Package: pcaMethods (via r-universe)

November 1, 2026

Maintainer Henning Redestig <henning.red@gmail.com>

License GPL (>= 3)

Title A collection of PCA methods

LinkingTo Rcpp

LazyLoad Yes

Author Wolfram Stacklies, Henning Redestig, Kevin Wright

SystemRequirements Rcpp

Description Provides Bayesian PCA, Probabilistic PCA, Nipals PCA, Inverse Non-Linear PCA and the conventional SVD PCA. A cluster based method for missing value estimation is included for comparison. BPCA, PPCA and NipalsPCA may be used to perform PCA on incomplete data as well as for accurate missing value estimation. A set of methods for printing and plotting the results is also provided. All PCA methods make use of the same data structure (pcaRes) to provide a common interface to the PCA results. Initiated at the Max-Planck Institute for Molecular Plant Physiology, Golm, Germany.

Version 2.4.0

URL https://github.com/hredestig/pcamethods

BugReports https://github.com/hredestig/pcamethods/issues

Encoding UTF-8

Depends Biobase, methods

Imports BiocGenerics, Rcpp (>= 0.11.3), MASS

Suggests matrixStats, lattice, ggplot2

Collate 'derrorHierarchic.R' 'errorHierarchic.R' 'AllClasses.R' 'AllGenerics.R' 'BPCA_dostep.R' 'BPCA_initmodel.R' 'bpca.R' 'checkData.R' 'forkNlpcaNet.R' 'kEstimate.R' 'kEstimateFast.R' 'lineSearch.R' 'llsImpute.R' 'methods-ExpressionSet.R' 'methods-nniRes.R' 'methods-pcaRes.R' 'nipalsPca.R' 'nlpca.R' 'optiAlgCgd.R' 'orth.R' 'pca.R' 'pcaMethods-package.R' 'ppca.R' 'prep.R' 'repmat.R' 'robustPca.R' 'sortFeatures.R' 'svdImpute.R' 'vector2matrices.R' 'xval.R'

biocViews Bayesian

RoxygenNote 6.1.1

Repository Bioconductor 3.23

Date/Publication 2026-04-28 12:31:56 UTC

RemoteUrl https://github.com/bioc/pcaMethods

RemoteRef RELEASE_3_23

RemoteSha 4b5f83b37ce995d7f48c07f12f4e72b829c0d884

Contents

asExprSet . . . 4
biplot-methods . . . 4
bpca . . . 5
BPCA_dostep . . . 8
BPCA_initmodel . . . 8
center,pcaRes-method . . . 9
centered,pcaRes-method . . . 10
checkData . . . 10
completeObs,nniRes-method . . . 11
cvseg . . . 12
cvstat,pcaRes-method . . . 13
deletediagonals . . . 13
derrorHierarchic . . . 14
dim.pcaRes . . . 14
DModX,pcaRes-method . . . 15
errorHierarchic . . . 16
fitted-methods . . . 17
forkNlpcaNet . . . 18
getHierarchicIdx . . . 18
helix . . . 19
kEstimate . . . 19
kEstimateFast . . . 22
leverage,pcaRes-method . . . 23
lineSearch . . . 24
linr . . . 25
listPcaMethods . . . 25
llsImpute . . . 26
loadings,ANY-method . . . 28
loadings,pcaRes-method . . . 28
loadings.pcaRes . . . 29
metaboliteData . . . 29
metaboliteDataComplete . . . 30
method,pcaRes-method . . . 31
nipalsPca . . . 31
nlpca . . . 32
nmissing,pcaRes-method . . . 34

nni . . . 35
nniRes . . . 36
nObs,pcaRes-method . . . 37
nP,pcaRes-method . . . 37
nPcs,pcaRes-method . . . 38
nVar,pcaRes-method . . . 38
optiAlgCgd . . . 39
orth . . . 40
pca . . . 40
pcaMethods . . . 42
pcaMethods-deprecated . . . 43
pcaNet . . . 43
pcaRes . . . 45
plot.pcaRes . . . 46
plotPcs . . . 47
ppca . . . 48
predict-methods . . . 50
prep . . . 51
Q2 . . . 52
R2cum,pcaRes-method . . . 54
R2VX,pcaRes-method . . . 55
rediduals-methods . . . 55
repmat . . . 56
RnipalsPca . . . 57
robustPca . . . 58
robustSvd . . . 60
scaled,pcaRes-method . . . 61
scl,pcaRes-method . . . 62
scores,pcaRes-method . . . 62
scores.pcaRes . . . 63
sDev,pcaRes-method . . . 64
show-methods . . . 64
showNniRes . . . 65
simpleEllipse . . . 65
slplot,pcaRes-method . . . 66
sortFeatures . . . 67
summary . . . 68
svdImpute . . . 69
svdPca . . . 70
tempFixNas . . . 71
vector2matrices,matrix-method . . . 72
vector2matrices,nlpcaNet-method . . . 72
wasna,pcaRes-method . . . 73
weightsAccount . . . 74

Index **75**

asExprSet *Convert pcaRes object to an expression set*

Description

This function can be used to conveniently replace the expression matrix in an ExpressionSet with the completed data from a pcaRes object.

Usage

```
asExprSet(object, exprSet)
```

Arguments

object	pcaRes – The object containing the completed data.
exprSet	ExpressionSet – The object passed on to pca for missing value estimation.

Details

This is not a standard as function as pcaRes object alone not can be converted to an ExpressionSet (the pcaRes object does not hold any phenoData for example).

Value

An object without missing values of class ExpressionSet.

