance matrix
c1	tuning parameter of the loss function for MM-estimation
SMu	location of the initial S-estimate
SGamma	shape of the initial S-estimate
SSigma	covariance matrix of the initial S-estimate
b	tuning parameters used in Tukey biweight loss function for S-estimation, as determined by bdp
W	scaled weights
outflag	outlier flags

# **Examples**

```
Y <- matrix(rnorm(50*5), ncol=5)
(MMests <- MMest_loccov(Y))

(Sests <- Sest_loccov(Y, bdp = 0.25))

Y1 <- matrix(rnorm(50*5), ncol=5)
Y2 <- matrix(rnorm(50*5), ncol=5)
Ybig <- rbind(Y1,Y2)
grp <- c(rep(1,50),rep(2,50))
(MMests <- MMest_twosample(Ybig, grp))</pre>
```

MMest\_multireg

MM-Estimates for Multivariate Regression

# Description

Computes MM-Estimates of multivariate regression, using initial S-estimates

# Usage

```
## S3 method for class 'formula'
MMest_multireg(formula, data=NULL, ...)

## Default S3 method:
MMest_multireg(X, Y, int = TRUE, control=MMcontrol(...),
na.action=na.omit, ...)
```

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## Arguments

formula	an object of class formula; a symbolic description of the model to be fit.
data	data frame from which variables specified in formula are to be taken.
X	a matrix or data frame containing the explanatory variables (possibly including intercept).
Υ	a matrix or data frame containing the response variables.
int	logical: if TRUE an intercept term is added to the model (unless it is already present in $\boldsymbol{X}$ )
control	a list with control parameters for tuning the MM-estimate and its computing algorithm, see ${\tt MMcontrol}()$ .
na.action	a function which indicates what should happen when the data contain NAs. Defaults to ${\tt na.omit}$ .
	allows for specifying control parameters directly instead of via control

#### **Details**

This function is called by FRBmultiregMM.

The MM-estimates are defined by first computing S-estimates of regression, then fixing the scale component of the error covariance estimate, and finally re-estimating the regression coefficients and the shape part of the error covariance by more efficient M-estimates (see Tatsuoka and Tyler (2000) for MM-estimates in the special case of location/scatter estimation, and Van Aelst and Willems (2005) for S-estimates of multivariate regression). Tukey's biweight is used for the loss functions. By default, the first loss function (in the S-estimates) is tuned in order to obtain 50% breakdown point. The default tuning of the second loss function (M-estimates) ensures 95% efficiency at the normal model for the coefficient estimates. The desired efficiency can be changed via argument control.

The computation of the S-estimates is performed by a call to Sest\_multireg, which uses the fast-S algorithm. See MMcontrol() to see or change the tuning parameters for this algorithm. The M-estimate part is computed through iteratively reweighted least squares (RWLS).

Apart from the MM-estimate of the regression coefficients, the function returns both the MM-estimate of the error covariance Sigma and the corresponding shape estimate Gamma (which has determinant equal to 1). Additionally, the initial S-estimates are returned as well (their Gaussian efficiency is usually lower than the MM-estimates but they may have a lower bias).

The returned object inherits from class mlm such that the standard coef, residuals, fitted and predict functions can be used.

## Value

An object of class FRBmultireg which extends class mlm and contains at least the following components:

coefficients MM-estimates of the regression coefficients residuals the residuals, that is response minus fitted values

fitted.values the fitted values.

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Sigma	MM-estimate of the error covariance matrix
Gamma	MM-estimate of the error shape matrix
scale	S-estimate of the size of the multivariate errors
weights	implicit weights corresponding to the MM-estimates (i.e. final weights in the RWLS procedure)
outFlag	outlier flags: 1 if the robust distance of the residual exceeds the .975 quantile of (the square root of) the chi-square distribution with degrees of freedom equal to the dimension of the responses; 0 otherwise
c0, b, c1	tuning parameters of the loss functions (depend on control parameters bdp and eff)
method	a list with following components: $est = character string indicating that GS-estimates were used, bdp = a copy of the bdp argument, eff a copy of the eff argument$
control	a copy of the control argument
SBeta	S-estimate of the regression coefficient matrix
SSigma	S-estimate of the error covariance matrix
SGamma	S-estimate of the error shape matrix

# Author(s)

Gert Willems, Stefan Van Aelst and Ella Roelant

## References

- K.S. Tatsuoka and D.E. Tyler (2000), The uniqueness of S and M-functionals under non-elliptical distributions. *The Annals of Statistics*, **28**, 1219–1243.
- S. Van Aelst and G. Willems (2005), Multivariate regression S-estimators for robust estimation and inference. *Statistica Sinica*, **15**, 981–1001.
- S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

