# Package: ICtest (via r-universe)

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Type Package
<b>Title</b> Estimating and Testing the Number of Interesting Components in Linear Dimension Reduction
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<b>Description</b> For different linear dimension reduction methods like principal components analysis (PCA), independent components analysis (ICA) and supervised linear dimension reduction tests and estimates for the number of interesting components (ICs) are provided.
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components

Generic Components Extraction Function

# **Description**

Function to extract components from an object. If the object is of class ictest or ladle the user can choose if all components are extracted or only those which were interesting under the null hypothesis.

# Usage

```
components(x, ...)
## S3 method for class 'ictest'
components(x, which = "all", ...)
## S3 method for class 'ladle'
components(x, which = "all", ...)
```

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# **Arguments**

x an object which has a components method, like for example an ictest object.

which for an object of class ictest. If "all", then all components S in the ictest object

are extracted. If "k", then only the first k components are extracted, where the value of k is taken from the ictest object. This is only meaningful if k was at

least 1.

... arguments passed on to other methods.

#### Value

a matrix with the components.

## Author(s)

Klaus Nordhausen

## **Examples**

```
n <- 200
X <- cbind(rnorm(n, sd = 2), rnorm(n, sd = 1.5), rnorm(n), rnorm(n), rnorm(n))
TestCov <- PCAasymp(X, k = 2)
head(components(TestCov))
head(components(TestCov, which = "k"))</pre>
```

covSIR

Supervised Scatter Matrix as Used in Sliced Inverse Regression

# Description

Sliced Inverse Regression (SIR) can be seen as special case of Supervised ICS (SICS) and this function gives the supervised scatter matrix for SIR

#### Usage

```
covSIR(X, y, h = 10, ...)
```

#### **Arguments**

X a numeric data matrix.

y a numeric response vector.

h the number of slices.

... arguments passed on to quantile.

FOBIasymp

#### **Details**

This supervised scatter matrix is usually used as the second scatter matrix in SICS to obtain a SIR type supervised linear dimension reduction. For that purpose covSIR first divides the response y into h slices using the corresponding quantiles as cut points. Then for each slice the mean vector of X is computed and the resulting supervised scatter matrix consist of the covariance matrix of these mean vectors.

The function might have problems if the sample size is too small.

#### Value

a supervised scatter matrix

#### Author(s)

Klaus Nordhausen

#### References

Liski, E., Nordhausen, K. and Oja, H. (2014), Supervised invariant coordinate selection, Statistics: A Journal of Theoretical and Applied Statistics, **48**, 711–731. <doi:10.1080/02331888.2013.800067>.

Nordhausen, K., Oja, H. and Tyler, D.E. (2022), Asymptotic and Bootstrap Tests for Subspace Dimension, Journal of Multivariate Analysis, 188, 104830. <doi:10.1016/j.jmva.2021.104830>.

# See Also

ics

# **Examples**

```
X <- matrix(rnorm(1000), ncol = 5)
eps <- rnorm(200, sd = 0.1)
y <- 2 + 0.5 * X[, 1] + 2 * X[, 3] + eps
covSIR(X, y)</pre>
```

**FOBIasymp** 

Testing for the Number of Gaussian Components in NGCA or ICA Using FOBI

# **Description**

In non-gaussian component analysis (NGCA) and independent components analysis (ICA) gaussian components are considered as uninteresting. The function tests, based on FOBI, if there are p-k gaussian components where p is the dimension of the data. The function offers three different test versions.

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#### Usage

FOBIasymp(X, k, type = "S3", model = "NGCA", method = "satterthwaite")

#### **Arguments**

X numeric data matrix.

k the number of non-gaussian components under the null.

type which of the three tests to perform. Options are "S1", "S2" and "S3". For the

differences see the details section.

model What is the underlying assumption of the non-gaussian parts. Options are gen-

eral "NGCA" model and "ICA" model.

method if type = "S1" the teststatistic has as limiting distribution a weighted sum of

chisquare distributions. To compute the p-value then the function used is pchisqsum. The method argument specifies which method pchisqsum uses for the computation. Options are "satterthwaite", "integration" and "saddlepoint".

#### **Details**

The function jointly diagonalizes the regular covariance and the matrix of fourth moments. Note however that in this case the matrix of fourth moments is not made consistent under the normal model by dividing it by p+2, as for example done by the function cov4 where p denotes the dimension of the data. Therefore the eigenvalues of this generalized eigenvector-eigenvalue problem which correspond to normally distributed components should be p+2.

Given eigenvalues  $d_1, ..., d_p$  the function thus orders the components in decending order according to the values of  $(d_i - (p+2))^2$ .

Under the null it is then assumed that the first k interesting components are mutually independent and non-normal and the last p-k are gaussian.

Three possible tests are then available to test this null hypothesis for a sample of size n:

1. type="S1": The test statistic T is the variance of the last p-k eigenvalues around p+2:

$$T = n \sum_{i=k+1}^{p} (d_i - (p+2))^2$$

the limiting distribution of which under the null is the sum of two weighted chisquare distributions with weights:

$$w_1 = 2\sigma_1/(p-k)$$
 and  $w_2 = 2\sigma_1/(p-k) + \sigma_2$ .

and degrees of freedom:

$$df_1 = (p - k - 1)(p - k + 2)/2$$
 and  $df_2 = 1$ .

2. type="S2": Another possible version for the test statistic is a scaled sum of the variance of the eigenvalues around the mean plus the variance around the expected value under normality (p+2). Denote  $VAR_{dpk}$  as the variance of the last p-k eigenvalues and  $VAR2_{dpk}$  as the variance of these eigenvalues around p+2. Then the test statistic is:

$$T = (n(p-k)VAR_{dpk})/(2\sigma_1) + (nVAR_{dpk})/(2\sigma_1/(p-k) + \sigma_2)$$

This test statistic has a limiting chisquare distribution with (p - k - 1)(p - q + 2)/2 + 1 degrees of freedom.

3. type="S3": The third possible test statistic just checks the equality of the last p-k eigenvalues using only the first part of the test statistic of type="S2". The test statistic is then:

$$T = (n(p-k)VAR_{dpk})/(2\sigma_1)$$

and has a limiting chisquare distribution with (p-k-1)(p-q+2)/2 degrees of freedom.

The constants  $\sigma_1$  and  $\sigma_2$  depend on the underlying model assumptions as specified in argument model and are estimated from the data.

#### Value

A list of class ictest inheriting from class htest containing:

statistic the value of the test statistic.
p.value the p-value of the test.

parameter the degrees of freedom of the test or the degrees of freedoms and the correspond-

ing weights of the test in case the test has as its limiting distribution a weighted

sum of chisquare distributions.

method character string denoting which test was performed.

data.name character string giving the name of the data.

alternative character string specifying the alternative hypothesis.

k the number or non-gaussian components used in the testing problem.

W the transformation matrix to the independent components. Also known as un-

mixing matrix.

S data matrix with the centered independent components.

D the underlying FOBI eigenvalues.

MU the location of the data which was substracted before calculating the independent

components.

sigma1 the asymptotic constant sigma1 needed for the asymptotic test(s).
sigma2 the asymptotic constant sigma2 needed for the asymptotic test(s).

type the value of type.
model the value of model.

## Author(s)

Klaus Nordhausen

# References

Nordhausen, K., Oja, H. and Tyler, D.E. (2022), Asymptotic and Bootstrap Tests for Subspace Dimension, Journal of Multivariate Analysis, 188, 104830. <doi:10.1016/j.jmva.2021.104830>.

Nordhausen, K., Oja, H., Tyler, D.E. and Virta, J. (2017), Asymptotic and Bootstrap Tests for the Dimension of the Non-Gaussian Subspace, Signal Processing Letters, 24, 887–891. <doi:10.1109/LSP.2017.2696880 >.

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## See Also

```
FOBI, FOBIboot
```

## **Examples**

```
n <- 1500
S <- cbind(runif(n), rchisq(n, 2), rexp(n), rnorm(n), rnorm(n), rnorm(n))
A <- matrix(rnorm(36), ncol = 6)
X <- S %*% t(A)

FOBIasymp(X, k = 2)
FOBIasymp(X, k = 3, type = "S1")
FOBIasymp(X, k = 0, type = "S2", model = "ICA")</pre>
```

**FOBIboot** 

Boostrap-based Testing for the Number of Gaussian Components in ICA Using FOBI

# **Description**

In independent components analysis (ICA) gaussian components are considered as uninteresting. The function uses boostrappping tests, based on FOBI, to decide if there are p-k gaussian components where p is the dimension of the data. The function offers two different boostrapping strategies.

# Usage

```
FOBIboot(X, k, n.boot = 200, s.boot = "B1")
```

#### **Arguments**

X a numeric data matrix with p>1 columns.

k the number of non-gaussian components under the null.

n.boot number of bootstrapping samples.

s.boot bootstrapping strategy to be used. Possible values are "B1", "B2". See details

for further information.