Author(s)

Wolfram Stacklies
CAS-MPG Partner Institute for Computational Biology, Shanghai, China

biplot-methods *Plot a overlaid scores and loadings plot*

Description

Visualize two-components simultaneously

Usage

```
## S3 method for class 'pcaRes'
biplot(x, choices = 1:2, scale = 1,
  pc.biplot = FALSE, ...)

## S4 method for signature 'pcaRes'
biplot(x, choices = 1:2, scale = 1,
  pc.biplot = FALSE, ...)
```

Arguments

x	a pcaRes object
choices	which two pcs to plot
scale	The variables are scaled by λ^{scale} and the observations are scaled by λ^{scale} where lambda are the singular values as computed by princomp. Normally $0 \leq scale \leq 1$, and a warning will be issued if the specified 'scale' is outside this range.
pc.biplot	If true, use what Gabriel (1971) refers to as a "principal component biplot", with $\lambda = 1$ and observations scaled up by sqrt(n) and variables scaled down by sqrt(n). Then the inner products between variables approximate covariances and distances between observations approximate Mahalanobis distance.
...	optional arguments to be passed to biplot.default.

Details

This is a method for the generic function 'biplot'. There is considerable confusion over the precise definitions: those of the original paper, Gabriel (1971), are followed here. Gabriel and Odoroff (1990) use the same definitions, but their plots actually correspond to pc.biplot = TRUE.

Value

a plot is produced on the current graphics device.

Author(s)

Kevin Wright, Adapted from biplot.prcomp

See Also

prcomp, pca, princomp

Examples

```
data(iris)
pcIr <- pca(iris[,1:4])
biplot(pcIr)
```

---

bpca *Bayesian PCA missing value estimation*

Description

Implements a Bayesian PCA missing value estimator. The script is a port of the Matlab version provided by Shigeyuki OBA. See also http://ishiilab.jp/member/oba/tools/BPCAFill.html. BPCA combines an EM approach for PCA with a Bayesian model. In standard PCA data far from the training set but close to the principal subspace may have the same reconstruction error. BPCA defines a likelihood function such that the likelihood for data far from the training set is much lower, even if they are close to the principal subspace.

Usage

```
bpca(Matrix, nPcs = 2, maxSteps = 100, verbose = interactive(),
  threshold = 1e-04, ...)
```

Arguments

Matrix	matrix – Pre-processed matrix (centered, scaled) with variables in columns and observations in rows. The data may contain missing values, denoted as NA.
nPcs	numeric – Number of components used for re-estimation. Choosing few components may decrease the estimation precision.
maxSteps	numeric – Maximum number of estimation steps.
verbose	boolean – BPCA prints the number of steps and the increase in precision if set to TRUE. Default is interactive().
threshold	convergence threshold
...	Reserved for future use. Currently no further parameters are used

Details

Scores and loadings obtained with Bayesian PCA slightly differ from those obtained with conventional PCA. This is because BPCA was developed especially for missing value estimation. The algorithm does not force orthogonality between factor loadings, as a result factor loadings are not necessarily orthogonal. However, the BPCA authors found that including an orthogonality criterion made the predictions worse.

The authors also state that the difference between real and predicted Eigenvalues becomes larger when the number of observation is smaller, because it reflects the lack of information to accurately determine true factor loadings from the limited and noisy data. As a result, weights of factors to predict missing values are not the same as with conventional PCA, but the missing value estimation is improved.

BPCA works iteratively, the complexity is growing with $O(n^3)$ because several matrix inversions are required. The size of the matrices to invert depends on the number of components used for re-estimation.

Finding the optimal number of components for estimation is not a trivial task; the best choice depends on the internal structure of the data. A method called kEstimate is provided to estimate the optimal number of components via cross validation. In general few components are sufficient for reasonable estimation accuracy. See also the package documentation for further discussion about on what data PCA-based missing value estimation makes sense.

It is not recommended to use this function directely but rather to use the pca() wrapper function.

There is a difference with respect the interpretation of rows (observations) and columns (variables) compared to matlab implementation. For estimation of missing values for microarray data, the suggestion in the original bpca is to intepret genes as observations and the samples as variables. In pcaMethods however, genes are interpreted as variables and samples as observations which arguably also is the more natural interpretation. For bpca behavior like in the matlab implementation, simply transpose your input matrix.

Details about the probabilistic model underlying BPCA are found in Oba et. al 2003. The algorithm uses an expectation maximation approach together with a Bayesian model to approximate the

principal axes (eigenvectors of the covariance matrix in PCA). The estimation is done iteratively, the algorithm terminates if either the maximum number of iterations was reached or if the estimated increase in precision falls below $1e^{-4}$.

Complexity: The relatively high complexity of the method is a result of several matrix inversions required in each step. Considering the case that the maximum number of iteration steps is needed, the approximate complexity is given by the term

$$maxSteps \cdot row_{miss} \cdot O(n^3)$$

Where row_{miss} is the number of rows containing missing values and $O(n^3)$ is the complexity for inverting a matrix of size $components$. Components is the number of components used for re-estimation.

Value

Standard PCA result object used by all PCA-based methods of this package. Contains scores, loadings, data mean and more. See pcaRes for details.

Note

Requires MASS.

Author(s)

Wolfram Stacklies

References

Shigeyuki Oba, Masa-aki Sato, Ichiro Takemasa, Morito Monden, Ken-ichi Matsubara and Shin Ishii. A Bayesian missing value estimation method for gene expression profile data. *Bioinformatics, 19(16):2088-2096, Nov 2003*.

See Also

ppca, svdImpute, prcomp, nipalsPca, pca, pcaRes. kEstimate.

Examples

```
## Load a sample metabolite dataset with 5\% missig values (metaboliteData)e
data(metaboliteData)
## Perform Bayesian PCA with 2 components
pc <- pca(t(metaboliteData), method="bpca", nPcs=2)
## Get the estimated principal axes (loadings)
loadings <- loadings(pc)
## Get the estimated scores
scores <- scores(pc)
## Get the estimated complete observations
cObs <- completeObs(pc)
## Now make a scores and loadings plot
slplot(pc)
```

BPCA_dostep *Do BPCA estimation step*

Description

The function contains the actual implementation of the BPCA component estimation. It performs one step of the BPCA EM algorithm. It is called 'maxStep' times from within the main loop in BPCAestimate.

Usage

```
BPCA_dostep(M, y)
```

Arguments

M	Data structure containing all needed information. See the source documentation of BPCA_initmodel for details
y	Numeric original data matrix

Details

This function is NOT intended to be run standalone.