# See Also

FRBmultiregMM, MMboot\_multireg, Sest\_multireg, MMcontrol

# **Examples**

```
data(schooldata)
school.x <- data.matrix(schooldata[,1:5])
school.y <- data.matrix(schooldata[,6:8])
## compute 95% efficient MM-estimates
MMres <- MMest_multireg(school.x,school.y)
## or using the formula interface</pre>
```

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```
MMres <- MMest_multireg(cbind(reading,mathematics,selfesteem)~., data=schooldata)</pre>
## the MM-estimate of the regression coefficient matrix:
MMres$coefficients
## or alternatively
coef(MMres)
## Do plots
    n <- nrow(schooldata)</pre>
    oldpar <- par(mfrow=c(2,1))</pre>
    ## the estimates can be considered as weighted least squares estimates with the
    ## following implicit weights
    plot(1:n, MMres$weights)
    ## Sres$outFlag tells which points are outliers based on whether or not their
    ## robust distance exceeds the .975 chi-square cut-off:
    plot(1:n, MMres$outFlag)
    ## (see also the diagnostic plot in plotDiag())
    par(oldpar)
```

plot.FRBhot

Plot Method for Objects of class 'FRBhot'

# **Description**

Plot function for FRBhot objects: plots the bootstrap histogram of the null distribution, and the simultaneous confidence limits (scaled)

## Usage

```
## S3 method for class 'FRBhot' plot(x,...)
```

# **Arguments**

x an R object of class FRBhot, typically created by FRBhotellingS or FRBhotellingMM
... potentially more arguments

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#### **Details**

This generic plot function presents two graphs. The first (top panel) is a histogram representing the test statistics in the bootstrap samples, which estimate the null distribution. A red line indicates the test statistic in the original sample (but is not shown when this value exceeds 100).

The second (bottom panel) displays the simultaneous confidence intervals based on the same bootstrap result. The intervals are scaled such that they all have the same length. Furthermore, in case of the one-sample test the intervals are shown relative to the hypothesized value mu0. Such visualization is meant to easily recognize the extent to which each variable is responsible for the overall deviation from the hypothesized value.

#### Value

Returns invisibly the first argument.

#### Author(s)

Gert Willems, Ella Roelant and Stefan Van Aelst

#### References

• S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

#### See Also

```
FRBhotellingS, FRBhotellingMM
```

## **Examples**

```
## One sample robust Hotelling test
data(ForgedBankNotes)
samplemean <- apply(ForgedBankNotes, 2, mean)</pre>
res = FRBhotellingS(ForgedBankNotes, mu0=samplemean,R=99)
plot(res)
## Note that the test rejects the hypothesis that the true mean equals the
## sample mean; this is due to outliers in the data (i.e. the robustly estimated
## center apparently significantly differs from the non-robust sample mean.
## It is clear from the scaled simultaneous confidence limits that the rejection
## of the hypothesis is due to the differences in variables Bottom and Diagonal
## For comparison, the hypothesis would be accepted if only the first three
## variables were considered:
res = FRBhotellingS(ForgedBankNotes[,1:3], mu0=samplemean[1:3],R=99)
plot(res)
## Two sample robust Hotelling test
data(hemophilia, package="rrcov")
```

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```
res <- FRBhotellingMM(cbind(AHFactivity, AHFantigen) ~ gr, data=hemophilia, R=99) plot(res)

## From the confidence limits it can be seen that the significant difference
## is mainly caused by the AHFactivity variable.

## the red line on the histogram indicates the test statistic value in the original
## sample (it is omitted if the statistic exceeds 100)
```

plot.FRBmultireg

Plot Method for Objects of class 'FRBmultireg'

# **Description**

Plot function for objects of class FRBmultireg. It produces histograms for the bootstrap estimates for all (or a selection) of the regression coefficients, based on Fast and Robust Bootstrap and with visualization of bootstrap confidence limits.

## Usage

```
## S3 method for class 'FRBmultireg'
plot(x, expl, resp, confmethod = c("BCA","basic"), onepage = TRUE, ...)
```

#### **Arguments**

X	an Robject of class FRBmultireg, typically created by FRBmultiregS, FRBmultiregMM or FRBmultiregGS
expl	optional; vector specifying the explanatory variables to be shown (either by index or by variable name)
resp	optional; vector specifying the response variables to be shown (either by index or by variable name)
confmethod	which kind of bootstrap confidence intervals to be displayed: 'BCA'= bias corrected and accelerated method, 'basic'= basic bootstrap method
onepage	logical: if TRUE, all requested histograms are plotted on one page; if FALSE, separate pages are used for each response variable
	potentially more arguments to be passed

### **Details**

With p and q the number of explanatory resp. response variables specified, the function by default (i.e. if onepage=TRUE) plots a p by q matrix of histograms, showing the bootstrap recalculations of the corresponding entry in the regression coefficient matrix as provided in x. The original estimates for the coefficients are indicated by dotted lines, while the solid lines are the bootstrap confidence limits. In case the interval does not contain zero, the plot title is printed in red and a star is added, indicating significance.

