Package 'rospca'

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Title Robust Sparse PCA using the ROSPCA Algorithm

Description Implementation of robust sparse PCA using the ROSPCA algorithm of Hubert et al. (2016) [<DOI:10.1080/00401706.2015.1093962>](https://doi.org/10.1080/00401706.2015.1093962).

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Depends $R (= 2.14.0)$

Imports stats, graphics, parallel, mrfDepth (>= 1.0.5), robustbase (>= 0.92-6), pcaPP, rrcov, elasticnet, mvtnorm, pracma

License GPL $(>= 2)$

URL <https://github.com/TReynkens/rospca>

BugReports <https://github.com/TReynkens/rospca/issues>

ByteCompile yes

NeedsCompilation no

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angle *Standardised last principal angle*

Description

Standardised last principal angle between the subspaces generated by the columns of A and B.

Usage

angle(A, B)

Arguments

Details

We compute the last principal angle between the subspaces generated by the columns of A and B using the algorithm in Bjorck and Golub (1973). This angle takes values between 0 and $\pi/2$. We divide it by $\pi/2$ to make it take values between 0 and 1, where 0 indicates that the subspaces are close.

Value

Standardised last principal angle between A and B.

Author(s)

Tom Reynkens

References

Bjorck, A. and Golub, G. H. (1973), "Numerical Methods for Computing Angles Between Linear Subspaces," *Mathematics of Computation*, 27, 579–594.

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Examples

```
tmp <- dataGen(m=1)
P <- eigen(tmp$R)$vectors[,1:2]
PP <- rospca(tmp$data[[1]], k=2)$loadings
angle(P, PP)
```
dataGen *Generate sparse data with outliers*

Description

Generate sparse data with outliers using simulation scheme detailed in Hubert et al. (2016).

Usage

dataGen(m = 100, n = 100, p = 10, a = $c(0.9, 0.5, 0)$, bLength = 4, SD = $c(10.5, 2)$, $eps = 0$, seed = TRUE)

Arguments

Details

Firstly, we generate a correlation matrix such that it has sparse eigenvectors. We design the correlation matrix to have $length(a) = k + 1$ groups of variables with no correlation between variables from different groups. The first k groups consist of blength variables each. The correlation between the different variables of the group is equal to $a[1]$ for group 1, The $(k+1)$ th group contains the remaining $p - k \times bLength$ variables, which we specify to have correlation a[k+1]. Secondly, the correlation matrix R is transformed into the covariance matrix $\Sigma = V^{0.5} \cdot R \cdot V^{0.5}$, where $V = diag(SD²)$.

Thirdly, the n observations are generated from a p-variate normal distribution with mean the p variate zero-vector and covariance matrix Σ. Standard normally distributed noise terms are also added to each of the p variables to make the sparse structure of the data harder to detect.

Finally, $(100 \times eps)$ % of the data points are randomly replaced by outliers. These outliers are generated from a *p*-variate normal distribution as in Croux et al. (2013).

The *i*th eigenvector of R, for $i = 1, ..., k$, is given by a (sparse) vector with the (*bLength* × (*i* − $(1) + 1$)th till the $(bLength \times i)$ th elements equal to $1/\sqrt{bLength}$ and all other elements equal to zero.

See Hubert et al. (2016) for more details.

Value

A list with components:

Author(s)

Tom Reynkens

References

Hubert, M., Reynkens, T., Schmitt, E. and Verdonck, T. (2016). "Sparse PCA for High-Dimensional Data with Outliers," *Technometrics*, 58, 424–434.

Croux, C., Filzmoser, P., and Fritz, H. (2013), "Robust Sparse Principal Component Analysis," *Technometrics*, 55, 202–214.

Examples

 $X \le -$ dataGen(m=1, n=100, p=10, eps=0.2, bLength=4)\$data[[1]] resR <- robpca(X, k=2, skew=FALSE) diagPlot(resR)

diagPlot *Diagnostic plot for PCA*

Description

Make diagnostic plot using the output from robpca or rospca.

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Usage

diagPlot(res, title = "Robust PCA", col = "black", pch = 16, labelOut = TRUE, id = 3)

Arguments

Details

The diagnostic plot contains the score distances on the x-axis and the orthogonal distances on the y-axis. To detect outliers, cut-offs for both distances are added, see Hubert et al. (2005).