Value

Updated version of the data structure

Author(s)

Wolfram Stacklies

BPCA_initmodel *Initialize BPCA model*

Description

Model initialization for Bayesian PCA. This function is NOT inteded to be run separately!

Usage

```
BPCA_initmodel(y, components)
```

Arguments

y	numeric matrix containing missing values. Missing values are denoted as 'NA'
components	Number of components used for estimation

Details

The function calculates the initial Eigenvectors by use of SVD from the complete rows. The data structure M is created and initial values are assigned.

Value

List containing

`rows`	Row number of input matrix
`cols`	Column number of input matrix
`comps`	Number of components to use
`yest`	(working variable) current estimate of complete data
`row_miss`	(Array) Indizes of rows containing missing values
`row_nomiss`	(Array) Indices of complete rows (such with no missing values)
`nans`	Matrix of same size as input data. TRUE if `input` == `NA`, false otherwise
`mean`	Column wise data mean
`PA`	(d x k) Estimated principal axes (eigenvectors, loadings) The matrix ROWS are the vectors
`tau`	Estimated precision of the residual error
`scores`	Estimated scores

Further elements are: galpha0, balpha0, alpha, gmu0, btau0, gtau0, SigW. These are working variables or constants.

Author(s)

Wolfram Stacklies

`center,pcaRes-method` *Get the centers of the original variables*

Description

Get the centers of the original variables

Usage

```
center(object, ...)
```

Arguments

`object`	pcaRes object
`...`	Not used

Value

Vector with the centers

Author(s)

Henning Redestig

`centered,pcaRes-method` *Check centering was part of the model*

Description

Check centering was part of the model

Usage

```
centered(object, ...)
```

Arguments

`object`	pcaRes object
`...`	Not used

Value

TRUE if model was centered

Author(s)

Henning Redestig

`checkData` *Do some basic checks on a given data matrix*

Description

Check a given data matrix for consistency with the format required for further analysis. The data must be a numeric matrix and not contain:

- Inf values
- NaN values
- Rows or columns that consist of NA only

Usage

```
checkData(data, verbose = FALSE)
```

Arguments

data	matrix – Data to check.
verbose	boolean – If TRUE, the function prints messages whenever an error in the data set is found.

Value

isValid — boolean – TRUE if no errors were found, FALSE otherwise. isValid contains a set of attributes, these are:

- isNumeric - TRUE if data is numeric, false otherwise
- isInfinite - TRUE if data contains 'Inf' values, false otherwise
- isNaN - TRUE if data contains 'NaN' values, false otherwise
- isMatrix - TRUE if the data is in matrix format, FALSE otherwise
- naRows - TRUE if data contains rows in which all elements are 'NA', FALSE otherwise
- naCols - TRUE if data contains columns in which all elements are 'NA', FALSE otherwise

Author(s)

Wolfram Stacklies

---

completeObs,nniRes-method

Get the original data with missing values replaced with predicted values.

Description

Get the original data with missing values replaced with predicted values.

Usage

```
completeObs(object, ...)
```

Arguments

object	object to fetch complete data from
...	Not used

Value

Completed data (matrix)

Author(s)

Henning Redestig

`cvseg` *Get CV segments*

Description

Get cross-validation segments that have (as far as possible) the same ratio of all classes (if classes are present)

Usage

```
cvseg(x, fold = 7, seed = NULL)
```

Arguments

`x`	a factor, character or numeric vector that describes class membership of a set of items, or, a numeric vector indicating unique indices of items, or, a numeric of length 1 that describes the number of items to segment (without any classes)
`fold`	the desired number of segments
`seed`	randomization seed for reproducibility

Value

a list where each element is a set of indices that defines the CV segment.

Author(s)

Henning Redestig

See Also

the `cvsegments` function in the `pls` package

Examples

```
seg <- cvseg(iris$Species, 10)
sapply(seg, function(s) table(iris$Species[s]))
cvseg(20, 10)
```

cvstat,pcaRes-method *Get cross-validation statistics (e.g. Q^2).*

Description

Get cross-validation statistics (e.g. Q^2).

Usage

```
cvstat(object, ...)
```

Arguments

object	pcaRes object
...	not used

Value

vector CV statistics

Author(s)

Henning Redestig

deletediagonals *Delete diagonals*

Description

Replace a diagonal of elements of a matrix with NA

Usage

```
deletediagonals(x, diagonals = 1)
```

Arguments

x	The matrix
diagonals	The diagonal to be replaced, i.e. the first, second and so on when looking at the fat version of the matrix (transposed or not) counting from the bottom. Can be a vector to delete more than one diagonal.

Details

Used for creating artifical missing values in matrices without causing any full row or column to be completely missing

Value

The original matrix with some values missing

Author(s)

Henning Redestig

`derrorHierarchic` *Later*

Description

Later

Usage

```
derrorHierarchic(nlnet, trainIn, trainOut)
```

Arguments

`nlnet`	the nlnet
`trainIn`	training data
`trainOut`	fitted data

Value

derror

Author(s)

Henning Redestig, Matthias Scholz

`dim.pcaRes` *Dimensions of a PCA model*

Description

Dimensions of a PCA model

Usage

```
## S3 method for class 'pcaRes'
dim(x)
```

Arguments

x	a pcaRes object

Value

Get the dimensions of this PCA model

Author(s)

Henning Redestig

DModX,pcaRes-method *DModX*

Description

Distance to the model of X-space.