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However, if p and/or q are large, the histograms may not fit on the page and an attempt to do it may result in an error. Therefore, the function first tries whether it fits (the outcome is platform-dependent), and if not it reduces p and/or q until all plots do fit on the page. Hence, only a selection may be shown and the user is given a warning in that case.

If onepage=FALSE, separate pages are used for each response variable and the user is prompted for page change. In case the number (p) of explanatory variables is very large, the function again may show only a selection.

#### Value

Returns invisibly the first argument.

## Author(s)

Gert Willems and Ella Roelant

#### References

- S. Van Aelst and G. Willems (2005). Multivariate regression S-estimators for robust estimation and inference. *Statistica Sinica*, **15**, 981-1001.
- S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

#### See Also

```
FRBmultiregS, FRBmultiregMM, FRBmultiregGS, summary.FRBmultireg
```

# **Examples**

```
data(schooldata)
school.x <- data.matrix(schooldata[,1:5])
school.y <- data.matrix(schooldata[,6:8])

Sres <- FRBmultiregS(school.x, school.y, R=999, bdp = 0.25, conf = 0.99)

plot(Sres)

## the plot command above selected a subset, since otherwise an error may occur;
## as may happen when you explicitely ask for all coefficients to be plotted on one page:

plot(Sres, expl=1:6, resp=1:3)

## use separate pages for each response in case of many covariates:
plot(Sres, onepage=FALSE)

## perhaps specify some specific variables of interest:
plot(Sres, expl=c("education", "occupation"), resp=c("selfesteem", "reading"))

## or (the same):
plot(Sres, expl=2:3, resp=c(3,1))</pre>
```

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plot.FRBpca

Plot Method for Objects of class 'FRBpca'

# Description

Plot functions for FRBpca objects: plots PC variances, PC angles and PC loadings, with bootstrap inference

# Usage

# Arguments

x	an R object of class FRBpca, typically created by FRBpcaS or FRBpcaMM
which	integer number(s) between 1 and 3 to specify which plot is desired $(1 = variances; 2 = angles; 3 = loadings)$
pcs.loadings	integer number(s) indicating for which of the PCs the loadings should be shown (in case the which argument contains $2$ )
cumul	integer between 0 and 2: $0 = \text{screeplot}$ , i.e. the variances of the PCs are shown; $1 = \text{the cumulative variances (percentage) of the PCs are shown; } 2 = (\text{default})$ both plots are shown on the same page
confmethod	which kind of bootstrap confidence intervals to be displayed: 'BCA'= bias corrected and accelerated method, 'basic'= basic bootstrap method
npcs	number of PCs to be included in screeplot/cumulative variances plot
pcs	PCs to consider in plot; defaults to first 12 (maximally) for plotFRBangles; defaults to first 5 for plotFRBloading (each PC is on a separate page here)
nvars	number of variables for which loadings should be shown in each PC; the loadings are shown in decreasing order in each PC
	potentially more arguments

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#### **Details**

The generic plot function calls plotFRBvars, plotFRBangles and plotFRBloadings, according to which of these are respectively specified in argument which, and displays the plots on separate pages (the user is prompted for each new page). The PCs for which the loadings should be plotted can be specified through the pcs.loadings argument. The other arguments are set to their default values by plot.

The solid curves displayed by plotFRBvars indicate the actual estimates of the variances (or percentages), while the dashed curves represent the confidence limits as computed by FRBpcaS or FRBpcaMM.

plotFRBangles plots, for each PC, histograms of the angles between the bootstrapped PC and the original PC estimate. The angles are in radians, between 0 and pi/2. These limits are indicated by the red vertical lines. Angles close to zero correspond to bootstrapped PCs closely aligned with the original PC, while an angle close to pi/2 means the bootstrapped PC is roughly perpendicular to the original estimate (hence a large number of angles close to pi/2 implies high variability). If the number of PCs specified in pcs is very large (usually larger than the default settings), the histograms may not fit on one page and a selection will be made (the user will be given a warning in that case).

In plotFRBloadings, the red dots represent the loadings, which are between -1 and 1. The square brackets indicate the confidence limits as computed by FRBpcaS or FRBpcaMM. Only the loadings of the first nvars variables are shown, where the variables were ordered according to the absolute value of the loading (i.e. only the nvars most important variables for that particular PC are shown).