Author(s)

Tom Reynkens, based on R code from Valentin Todorov for the diagnostic plot in rrcov (released under GPL-3).

References

Hubert, M., Rousseeuw, P. J., and Vanden Branden, K. (2005), "ROBPCA: A New Approach to Robust Principal Component Analysis," *Technometrics*, 47, 64–79.

Examples

```
X \le - dataGen(m=1, n=100, p=10, eps=0.2, bLength=4)$data[[1]]
resR <- robpca(X, k=2, skew=FALSE)
diagPlot(resR)
```


Description

Glass data of Lemberge et al. (2000) containing Electron Probe X-ray Microanalysis (EPXMA) intensities for different wavelengths of 16–17th century archaeological glass vessels. This dataset was also used in Hubert et al. (2005).

Usage

data(Glass)

Format

A data frame with 180 observations and 750 variables. These variables correspond to EPXMA intensities for different wavelengths and are indicated by V1, V2, ..., V750.

Source

Lemberge, P., De Raedt, I., Janssens, K. H., Wei, F., and Van Espen, P. J. (2000), "Quantitative Z-Analysis of the 16–17th Century Archaelogical Glass Vessels using PLS Regression of EPXMA and µ-XRF Data," *Journal of Chemometrics*, 14, 751–763.

References

Hubert, M., Rousseeuw, P. J., and Vanden Branden, K. (2005), "ROBPCA: A New Approach to Robust Principal Component Analysis," *Technometrics*, 47, 64–79.

Examples

```
data(Glass)
res <- robpca(Glass, k=4, alpha=0.5)
matplot(res$loadings, type="l", lty=1)
```
robpca *ROBust PCA algorithm*

Description

ROBPCA algorithm of Hubert et al. (2005) including reweighting (Engelen et al., 2005) and possible extension to skewed data (Hubert et al., 2009).

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Usage

robpca $(x, k = 0, kmax = 10, alpha = 0.75, h = NULL, mcd = FALSE,$ ndir = "all", skew = $FALSE, ...$)

Arguments

Details

This function is based extensively on PcaHubert from rrcov and there are two main differences:

The outlyingness measure that is used for non-skewed data (skew=FALSE) is the Stahel-Donoho measure as described in Hubert et al. (2005) which is also used in [PcaHubert](#page-0-0). The implementation in mrfDepth (which is used here) is however much faster than the one in [PcaHubert](#page-0-0) and hence more, or even all, directions can be considered when computing the outlyingness measure.

Moreover, the extension for skewed data of Hubert et al. (2009) (skew=TRUE) is also implemented here, but this is not included in [PcaHubert](#page-0-0).

For an extensive description of the ROBPCA algorithm we refer to Hubert et al. (2005) and to [PcaHubert](#page-0-0).

When mcd=TRUE and $n < 5 \times p$, we do not apply the full ROBPCA algorithm. The loadings and eigenvalues are then computed as the eigenvectors and eigenvalues of the MCD estimator applied to the data set after the SVD step.

Value

A list with components:

Author(s)

Tom Reynkens, based on R code from Valentin Todorov for PcaHubert in rrcov (released under GPL-3) and Matlab code from Katrien Van Driessen (for the univariate MCD).

References

Hubert, M., Rousseeuw, P. J., and Vanden Branden, K. (2005), "ROBPCA: A New Approach to Robust Principal Component Analysis," *Technometrics*, 47, 64–79.

Engelen, S., Hubert, M. and Vanden Branden, K. (2005), "A Comparison of Three Procedures for Robust PCA in High Dimensions", *Austrian Journal of Statistics*, 34, 117–126.

Hubert, M., Rousseeuw, P. J., and Verdonck, T. (2009), "Robust PCA for Skewed Data and Its Outlier Map," *Computational Statistics & Data Analysis*, 53, 2264–2274.

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See Also

[PcaHubert](#page-0-0), [outlyingness](#page-0-0), [adjOutl](#page-0-0)

Examples

X <- dataGen(m=1, n=100, p=10, eps=0.2, bLength=4)\$data[[1]]

resR <- robpca(X, k=2) diagPlot(resR)

rospca *RObust Sparse PCA algorithm*

Description

Sparse robust PCA algorithm based on the ROBPCA algorithm of Hubert et al. (2005).

