Package: epca (via r-universe)

September 14, 2024

Type Package Title Exploratory Principal Component Analysis Version 1.1.0 Date 2023-07-10 Description Exploratory principal component analysis for large-scale dataset, including sparse principal component analysis and sparse matrix approximation. URL <https://github.com/fchen365/epca> BugReports <https://github.com/fchen365/epca/issues> License GPL-3 Depends R ($> = 3.5$), Imports clue, irlba, Matrix, GPArotation, Suggests elasticnet, ggcorrplot, tidyverse, rmarkdown, reshape2, markdown, RSpectra, matlabr, knitr, PMA, testthat (>= 3.0.0) Roxygen list(markdown = TRUE) VignetteBuilder knitr, rmarkdown Encoding UTF-8 RoxygenNote 7.2.3 Repository https://fchen365.r-universe.dev RemoteUrl https://github.com/fchen365/epca RemoteRef HEAD RemoteSha d61352c653c533870b4599847f1a6389ff2a7a14

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epca-package *Exploratory Principal Component Analysis*

Description

epca is for comprehending any data matrix that contains *low-rank* and *sparse* underlying signals of interest. The package currently features two key tools: (1) sca for sparse principal component analysis and (2) sma for sparse matrix approximation, a two-way data analysis for simultaneously row and column dimensionality reductions.

References

Chen, F. and Rohe K. (2020) "A New Basis for Sparse PCA".

Given a p x k matrix x, finds the orthogonal matrix (rotation) that minimizes the [absmin.criteria.](#page-2-1)

Usage

```
absmin(x, r0 = diag(ncol(x)), normalize = FALSE,eps = 1e-05, maxit = 1000L)
```
Arguments

Value

A list with three elements:

See Also

GPArotation::GPForth

Description

Calculate the absmin criteria. This is a helper function for [absmin.](#page-2-2)

Usage

absmin.criteria(x)

Arguments

x a matrix or Matrix, initial factor loadings matrix for which the rotation criterian is to be optimized.

cpve *Cumulative Proportion of Variance Explained (CPVE)*

Description

Calculate the CPVE.

Usage

 c pve $(x, v, is.cov = FALSE)$

Arguments

Value

a numeric vector of length $ncol(v)$, the i-th value is the CPVE of the first i columns in v.

See Also

[pve](#page-13-1)

```
## use the "swiss" data
## find two sparse PCs
s.sca <- sca(swiss, 2, gamma = sqrt(ncol(swiss)))
ld <- loadings(s.sca)
cpve(as.matrix(swiss), ld)
```


Compute the distance between two matrices. The distance between two matrices is defined as the sum of distances between column pairs. This function matches the columns of two matrices, such that the matrix distance (i.e., the sum of paired column distances) is minimized. This is accomplished by solving an optimization over column permutation. Given two matrices, x and y, find permutation p() that minimizes sum_i similarity($x[$,p(i)], $y[$,i]), where the similarity() can be "euclidean" distance, 1 - "cosine", or "maximum" difference (manhattan distance). The solution is computed by [clue::solve_LSAP\(\)](#page-0-0).

Usage

 $dist.matrix(x, y, method = "euclidean")$

Arguments

Value

a list of four components:

See Also

[clue::solve_LSAP](#page-0-0)

```
x \leftarrow diag(4)y \le -x + \text{norm}(16, \text{ sd} = 0.05) # add some noise
y = t(t(y) / sqrt(colsums(y \land 2))) ## normalize the columns
## euclidian distance between column pairs, with minimal matches
dist.matrix(x, y, "euclidean")
```


Matrix Distance

Usage

distance(x, y, method = "euclidean")

Arguments

Value

numeric, the distance between two matrices.

exp.frac *Calculate fractional exponent/power*

Description

Calculate fractional exponent/power, a^(num/den), where a could be negative.

Usage

S3 method for class 'frac' exp(a, num, den)

Arguments

Value

numeric, the evaluated a^(num/den)

Perform hard-thresholding given the cut-off value.

Usage

hard(x, t)

Arguments

Matrix Inner Product

Description

Calculate the custom matrix inner product z of two matrices, x and y, where $z[i,j] = \text{FUN}(x[,i],$ y[,j]).

Usage

 $inner(x, y, FUN = "crossprod", ...)$

Arguments

Value

matrix, inner product of x and y.

Examples

```
x \le - matrix(1:6, 2, 3)
y <- matrix(7:12, 2, 3)
## The default is equivalent to `crossprod(x, y)`
inner(x, y)
## We can compute the pair-wise Euclidean distance of columns.
EuclideanDistance = function(x, y) crossprod(x, y)^2
inner(x, y, EuclideanDistance)
```
labelCluster *Label Cluster*

Description

Assign cluster labels to each row from the membership matrix.