## **Details**

As in FOBIasymp the function jointly diagonalizes the regular covariance and the matrix of fourth moments. Note that in this case the matrix of fourth moments is not made consistent under the normal model by dividing it by p+2, as for example done by the function cov4 where p denotes the dimension of the data. Therefore the eigenvalues of this generalized eigenvector-eigenvalue problem which correspond to normally distributed components should be p+2. Given eigenvalues  $d_1, ..., d_p$  the function thus orders the components in descending order according to the values of  $(d_i - (p+2))^2$ .

Under the null it is then assumed that the first k interesting components are mutually independent and non-normal and the last p-k components are gaussian.

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Let  $d_1, ..., d_p$  be the ordered eigenvalues, W the correspondingly ordered unmixing matrix,  $s_i = W(x_i - MU)$  the corresponding source vectors which give the source matrix S which can be decomposed into  $S_1$  and  $S_2$  where  $S_1$  is the matrix with the k non-gaussian components and  $S_2$  the matrix with the gaussian components (under the null).

The test statistic is then  $T = n \sum_{i=k+1}^{p} (d_i - (p+2))^2$ 

Two possible bootstrap tests are provided for testing that the last p-k components are gaussian and independent from the first k components:

- 1. s.boot="B1": The first strategy has the following steps:
  - (a) Take a bootstrap sample  $S_1^*$  of size n from  $S_1$ .
  - (b) Take a bootstrap sample  $S_2^*$  consisting of a matrix of standard normally distributed elements.
  - (c) Combine  $S^* = (S_1^*, S_2^*)$  and create  $X^* = S^*W$ .
  - (d) Compute the test statistic based on  $X^*$ .
  - (e) Repeat the previous steps n. boot times.

Note that in this bootstrapping test the assumption of "independent components" is not used, it is only used that the last p-k components are gaussian and independent from the first k components. Therefore this strategy can be applied in an independent component analysis (ICA) framework and in a non-gaussian components analysis (NGCA) framework.

- 2. s.boot="B2": The second strategy has the following steps:
  - (a) Take a bootstrap sample  $S_1^*$  of size n from  $S_1$  where the subsampling is done separately for each independent component.
  - (b) Take a bootstrap sample  $S_2^*$  consisting of a matrix of standard normally distributed elements.
  - (c) Combine  $S^* = (S_1^*, S_2^*)$  and create  $X^* = S^*W$ .
  - (d) Compute the test statistic based on  $X^*$ .
  - (e) Repeat the previous steps n. boot times.

This bootstrapping strategy assumes a full ICA model and cannot be used in an NGCA framework.

## Value

A list of class ictest inheriting from class htest containing:

statistic the value of the test statistic.

p.value the p-value of the test.

parameter the number of boostrapping samples used to obtain the p-value.

method character string which test was performed.
data.name character string giving the name of the data.

alternative character string specifying the alternative hypothesis.

k the number or non-gaussian components used in the testing problem.

W the transformation matrix to the independent components. Also known as un-

mixing matrix.

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S data matrix with the centered independent componen	ts.
--	-----

D the underlying FOBI eigenvalues.

MU the location of the data which was substracted before calculating the independent

components.

s.boot character string which boostrapping strategy was used.

#### Author(s)

Klaus Nordhausen

#### References

Nordhausen, K., Oja, H. and Tyler, D.E. (2022), Asymptotic and Bootstrap Tests for Subspace Dimension, Journal of Multivariate Analysis, 188, 104830. <doi:10.1016/j.jmva.2021.104830>.

Nordhausen, K., Oja, H., Tyler, D.E. and Virta, J. (2017), Asymptotic and Bootstrap Tests for the Dimension of the Non-Gaussian Subspace, Signal Processing Letters, 24, 887–891. <doi:10.1109/LSP.2017.2696880 >.

#### See Also

```
FOBI, FOBIasymp
```

#### **Examples**

```
n <- 1500
S <- cbind(runif(n), rchisq(n, 2), rexp(n), rnorm(n), rnorm(n), rnorm(n))
A <- matrix(rnorm(36), ncol = 6)
X <- S %*% t(A)

FOBIboot(X, k = 2)
FOBIboot(X, k = 3, s.boot = "B1")
FOBIboot(X, k = 0, s.boot = "B2")</pre>
```

FOBIladle

Ladle Estimate to Estimate the Number of Gaussian Components in ICA or NGCA

# Description

The ladle estimator uses the eigenvalues and eigenvectors of FOBI to estimate the number of Gaussian components in ICA or NGCA.

#### Usage

```
FOBIladle(X, n.boot = 200,

ncomp = ifelse(ncol(X) > 10, floor(ncol(X)/log(ncol(X))), ncol(X) - 1))
```

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#### **Arguments**

X numeric data matrix.

n.boot number of bootstrapping samples to be used.

ncomp The number of components among which the ladle estimator is to be searched.

The default here follows the recommendation of Luo and Li 2016.

#### **Details**

The model here assumes that in ICA or NGCA there are k non-gaussian components and p-k gaussian components. The idea is then to decide which eigenvalues differ from p+2. The ladle estimate for this purpose combines the values of the scaled eigenvalues and the variation of the eigenvectors based on bootstrapping. The idea there is that for distinct eigenvales the variation of the eigenvectors is small and for equal eigenvalues the corresponding eigenvectors have large variation.

This measure is then computed assuming k=0,..., ncomp and the ladle estimate for k is the value where the measure takes its minimum.

#### Value

A list of class ladle containing:

method the string FOBI.

k the estimated number of non-gaussian components.

fn vector giving the measures of variation of the eigenvectors using the bootstrapped

eigenvectors for the different number of components.

phin normalized eigenvalues of the FOBI matrix.

gn the main criterion for the ladle estimate - the sum of fn and phin. k is the value

where gn takes its minimum

lambda the eigenvalues of the FOBI matrix.

W the transformation matrix to the independent components. Also known as un-

mixing matrix.

S data matrix with the centered independent components.

MU the location of the data which was substracted before calculating the independent

components.

data.name the name of the data for which the ladle estimate was computed.

#### Author(s)

Klaus Nordhausen

#### References

Luo, W. and Li, B. (2016), Combining Eigenvalues and Variation of Eigenvectors for Order Determination, Biometrika, 103. 875–887. <doi:10.1093/biomet/asw051>

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#### See Also

```
ladleplot
```

## **Examples**

```
n <- 1000
X <- cbind(rexp(n), rt(n,5), rnorm(n), rnorm(n), rnorm(n), rnorm(n))
test <- FOBIladle(X)
test
summary(test)
plot(test)
ladleplot(test)</pre>
```

ggladleplot

Ladle Plot for an Object of Class ladle Using ggplot2

## **Description**

The ladle plot is a measure to decide about the number of interesting components. Of interest for the ladle criterion is the minimum. The function here offers however also to plot other criterion values which are part of the actual ladle criterion.

#### Usage

#### Arguments

```
x an object of class ladle.

crit the criterion to be plotted, options are "gn", "fn", "phin" and "lambda".

type plotting type.

ylab default ylab value.

xlab default xlab value.

main default title.

... other arguments for the plotting functions.
```

## **Details**

The main criterion of the ladle is the scaled sum of the eigenvalues and the measure of variation of the eigenvectors up to the component of interest.

The sum is denoted "gn" and the individual parts are "fn" for the measure of the eigenvector variation and "phin" for the scaled eigenvalues. The last option "lambda" corresponds to the unscaled eigenvalues yielding then a screeplot.

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#### Author(s)

Klaus Nordhausen, Joni Virta

#### References

Luo, W. and Li, B. (2016), Combining Eigenvalues and Variation of Eigenvectors for Order Determination, Biometrika, 103. 875–887. <doi:10.1093/biomet/asw051>

#### See Also

```
FOBIladle, PCAladle, SIRladle
```

#### **Examples**

```
n <- 1000
X <- cbind(rexp(n), rt(n,5), rnorm(n), rnorm(n), rnorm(n), rnorm(n))
test <- FOBIladle(X)
ggladleplot(test)
ggladleplot(test, crit="fn")
ggladleplot(test, crit="phin")
ggladleplot(test, crit="lambda")</pre>
```

ggplot.ictest

Scatterplot Matrix for a ictest Object using ggplot2

# Description

For an object of class ictest, plots either the pairwise scatter plot matrix using ggpairs from GGally, or the time series plots of the underlying components using ggplot2. The user can choose if only the components considered interesting or all of them should be plotted. Aesthetics can be passed to ggpairs as well.

# Usage

#### **Arguments**

data	object of class ictest
mapping	aesthetic mapping, see documentation fo

aesthetic mapping, see documentation for ggpairs. If x has the class mts then

this argument is not used.

mapvar data.frame of the external variables used by the aesthetic mappings. If x has the

class mts then this argument is not used.

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which	if "all", then all components of S in the ictest object are plotted. If "k", then only the first k components are plotted, where the value of k is taken from the ictest object. This is only meaningful if k was at least 2.
• • •	arguments passed on to ggpairs. If the component matrix has the class mts, xts or zoo then this argument is not used.
environment	not used but needed for consistency.