Usage

rospca(X, k, kmax = 10, alpha = 0.75, h = NULL, ndir = "all", grid = TRUE, $lambda = 10^(-6)$, sparse = "varnum", para, stand = TRUE, skew = FALSE)

Arguments

Details

The ROSPCA algorithm consists of an outlier detection part (step 1), and a sparsification part (steps 2 and 3). We give an overview of these steps here and refer to Hubert et al. (2016) for more details.

Step 1: This is a robustness step similar to ROBPCA. When a standardisation is appropriate, the variables are first robustly standardised by means of the componentwise median and the Q_n . Using the singular value decomposition (SVD) of the resulting data matrix, the p -dimensional data space is reduced to the affine subspace spanned by the n observations. Then, the subset of the h observations with smallest outlyingness is selected (H_0) . Thereafter, a reweighting step is applied: given the orthogonal distances to the preliminary PCA subspace determined by the observations in H_0 , all observations with orthogonal distances (ODs) smaller than the corresponding cut-off are kept (H_1) .

Step 2: First, the data points with indices in H_1 are standardised using the componentwise median and the Q_n and sparse PCA is applied to them. Then, an additional reweighting step is performed which incorporates information about the sparse structure of the data. Variables with zero loadings on all k PCs are discarded and then the orthogonal distances to the estimated sparse PCA subspace are computed. This yields an index set H_2 of observations with orthogonal distance smaller than the cut-off corresponding to these new orthogonal distances. Thereafter, the subset of observations with indices in H_2 is standardised using the componentwise median and the Q_n of the observations in H_1 (the same standardisation as in the first time sparse PCA is applied) and sparse PCA is applied to them which gives sparse loadings. Adding the discarded zero loadings again gives the loadings matrix P_2 .

Step 3: In the last step, the eigenvalues are estimated robustly by applying the Q_n^2 estimator on the scores of the observations with indices in H_2 . In order to robustly estimate the centre, the score distances are computed and all observations of $H₂$ with a score distance smaller than the corresponding cut-off are considered, this is the set H_3 . Then, the centre is estimated by the mean of these observations. Finally, the estimates of the eigenvalues are recomputed as the sample variance of the (new) scores of the observations with indices in H_3 . The eigenvalues are sorted in descending order, so the order of the PCs may change. The columns of the loadings and scores matrices are changed accordingly.

Note that when it is not necessary to standardise the data, they are only centred as in the scheme above, but not scaled.

In contrast to Hubert et al. (2016), we allow for SPCA (Zou et al., 2006) to be used as the sparse PCA method inside ROSPCA (grid=FALSE). Moreover, we also include a skew-adjusted version of ROSPCA (skew=TRUE) similar to the skew-adjusted version of ROBPCA (Hubert et al., 2009). This adjusted version is not detailed in Hubert et al. (2016).

Value

A list with components:

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Author(s)

Tom Reynkens, based on R code from Valentin Todorov for PcaHubert in rrcov (released under GPL-3) and Matlab code from Katrien Van Driessen (for the univariate MCD).

References

Hubert, M., Reynkens, T., Schmitt, E. and Verdonck, T. (2016). "Sparse PCA for High-Dimensional Data with Outliers," *Technometrics*, 58, 424–434.

Hubert, M., Rousseeuw, P. J., and Vanden Branden, K. (2005), "ROBPCA: A New Approach to Robust Principal Component Analysis," *Technometrics*, 47, 64–79.

Hubert, M., Rousseeuw, P. J., and Verdonck, T. (2009), "Robust PCA for Skewed Data and Its Outlier Map," *Computational Statistics & Data Analysis*, 53, 2264–2274.

Croux, C., Filzmoser, P., and Fritz, H. (2013), "Robust Sparse Principal Component Analysis," *Technometrics*, 55, 202–214.

Zou, H., Hastie, T., and Tibshirani, R. (2006), "Sparse Principal Component Analysis," *Journal of Computational and Graphical Statistics*, 15, 265–286.