Usage

labelCluster(x, ties.method = "random")

Arguments

Value

integer vector of the same length as x. Each entry is one of $1, 2, ..., \text{ncol}(x)$.

misClustRate *Mis-Classification Rate (MCR)*

Description

Compute the empirical MCR, assuming that #cluster = #block, This calculation allows a permutation on clusters.

Usage

```
misClustRate(cluster, truth)
```


norm. Lp $\qquad \qquad \qquad 9$

Arguments

Value

numeric, the MCR.

Examples

```
truth = rep(1:3, each = 30)cluster = rep(3:1, times = c(25, 32, 33))
misClustRate(cluster, truth)
```
norm.Lp *Element-wise Matrix Norm*

Description

Compute element-wise matrix Lp-norm. This is a helper function to [shrinkage\(\)](#page-18-1).

Usage

norm. $Lp(x, p = 1)$

Arguments

Value

numeric(1), the absolute sum of all elements.

Perform column permutation of block membership matrix for aesthetic visualization. That is, the k-th column gives k-th cluster. This is done by ranking the column sums of squares (by default).

Usage

 $permColumn(x, s = 2)$

Arguments

Description

The pitprops data is a correlation matrix that was calculated from 180 observations. There are 13 explanatory variables. Jeffers (1967) tried to interpret the first six PCs. This is a classical example showing the difficulty of interpreting principal components.

References

Jeffers, J. (1967) "Two case studies in the application of principal component", *Applied Statistics*, 16, 225-236.

```
## NOT TEST
data(pitprops)
ggcorrplot::ggcorrplot(pitprops)
```


Perform the polar decomposition of an n x p $(n > p)$ matrix x into two parts: u and h, where u is an $n \times p$ unitary matrix with orthogonal columns (i.e. crossprod(u) is the identity matrix), and h is a p x p positive-semidefinite Hermitian matrix. The function returns the u matrix. This is a helper function of $prs()$.

Usage

polar(x)

Arguments

x a matrix or Matrix, which is presumed full-rank.

Value

a matrix of the unitary part of the polar decomposition.

References

Chen, F. and Rohe, K. (2020) "A New Basis for Sparse Principal Component Analysis."

Examples

 $x \le -$ matrix(1:6, nrow = 3) polar_x <- polar(x)

print.sca *Print SCA*

Description

Print SCA

Usage

```
## S3 method for class 'sca'
print(x, verbose = FALSE, ...)
```
Arguments

Value

Print an sca object interactively.

print.sma *Print SMA*

Description

Print SMA

Usage

S3 method for class 'sma' $print(x,$ verbose = $FALSE, ...)$

Arguments

Value

Print an sma object interactively.

prs *Polar-Rotate-Shrink*

Description

This function is a helper function of [sma\(\)](#page-19-1). It performs polar docomposition, orthogonal rotation, and soft-thresholding shrinkage in order. The three steps together enable sparse estimates of the SMA and SCA.

Usage

prs(x, z.hat, gamma, rotate, shrink, normalize, order, flip, epsilon)

Arguments

Details

rotate: The rotate option specifies the rotation technique to use. Currently, there are two build-in options—"varimax" and "absmin". The "varimax" rotation maximizes the element-wise L4 norm of the rotated matrix. It is faster and computationally more stable. The "absmin" rotation minimizes the absolute sum of the rotated matrix. It is sharper (as it directly minimizes the L1 norm) but slower and computationally less stable.

shrink: The shrink option specifies the shrinkage operator to use. Currently, there are two build-in options—"soft"- and "hard"-thresholding. The "soft"-thresholding universally reduce all elements and sets the small elements to zeros. The "hard"-thresholding only sets the small elements to zeros.

normalize: The argument normalize gives an indication of if and how any normalization should be done before rotation, and then undone after rotation. If normalize is FALSE (the default) no normalization is done. If normalize is TRUE then Kaiser normalization is done. (So squared row entries of normalized x sum to 1.0. This is sometimes called Horst normalization.) For rotate="absmin", if normalize is a vector of length equal to the number of indicators (i.e., the number of rows of x), then the columns are divided by normalize before rotation and multiplied by normalize after rotation. Also, If normalize is a function then it should take x as an argument and return a vector which is used like the vector above.

order: In PCA (and SVD), the principal components (and the singular vectors) are ordered. For this, we order the sparse components (i.e., the columns of z or y) by their explained variance in the data, which is defined as sum($(x % * % y)^2$), where y is a column of the sparse component. Note: not to be confused with the cumulative proportion of variance explained by y (and z), particularly when y (and z) is may not be strictly orthogonal.

flip: The argument flip gives an indication of if and the columns of estimated sparse component should be flipped. Note that the estimated (sparse) loadings, i.e., the weights on original variables, are column-wise invariant to a sign flipping. This is because flipping of a principal direction does not influence the amount of the explained variance by the component. If flip=TRUE, then the columns of loadings will be flip accordingly, such that each column is positive-skewed. This means that for each column, the sum of cubic elements (i.e., $sum(x^3)$) are non-negative.