#### Value

Returns invisibly the first argument.

## Author(s)

Gert Willems and Ella Roelant

## References

• S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

#### See Also

```
FRBpcaS, FRBpcaMM, summary.FRBpca
```

# **Examples**

```
data(ForgedBankNotes)

MMpcares <- FRBpcaMM(ForgedBankNotes, R=999, conf=0.95)
plot(MMpcares)

## a closer look at the screeplot, specifying basic bootstrap intervals
plotFRBvars(MMpcares, cumul=0, confmethod="basic")</pre>
```

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```
## plots the bootstrap angles for the first PC only
plotFRBangles(MMpcares, pcs=1)

## plots the loadings, with basic bootstrap intervals, for *all* the PCs
plotFRBloadings(MMpcares, confmethod="basic", pcs=1:ncol(ForgedBankNotes))
```

Sboot\_loccov

Fast and Robust Bootstrap for S-estimates of location/covariance

## **Description**

Calculates bootstrapped S-estimates using the Fast and Robust Bootstrap method.

## Usage

```
Sboot_loccov(Y, R = 999, ests = Sest_loccov(Y))
```

## **Arguments**

Y matrix or data frame.

R number of bootstrap samples. Default is R=999.

ests original S-estimates as returned by Sest\_loccov().

# **Details**

This function is called by FRBpcaS and FRBhotellingS, it is typically not to be used on its own. It requires the S-estimates of multivariate location and scatter/shape (the result of Sest\_loccov applied on Y), supplied through the argument ests. If ests is not provided, Sest\_loccov calls the implementation of the multivariate S-estimates in package **rrcov** of Todorov and Filzmoser (2009) with default arguments.

For multivariate data the fast and robust bootstrap was developed by Salibian-Barrera, Van Aelst and Willems (2006).

The value centered gives a matrix with R columns and p+p\*p rows (p is the number of variables in Y), containing the recalculated estimates of the S-location and -covariance. Each column represents a different bootstrap sample. The first p rows are the location estimates and the next p\*p rows are the covariance estimates (vectorized). The estimates are centered by the original estimates, which are also returned through Sest.

#### Value

#### A list containing:

centered recalculated estimates of location and covariance (centered by original esti-

mates)

Sest original estimates of location and covariance

Sboot\_multireg

#### Author(s)

Gert Willems, Ella Roelant and Stefan Van Aelst

#### References

- M. Salibian-Barrera, S. Van Aelst and G. Willems (2006) PCA based on multivariate MM-estimators with fast and robust bootstrap. *Journal of the American Statistical Association*, 101, 1198–1211.
- M. Salibian-Barrera, S. Van Aelst and G. Willems (2008) Fast and robust bootstrap. *Statistical Methods and Applications*, **17**, 41–71.
- V. Todorov and P. Filzmoser (2009), An Object Oriented Framework for Robust Multivariate Analysis. *Journal of Statistical Software*, **32**(3), 1–47. doi:10.18637/jss.v032.i03.
- S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

#### See Also

```
FRBpcaS, FRBhotellingS, MMboot_loccov
```

# Examples

```
Y <- matrix(rnorm(50*5), ncol=5)
Sests <- Sest_loccov(Y, bdp = 0.25)
bootresult <- Sboot_loccov(Y, R = 1000, ests = Sests)</pre>
```

Sboot\_multireg

Fast and Robust Bootstrap for S-Estimates of Multivariate Regression

# **Description**

Calculates bootstrapped S-estimates of multivariate regression and corresponding bootstrap confidence intervals using the Fast and Robust Bootstrap method.

# Usage