Usage

```
DModX(object, dat, newdata=FALSE, type=c("normalized","absolute"), ...)
```

Arguments

object	a pcaRes object
dat	the original data, taken from completeObs if left missing.
newdata	logical indicating if this data was part of the training data or not. If it was, it is adjusted by a near one factor $v = (N/(N - A - A0))^-1$
type	if absolute or normalized values should be given. Normalized values are adjusted to the the total RSD of the model.
...	Not used

Details

Measures how well described the observations are, i.e. how well they fit in the mode. High DModX indicate a poor fit. Defined as:

$$\frac{\sqrt{\frac{SSE_i}{K-A}}}{\sqrt{\frac{SSE}{(N-A-A_0)(K-A)}}}$$

For observation i, in a model with A components, K variables and N obserations. SSE is the squared sum of the residuals. A_0 is 1 if model was centered and 0 otherwise. DModX is claimed to be approximately F-distributed and can therefore be used to check if an observation is significantly far away from the PCA model assuming normally distributed data.

Pass original data as an argument if the model was calculated with completeObs=FALSE.

Value

A vector with distances from observations to the PCA model

Author(s)

Henning Redestig

References

Introduction to Multi- and Megavariate Data Analysis using Projection Methods (PCA and PLS), L. Eriksson, E. Johansson, N. Kettaneh-Wold and S. Wold, Umetrics 1999, p. 468

Examples

```
data(iris)
pcIr <- pca(iris[,1:4])
with(iris, plot(DModX(pcIr)~Species))
```

---

errorHierarchic *Later*

Description

Later

Usage

```
errorHierarchic(nlnet, trainIn, trainOut)
```

Arguments

nlnet	The nlnet
trainIn	training data
trainOut	fitted data

Value

error

Author(s)

Henning Redestig, Matthias Scholz

`fitted-methods` *Extract fitted values from PCA.*

Description

Fitted values of a PCA model

Usage

```
## S3 method for class 'pcaRes'
fitted(object, data = NULL, nPcs = nP(object),
  pre = TRUE, post = TRUE, ...)

## S4 method for signature 'pcaRes'
fitted(object, data = NULL, nPcs = nP(object),
  pre = TRUE, post = TRUE, ...)
```

Arguments

`object`	the `pcaRes` object of interest.
`data`	For standard PCA methods this can safely be left null to get scores x loadings but if set, then the scores are obtained by projecting provided data onto the loadings. If data contains missing values the result will be all NA. Non-linear PCA is an exception, here if data is NULL then data is set to the completeObs and propaged through the network.
`nPcs`	The number of PC's to consider
`pre`	pre-process `data` based on the pre-processing chosen for the PCA model
`post`	unpre-process the final data (add the center back etc to get the final estimate)
`...`	Not used

Details

This function extracts the fitted values from a pcaResobject. For PCA methods like SVD, Nipals, PPCA etc this is basically just the scores multipled by the loadings and adjusted for pre-processing. for non-linear PCA the original data is propagated through the network to obtain the approximated data.

Value

A matrix representing the fitted data

Author(s)

Henning Redestig

Examples

```
pc <- pca(iris[,1:4], nPcs=4, center=TRUE, scale="uv")
sum( (fitted(pc) - iris[,1:4])^2 )
```

`forkNlpcaNet` *Complete copy of nlpca net object*

Description

Complete copy of nlpca net object

Usage

```
forkNlpcaNet(nlnet)
```

Arguments

`nlnet`	a nlnet

Value

A copy of the input nlnet

Author(s)

Henning Redestig

`getHierarchicIdx` *Index in hiearchy*

Description

Index in hiearchy

Usage

```
getHierarchicIdx(hierarchicNum)
```

Arguments

`hierarchicNum`	A number

Value

...

Author(s)

Henning Redestig, Matthias Scholz

helix *A helix structured toy data set*

Description

Simulated data set looking like a helix

Usage

```
data(helix)
```

Details

A matrix containing 1000 observations (rows) and three variables (columns).

Author(s)

Henning Redestig

References

Matthias Scholz, Fatma Kaplan, Charles L. Guy, Joachim Kopka and Joachim Selbig. - Non-linear PCA: a missing data approach. *Bioinformatics 2005 21(20):3887-3895*

kEstimate *Estimate best number of Components for missing value estimation*

Description

Perform cross validation to estimate the optimal number of components for missing value estimation. Cross validation is done for the complete subset of a variable.

Usage

```
kEstimate(Matrix, method = "ppca", evalPcs = 1:3, segs = 3,
  nruncv = 5, em = "q2", allVariables = FALSE,
  verbose = interactive(), ...)
```

Arguments

Matrix	matrix – numeric matrix containing observations in rows and variables in columns
method	character – of the methods found with pcaMethods() The option llsImputeAll calls llsImpute with the allVariables = TRUE parameter.
evalPcs	numeric – The principal components to use for cross validation or the number of neighbour variables if used with llsImpute. Should be an array containing integer values, eg. evalPcs = 1:10 or evalPcs = c(2,5,8). The NRMSEP or Q2 is calculated for each component.
segs	numeric – number of segments for cross validation
nruncv	numeric – Times the whole cross validation is repeated
em	character – The error measure. This can be nrmsep or q2
allVariables	boolean – If TRUE, the NRMSEP is calculated for all variables, If FALSE, only the incomplete ones are included. You maybe want to do this to compare several methods on a complete data set.
verbose	boolean – If TRUE, some output like the variable indexes are printed to the console each iteration.
...	Further arguments to pca or nni

Details

The assumption hereby is that variables that are highly correlated in a distinct region (here the non-missing observations) are also correlated in another (here the missing observations). This also implies that the complete subset must be large enough to be representative. For each incomplete variable, the available values are divided into a user defined number of cv-segments. The segments have equal size, but are chosen from a random equal distribution. The non-missing values of the variable are covered completely. PPCA, BPCA, SVDimpute, Nipals PCA, llsImpute an NLPCA may be used for imputation.

The whole cross validation is repeated several times so, depending on the parameters, the calculations can take very long time. As error measure the NRMSEP (see Feten et. al, 2005) or the Q2 distance is used. The NRMSEP basically normalises the RMSD between original data and estimate by the variable-wise variance. The reason for this is that a higher variance will generally lead to a higher estimation error. If the number of samples is small, the variable - wise variance may become an unstable criterion and the Q2 distance should be used instead. Also if variance normalisation was applied previously.