#### **Details**

If the component matrix has the class mts, xts or zoo then a time series plot will be plotted using ggplot2. Otherwise, a pairwise scatter plot matrix will be plotted using GGally.

#### Author(s)

Klaus Nordhausen, Joni Virta

#### See Also

```
plot.ictest, pairs
```

# **Examples**

```
# The data
X <- iris[, 1:4]

# The aesthetics variables
mapvar <- data.frame(iris[, 5])
colnames(mapvar) <- "species"

TestCov <- PCAasymp(X, k = 2)
ggplot(TestCov)
ggplot(TestCov, aes(color = species), mapvar = mapvar, which = "k")</pre>
```

ggplot.ladle

Scatterplot Matrix for a ladle Object using ggplot2

## **Description**

For an object of class ladle, plots either the pairwise scatter plot matrix using ggpairs from GGally, or the time series plots of the underlying components using ggplot2. The user can choose if only the components considered interesting or all of them should be plotted. Aesthetics can be passed to ggpairs as well.

#### Usage

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# **Arguments**

data	object of class ladle
mapping	aesthetic mapping, see documentation for $ggpairs$ . If x has the class $mts$ then this argument is not used.
mapvar	data.frame of the external variables used by the aesthetic mappings. If $x$ has the class $mts$ then this argument is not used.
which	if "all", then all components of S in the ladle object are plotted. If "k", then only the first k components are plotted, where the value of k is taken from the ladle object. This is only meaningful if k was at least $2$ .
• • •	arguments passed on to ggpairs. If the component matrix has the class mts, xts or zoo then this argument is not used.
environment	not used but needed for consistency.

#### **Details**

If the component matrix has the class mts, xts or zoo then a time series plot will be plotted using ggplot2. Otherwise, a pairwise scatter plot matrix will be plotted using GGally.

# Author(s)

Klaus Nordhausen, Joni Virta

# See Also

```
plot.ladle, pairs
```

```
# The data
X <- as.matrix(iris[, 1:4])

# The aesthetics variables
mapvar <- data.frame(iris[, 5])
colnames(mapvar) <- "species"

ladle_res <- PCAladle(X)

# The estimate
summary(ladle_res)

# Plots of the components
ggplot(ladle_res)
ggplot(ladle_res, aes(color = species), mapvar = mapvar, which = "k")</pre>
```

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ggscreeplot	ggplot2-style screeplot

# **Description**

A generic method for ggplot2-style screeplots.

## Usage

```
ggscreeplot(x, ...)
```

# **Arguments**

x An object of an appropriate class.

... Additional arguments.

## Author(s)

Joni Virta, Klaus Nordhausen

```
ggscreeplot.ictest Screeplot for an ictest Object Using ggplot2
```

# **Description**

Plots the criterion values of an ictest object against its index number using ggplot2. Two versions of this screeplot are available.

# Usage

# **Arguments**

```
x object of class ictest.
type barplot if a barplot or lines if a line plot is preferred.
main main title of the plot.
ylab y-axis label.
xlab x-axis label.
... arguments passed to and from methods.
```

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#### Author(s)

Klaus Nordhausen, Joni Virta

#### See Also

```
screeplot.ictest
```

# **Examples**

```
n <- 200
X <- cbind(rnorm(n, sd = 2), rnorm(n, sd = 1.5), rnorm(n), rnorm(n), rnorm(n))
TestCov <- PCAasymp(X, k = 2)
ggscreeplot(TestCov)</pre>
```

**ICSboot** 

Boostrap-based Testing for the Number of Gaussian Components in NGCA Using Two Scatter Matrices

# **Description**

In independent components analysis (ICA) gaussian components are considered as uninteresting. The function uses boostrappping tests, based on ICS using any combination of two scatter matrices, to decide if there are p-k gaussian components where p is the dimension of the data. The function offers two different boostrapping strategies.

# Usage

```
ICSboot(X, k, S1=cov, S2=cov4, S1args=NULL, S2args=NULL, n.boot = 200, s.boot = "B1")
```

# Arguments

Χ	a numeric data matrix with p>1 columns.
k	the number of non-gaussian components under the null.
S1	name of the first scatter matrix function. Can only return a matrix. Default is cov
•	
S2	name of the second scatter matrix function. Can only return a matrix. Default is cov4
S1args	list with optional additional arguments for S1.
S2args	list with optional additional arguments for S2.
n.boot	number of bootstrapping samples.
s.boot	bootstrapping strategy to be used. Possible values are "B1", "B2". See details for further information.

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#### **Details**

While in FOBIasymp and FOBIboot the two scatters used are always cov and cov4 this function can be used with any two scatter functions. In that case however the value of the Gaussian eigenvalues are in general not known and depend on the scatter functions used. Therefore the test uses as test statistic the k successive eigenvalues with the smallest variance. Which means the default here might differ from FOBIasymp and FOBIboot.

Given eigenvalues  $d_1, ..., d_p$  the function thus orders the components in descending order according to the "variance" criterion .

Under the null it is then assumed that the first k interesting components are mutually independent and non-normal and the last p-k components are gaussian.

Let  $d_1, ..., d_p$  be the ordered eigenvalues, W the correspondingly ordered unmixing matrix,  $s_i = W(x_i - MU)$  the corresponding source vectors which give the source matrix S which can be decomposed into  $S_1$  and  $S_2$  where  $S_1$  is the matrix with the k non-gaussian components and  $S_2$  the matrix with the gaussian components (under the null).

Two possible bootstrap tests are provided for testing that the last p-k components are gaussian and independent from the first k components:

- 1. s.boot="B1": The first strategy has the following steps:
  - (a) Take a bootstrap sample  $S_1^*$  of size n from  $S_1$ .
  - (b) Take a bootstrap sample  $S_2^*$  consisting of a matrix with gaussian random variables having  $cov(S_2)$ .
  - (c) Combine  $S^* = (S_1^*, S_2^*)$  and create  $X^* = S^*W$ .
  - (d) Compute the test statistic based on  $X^*$ .
  - (e) Repeat the previous steps n. boot times.

Note that in this bootstrapping test the assumption of "independent components" is not used, it is only used that the last p-k components are gaussian and independent from the first k components. Therefore this strategy can be applied in an independent component analysis (ICA) framework and in a non-gaussian components analysis (NGCA) framework.

- 2. s.boot="B2": The second strategy has the following steps:
  - (a) Take a bootstrap sample  $S_1^*$  of size n from  $S_1$  where the subsampling is done separately for each independent component.
  - (b) Take a bootstrap sample  $S_2^*$  consisting of a matrix with gaussian random variables having  $cov(S_2)$
  - (c) Combine  $S^* = (S_1^*, S_2^*)$  and create  $X^* = S^*W$ .
  - (d) Compute the test statistic based on  $X^*$ .
  - (e) Repeat the previous steps n. boot times.

This bootstrapping strategy assumes a full ICA model and cannot be used in an NGCA framework. Note that when the goal is to recover the non-gaussian independent components both scatters used must have the independence property.

#### Value

A list of class ictest inheriting from class htest containing:

statistic the value of the test statistic.

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p.value	the p-value of the test.
parameter	the number of boostrapping samples used to obtain the p-value.
method	character string which test was performed and which scatters were used.
data.name	character string giving the name of the data.
alternative	character string specifying the alternative hypothesis.
k	the number or non-gaussian components used in the testing problem.
W	the transformation matrix to the independent components. Also known as unmixing matrix.
S	data matrix with the centered independent components.
D	the underlying eigenvalues.
MU	the location of the data which was substracted before calculating the independent components.
s.boot	character string which boostrapping strategy was used.

## Author(s)

Klaus Nordhausen

#### References

Nordhausen, K., Oja, H. and Tyler, D.E. (2022), Asymptotic and Bootstrap Tests for Subspace Dimension, Journal of Multivariate Analysis, 188, 104830. <doi:10.1016/j.jmva.2021.104830>.

Nordhausen, K., Oja, H., Tyler, D.E. and Virta, J. (2017), Asymptotic and Bootstrap Tests for the Dimension of the Non-Gaussian Subspace, Signal Processing Letters, 24, 887–891. <doi:10.1109/LSP.2017.2696880>.

Radojicic, U. and Nordhausen, K. (2020), Non-Gaussian Component Analysis: Testing the Dimension of the Signal Subspace. In Maciak, M., Pestas, M. and Schindler, M. (editors) "Analytical Methods in Statistics. AMISTAT 2019", 101–123, Springer, Cham. <doi:10.1007/978-3-030-48814-7\_6>.