```
Sboot_multireg(X, Y, R = 999, conf=0.95, ests = Sest_multireg(X, Y))
```

## **Arguments**

X	a matrix or data frame containing the explanatory variables (possibly including intercept).
Υ	a matrix or data frame containing the response variables.
R	number of bootstrap samples. Default is R=999.
conf	level of the bootstrap confidence intervals. Default is conf=0.95.
ests	S-estimates as returned by Sest_multireg().

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#### **Details**

Called by FRBmultiregS and typically not to be used on its own. It requires the result of Sest\_multireg applied on X and Y, supplied through the argument ests. If ests is not provided, Sest\_multireg will be called with default arguments.

The fast and robust bootstrap was first developed by Salibian-Barrera and Zamar (2002) for univariate regression MM-estimators and extended to multivariate regression by Van Aelst and Willems (2005).

The value centered gives a matrix with R columns and p\*q+q\*q rows (p is the number of explanatory variables and q the number of response variables), containing the recalculated S-estimates of the regression coefficients and the error covariance matrix. Each column represents a different bootstrap sample. The first p\*q rows are the coefficient estimates, the next q\*q rows represent the covariance estimate (the estimates are vectorized, i.e. columns stacked on top of each other). The estimates are centered by the original estimates, which are also returned through vecest in vectorized form.

The output list further contains bootstrap standard errors, as well as so-called basic bootstrap confidence intervals and bias corrected and accelerated (BCa) confidence intervals (Davison and Hinkley, 1997, p.194 and p.204 respectively). Also in the output are p-values defined as 1 minus the smallest confidence level for which the confidence intervals would include the (hypothesised) value of zero. Both BCa and basic bootstrap p-values are given. These are only useful for the regression coefficient estimates (not really for the covariance estimates).

Bootstrap samples which contain less than p distinct observations with positive weights are discarded (a warning is given if this happens). The number of samples actually used is returned via ROK.

#### Value

A list containing the following components:

centered	a matrix of all fast/robust bootstrap recalculations where the recalculations are centered by original estimates (see Details)
vecest	a vector containing the original estimates (see Details)
SE	bootstrap standard errors for the estimates in vecest
cov	bootstrap covariance matrix for the estimates in vecest
CI.bca	a matrix containing bias corrected and accelerated confidence intervals corresponding to the estimates in vecest (first column are lower limits, second column are upper limits)
CI.basic	a matrix containing basic bootstrap intervals corresponding to the estimates in vecest (first column are lower limits, second column are upper limits)
p.bca	a vector containing p-values based on the bias corrected and accelerated confidence intervals (corresponding to the estimates in vecest)
p.basic	a vector containing p-values based on the basic bootstrap intervals (corresponding to the estimates in vecest)
ROK	number of bootstrap samples actually used (i.e. not discarded due to too few distinct observations with positive weight)

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#### Author(s)

Gert Willems, Ella Roelant and Stefan Van Aelst

#### References

- A.C. Davison, D.V. Hinkley (1997) Bootstrap methods and their application. Cambridge University Press.
- M. Salibian-Barrera, S. Van Aelst and G. Willems (2008) Fast and robust bootstrap. *Statistical Methods and Applications*, **17**, 41–71.
- M. Salibian-Barrera, R.H. Zamar (2002) Bootstrapping robust estimates of regression. *The Annals of Statistics*, **30**, 556–582.
- S. Van Aelst and G. Willems (2005) Multivariate regression S-estimators for robust estimation and inference. *Statistica Sinica*, **15**, 981–1001.
- S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

#### See Also

```
FRBmultiregS, Sest_multireg, MMboot_multireg
```

# **Examples**

```
data(schooldata)
school.x <- data.matrix(schooldata[,1:5])
school.y <- data.matrix(schooldata[,6:8])

#computes 1000 bootstrap recalculations starting from the S-estimator
#obtained from Sest_multireg()
bootres <- Sboot_multireg(school.x,school.y,R=1000)</pre>
```

Sboot\_twosample

Fast and Robust Bootstrap for Two-Sample S-estimates of Location and Covariance

# **Description**

Calculates bootstrapped two-sample S-estimates using the Fast and Robust Bootstrap method.

## Usage

```
Sboot_twosample(X, groups, R = 999, ests = Sest_twosample(X, groups))
```

# **Arguments**

Χ	matrix or data frame.
groups	vector of 1's and 2's, indicating group numbers.
R	number of bootstrap samples. Default is R=999.
ests	original two-sample S-estimates as returned by Sest_twosample().

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#### **Details**

This function is called by FRBhotellingS, it is typically not to be used on its own. It requires the result of Sest\_twosample applied on X, supplied through the argument ests. If ests is not provided, Sest\_twosample will be called with default arguments.

The fast and robust bootstrap was first developed by Salibian-Barrera and Zamar (2002) for univariate regression MM-estimators and extended to the two sample setting by Roelant et al. (2008).

The value centered gives a matrix with R columns and 2 \* p + p \* p rows (p is the number of variables in X), containing the recalculated estimates of the S-location for the first and second center and common S-covariance. Each column represents a different bootstrap sample. The first p rows are the location estimates of the first center, the next p rows are the location estimates of the second center and the last p \* p rows are the common covariance estimates (vectorized). The estimates are centered by the original estimates, which are also returned through Sest.

#### Value

## A list containing:

centered recalculated estimates of location of first and second center and covariance (cen-

tered by original estimates)

Sest original estimates of first and second center and common covariance

#### Author(s)

Ella Roelant, Gert Willems and Stefan Van Aelst

## References

- E. Roelant, S. Van Aelst and G. Willems, (2008) Fast Bootstrap for Robust Hotelling Tests, COMPSTAT 2008: Proceedings in Computational Statistics (P. Brito, Ed.) Heidelberg: Physika-Verlag, 709–719.
- M. Salibian-Barrera, S. Van Aelst and G. Willems (2008) Fast and robust bootstrap. *Statistical Methods and Applications*, **17**, 41–71.
- M. Salibian-Barrera, R.H. Zamar (2002) Bootstrapping robust estimates of regression. *The Annals of Statistics*, **30**, 556–582.
- S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

#### See Also