The method proceeds variable - wise, the NRMSEP / Q2 distance is calculated for each incomplete variable and averaged afterwards. This allows to easily see for wich set of variables missing value imputation makes senes and for wich set no imputation or something like mean-imputation should be used. Use kEstimateFast or Q2 if you are not interested in variable wise CV performance estimates.

Run time may be very high on large data sets. Especially when used with complex methods like BPCA or Nipals PCA. For PPCA, BPCA, Nipals PCA and NLPCA the estimation method is called $(v_{miss} \cdot segs \cdot nruncv \cdot)$ times as the error for all numbers of principal components can be calculated at once. For LLSimpute and SVDimpute this is not possible, and the method is called $(v_{miss} \cdot segs \cdot nruncv \cdot length(evalPcs))$ times. This should still be fast for LLSimpute because the method

allows to choose to only do the estimation for one particular variable. This saves a lot of iterations. Here, v_{miss} is the number of variables showing missing values.

As cross validation is done variable-wise, in this function Q2 is defined on single variables, not on the entire data set. This is Q2 is calculated as as $\frac{\sum(x-xe)^2}{\sum(x^2)}$, where x is the currently used variable and xe it's estimate. The values are then averaged over all variables. The NRMSEP is already defined variable-wise. For a single variable it is then $\sqrt{(\frac{\sum(x-xe)^2}{(n \cdot var(x))})}$, where x is the variable and xe it's estimate, n is the length of x. The variable wise estimation errors are returned in parameter variableWiseError.

Value

A list with:

`bestNPcs` number of PCs or k for which the minimal average NRMSEP or the maximal Q2 was obtained.

`eError` an array of of size length(evalPcs). Contains the average error of the cross validation runs for each number of components.

`variableWiseError` Matrix of size `incomplete_variables` x length(evalPcs). Contains the NRMSEP or Q2 distance for each variable and each number of PCs. This allows to easily see for wich variables imputation makes sense and for which one it should not be done or mean imputation should be used.

`evalPcs` The evaluated numbers of components or number of neighbours (the same as the evalPcs input parameter).

`variableIx` Index of the incomplete variables. This can be used to map the variable wise error to the original data.

Author(s)

Wolfram Stacklies

See Also

`kEstimateFast`, `Q2`, `pca`, `nni`.

Examples

```
## Load a sample metabolite dataset with 5\% missing values (metaboliteData)
data(metaboliteData)
# Do cross validation with ppca for component 2:4
esti <- kEstimate(metaboliteData, method = "ppca", evalPcs = 2:4, nruncv=1, em="nrmsep")
# Plot the average NRMSEP
barplot(drop(esti$eError), xlab = "Components",ylab = "NRMSEP (1 iterations)")
# The best result was obtained for this number of PCs:
print(esti$bestNPcs)
# Now have a look at the variable wise estimation error
barplot(drop(esti$variableWiseError[, which(esti$evalPcs == esti$bestNPcs)]),
        xlab = "Incomplete variable Index", ylab = "NRMSEP")
```

kEstimateFast *Estimate best number of Components for missing value estimation*

Description

This is a simple estimator for the optimal number of componets when applying PCA or LLSimpute for missing value estimation. No cross validation is performed, instead the estimation quality is defined as Matrix[!missing] - Estimate[!missing]. This will give a relatively rough estimate, but the number of iterations equals the length of the parameter evalPcs.
Does not work with LLSimpute!! As error measure the NRMSEP (see Feten et. al, 2005) or the Q2 distance is used. The NRMSEP basically normalises the RMSD between original data and estimate by the variable-wise variance. The reason for this is that a higher variance will generally lead to a higher estimation error. If the number of samples is small, the gene - wise variance may become an unstable criterion and the Q2 distance should be used instead. Also if variance normalisation was applied previously.

Usage

```
kEstimateFast(Matrix, method = "ppca", evalPcs = 1:3, em = "nrmsep",
  allVariables = FALSE, verbose = interactive(), ...)
```

Arguments

Matrix	matrix – numeric matrix containing observations in rows and variables in columns
method	character – a valid pca method (see pca).
evalPcs	numeric – The principal components to use for cross validation or cluster sizes if used with llsImpute. Should be an array containing integer values, eg. evalPcs = 1:10 or evalPcs = C(2,5,8).The NRMSEP is calculated for each component.
em	character – The error measure. This can be nrmsep or q2
allVariables	boolean – If TRUE, the NRMSEP is calculated for all variables, If FALSE, only the incomplete ones are included. You maybe want to do this to compare several methods on a complete data set.
verbose	boolean – If TRUE, the NRMSEP and the variance are printed to the console each iteration.
...	Further arguments to pca

Value

list Returns a list with the elements:

- minNPcs - number of PCs for which the minimal average NRMSEP was obtained
- eError - an array of of size length(evalPcs). Contains the estimation error for each number of components.
- evalPcs - The evaluated numbers of components or cluster sizes (the same as the evalPcs input parameter).

Author(s)

Wolfram Stacklies

See Also

kEstimate.

Examples

```
data(metaboliteData)
# Estimate best number of PCs with ppca for component 2:4
esti <- kEstimateFast(t(metaboliteData), method = "ppca", evalPcs = 2:4, em="nrmsep")
barplot(drop(esti$eError), xlab = "Components",ylab = "NRMSEP (1 iterations)")
# The best k value is:
print(esti$minNPcs)
```

---

leverage,pcaRes-method

Extract leverages of a PCA model

Description

The leverages of PCA model indicate how much influence each observation has on the PCA model. Observations with high leverage has caused the principal components to rotate towards them. It can be used to extract both "unimportant" observations as well as picking potential outliers.