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Value

a matrix of the sparse estimate, of the same dimension as crossprod(x, z.hat).

References

Chen, F. and Rohe, K. (2020) "A New Basis for Sparse Principal Component Analysis."

See Also

[sma,](#page-19-1) [sca,](#page-15-1) [polar,](#page-10-1) [rotation,](#page-14-1) [shrinkage](#page-18-1)

pve *Proportion of Variance Explained (PVE)*

Description

Calculate the Proportion of variance explained by a set of linear transformation, (e.g. eigenvectors).

Usage

 $pve(x, v, is.cov = FALSE)$

Arguments

Value

a numeric value between 0 and 1, the proportion of total variance in x explained by the PCs whose loadings are in v.

References

Shen, H., & Huang, J. Z. (2008). "Sparse principal component analysis via regularized low rank matrix approximation." *Journal of multivariate analysis*, 99(6), 1015-1034.

```
## use the "swiss" data
## find two sparse PCs
s.sca <- sca(swiss, 2, gamma = sqrt(ncol(swiss)))
ld <- loadings(s.sca)
pve(as.matrix(swiss), ld)
```


Find the root matrix (x) from the Gram matrix (i.e., c rossprod(x)). This is also useful when the input is a covariance matrix, up to a scaling factor of n-1, where n is the sample size.

Usage

rootmatrix(x)

Arguments

x a symmetric matrix (will trigger error if not symmetric).

Description

Perform varimax rotation. Flip the signs of columns so that the resulting matrix is positive-skewed.

Usage

```
rotation(
  x,
  rotate = c("varimax", "absmin"),
 normalize = FALSE,
 flip = TRUE,eps = 1e-06
\mathcal{E}
```
Arguments

Details

rotate: The rotate option specifies the rotation technique to use. Currently, there are two build-in options—"varimax" and "absmin". The "varimax" rotation maximizes the element-wise L4 norm of the rotated matrix. It is faster and computationally more stable. The "absmin" rotation minimizes the absolute sum of the rotated matrix. It is sharper (as it directly minimizes the L1 norm) but slower and computationally less stable.

normalize: The argument normalize gives an indication of if and how any normalization should be done before rotation, and then undone after rotation. If normalize is FALSE (the default) no normalization is done. If normalize is TRUE then Kaiser normalization is done. (So squared row entries of normalized x sum to 1.0. This is sometimes called Horst normalization.) For rotate="absmin", if normalize is a vector of length equal to the number of indicators (i.e., the number of rows of x), then the columns are divided by normalize before rotation and multiplied by normalize after rotation. Also, If normalize is a function then it should take x as an argument and return a vector which is used like the vector above.

flip: The argument flip gives an indication of if and the columns of estimated sparse component should be flipped. Note that the estimated (sparse) loadings, i.e., the weights on original variables, are column-wise invariant to a sign flipping. This is because flipping of a principal direction does not influence the amount of the explained variance by the component. If flip=TRUE, then the columns of loadings will be flip accordingly, such that each column is positive-skewed. This means that for each column, the sum of cubic elements (i.e., $\text{sum}(x^3)$) are non-negative.

Value

the rotated matrix of the same dimension as x.

References

Chen, F. and Rohe, K. (2020) "A New Basis for Sparse Principal Component Analysis."

See Also

[prs,](#page-11-1) [varimax](#page-22-1)

Examples

```
## use the "swiss" data
fa \le factanal( \sim., 2, data = swiss, rotation = "none")
rotation(loadings(fa))
```
sca *Sparse Component Analysis*

Description

sca performs sparse principal components analysis on the given numeric data matrix. Choices of rotation techniques and shrinkage operators are available.