```
FRBhotellingS
```

# **Examples**

```
Y1 <- matrix(rnorm(50*5), ncol=5)
Y2 <- matrix(rnorm(50*5), ncol=5)
Ybig <- rbind(Y1,Y2)
grp <- c(rep(1,50),rep(2,50))
Sests <- Sest_twosample(Ybig, grp, bdp=0.25)
```

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bootresult <- Sboot\_twosample(Ybig,grp,R=1000,ests=Sests)</pre>

schooldata

School Data

# **Description**

School Data, from Charnes et al. (1981). The aim is to explain scores on 3 different tests from 70 school sites by means of 5 explanatory variables.

#### **Usage**

data(schooldata)

#### **Format**

A data frame with 70 observations on the following 8 variables.

education education level of mother as measured in terms of percentage of high school graduates among female parents

occupation highest occupation of a family member according to a pre-arranged rating scale

visit parental visits index representing the number of visits to the school site

counseling parent counseling index calculated from data on time spent with child on school-related topics such as reading together, etc.

teacher number of teachers at a given site

reading total reading score as measured by the Metropolitan Achievement Test mathematics total mathematics score as measured by the Metropolitan Achievement Test selfesteem Coopersmith Self-Esteem Inventory, intended as a measure of self-esteem

## **Source**

Charnes et al. (1981)

## References

A. Charnes, W.W. Cooper and E. Rhodes (1981) Evaluating Program and Managerial Efficiency: An Application of Data Envelopment Analysis to Program Follow Through. *Management Science*, 27, 668-697.

### **Examples**

data(schooldata)

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Sco			

Tuning parameters for multivariate S, MM and GS estimates

## **Description**

Tuning parameters for multivariate S, MM and GS estimates as used in FRB functions for multivariate regression, PCA and Hotelling tests. Mainly regarding the fast-(G)S algorithm.

#### **Usage**

# **Arguments**

nsamp	number of random subsamples to be used in the fast-(G)S algorithm
k	number of initial concentration steps performed on each subsample candidate
bestr	number of best candidates to keep for full iteration (i.e. concentration steps until convergence)
convTol	relative convergence tolerance for estimates used in (G)S-concentration iteration
maxIt	maximal number of steps in (G)S-concentration iteration
bdp	breakdown point of the MM-estimates; usually equals 0.5
eff	Gaussian efficiency of the MM-estimates; usually set at 0.95
shapeEff	logical; if TRUE, eff is with regard to shape-efficiency, otherwise location-efficiency
convTol.MM	relative convergence tolerance for estimates used in MM-iteration
maxIt.MM	maximal number of steps in MM-iteration
fastScontrols	the tuning parameters of the initial S-estimate
	allows for any individual parameter from Scontrol to be set directly

# **Details**

The default number of random samples is lower for GS-estimates than for S-estimates, because computations regarding the former are more demanding.

## Value

A list with the tuning parameters as set by the arguments.

# Author(s)

Gert Willems and Ella Roelant

Sest\_multireg

## References

• S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

#### See Also

```
{\tt GSest\_multireg, Sest\_multireg, MMest\_multireg, Sest\_twosample, MMest\_twosample, FRBpcaS, ...}
```

# **Examples**

```
## Show the default settings:
str(Scontrol())
str(MMcontrol())
str(GScontrol())
```

Sest\_multireg

S-Estimates for Multivariate Regression

## **Description**

Computes S-Estimates of multivariate regression based on Tukey's biweight function using the fast-S algorithm.

# Usage

```
## S3 method for class 'formula'
Sest_multireg(formula, data=NULL, ...)