Usage

```
## S4 method for signature 'pcaRes'
leverage(object)
```

Arguments

object	a pcaRes object

Details

Defined as $Tr(T(T'T)^{-1}T')$

Value

The observation leverages as a numeric vector

Author(s)

Henning Redestig

References

Introduction to Multi- and Megavariate Data Analysis using Projection Methods (PCA and PLS), L. Eriksson, E. Johansson, N. Kettaneh-Wold and S. Wold, Umetrics 1999, p. 466

Examples

```
data(iris)
pcIr <- pca(iris[,1:4])
## versicolor has the lowest leverage
with(iris, plot(leverage(pcIr)~Species))
```

`lineSearch` *Line search for conjugate gradient*

Description

Line search for conjugate gradient

Usage

```
lineSearch(nlnet, dw, e0, ttGuess, trainIn, trainOut, verbose)
```

Arguments

`nlnet`	The nlnet
`dw`	..
`e0`	..
`ttGuess`	..
`trainIn`	Training data
`trainOut`	Fitted data
`verbose`	logical, print messages

Value

...

Author(s)

Henning Redestig, Matthias Scholz

linr *Linear kernel*

Description

Linear kernel

Usage

```
linr(x)
```

Arguments

x	datum

Value

Input value

Author(s)

Henning Redestig, Matthias Scholz

listPcaMethods *List PCA methods*

Description

Vector with current valid PCA methods

Usage

```
listPcaMethods(which = c("all", "linear", "nonlinear"))
```

Arguments

which	the type of methods to get. E.g. only get the PCA methods based on the classical model where the fitted data is a direct multiplication of scores and loadings.

Value

A character vector with the current methods for doing PCA

Author(s)

Henning Redestig

`llsImpute` *LLSimpute algorithm*

Description

Missing value estimation using local least squares (LLS). First, k variables (for Microarrya data usually the genes) are selected by pearson, spearman or kendall correlation coefficients. Then missing values are imputed by a linear combination of the k selected variables. The optimal combination is found by LLS regression. The method was first described by Kim et al, Bioinformatics, 21(2),2005.

Usage

```
llsImpute(Matrix, k = 10, center = FALSE, completeObs = TRUE,
  correlation = "pearson", allVariables = FALSE, maxSteps = 100,
  xval = NULL, verbose = FALSE, ...)
```

Arguments

`Matrix`	`matrix` – Data containing the variables (genes) in columns and observations (samples) in rows. The data may contain missing values, denoted as `NA`.
`k`	`numeric` – Cluster size, this is the number of similar genes used for regression.
`center`	`boolean` – Mean center the data if TRUE
`completeObs`	`boolean` – Return the estimated complete observations if TRUE. This is the input data with NA values replaced by the estimated values.
`correlation`	`character` – How to calculate the distance between genes. One out of pearson | kendall | spearman , see also help("cor").
`allVariables`	`boolean` – Use only complete genes to do the regression if TRUE, all genes if FALSE.
`maxSteps`	`numeric` – Maximum number of iteration steps if allGenes = TRUE.
`xval`	`numeric` Use LLSimpute for cross validation. xval is the index of the gene to estimate, all other incomplete genes will be ignored if this parameter is set. We do not consider them in the cross-validation.
`verbose`	`boolean` – Print step number and relative change if TRUE and allVariables = TRUE
`...`	Reserved for parameters used in future version of the algorithm

Details

Missing values are denoted as `NA`
It is not recommended to use this function directely but rather to use the nni() wrapper function. The methods provides two ways for missing value estimation, selected by the `allVariables` option. The first one is to use only complete variables for the regression. This is preferable when the number of incomplete variables is relatively small.

The second way is to consider all variables as candidates for the regression. Hereby missing values are initially replaced by the columns wise mean. The method then iterates, using the current estimate as input for the regression until the change between new and old estimate falls below a threshold (0.001).

Value

`nniRes`	Standard nni (nearest neighbour imputation) result object of this package. See `nniRes` for details.

Note

Each step the generalized inverse of a `miss` x k matrix is calculated. Where `miss` is the number of missing values in variable j and k the number of neighbours. This may be slow for large values of k and / or many missing values. See also help("ginv").

Author(s)

Wolfram Stacklies

References

Kim, H. and Golub, G.H. and Park, H. - Missing value estimation for DNA microarray gene expression data: local least squares imputation. *Bioinformatics, 2005; 21(2):187-198.*

Troyanskaya O. and Cantor M. and Sherlock G. and Brown P. and Hastie T. and Tibshirani R. and Botstein D. and Altman RB. - Missing value estimation methods for DNA microarrays. *Bioinformatics. 2001 Jun;17(6):520-525.*

See Also

`pca`, `nniRes`, `nni`.

Examples

```
## Load a sample metabolite dataset (metaboliteData) with already 5\% of
## data missing
data(metaboliteData)
## Perform llsImpute using k = 10
## Set allVariables TRUE because there are very few complete variables
result <- llsImpute(metaboliteData, k = 10, correlation="pearson", allVariables=TRUE)
## Get the estimated complete observations
cObs <- completeObs(result)
```

loadings,ANY-method *Crude way to unmask the function with the same name from* stats

Description

Crude way to unmask the function with the same name from stats

Usage

```
## S4 method for signature 'ANY'
loadings(object, ...)
```

Arguments

object	any object
...	not used

Value

The loadings

Author(s)

Henning Redestig

loadings,pcaRes-method *Get loadings from a pcaRes object*

Description

Get loadings from a pcaRes object

Usage

```
## S4 method for signature 'pcaRes'
loadings(object, ...)
```

Arguments

object	a pcaRes object
...	not used

Value

The loadings as a matrix

Author(s)

Henning Redestig

See Also

loadings.pcaRes

---

loadings.pcaRes *Get loadings from a pcaRes object*

Description

Get loadings from a pcaRes object

Usage

```
## S3 method for class 'pcaRes'
loadings(object, ...)
```

Arguments

object	a pcaRes object
...	not used

Value

The loadings as a matrix

Author(s)

Henning Redestig

---

metaboliteData *A incomplete metabolite data set from an Arabidopsis coldstress experiment*

Description

A incomplete subset from a larger metabolite data set. This is the original, complete data set and can be used to compare estimation results created with the also provided incomplete data (called metaboliteData).

Details

A matrix containing 154 observations (rows) and 52 metabolites (columns). The data contains 5% of artificially created uniformly distributed misssing values. The data was created during an in house Arabidopsis coldstress experiment.