See Also

[PcaHubert](#page-0-0), [robpca](#page-5-1), [outlyingness](#page-0-0), [adjOutl](#page-0-0), [sPCAgrid](#page-0-0), [spca](#page-0-0)

Examples

X <- dataGen(m=1, n=100, p=10, eps=0.2, bLength=4)\$data[[1]]

```
resRS <- rospca(X, k=2, lambda=0.4, stand=TRUE)
diagPlot(resRS)
```
selectLambda *Selection of sparsity parameter using IC*

Description

Selection of the sparsity parameter for ROSPCA and SCoTLASS using BIC of Hubert et al. (2016), and for SRPCA using BIC of Croux et al. (2013).

Usage

selectLambda(X, k, kmax = 10, method = "ROSPCA", lmin = 0, lmax = 2, lstep = 0.02 , $alpha = 0.75$, stand = TRUE, skew = FALSE, multicore = FALSE, $mc.core$ = NULL, $P = NULL$, $ndir = "all")$

Arguments

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Details

We select an optimal value of λ for a certain method on a certain dataset by looking at an equidistant grid of λ values. For each value of λ , we apply the method on the dataset using this sparsity parameter, and compute an Information Criterion (IC). The optimal value of λ is then the one corresponding to the minimal IC. The ICs we consider are the BIC of for Hubert et al. (2016) for ROSPCA and SCoTLASS, and the BIC of Croux et al. (2013) for SRPCA. The BIC of Hubert et al. (2016) is defined as

$$
BIC(\lambda) = \ln(1/(h_1 p) \sum_{i=1}^{h_1} OD_{(i)}^2(\lambda)) + df(\lambda) \ln(h_1 p)/(h_1 p),
$$

where h_1 is the size of H_1 (the subset of observations that are kept in the non-sparse reweighting step) and $OD_{(i)}(\lambda)$ is the *i*th smallest orthogonal distance for the model when using λ as the sparsity parameter. The degrees of freedom $df(\lambda)$ are the number of non-zero loadings when λ is used as the sparsity parameter.

Value

A list with components:

Author(s)

Tom Reynkens

References

Hubert, M., Reynkens, T., Schmitt, E. and Verdonck, T. (2016). "Sparse PCA for High-Dimensional Data with Outliers," *Technometrics*, 58, 424–434.

Croux, C., Filzmoser, P., and Fritz, H. (2013), "Robust Sparse Principal Component Analysis," *Technometrics*, 55, 202–214.

See Also

[selectPlot,](#page-13-1) [mclapply,](#page-0-0) [angle](#page-1-1)

Examples

 $X \le -$ dataGen(m=1, n=100, p=10, eps=0.2, bLength=4)\$data[[1]]

```
sl <- selectLambda(X, k=2, method="ROSPCA", lstep=0.1)
selectPlot(sl)
```
selectPlot *Selection plot*

Description

Plot Information Criterion (IC) versus values of the sparsity parameter λ .

Usage

selectPlot(sl, indicate = TRUE, main = NULL)

Arguments

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Author(s)

Tom Reynkens

References

Hubert, M., Reynkens, T., Schmitt, E. and Verdonck, T. (2016). "Sparse PCA for High-Dimensional Data with Outliers," *Technometrics*, 58, 424–434.

See Also

[selectLambda](#page-11-1)

Examples

```
X \le - dataGen(m=1, n=100, p=10, eps=0.2, bLength=4)$data[[1]]
sl <- selectLambda(X, k=2, method="ROSPCA", lstep=0.1)
selectPlot(sl)
```
zeroMeasure *Zero measure*

Description

Compute the average zero measures and total zero measure for a list of matrices.

Usage

```
zeroMeasure(Plist, P, prec = 10^(-5))
```
Arguments

Details

The *zero measure* is a way to compare how correctly a PCA method estimates the sparse loadings matrix P. For each element of an estimated loadings matrix, it is equal to one if the estimated and true value are both zero or both non-zero, and zero otherwise. We then take the average zero measure over all elements of an estimated loadings matrix and over all estimated loadings matrices which we call the *total zero measure*.

Value

A list with components:

Author(s)

Tom Reynkens

References

Hubert, M., Reynkens, T., Schmitt, E. and Verdonck, T. (2016). "Sparse PCA for High-Dimensional Data with Outliers," *Technometrics*, 58, 424–434.

Examples

```
P \leftarrow \text{cbind}(c(1,1), c(0,1))Plist <- list(matrix(1,2,2), P)
```
zeroMeasure(Plist, P)

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