## Default S3 method:
Sest_multireg(X, Y, int = TRUE, bdp = 0.5, control=Scontrol(...),
na.action=na.omit, ...)
```

# **Arguments**

formula	an object of class formula; a symbolic description of the model to be fit.
data	data frame from which variables specified in formula are to be taken.
X	a matrix or data frame containing the explanatory variables (possibly including intercept).
Υ	a matrix or data frame containing the response variables.
int	logical: if TRUE an intercept term is added to the model (unless it is already present in X).
bdp	required breakdown point. Should have $0 < bdp \le 0.5$ , the default is 0.5.
control	a list with control parameters for tuning the computing algorithm, see Scontrol().
na.action	a function which indicates what should happen when the data contain NAs. Defaults to na.omit.
	allows for specifying control parameters directly instead of via control.

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#### **Details**

This function is called by FRBmultiregS.

S-estimates for multivariate regression were discussed in Van Aelst and Willems (2005). The algorithm used here is a multivariate version of the fast-S algorithm introduced by Salibian-Barrera and Yohai (2006). See Scontrol for the adjustable tuning parameters of this algorithm.

Apart from the regression coefficients, the function returns both the error covariance matrix estimate Sigma and the corresponding shape estimate Gamma (which has determinant equal to 1). The scale is determined by  $det(Sigma)^{1/2/q}$ , with q the number of response variables.

The returned object inherits from class mlm such that the standard coef, residuals, fitted and predict functions can be used.

#### Value

An object of class FRBmultireg which extends class mlm and contains at least the following components:

coefficients S-estimates of the regression coefficients

residuals the residuals, that is response minus fitted values

fitted.values the fitted values.

Gamma S-estimate of the error shape matrix
Sigma S-estimate of the error covariance matrix
scale S-estimate of the size of the multivariate errors

weights implicit weights corresponding to the S-estimates (i.e. final weights in the

RWLS procedure at the end of the fast-S algorithm)

outFlag outlier flags: 1 if the robust distance of the residual exceeds the .975 quantile of

(the square root of) the chi-square distribution with degrees of freedom equal to

the dimension of the responses; 0 otherwise

b, c tuning parameters used in Tukey biweight loss function, as determined by bdp method a list with following components: est = character string indicating that GS-

estimates were used and bdp = a copy of the bdp argument

control a copy of the control argument

## Author(s)

Gert Willems, Stefan Van Aelst and Ella Roelant

# References

- M. Salibian-Barrera and V. Yohai (2006) A fast algorithm for S-regression estimates. *Journal of Computational and Graphical Statistics*, **15**, 414–427.
- S. Van Aelst and G. Willems (2005) Multivariate regression S-estimators for robust estimation and inference. *Statistica Sinica*, **15**, 981–1001
- S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

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# See Also

```
FRBmultiregS, Sboot_multireg, MMest_multireg, Scontrol
```

## **Examples**

```
data(schooldata)
school.x <- data.matrix(schooldata[,1:5])</pre>
school.y <- data.matrix(schooldata[,6:8])</pre>
## compute 25% breakdown S-estimates
Sres <- Sest_multireg(school.x,school.y, bdp=0.25)</pre>
    ## or using the formula interface
  Sres <- Sest_multireg(cbind(reading, mathematics, selfesteem)~., data=schooldata, bdp=0.25)</pre>
    ## the regression coefficients:
    Sres$coefficients
    ## or alternatively
    coef(Sres)
   n <- nrow(schooldata)</pre>
    oldpar <- par(mfrow=c(2,1))</pre>
    ## the estimates can be considered as weighted least squares estimates with the
    ## following implicit weights
    plot(1:n, Sres$weights)
    ## Sres$outFlag tells which points are outliers based on whether or not their
    ## robust distance exceeds the .975 chi-square cut-off:
   plot(1:n, Sres$outFlag)
    ## (see also the diagnostic plot in plotDiag())
    par(oldpar)
```

summary.FRBhot

Summary Method for Objects of Class 'FRBhot'

# **Description**

Summary method for objects of class FRBhot, and print method of the summary object.

# Usage

```
## S3 method for class 'FRBhot'
summary(object, digits = 5, ...)
## S3 method for class 'summary.FRBhot'
print(x, ...)
```

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# Arguments

object	an R object of class FRBhot, typically created by FRBhotellingS or FRBhotellingMM
digits	number of digits for printing (default is 5)
X	an R object of class summary. FRBhot, resulting from summary (FRBhotellingS(),) or summary (FRBhotellingMM(),)
	potentially more arguments to be passed to methods

# **Details**

The print method here displays the value of the test statistic and the corresponding bootstrap p-value. It also presents the simultaneous confidence intervals for the components of the location vector (or difference between the two location vectors), and the robust estimates for the location vector(s) and covariance matrix.

## Value

summary. FRBhot simply returns its two arguments in a list.

## Author(s)

Gert Willems, Ella Roelant and Stefan Van Aelst

# References

• S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

## See Also

```
FRBhotellingS, FRBhotellingMM, plot.FRBhot
```

# **Examples**

```
data(ForgedBankNotes)
samplemean <- apply(ForgedBankNotes, 2, mean)
res = FRBhotellingS(ForgedBankNotes, mu0=samplemean)
summary(res) # -> print.summary.FRBhot() method
```

Summary Method for Objects of Class 'FRBmultireg' summary.FRBmultireg

## **Description**

Summary method for objects of class FRBmultireg, and print method of the summary object.

# Usage