#### See Also

```
ics, FOBIboot, FOBIasymp
```

```
n <- 750
S <- cbind(runif(n), rchisq(n, 2), rexp(n), rnorm(n), rnorm(n),
A <- matrix(rnorm(36), ncol = 6)
X <- S %*% t(A)
# n.boot is small for demonstration purpose, should be larger
ICSboot(X, k=1, n.boot=20)
if(require("ICSNP")){
myTyl <- function(X,...) HR.Mest(X,...)$scatter
myT <- function(X,...) tM(X,...)$V</pre>
```

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```
# n.boot is small for demonstration purpose, should be larger
ICSboot(X, k=3, S1=myT, S2=myTyl, s.boot = "B2", n.boot=20)
}
```

ladle

Ladle estimate for an arbitrary matrix

# Description

The ladle estimates the rank of a symmetric matrix S by combining the classical screeplot with an estimate of the rank from the bootstrap eigenvector variability of S.

# Usage

```
ladle(x, S, n.boots = 200, ...)
```

## **Arguments**

x n x p data matrix.

S Function for computing a q x q symmetric matrix from the data x.

n.boots The number of bootstrap samples.
... Further parameters passed to S

#### **Details**

Assume that the eigenvalues of the population version of S are  $\lambda_1 >= ... >= \lambda_k > \lambda_k + 1 = ... = \lambda_p$ . The ladle estimates the true value of k (for example the rank of S) by combining the classical screeplot with estimate of k from the bootstrap eigenvector variability of S.

For applying the ladle to either PCA, FOBI or SIR, see the dedicated functions PCAladle, FOBIladle, SIRladle.

## Value

A list of class ladle containing:

method The string "general".

k The estimated value of k.

fn A vector giving the measures of variation of the eigenvectors using the boot-

strapped eigenvectors for the different number of components.

phin The normalized eigenvalues of the S matrix.

gn The main criterion for the ladle estimate - the sum of fn and phin. k is the value

where gn takes its minimum.

lambda The eigenvalues of the covariance matrix.

data.name The name of the data for which the ladle estimate was computed.

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#### Author(s)

Joni Virta

#### References

Luo, W. and Li, B. (2016), Combining Eigenvalues and Variation of Eigenvectors for Order Determination, Biometrika, 103. 875-887. <doi:10.1093/biomet/asw051>

#### See Also

```
PCAladle, FOBIladle, SIRladle
```

# **Examples**

```
# Function for computing the left CCA matrix
S_CCA <- function(x, dim){</pre>
  x1 <- x[, 1:dim]
  x2 <- x[, -(1:dim)]
  stand <- function(x){</pre>
    x <- as.matrix(x)</pre>
    x \leftarrow sweep(x, 2, colMeans(x), "-")
    eigcov <- eigen(cov(x), symmetric = TRUE)</pre>
    x%*%(eigcov$vectors%*%diag((eigcov$values)^(-1/2))%*%t(eigcov$vectors))
  x1stand <- stand(x1)
  x2stand <- stand(x2)
  crosscov <- cov(x1stand, x2stand)</pre>
  tcrossprod(crosscov)
}
# Toy data with two canonical components
x1 <- matrix(rnorm(n*5), n, 5)</pre>
x2 \leftarrow cbind(x1[, 1] + rnorm(n, sd = sqrt(0.5)),
             -1*x1[, 1] + x1[, 2] + rnorm(n, sd = sqrt(0.5)),
             matrix(rnorm(n*3), n, 3))
x \leftarrow cbind(x1, x2)
# The ladle estimate
ladle_1 \leftarrow ladle(x, S_CCA, dim = 5)
ladleplot(ladle_1)
```

ladleplot

Ladle Plot for an Object of Class ladle

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## **Description**

The ladle plot is a measure to decide about the number of interesting components. Of interest for the ladle criterion is the minimum. The function here offers however also to plot other criterion values which are part of the actual ladle criterion.

## Usage

## Arguments

```
x an object of class ladle.

crit the criterion to be plotted, options are "gn", "fn", "phin" and "lambda".

type plotting type.

ylab default ylab value.

xlab default xlab value.

main default title.

... other arguments for the plotting functions.
```

#### **Details**

The main criterion of the ladle is the scaled sum of the eigenvalues and the measure of variation of the eigenvectors up to the component of interest.

The sum is denoted "gn" and the individual parts are "fn" for the measure of the eigenvector variation and "phin" for the scaled eigenvalues. The last option "lambda" corresponds to the unscaled eigenvalues yielding then a screeplot.

#### Author(s)

Klaus Nordhausen

# References

Luo, W. and Li, B. (2016), Combining Eigenvalues and Variation of Eigenvectors for Order Determination, Biometrika, 103. 875–887. <doi:10.1093/biomet/asw051>

#### See Also

```
FOBIladle, PCAladle, SIRladle
```

```
n <- 1000
X <- cbind(rexp(n), rt(n,5), rnorm(n), rnorm(n), rnorm(n), rnorm(n))
test <- FOBIladle(X)
ladleplot(test)
ladleplot(test, crit="fn")</pre>
```

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```
ladleplot(test, crit="phin")
ladleplot(test, crit="lambda")
```

**NGPP** 

Non-Gaussian Projection Pursuit

#### **Description**

Estimates k non-Gaussian signal components using projection pursuit. The projection index can be chosen among convex combinations of squares of one or several standard projection indices used in ICA.

## Usage

```
NGPP(X, k, nl = c("skew", "pow3"), alpha = 0.8, method = "symm", eps = 1e-6, verbose = FALSE, maxiter = 100)
```

# Arguments

X	Numeric matrix with n rows corresponding to the observations and p columns corresponding to the variables.
k	Number of components to estimate, $1 \le k \le p$ .
nl	Vector of non-linearities, a convex combination of the corresponding squared objective functions of which is then used as the projection index. The choices include "skew" (skewness), "pow3" (excess kurtosis), "tanh" $(log(cosh))$ and "gauss" (Gaussian function).
alpha	Vector of positive weights between 0 and 1 given to the non-linearities. The length of alpha should be either one less than the number of non-linearities in which case the missing weight is chosen so that alpha sums to one, or equal to the number of non-linearities in which case the weights are used as such. No boundary checks for the weights are done.
method	If "symm" the k signals are estimated simultaneously (symmetric projection pursuit) and if "defl" they are estimated one-by-one (deflation-based projection pursuit).
eps	Convergence tolerance.
verbose	If TRUE the numbers of iterations will be printed.
maxiter	Maximum number of iterations.

# **Details**

It is assumed that the data is a random sample from the model x=m+As where the latent vector  $s=(s_1^T,s_2^T)^T$  consists of k-dimensional non-Gaussian subvector (the signal) and p-k-dimensional Gaussian subvector (the noise) and the components of s are mutually independent. Without loss of generality we further assume that the components of s have zero means and unit variances.

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The objective is to estimate an inverse for the mixing matrix A and in non-Gaussian projection pursuit this is done by first standardizaing the observations and then finding mutually orthogonal directions maximizing a convex combination of the chosen squared objective functions.

After estimation the found signals are ordered in decreasing order with respect to their objective function values.

#### Value

A list with class 'bss' containing the following components:

W	Estimated unmixing matrix
S	Matrix of size $n \times k$ containing the estimated signals.
D	Vector of the objective function values of the signals
MU	Location vector of the data which was substracted before estimating the signal components.

# Author(s)

Joni Virta

#### References

Virta, J., Nordhausen, K. and Oja, H., (2016), Projection Pursuit for non-Gaussian Independent Components, <a href="https://arxiv.org/abs/1612.05445">https://arxiv.org/abs/1612.05445</a>.

#### See Also

```
NGPPsim, NGPPest, fICA
```

```
# Simulated data with 2 signals

n <- 500
S <- cbind(rexp(n), runif(n), rnorm(n))
A <- matrix(rnorm(9), ncol = 3)
X <- S %*% t(A)

res <- NGPP(X, 2)
res$W %*% A

# Iris data

X <- as.matrix(iris[, 1:4])

res <- NGPP(X, 2, nl = c("pow3", "tanh"), alpha = 0.5)
plot(res, col = iris[, 5])</pre>
```

24 NGPPest

NGPPest Signal Subspace Dimension Testing Using non-Gaussian Projection Pursuit	NGPPest	Signal Subspace Dimension Testing Using non-Gaussian Projection Pursuit
---	---------	---

#### **Description**

Estimates the dimension of the signal subspace using NGPP to conduct sequential hypothesis testing. The test statistic is a multivariate extension of the classical Jarque-Bera statistic and the distribution of it under the null hypothesis is obtained by simulation.

## Usage

```
NGPPest(X, nl = c("skew", "pow3"), alpha = 0.8, N = 500, eps = 1e-6, verbose = FALSE, maxiter = 100)
```

#### **Arguments**

X	Numeric matrix with n rows corresponding to the observations and p columns corresponding to the variables.
nl	Vector of non-linearities, a convex combination of the corresponding squared objective functions of which is then used as the projection index. The choices include "skew" (skewness), "pow3" (excess kurtosis), "tanh" $(log(cosh))$ and "gauss" (Gaussian function).
alpha	Vector of positive weights between 0 and 1 given to the non-linearities. The length of alpha should be either one less than the number of non-linearities in which case the missing weight is chosen so that alpha sums to one, or equal to the number of non-linearities in which case the weights are used as such. No boundary checks for the weights are done.
N	Number of normal samples to be used in simulating the distribution of the test statistic under the null hypothesis.
eps	Convergence tolerance.
verbose	If TRUE the numbers of iterations will be printed.
maxiter	Maximum number of iterations.