Usage

```
sca(
 x,
 k = min(5, dim(x)),gamma = NULL,is.cov = FALSE,
 rotate = c("varimax", "absmin"),
  shrink = c("soft", "hard"),
 center = TRUE,
  scale = FALSE,
 normalize = FALSE,
 order = TRUE,
 flip = TRUE,max.iter = 1000,
 epsilon = 1e-05,
 quiet = TRUE\mathcal{L}
```
Arguments

 sca 17

Details

rotate: The rotate option specifies the rotation technique to use. Currently, there are two build-in options—"varimax" and "absmin". The "varimax" rotation maximizes the element-wise L4 norm of the rotated matrix. It is faster and computationally more stable. The "absmin" rotation minimizes the absolute sum of the rotated matrix. It is sharper (as it directly minimizes the L1 norm) but slower and computationally less stable.

shrink: The shrink option specifies the shrinkage operator to use. Currently, there are two build-in options—"soft"- and "hard"-thresholding. The "soft"-thresholding universally reduce all elements and sets the small elements to zeros. The "hard"-thresholding only sets the small elements to zeros.

normalize: The argument normalize gives an indication of if and how any normalization should be done before rotation, and then undone after rotation. If normalize is FALSE (the default) no normalization is done. If normalize is TRUE then Kaiser normalization is done. (So squared row entries of normalized x sum to 1.0. This is sometimes called Horst normalization.) For rotate="absmin", if normalize is a vector of length equal to the number of indicators (i.e., the number of rows of x), then the columns are divided by normalize before rotation and multiplied by normalize after rotation. Also, If normalize is a function then it should take x as an argument and return a vector which is used like the vector above.

order: In PCA (and SVD), the principal components (and the singular vectors) are ordered. For this, we order the sparse components (i.e., the columns of z or y) by their explained variance in the data, which is defined as sum($(x$ $x \times x$ y) 2), where y is a column of the sparse component. Note: not to be confused with the cumulative proportion of variance explained by y (and z), particularly when y (and z) is may not be strictly orthogonal.

flip: The argument flip gives an indication of if and the columns of estimated sparse component should be flipped. Note that the estimated (sparse) loadings, i.e., the weights on original variables, are column-wise invariant to a sign flipping. This is because flipping of a principal direction does not influence the amount of the explained variance by the component. If flip=TRUE, then the columns of loadings will be flip accordingly, such that each column is positive-skewed. This means that for each column, the sum of cubic elements (i.e., $sum(x^3)$) are non-negative.

Value

an sca object that contains:

References

Chen, F. and Rohe, K. (2020) "A New Basis for Sparse Principal Component Analysis."

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See Also

[sma,](#page-19-1) [prs](#page-11-1)

Examples

```
## ------ example 1 ------
## simulate a low-rank data matrix with some additive Gaussian noise
n < -300p <- 50
k <-5 ## rank
z <- shrinkage(polar(matrix(runif(n * k), n, k)), sqrt(n))
b \leftarrow diag(5) * 3y <- shrinkage(polar(matrix(runif(p * k), p, k)), sqrt(p))
e \le - matrix(rnorm(n * p, sd = .01), n, p)
x \leftarrow scale(z %* % b %* % t(y) + e)## perform sparse PCA
s.sca \leq sca(x, k)s.sca
## ------ example 2 ------
## use the `pitprops` data from the `elasticnet` package
data(pitprops)
## find 6 sparse PCs
s.sca <- sca(pitprops, 6, gamma = 6, is.cov = TRUE)
print(s.sca, verbose = TRUE)
```
shrinkage *Shrinkage*

Description

Shrink a matrix using soft-thresholding or hard-thresholding.

Usage

```
shrinkage(x, gamma, shrink = c("soft", "hard"), epsilon = 1e-11)
```
Arguments

Details

A binary search to find the cut-off value.

shrink: The shrink option specifies the shrinkage operator to use. Currently, there are two build-in options—"soft"- and "hard"-thresholding. The "soft"-thresholding universally reduce all elements and sets the small elements to zeros. The "hard"-thresholding only sets the small elements to zeros.

Value

a list with two components:

References

Chen, F. and Rohe, K. (2020) "A New Basis for Sparse Principal Component Analysis."

See Also

[prs](#page-11-1)

Examples

 $x \le$ matrix(1:6, nrow = 3) shrink_x <- shrinkage(x, 1)

sma *Sparse Matrix Approximation*

Description

Perform the sparse matrix approximation (SMA) of a data matrix x as three multiplicative components: z , b , and $t(y)$, where z and y are sparse, and b is low-rank but not necessarily diagonal.