Author(s)

Wolfram Stacklies

References

Matthias Scholz, Fatma Kaplan, Charles L. Guy, Joachim Kopka and Joachim Selbig. - Non-linear PCA: a missing data approach.*Bioinformatics 2005 21(20):3887-3895*

See Also

metaboliteDataComplete

`metaboliteDataComplete` *A complete metabolite data set from an Arabidopsis coldstress experiment*

Description

A complete subset from a larger metabolite data set. This is the original, complete data set and can be used to compare estimation results created with the also provided incomplete data (called metaboliteData). The data was created during an in house Arabidopsis coldstress experiment.

Details

A matrix containing 154 observations (rows) and 52 metabolites (columns).

Author(s)

Wolfram Stacklies

References

Matthias Scholz, Fatma Kaplan, Charles L. Guy, Joachim Kopka and Joachim Selbig. - Non-linear PCA: a missing data approach.*Bioinformatics 2005 21(20):3887-3895*

See Also

metaboliteData

method,pcaRes-method *Get the used PCA method*

Description

Get the used PCA method

Usage

```
method(object, ...)
```

Arguments

object	pcaRes object
...	Not used

Value

The used pca method

Author(s)

Henning Redestig

nipalsPca *NIPALS PCA*

Description

PCA by non-linear iterative partial least squares

Usage

```
nipalsPca(Matrix, nPcs = 2, varLimit = 1, maxSteps = 5000,
  threshold = 1e-06, ...)
```

Arguments

Matrix	Pre-processed (centered, scaled) numerical matrix samples in rows and variables as columns.
nPcs	Number of components that should be extracted.
varLimit	Optionally the ratio of variance that should be explained. nPcs is ignored if varLimit < 1
maxSteps	Defines how many iterations can be done before algorithm should abort (happens almost exclusively when there were some wrong in the input data).

threshold	The limit condition for judging if the algorithm has converged or not, specifically if a new iteration is done if $(T_{old} - T)^T (T_{old} - T) >$ limit.
...	Only used for passing through arguments.

Details

Can be used for computing PCA on a numeric matrix using either the NIPALS algorithm which is an iterative approach for estimating the principal components extracting them one at a time. NIPALS can handle a small amount of missing values. It is not recommended to use this function directely but rather to use the pca() wrapper function.

Value

A pcaRes object.

Author(s)

Henning Redestig

References

Wold, H. (1966) Estimation of principal components and related models by iterative least squares. In Multivariate Analysis (Ed., P.R. Krishnaiah), Academic Press, NY, 391-420.

See Also

prcomp, princomp, pca

Examples

```
data(metaboliteData)
mat <- prep(t(metaboliteData))
pc <- nipalsPca(mat, nPcs=2)
## better use pca()
pc <- pca(t(metaboliteData), method="nipals", nPcs=2)
```

---

nlpca *Non-linear PCA*

Description

Neural network based non-linear PCA

Usage

```
nlpca(Matrix, nPcs = 2, maxSteps = 2 * prod(dim(Matrix)),
  unitsPerLayer = NULL, functionsPerLayer = NULL,
  weightDecay = 0.001, weights = NULL, verbose = interactive(), ...)
```

Arguments

Matrix	matrix — Preprocessed data with the variables in columns and observations in rows. The data may contain missing values, denoted as NA
nPcs	numeric – Number of components to estimate. The preciseness of the missing value estimation depends on thenumber of components, which should resemble the internal structure of the data.
maxSteps	numeric – Number of estimation steps. Default is based on a generous rule of thumb.
unitsPerLayer	The network units, example: c(2,4,6) for two input units 2feature units (principal components), one hidden layer fornon-linearity and three output units (original amount ofvariables).
functionsPerLayer	The function to apply at each layer eg. c("linr", "tanh", "linr")
weightDecay	Value between 0 and 1.
weights	Starting weights for the network. Defaults to uniform random values but can be set specifically to make algorithm deterministic.
verbose	boolean – nlpca prints the number of steps and warning messages if set to TRUE. Default is interactive().
...	Reserved for future use. Not passed on anywhere.

Details

Artificial Neural Network (MLP) for performing non-linear PCA. Non-linear PCA is conceptually similar to classical PCA but theoretically quite different. Instead of simply decomposing our matrix (X) to scores (T) loadings (P) and an error (E) we train a neural network (our loadings) to find a curve through the multidimensional space of X that describes a much variance as possible. Classical ways of interpreting PCA results are thus not applicable to NLPCA since the loadings are hidden in the network. However, the scores of components that lead to low cross-validation errors can still be interpreted via the score plot. Unfortunately this method depend on slow iterations which currently are implemented in R only making this method extremely slow. Furthermore, the algorithm does not by itself decide when it has converged but simply does 'maxSteps' iterations.

Value

Standard PCA result object used by all PCA-basedmethods of this package. Contains scores, loadings, data meanand more. See pcaRes for details.

Author(s)

Based on a matlab script by Matthias Scholz and ported to R by Henning Redestig

References

Matthias Scholz, Fatma Kaplan, Charles L Guy, Joachim Kopkaand Joachim Selbig. Non-linear PCA: a missing data approach. *Bioinformatics, 21(20):3887-3895, Oct 2005*

Examples

```
## Data set with three variables where data points constitute a helix
data(helix)
helixNA <- helix
## not a single complete observation
helixNA <- t(apply(helix, 1, function(x) { x[sample(1:3, 1)] <- NA; x}))
## 50 steps is not enough, for good estimation use 1000
helixNlPca <- pca(helixNA, nPcs=1, method="nlpca", maxSteps=50)
fittedData <- fitted(helixNlPca, helixNA)
plot(fittedData[which(is.na(helixNA))], helix[which(is.na(helixNA))])
## compared to solution by Nipals PCA which cannot extract non-linear patterns
helixNipPca <- pca(helixNA, nPcs=2)
fittedData <- fitted(helixNipPca)
plot(fittedData[which(is.na(helixNA))], helix[which(is.na(helixNA))])
```

---

nmissing,pcaRes-method

Missing values

Description

Missing values

Usage

```
nmissing(object, ...)
```

Arguments

object	pcaRes object
...	Not used

Value

Get the number of missing values

Author(s)

Henning Redestig

nni *Nearest neighbour imputation*

Description

Wrapper function for imputation methods based on nearest neighbour clustering. Currently llsImpute only.