#### **Details**

It is assumed that the data is a random sample from the model x=m+As where the latent vector  $s=(s_1^T,s_2^T)^T$  consists of k-dimensional non-Gaussian subvector (the signal) and p-k-dimensional Gaussian subvector (the noise) and the components of s are mutually independent. Without loss of generality we further assume that the components of s have zero means and unit variances.

The algorithm first estimates full p components from the data using deflation-based NGPP with the chosen non-linearities and weighting and then tests the null hypothesis  $H_0: k_{true} \leq k$  for each  $k=0,\ldots,p-1$ . The testing is based on the fact that under the null hypothesis  $H_0: k_{true} \leq k$  the distribution of the final p-k components is standard multivariate normal and the significance of the test can be obtained by comparing the objective function value of the (k+1)th estimated

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components to the same quantity estimated from N samples of size n from (p-k)-dimensional standard multivariate normal distribution.

Note that if maxiter is reached at any step of the algorithm it will use the current estimated direction and continue to the next step.

#### Value

A list with class 'icest' containing the following components:

statistic Test statistic, i.e. the objective function values of all estimated component. p.value Obtained vector of p-values.

parameter Number N of simulated normal samples.

method Character string "Estimation the signal subspace dimension using NGPP".

data. name Character string giving the name of the data.

W Estimated unmixing matrix

S Matrix of size  $n \times p$  containing the estimated signals. D Vector of the objective function values of the signals

MU Location vector of the data which was substracted before estimating the signal

components.

conv Boolean vector telling for which components the algorithm converged (TRUE)

and for which not (FALSE).

#### Author(s)

Joni Virta

## References

Virta, J., Nordhausen, K. and Oja, H., (2016), Projection Pursuit for non-Gaussian Independent Components, <a href="https://arxiv.org/abs/1612.05445">https://arxiv.org/abs/1612.05445</a>>.

#### See Also

```
NGPP, NGPPsim
```

```
# Iris data

X <- as.matrix(iris[, 1:4])

# The number of simulations N should be increased in practical situations
# Now we settle for N = 100

res <- NGPPest(X, N = 100)
res$statistic
res$p.value
res$conv</pre>
```

26 NGPPsim

NGPPsim	Signal Subspace Dimension Testing Using non-Gaussian Projection Pursuit

# Description

Tests whether the true dimension of the signal subspace is less than or equal to a given k. The test statistic is a multivariate extension of the classical Jarque-Bera statistic and the distribution of it under the null hypothesis is obtained by simulation.

#### Usage

```
NGPPsim(X, k, nl = c("skew", "pow3"), alpha = 0.8, N = 1000, eps = 1e-6, verbose = FALSE, maxiter = 100)
```

# Arguments

_	
X	Numeric matrix with n rows corresponding to the observations and p columns corresponding to the variables.
k	Number of components to estimate, $1 \le k \le p$ .
nl	Vector of non-linearities, a convex combination of the corresponding squared objective functions of which is then used as the projection index. The choices include "skew" (skewness), "pow3" (excess kurtosis), "tanh" $(log(cosh))$ and "gauss" (Gaussian function).
alpha	Vector of positive weights between 0 and 1 given to the non-linearities. The length of alpha should be either one less than the number of non-linearities in which case the missing weight is chosen so that alpha sums to one, or equal to the number of non-linearities in which case the weights are used as such. No boundary checks for the weights are done.
N	Number of normal samples to be used in simulating the distribution of the test statistic under the null hypothesis.
eps	Convergence tolerance.
verbose	If TRUE the numbers of iterations will be printed.
maxiter	Maximum number of iterations.

#### **Details**

It is assumed that the data is a random sample from the model x=m+As where the latent vector  $s=(s_1^T,s_2^T)^T$  consists of k-dimensional non-Gaussian subvector (the signal) and p-k-dimensional Gaussian subvector (the noise) and the components of s are mutually independent. Without loss of generality we further assume that the components of s have zero means and unit variances.

To test the null hypothesis  $H_0: k_{true} \leq k$  the algorithm first estimates k+1 components using delfation-based NGPP with the chosen non-linearities and weighting. Under the null hypothesis the distribution of the final p-k components is standard multivariate normal and the significance of the test is obtained by comparing the objective function value of the (k+1)th estimated components to

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the same quantity estimated from N samples of size n from (p-k)-dimensional standard multivariate normal distribution.

Note that if maxiter is reached at any step of the algorithm it will use the current estimated direction and continue to the next step.

## Value

A list with class 'ictest', inheriting from the class 'hctest', containing the following components:

statistic Test statistic, i.e. the objective function value of the (k + 1)th estimated compo-

nent.

p.value Obtained *p*-value.

parameter Number N of simulated normal samples.

method Character string denoting which test was performed.

data. name Character string giving the name of the data.

alternative Alternative hypothesis, i.e. "There are less than p - k Gaussian components".

k Tested dimension k.

W Estimated unmixing matrix

S Matrix of size  $n \times (k+1)$  containing the estimated signals.

D Vector of the objective function values of the signals

MU Location vector of the data which was substracted before estimating the signal

components.

## Author(s)

Joni Virta

#### References

Virta, J., Nordhausen, K. and Oja, H., (2016), Projection Pursuit for non-Gaussian Independent Components, <a href="https://arxiv.org/abs/1612.05445">https://arxiv.org/abs/1612.05445</a>>.

# See Also

```
NGPP, NGPPest
```

```
# Simulated data with 2 signals and 2 noise components

n <- 200
S <- cbind(rexp(n), rbeta(n, 1, 2), rnorm(n), rnorm(n))
A <- matrix(rnorm(16), ncol = 4)
X <- S %*% t(A)

# The number of simulations N should be increased in practical situations
# Now we settle for N = 100</pre>
```

```
res1 <- NGPPsim(X, 1, N = 100)
res1
screeplot(res1)

res2 <- NGPPsim(X, 2, N = 100)
res2
screeplot(res2)</pre>
```

**PCAasymp** 

Testing for Subsphericity using the Covariance Matrix or Tyler's Shape Matrix

# Description

The function tests, assuming an elliptical model, that the last p-k eigenvalues of a scatter matrix are equal and the k interesting components are those with a larger variance. The scatter matrices that can be used here are the regular covariance matrix and Tyler's shape matrix.

## Usage

```
PCAasymp(X, k, scatter = "cov", ...)
```

#### **Arguments**

Χ	a numeric data matrix with p>1 columns.
k	the number of eigenvalues larger than the equal ones. Can be between 0 and p-2.
scatter	the scatter matrix to be used. Can be "cov" or "tyler". For "cov" the regular covariance matrix is computed and for "tyler" the function HR. Mest is used to compute Tyler's shape matrix.
	arguments passed on to HR. Mest if scatter = "tyler".

#### **Details**

The functions assumes an elliptical model and tests if the last p-k eigenvalues of PCA are equal. PCA can here be either be based on the regular covariance matrix or on Tyler's shape matrix.

For a sample of size n, the test statistic is

$$T = n/(2\bar{d}^2\sigma_1)\sum_{k+1}^{p}(d_i - \bar{d})^2,$$

where  $\bar{d}$  is the mean of the last p - k PCA eigenvalues.

The constant  $\sigma_1$  is for the regular covariance matrix estimated from the data whereas for Tyler's shape matrix it is simply a function of the dimension of the data.

The test statistic has a limiting chisquare distribution with (p - k - 1)(p - k + 2)/2 degrees of freedom.

Note that the regular covariance matrix is here divided by n and not by n-1.

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# Value

A list of class ictest inheriting from class htest containing:

statistic the value of the test statistic.
p.value the p-value of the test.

parameter the degrees of freedom of the test.

method character string which test was performed.
data.name character string giving the name of the data.

alternative character string specifying the alternative hypothesis.

k the number or larger eigenvalues used in the testing problem.

W the transformation matrix to the principal components.

S data matrix with the centered principal components.

D the underlying eigenvalues.

MU the location of the data which was substracted before calculating the principal

components.

SCATTER the computed scatter matrix.

sigma1 the asymptotic constant needed for the asymptotic test.

# Author(s)

Klaus Nordhausen

#### References

Nordhausen, K., Oja, H. and Tyler, D.E. (2022), Asymptotic and Bootstrap Tests for Subspace Dimension, Journal of Multivariate Analysis, 188, 104830. <doi:10.1016/j.jmva.2021.104830>.