Usage

```
sma(
  x,
 k = min(5, dim(x)),gamma = NULL,
  rotate = c("varimax", "absmin"),
  shrink = c("soft", "hard"),
  center = FALSE,
  scale = FALSE,
  normalize = FALSE,
```
 sma 21

```
order = FALSE,
flip = FALSE,
max.iter = 1000.
epsilon = 1e-05,
quiet = TRUE
```
Arguments

)

Details

rotate: The rotate option specifies the rotation technique to use. Currently, there are two build-in options—"varimax" and "absmin". The "varimax" rotation maximizes the element-wise L4 norm of the rotated matrix. It is faster and computationally more stable. The "absmin" rotation minimizes the absolute sum of the rotated matrix. It is sharper (as it directly minimizes the L1 norm) but slower and computationally less stable.

shrink: The shrink option specifies the shrinkage operator to use. Currently, there are two build-in options—"soft"- and "hard"-thresholding. The "soft"-thresholding universally reduce all elements and sets the small elements to zeros. The "hard"-thresholding only sets the small elements to zeros.

normalize: The argument normalize gives an indication of if and how any normalization should be done before rotation, and then undone after rotation. If normalize is FALSE (the default) no normalization is done. If normalize is TRUE then Kaiser normalization is done. (So squared row entries of normalized x sum to 1.0. This is sometimes called Horst normalization.) For rotate="absmin", if normalize is a vector of length equal to the number of indicators (i.e., the number of rows of

x), then the columns are divided by normalize before rotation and multiplied by normalize after rotation. Also, If normalize is a function then it should take x as an argument and return a vector which is used like the vector above.

order: In PCA (and SVD), the principal components (and the singular vectors) are ordered. For this, we order the sparse components (i.e., the columns of z or y) by their explained variance in the data, which is defined as sum($(x$ %*% y)^2), where y is a column of the sparse component. Note: not to be confused with the cumulative proportion of variance explained by y (and z), particularly when y (and z) is may not be strictly orthogonal.

flip: The argument flip gives an indication of if and the columns of estimated sparse component should be flipped. Note that the estimated (sparse) loadings, i.e., the weights on original variables, are column-wise invariant to a sign flipping. This is because flipping of a principal direction does not influence the amount of the explained variance by the component. If flip=TRUE, then the columns of loadings will be flip accordingly, such that each column is positive-skewed. This means that for each column, the sum of cubic elements (i.e., $sum(x^3)$) are non-negative.

Value

an sma object that contains:

n.iter integer, the number of iteration taken.

References

Chen, F. and Rohe, K. (2020) "A New Basis for Sparse Principal Component Analysis."

See Also

[sca,](#page-15-1) [prs](#page-11-1)

```
## simulate a rank-5 data matrix with some additive Gaussian noise
n < -300p \le -50k < -5 ## rank
z <- shrinkage(polar(matrix(runif(n * k), n, k)), sqrt(n))
b \leftarrow diag(5) * 3y <- shrinkage(polar(matrix(runif(p * k), p, k)), sqrt(p))
e \le - matrix(rnorm(n \times p, sd = .01), n, p)
x \le - scale(z %*% b %*% t(y) + e)
```

```
## perform sparse matrix approximation
s.sma \leq sma(x, k)s.sma
```
soft *Soft-thresholding*

Description

Perform soft-thresholding given the cut-off value.

Usage

soft(x, t)

Arguments

Description

This is a re-implementation of [stats::varimax,](#page-0-0) which (1) adds a parameter for the maximum number of iterations, (2) sets the default normalize parameter to FALSE, (3) outputs the number of iteration taken, and (4) returns regular matrix rather than in loadings class.

Usage

```
varimax(x, normalize = FALSE,eps = 1e-05, maxit = 1000L)
```
Arguments

Value

A list with three elements:

See Also

[stats::varimax](#page-0-0)

varimax.criteria *The varimax criterion*

Description

Calculate the varimax criterion

Usage

varimax.criteria(x)

Arguments

x a matrix or Matrix.

Value

a numeric of evaluated varimax criterion.

References

[Varimax rotation \(Wikipedia\)](https://en.wikipedia.org/wiki/Varimax_rotation)

```
## use the "swiss" data
fa \le factanal( \sim., 2, data = swiss, rotation = "none")
lds <- loadings(fa)
## compute varimax criterion:
varimax.criteria(lds)
## compute varimax criterion (after the varimax rotation):
rlds <- rotation(lds, rotate = "varimax")
varimax.criteria(rlds)
```


This is a helper function for [absmin](#page-2-2) and is not to be used directly by users.

Usage

```
vgQ.absmin(x)
```
Arguments

x a matrix or Matrix, initial factor loadings matrix for which the rotation criterian is to be optimized.

Value

a list required by GPArotation::GPForth for the absmin rotation.

Examples

Not run: ## NOT RUN ## NOT for users to call.

End(Not run)

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