```
## S3 method for class 'FRBmultireg'
summary(object, confmethod = c("BCA", "basic", "both"), digits = 3,
print.CI=FALSE, sep="", ...)
## S3 method for class 'summary.FRBmultireg'
print(x, ...)
```

#### **Arguments**

object an Robject of class FRBmultireg, typically created by FRBmultiregS, FRBmultiregMM

or FRBmultiregGS

confmethod which kind of bootstrap confidence intervals to be displayed: 'BCA'= bias cor-

rected and accelerated method, 'basic'= basic bootstrap method, 'both'=both

kinds of confidence intervals

digits number of digits for printing (default is 3)

print.CI logical: Should Confidence intervals be printed? Symmbol to separate columns in output. Default is "" sep

an Robject of class summary.FRBmultireg, resulting for example from summary(FRBmultiregS(),...)

potentially more arguments to be passed to methods

## **Details**

Χ

The print method displays in a "familiar way" the components of the summary object, which are listed in the Value section.

## Value

summary returns an object of class summary. FRBmultireg, which contains the following components:

the names of the response variables in the fitted model responses covariates the names of the covariates (predictors) in the fitted model

a data frame containing the coefficient estimates and their bootstrap standard Betawstd

errors

estimate for the error covariance matrix Sigma

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table.bca	a list with for each response variable a matrix containing the estimates, standard errors, lower and upper limits of the BCa confidence intervals, p-values and a significance code (only present when confmethod="BCA" or confmethod="both")
table.basic	a list with for each response variable a matrix containing the estimates, standard errors, lower and upper limits of the basic bootstrap confidence intervals, p-values and a significance code (only present when confmethod="basic" or confmethod="both")
method	multivariate regression method that was used
conf	confidence level that was used
digits	number of digits for printing

## Author(s)

Gert Willems, Ella Roelant and Stefan Van Aelst

#### References

• S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

# See Also

```
{\tt FRB multiregSS, FRB multiregMM, FRB multiregGS, print. FRB multireg, plot. FRB multireg}
```

## **Examples**

```
data(schooldata)

MMres <- FRBmultiregMM(cbind(reading,mathematics,selfesteem)~., data=schooldata,
R=199, conf = 0.99,nsamp=200)
summary(MMres) # -> print.summary.FRBmultireg() method

GSres <- FRBmultiregGS(cbind(reading,mathematics,selfesteem)~., data=schooldata,
bdp = 0.25,R=199,nsamp=50)
summary(GSres, confmethod="both") # -> print.summary.FRBmultireg() method
```

summary.FRBpca

Summary Method for Objects of Class 'FRBpca'

# **Description**

Summary method for objects of class FRBpca, and print method of the summary object.

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## Usage

```
## S3 method for class 'FRBpca'
summary(object, confmethod = c("BCA", "basic", "both"), digits = 3, ...)
## S3 method for class 'summary.FRBpca'
print(x, ...)
```

# Arguments

object an R object of class FRBpca, typically created by FRBpcaS or FRBpcaMM

which kind of bootstrap confidence intervals to be displayed: 'BCA'= bias corrected and accelerated method, 'basic'= basic bootstrap method, 'both'= both kinds of confidence intervals

digits number of digits for printing (default is 3)

x an R object of class summary.FRBpca, resulting from summary(FRBpcaS(),...) or summary(FRBpcaMM(),...)

potentially more arguments to be passed to methods

#### **Details**

The print method displays mostly the components of the summary object as listed in the Value section.

#### Value

summary returns an object of class summary. FRBpca, which contains the following components:

eigvals	eigenvalues of the shape estimate (variances of the principal components) with confidence limits
eigvecs	eigenvectors of the shape estimate (loadings of the principal components)
avgangle	bootstrap estimates of average angles between true and estimated eigenvectors
pvars	cumulative percentage of variance explained by first principal components with confidence limits
method	PCA method that was used
digits	number of digits for printing

# Author(s)

Gert Willems, Ella Roelant and Stefan Van Aelst

#### References

• S. Van Aelst and G. Willems (2013), Fast and robust bootstrap for multivariate inference: The R package FRB. *Journal of Statistical Software*, **53**(3), 1–32. doi:10.18637/jss.v053.i03.

## See Also

```
FRBpcaS, FRBpcaMM, print.FRBpca, plot.FRBpca
```

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# Examples

data(ForgedBankNotes)

MMpcares <- FRBpcaMM(ForgedBankNotes, R=999, conf=0.95)
summary(MMpcares) # -> print.summary.FRBpca() method

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