#### See Also

```
HR. Mest, PCAboot
```

```
n <- 200
X <- cbind(rnorm(n, sd = 2), rnorm(n, sd = 1.5), rnorm(n), rnorm(n), rnorm(n))
TestCov <- PCAasymp(X, k = 2)
TestCov
TestTyler <- PCAasymp(X, k = 1, scatter = "tyler")
TestTyler</pre>
```

30 PCAaug

PCAaug	Augmentation Estimate for PCA

#### **Description**

For p-variate data, the augmentation estimate for PCA assumes that the last p-k eigenvalues are equal. Combining information from the eigenvalues and eigenvectors of the covariance matrix the augmentation estimator yields an estimate for k.

#### Usage

```
PCAaug(X, noise = "median", naug = 1, nrep = 1, sigma2 = NULL, alpha = NULL)
```

## **Arguments**

X	numeric data matrix.
noise	name of the method to be used to estimate the noise variance. Options are "median", "last", "quantile" or "known". See details.
naug	number of components to be augmented.
nrep	number of repetitions for the augmentation procedure.
sigma2	value of the noise variance when noise = "known".
alpha	the quantile to be used when noise = "quantile".

## **Details**

The model here assumes that the eigenvalues of the covariance matrix are of the form  $\lambda_1 \ge ... \ge \lambda_k > \lambda_{k+1} = ... = \lambda_p$  and the goal is to estimate the value of k. The value  $\lambda_{k+1}$  corresponds then to the noise variance.

The augmented estimator adds for that purpose naug Gaussian components with the provided noise variance which needs to be provided (noise = "known") or estimated from the data. Three estimation methods are available. In the case of noise = "median" the estimate is the median of the eigenvalues of the covariance matrix, in the case of noise = "last" it corresponds to the last eigenvalue of the covariance matrix and in the case of noise = "quantile" it is the mean of the eigenvalues smaller or equal to the alpha-quantile of the eigenvalues of the covariance matrix.

The augmentation estimator uses then the augmented components to measure the variation of the eigenvalues. For a more stable result it is recommend to repeat the augmentation process several times and Lue and Li (2021) recommend to use for naug approximately p/5 or p/10 where p is the number of columns of X.

The augmented estimator for this purpose combines then the values of the scaled eigenvalues and the variation measured via augmentation. The main idea there is that for distinct eigenvales the variation of the eigenvectors is small and for equal eigenvalues the corresponding eigenvectors have large variation.

The augmented estimate for k is the value where the measure takes its minimum and can be also visualized as a ladle.

For further details see Luo and Li (2021) and Radojicic et al. (2021).

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#### Value

A list of class ladle containing:

method the string PCA.

k the estimated value of k.

fn vector giving the measures of variation of the eigenvectors using the bootstrapped

eigenvectors for the different number of components.

phin normalized eigenvalues of the covariance matrix.

gn the main criterion for the augmented estimate - the sum of fn and phin. k is the

value where gn takes its minimum

lambda the eigenvalues of the covariance matrix.

W the transformation matrix to the principal components.
S data matrix with the centered principal components.

MU the location of the data which was substracted before calculating the principal

components.

data.name the name of the data for which the augmented estimate was computed.

sigma2 the value used as noise variance when simulating the augmented components.

## Author(s)

Klaus Nordhausen

#### References

Luo, W. and Li, B. (2021), On Order Determination by Predictor Augmentation, Biometrika, 108, 557–574. <doi:10.1093/biomet/asaa077>

Radojicic, U., Lietzen, N., Nordhausen, K. and Virta, J. (2021), Dimension Estimation in Two-Dimensional PCA. In S. Loncaric, T. Petkovic and D. Petrinovic (editors) "Proceedings of the 12 International Symposium on Image and Signal Processing and Analysis (ISPA 2021)", 16–22. <doi:10.1109/ISPA52656.2021.9552114>

#### See Also

```
ladleplot, PCAladle
```

```
n <- 1000
Y <- cbind(rnorm(n, sd=2), rnorm(n,sd=2), rnorm(n), rnorm(n), rnorm(n), rnorm(n))
testPCA <- PCAaug(Y)
testPCA
summary(testPCA)
plot(testPCA)
ladleplot(testPCA)
ladleplot(testPCA, crit = "fn")
ladleplot(testPCA, crit = "lambda")
ladleplot(testPCA, crit = "phin")</pre>
```

32 PCAboot

**PCAboot** 

Bootstrap-Based Testing for Subsphericity

## **Description**

The function tests, assuming an elliptical model, that the last p-k eigenvalues of a scatter matrix are equal and the k interesting components are those with a larger variance. To obtain p-values two different bootstrapping strategies are available and the user can provide the scatter matrix to be used as a function.

#### Usage

```
PCAboot(X, k, n.boot = 200, s.boot = "B1", S = MeanCov, Sargs = NULL)
```

#### **Arguments**

Χ	a numeric data matrix with p>1 columns.
k	the number of eigenvalues larger than the equal ones. Can be between 0 and p-2.
n.boot	number of bootstrapping samples.
s.boot	bootstrapping strategy to be used. Possible values are "B1", "B2". See details for further information.
S	A function which returns a list that has as its first element a location vector and as the second element the scatter matrix.
Sargs	list of further arguments passed on to the function specified in S.

#### **Details**

Here the function S needs to return a list where the first argument is a location vector and the second one a scatter matrix.

The location is used to center the data and the scatter matrix is used to perform PCA.

Consider X as the centered data and denote by W the transformation matrix to the principal components. The corresponding eigenvalues from PCA are  $d_1,...,d_p$ . Under the null,  $d_k > d_{k+1} = ... = d_p$ . Denote further by  $\bar{d}$  the mean of the last p-k eigenvalues and by  $D^* = diag(d_1,...,d_k,\bar{d},...,\bar{d})$  a  $p \times p$  diagonal matrix. Assume that S is the matrix with principal components which can be decomposed into  $S_1$  and  $S_2$  where  $S_1$  contains the k interesting principal components and  $S_2$  the last p-k principal components.

For a sample of size n, the test statistic used for the boostrapping tests is

$$T = n/(\bar{d}^2) \sum_{k=1}^{p} (d_i - \bar{d})^2.$$

The function offers then two boostrapping strategies:

1. s.boot="B1": The first strategy has the following steps:

- (a) Take a bootstrap sample  $S^*$  of size n from S and decompose it into  $S_1^*$  and  $S_2^*$ .
- (b) Every observation in  $S_2^*$  is transformed with a different random orthogonal matrix.
- (c) Recombine  $S^* = (S_1^*, S_2^*)$  and create  $X^* = S^*W$ .
- (d) Compute the test statistic based on  $X^*$ .
- (e) Repeat the previous steps n. boot times.
- 2. s.boot="B2": The second strategy has the following steps:
  - (a) Scale each principal component using the matrix D, i.e. Z = SD.
  - (b) Take a bootstrap sample  $Z^*$  of size n from Z.
  - (c) Every observation in  $Z^*$  is transformed with a different random orthogonal matrix.
  - (d) Recreate  $X^* = Z^*D^{*-1}W$ .
  - (e) Compute the test statistic based on  $X^*$ .
  - (f) Repeat the previous steps n. boot times.

To create the random orthogonal matrices the function rorth is used.

#### Value

A list of class ictest inheriting from class htest containing:

statistic	the value of the test statistic.
p.value	the p-value of the test.
parameter	the degrees of freedom of the test.
method	character string which test was performed.
data.name	character string giving the name of the data.
alternative	character string specifying the alternative hypothesis.
k	the number or larger eigenvalues used in the testing problem.
W	the transformation matrix to the principal components.
S	data matrix with the centered principal components.
D	the underlying eigenvalues.
MU	the location of the data which was substracted before calculating the principal components.
SCATTER	The computed scatter matrix.
scatter	character string denoting which scatter function was used.
s.boot	character string denoting which bootstrapping test version was used.

# Author(s)

Klaus Nordhausen

# References

Nordhausen, K., Oja, H. and Tyler, D.E. (2022), Asymptotic and Bootstrap Tests for Subspace Dimension, Journal of Multivariate Analysis, 188, 104830. <doi:10.1016/j.jmva.2021.104830>.

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## See Also

```
cov, MeanCov, PCAasymp
```

## **Examples**

```
n <- 200
X <- cbind(rnorm(n, sd = 2), rnorm(n, sd = 1.5), rnorm(n), rnorm(n), rnorm(n))
# for demonstration purpose the n.boot is chosen small, should be larger in real applications
TestCov <- PCAboot(X, k = 2, n.boot=30)
TestTM <- PCAboot(X, k = 1, n.boot=30, s.boot = "B2", S = "tM", Sargs = list(df=2))
TestTM</pre>
```

**PCAladle** 

Ladle Estimate for PCA

# Description

For p-variate data, the Ladle estimate for PCA assumes that the last p-k eigenvalues are equal. Combining information from the eigenvalues and eigenvectors of the covariance matrix the ladle estimator yields an estimate for k.

# Usage

#### **Arguments**

X numeric data matrix.

n.boot number of bootstrapping samples to be used.

ncomp The number of components among which the ladle estimator is to be searched.

The default here follows the recommendation of Luo and Li 2016.

#### **Details**

The model here assumes that the eigenvalues of the covariance matrix are of the form  $\lambda_1 \geq ... \geq \lambda_k > \lambda_{k+1} = ... = \lambda_p$  and the goal is to estimate the value of k. The ladle estimate for this purpose combines the values of the scaled eigenvalues and the variation of the eigenvectors based on bootstrapping. The idea there is that for distinct eigenvales the variation of the eigenvectors is small and for equal eigenvalues the corresponding eigenvectors have large variation.

This measure is then computed assuming k=0,..., ncomp and the ladle estimate for k is the value where the measure takes its minimum.

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# Value

A list of class ladle containing:

method	the string PCA.
k	the estimated value of k.
fn	vector giving the measures of variation of the eigenvectors using the bootstrapped eigenvectors for the different number of components.
phin	normalized eigenvalues of the covariance matrix.
gn	the main criterion for the ladle estimate - the sum of fn and phin. k is the value where gn takes its minimum
lambda	the eigenvalues of the covariance matrix.
W	the transformation matrix to the principal components.
S	data matrix with the centered principal components.
MU	the location of the data which was substracted before calculating the principal components.

# Author(s)

Klaus Nordhausen

data.name

#### References

Luo, W. and Li, B. (2016), Combining Eigenvalues and Variation of Eigenvectors for Order Determination, Biometrika, 103, 875–887. <doi:10.1093/biomet/asw051>

the name of the data for which the ladle estimate was computed.

#### See Also

```
ladleplot
```

```
n <- 1000
Y <- cbind(rnorm(n, sd=2), rnorm(n,sd=2), rnorm(n), rnorm(n), rnorm(n), rnorm(n))
testPCA <- PCAladle(Y)
testPCA
summary(testPCA)
plot(testPCA)
ladleplot(testPCA)
ladleplot(testPCA, crit = "fn")
ladleplot(testPCA, crit = "lambda")
ladleplot(testPCA, crit = "phin")</pre>
```

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PCAschott	Testing for Subsphericity using the Schott's test

#### **Description**

The test tests the equality of the last eigenvalues assuming normal distributed data using the regular covariance matrix.

#### Usage

```
PCAschott(X, k)
```

#### **Arguments**

X a numeric data matrix with p>1 columns.

k the number of eigenvalues larger than the equal ones. Can be between 0 and p-2.

#### **Details**

The functions assumes multivariate normal data and tests if the last p - k eigenvalues of PCA are equal.

#### Value

A list of class ictest inheriting from class htest containing:

statistic the value of the test statistic.
p.value the p-value of the test.

parameter the degrees of freedom of the test.

method character string which test was performed.
data.name character string giving the name of the data.

alternative character string specifying the alternative hypothesis.

k the number or larger eigenvalues used in the testing problem.

W the transformation matrix to the principal components.S data matrix with the centered principal components.

D the underlying eigenvalues.

MU the mean vector of the data which was substracted before calculating the princi-

pal components.

SCATTER the computed covariance matrix matrix.

# Author(s)

Klaus Nordhausen

plot.ictest 37

## References

Schott, J.R. (2006), A High-Dimensional Test for the Equality of the Smallest Eigenvalues of a Covariance Matrix, Journal of Multivariate Analysis, 97, 827–843. <a href="https://doi.org/10.1016/j.jmva.2005.05.003">doi:10.1016/j.jmva.2005.05.003</a>

#### See Also

```
PCAasymp, PCAboot
```

## **Examples**

```
n \leftarrow 200
 X \leftarrow cbind(rnorm(n, sd = 2), rnorm(n, sd = 1.5), rnorm(n), rnorm(n), rnorm(n))
 PCAschott(X, 2)
```

plot.ictest

Scatterplot Matrix for a ictest Object

## **Description**

For an object of class ictest, plots either the pairwise scatter plot matrix, or the time series plots of the underlying components. The user can choose if only the components considered interesting or all of them should be plotted.

#### Usage

```
## S3 method for class 'ictest'
plot(x, which = "all", ...)
```

## **Arguments**

x object of class ictest
 which if "all", then all components of S in the ictest object are plotted. If "k", then only the first k components are plotted, where the value of k is taken from the ictest object. This is only meaningful if k was at least 2.
 ... other arguments passed on to pairs if the components are a numeric matrix or to plot.ts, plot.zoo or plot.xts if the components are from the corresponding class.

## **Details**

If the component matrix has the class mts, xts or zoo, then a time series plot will be plotted. Otherwise, the pairwise scatter plot matrix will be plotted.

## Author(s)

Klaus Nordhausen

38 plot.ladle

## See Also

```
ggplot.ictest, pairs, plot.ts, plot.zoo, plot.xts
```

## **Examples**

```
n <- 200
X <- cbind(rnorm(n, sd = 2), rnorm(n, sd = 1.5), rnorm(n), rnorm(n), rnorm(n))
TestCov <- PCAasymp(X, k = 2)
plot(TestCov)
plot(TestCov, which = "k")</pre>
```

plot.ladle

Plotting an Object of Class ladle

## Description

An object of class ladle contains always the source components as estimated by the corresponding statistical method. This function either plots all of the components or only this considered interesting according to the ladle estimate.

## Usage

```
## S3 method for class 'ladle'
plot(x, which = "all", ...)
```

#### **Arguments**

x an object of class ladle.

which if "all", then all components of S in the ladle object are plotted. If "k", then only the k components are plotted, which are considered interesting according to the ladle estimator. This is only meaningful if the estimated 'k' is at least 2.

... other arguments passed on to pairs if the components are a numeric matrix or to plot.ts, plot.zoo or plot.xts if the components are from the corresponding class.

## **Details**

If the component matrix has the class mts, xts or zoo, then a time series plot will be plotted. Otherwise, the pairwise scatter plot matrix will be plotted.

#### Author(s)

Klaus Nordhausen

## See Also

```
pairs, plot.ts, plot.zoo, plot.xts
```

print.ladle 39

## **Examples**

```
n <- 1000
X <- cbind(rexp(n), rt(n,5), rnorm(n), rnorm(n), rnorm(n), rnorm(n))
test <- FOBIladle(X)
plot(test)</pre>
```

print.ladle

Printing an Object of Class ladle

# Description

Basic printing of an object of class ladle. Prints basically everything but the estimated components.

## Usage

```
## S3 method for class 'ladle'
print(x, ...)
```

## **Arguments**

x an object of class ladle.

... further arguments to be passed to or from methods.

## Author(s)

Klaus Nordhausen

## See Also

```
summary.ladle, plot.ladle, ladleplot, FOBIladle, PCAladle, SIRladle
```

```
n <- 1000
X <- cbind(rexp(n), rt(n,5), rnorm(n), rnorm(n), rnorm(n), rnorm(n))
test <- FOBIladle(X)
test</pre>
```

40 rOMEGA

rMU

Greek Letter mu Shaped Bivariate Data Generation

# Description

A function to generate bivariate data with the scatterplot resembling the greek letter mu.

# Usage

rMU(n)

## **Arguments**

n

the sample size.

## Value

A n times 2 matrix

## Author(s)

Klaus Nordhausen, Joni Virta

## **Examples**

```
x <- rMU(1000)
plot(x)</pre>
```

rOMEGA

Greek Letter Omega Shaped Bivariate Data Generation

# Description

A function to generate bivariate data with the scatterplot resembling the greek letter Omega.

## Usage

```
rOMEGA(n)
```

# Arguments

n

the sample size.

## Value

A n times 2 matrix

rorth 41

## Author(s)

Klaus Nordhausen, Joni Virta

# **Examples**

```
x <- rOMEGA(1000)
plot(x)</pre>
```

rorth

Random Orthogonal Matrix Creation Uniform WRT the Haar Measure.

## Description

A function to create a random orthogonal matrix uniformly distributed with respect to the Haar measure.

## Usage

rorth(k)

## **Arguments**

k

the desired numer of columns (=rows) of the orthogonal matrix.

## **Details**

The function fills a kxk matrix with N(0,1) random variables and perfroms then a QR decomposition using qr. If the diagonal elements of R are all positive the resulting orthogonal matrix Q is uniform distributed wrt to the Haar measure. Note that the function currently does not check if all diagonal measurements are indeed positive (however this will happen with probability 1 in theory).

## Value

An orthogonal k times k matrix

#### Author(s)

Klaus Nordhausen

#### References

Stewart, G.W. (1980), The efficient generation of random orthogonal matrices with an application to condition estimators, SIAM Journal on Numerical Analysis, 17, 403–409. <doi:10.1137/0717034>.

42 screeplot.ictest

## **Examples**

```
Orth <- rorth(4)
crossprod(Orth)
tcrossprod(Orth)</pre>
```

screeplot.ictest

Screeplot for an ictest Object

## **Description**

Plots the criterion values of an ictest object against its index number. Two versions of this screeplot are available.

## Usage

```
## S3 method for class 'ictest'
screeplot(x, type = "barplot", main = deparse(substitute(x)),
  ylab = "criterion", xlab = "component", ...)
```

## **Arguments**

```
x object of class ictest.
type barplot if a barplot or lines if a line plot is preferred.
main main title of the plot.
ylab y-axis label.
xlab x-axis label.
other arguments for the plotting functions.
```

#### Author(s)

Klaus Nordhausen

## See Also

```
ggscreeplot
```

```
n <- 200
X <- cbind(rnorm(n, sd = 2), rnorm(n, sd = 1.5), rnorm(n), rnorm(n), rnorm(n))
TestCov <- PCAasymp(X, k = 2)
screeplot(TestCov)</pre>
```

SIRasymp 43

SIRasymp	Testing the Subspace Dimension for Sliced Inverse Regression.

## **Description**

Using the two scatter matrices approach (SICS) for sliced inversion regression (SIR), the function tests if the last p-k components have zero eigenvalues, where p is the number of explaining variables. Hence the assumption is that the first k components are relevant for modelling the response y and the remaining components are not.

## Usage

```
SIRasymp(X, y, k, h = 10, ...)
```

# Arguments

Χ	a numeric data matrix of explaining variables.
у	a numeric vector specifying the response.
k	the number of relevant components under the null hypothesis.
h	the number of slices used in SIR. Passed on to function covSIR.
	other arguments passed on to covSIR.

## **Details**

Under the null the first k eigenvalues contained in D are non-zero and the remaining p-k are zero.

For a sample of size n, the test statistic T is then n times the sum of these last p-k eigenvalue and has under the null a chisquare distribution with (p-k)(h-k-1) degrees of freedom, therefore it is required that k < h-1.

## Value

A list of class ictest inheriting from class htest containing:

statistic	the value of the test statistic.
p.value	the p-value of the test.
parameter	the degrees of freedom of the test.
method	character string which test was performed.
data.name	character string giving the name of the data.
alternative	character string specifying the alternative hypothesis.
k	the number of non-zero eigenvalues used in the testing problem.
W	the transformation matrix to the underlying components.
S	data matrix with the centered underlying components.
D	the underlying eigenvalues.
MU	the location of the data which was substracted before calculating the compo-
	nents.

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## Author(s)

Klaus Nordhausen

#### References

Nordhausen, K., Oja, H. and Tyler, D.E. (2022), Asymptotic and Bootstrap Tests for Subspace Dimension, Journal of Multivariate Analysis, 188, 104830. <doi:10.1016/j.jmva.2021.104830>.

#### See Also

```
covSIR, SIRboot
```

## **Examples**

```
X <- matrix(rnorm(1000), ncol = 5)
eps <- rnorm(200, sd = 0.1)
y <- 2 + 0.5 * X[, 1] + 2 * X[, 3] + eps

SIRasymp(X, y, k = 0)
SIRasymp(X, y, k = 1)</pre>
```

SIRboot

Testing the Subspace Dimension for Sliced Inverse Regression Using Bootstrapping.

## **Description**

Using the two scatter matrices approach (SICS) for sliced inversion regression (SIR) the function tests if the last p-k components have zero eigenvalues, where p is the number of explaining variables. Hence the assumption is that the first k components are relevant for modelling the response y and the remaining components are not. The function performs bootstrapping to obtain a p-value.

## Usage

```
SIRboot(X, y, k, h = 10, n.boot = 200, ...)
```

## **Arguments**

X	a numeric data matrix of explaining variables.
У	a numeric vector specifying the response.
k	the number of relevant components under the null hypothesis.
h	the number of slices used in SIR. Passed on to function covSIR.
n.boot	number of bootstrapping samples.
	other arguments passed on to covSIR.

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#### **Details**

Under the null hypthesis the last p-k eigenvalue as given in D are zero. The test statistic is then the sum of these eigenvalues.

Denote W as the transformation matrix to the supervised invariant coordinates (SIC)  $s_i$ , i = 1, ..., n, i.e.

$$s_i = W(x_i - MU),$$

where MU is the location.

Let  $S_1$  be the submatrix of the SICs which are relevant and  $S_2$  the submatrix of the SICs which are irrelevant for the response y under the null.

The boostrapping has then the following steps:

- 1. Take a boostrap sample  $(y^*, S_1^*)$  of size n from  $(y, S_1)$ .
- 2. Take a boostrap sample  $S_2^*$  of size n from  $S_2$ .
- 3. Combine  $S^* = (S_1^*, S_2^*)$  and create  $X^* = S^*W$ .
- 4. Compute the test statistic based on  $X^*$ .
- 5. Repeat the previous steps n.boot times.

## Value

A list of class ictest inheriting from class htest containing:

statistic the value of the test statistic.

p.value the p-value of the test.

parameter the number of boostrapping samples used to compute the p-value.

method character string which test was performed.

data.name character string giving the name of the data.

alternative character string specifying the alternative hypothesis.

k the number of non-zero eigenvalues used in the testing problem.

the transformation matrix to the underlying components.data matrix with the centered underlying components.

D the underlying eigenvalues.

MU the location of the data which was substracted before calculating the compo-

nents.

## Author(s)

Klaus Nordhausen

## References

Nordhausen, K., Oja, H. and Tyler, D.E. (2022), Asymptotic and Bootstrap Tests for Subspace Dimension, Journal of Multivariate Analysis, 188, 104830. <doi:10.1016/j.jmva.2021.104830>.

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## See Also

```
covSIR, SIRasymp
```

#### **Examples**

```
X <- matrix(rnorm(1000), ncol = 5)
eps <- rnorm(200, sd = 0.1)
y <- 2 + 0.5 * X[, 1] + 2 * X[, 3] + eps

SIRboot(X, y, k = 0)
SIRboot(X, y, k = 1)</pre>
```

SIRladle

Ladle Estimate for SIR

## **Description**

In the supervised dimension reduction context with response y and explaining variables x, this functions provides the ladle estimate for the dimension of the central subspace for SIR.

## Usage

```
SIRladle(X, y, h = 10, n.boot = 200, \\ ncomp = ifelse(ncol(X) > 10, floor(ncol(X)/log(ncol(X))), ncol(X) - 1), ...)
```

## **Arguments**

Χ	numeric data matrix.
У	numeric response vector.
h	number of slices in SIR.
n.boot	number of bootstrapping samples to be used.
ncomp	The number of components among which the ladle estimator is to be searched. The default here follows the recommendation of Luo and Li 2016.
	arguments passed on to quantile.

## **Details**

The idea here is that the eigenvalues of the SIR-M matrix are of the form  $\lambda_1 \ge ... \ge \lambda_k > 0 = ... = 0$  and the eigenvectors of the non-zero eigenvalue span the central subspace.

The ladle estimate for k for this purpose combines the values of the scaled eigenvalues and the variation of the eigenvectors based on bootstrapping. The idea there is that for distinct eigenvales the variation of the eigenvectors is small and for equal eigenvalues the corresponding eigenvectors have large variation.

This measure is then computed assuming k=0,..., ncomp and the ladle estimate for k is the value where the measure takes its minimum.

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#### Value

A list of class ladle containing:

method the string SIR.

k the estimated value of k.

fn vector giving the measures of variation of the eigenvectors using the bootstrapped

eigenvectors for the different number of components.

phin normalized eigenvalues of the M matrix in the SIR case.

gn the main criterion for the ladle estimate - the sum of fn and phin. k is the value

where gn takes its minimum

lambda the eigenvalues of the M matrix in the SIR case.

W the transformation matrix to supervised components.S data matrix with the centered supervised components.

MU the location of the data which was substracted before calculating the supervised

components.

data.name the name of the data for which the ladle estimate was computed.

#### Author(s)

Klaus Nordhausen

#### References

Luo, W. and Li, B. (2016), Combining Eigenvalues and Variation of Eigenvectors for Order Determination, Biometrika, 103. 875–887. <doi:10.1093/biomet/asw051>

#### See Also

ladleplot

```
n <- 1000
X <- cbind(rnorm(n), rnorm(n), rnorm(n), rnorm(n), rnorm(n))
eps <- rnorm(n, sd=0.02)
y <- 4*X[,1] + 2*X[,2] + eps

test <- SIRladle(X, y)
test
summary(test)
plot(test)
pairs(cbind(y, components(test)))
ladleplot(test)
ladleplot(test, crit = "fn")
ladleplot(test, crit = "lambda")
ladleplot(test, crit = "phin")</pre>
```

48 summary.ladle

summary.ladle

Summarizing an Object of Class ladle

# Description

Summarizes an ladle object

# Usage

```
## S3 method for class 'ladle'
summary(object, ...)
```

# Arguments

object an object of class ladle.

... further arguments to be passed to or from methods.

# Author(s)

Klaus Nordhausen

## See Also

```
print.ladle, plot.ladle, ladleplot, FOBIladle, PCAladle, SIRladle
```

```
n <- 1000
X <- cbind(rexp(n), rt(n,5), rnorm(n), rnorm(n), rnorm(n), rnorm(n))
test <- FOBIladle(X)
summary(test)</pre>
```

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