Usage

```
nni(object, method = c("llsImpute"), subset = numeric(), ...)
```

Arguments

object	Numerical matrix with (or an object coercible to such) with samples in rows and variables as columns. Also takes ExpressionSet in which case the transposed expression matrix is used.
method	For convenience one can pass a large matrix but only use the variable specified as subset. Can be colnames or indices.
subset	Currently "llsImpute" only.
...	Further arguments to the chosen method.

Details

This method is wrapper function to llsImpute, See documentation for link{llsImpute}.

Value

A clusterRes object. Or a list containing a clusterRes object as first and an ExpressionSet object as second entry if the input was of type ExpressionSet.

Author(s)

Wolfram Stacklies

See Also

llsImpute, pca

Examples

```
data(metaboliteData)
llsRes <- nni(metaboliteData, k=6, method="llsImpute", allGenes=TRUE)
```

nniRes *Class for representing a nearest neighbour imputation result*

Description

This is a class representation of nearest neighbour imputation (nni) result

Details

Creating Objects

`new("nniRes", completeObs=[the estimated complete observations], k=[cluster size], nObs=[amount of observations],nVar=[amount of variables], centered=[was the data centered befor running LLSimpute], center=[original means], method=[method used to perform clustering], missing=[amount of NAs])`

Slots

completeObs "matrix", the estimated complete observations

nObs "numeric", amount of observations

nVar "numeric", amount of variables

correlation "character", the correlation method used (pearson, kendall or spearman)

centered "logical", data was centered or not

center "numeric", the original variable centers

k "numeric", cluster size

method "character", the method used to perform the clustering

missing "numeric", the total amount of missing values in original data

Methods

print Print function

Author(s)

Wolfram Stacklies

nObs,pcaRes-method *Get the number of observations used to build the PCA model.*

Description

Get the number of observations used to build the PCA model.

Usage

```
nObs(object, ...)
```

Arguments

object	pcaRes object
...	Not used

Value

Number of observations

Author(s)

Henning Redestig

nP,pcaRes-method *Get number of PCs*

Description

Get number of PCs

Usage

```
nP(object, ...)
```

Arguments

object	pcaRes object
...	not used

Value

Number of PCs

Author(s)

Henning Redestig

nPcs,pcaRes-method *Get number of PCs.*

Description

Get number of PCs.

Usage

```
nPcs(object, ...)
```

Arguments

object	pcaRes object
...	not used

Value

Number of PCs

Note

Try to use link{nP} instead since nPcs tend to clash with argument names.

Author(s)

Henning Redestig

nVar,pcaRes-method *Get the number of variables used to build the PCA model.*

Description

Get the number of variables used to build the PCA model.

Usage

```
nVar(object, ...)
```

Arguments

object	pcaRes object
...	Not used

Value

Number of variables

Author(s)

Henning Redestig

`optiAlgCgd` *Conjugate gradient optimization*

Description

Conjugate gradient optimization

Usage

```
optiAlgCgd(nlnet, trainIn, trainOut, verbose = FALSE)
```

Arguments

`nlnet`	The nlnet
`trainIn`	Training data
`trainOut`	fitted data
`verbose`	logical, print messages

Value

...

Author(s)

Henning Redestig, Matthias Scholz

orth *Calculate an orthonormal basis*

Description

ONB = orth(mat) is an orthonormal basis for the range of matrix mat. That is, ONB' * ONB = I, the columns of ONB span the same space as the columns of mat, and the number of columns of ONB is the rank of mat.

Usage

```
orth(mat, skipInac = FALSE)
```

Arguments

mat	matrix to calculate orthonormal base
skipInac	do not include components with precision below .Machine$double.eps if TRUE

Value

orthonormal basis for the range of matrix

Author(s)

Wolfram Stacklies

pca *Perform principal component analysis*

Description

Perform PCA on a numeric matrix for visualisation, information extraction and missing value imputation.

Usage

```
pca(object, method, nPcs = 2, scale = c("none", "pareto", "vector",
  "uv"), center = TRUE, completeObs = TRUE, subset = NULL,
  cv = c("none", "q2"), ...)
```

Arguments

object	Numerical matrix with (or an object coercible to such) with samples in rows and variables as columns. Also takes ExpressionSet in which case the transposed expression matrix is used. Can also be a data frame in which case all numberic variables are used to fit the PCA.
method	One of the methods reported by listPcaMethods(). Can be left missing in which case the svd PCA is chosen for data wihout missing values and nipalsPca for data with missing values
nPcs	Number of principal components to calculate.
scale	Scaling, see prep.
center	Centering, see prep.
completeObs	Sets the completeObs slot on the resulting pcaRes object containing the original data with but with all NAs replaced with the estimates.
subset	A subset of variables to use for calculating the model. Can be column names or indices.
cv	character naming a the type of cross-validation to be performed.
...	Arguments to prep, the chosen pca method and Q2.

Details

This method is wrapper function for the following set of pca methods:

svd: Uses classical prcomp. See documentation for svdPca.

nipals: An iterative method capable of handling small amounts of missing values. See documentation for nipalsPca.

rnipals: Same as nipals but implemented in R.

bpca: An iterative method using a Bayesian model to handle missing values. See documentation for bpca.

ppca: An iterative method using a probabilistic model to handle missing values. See documentation for ppca.

svdImpute: Uses expectation maximation to perform SVD PCA on incomplete data. See documentation for svdImpute.

Scaling and centering is part of the PCA model and handled by prep.

Value

A pcaRes object.

Author(s)

Wolfram Stacklies, Henning Redestig

References

Wold, H. (1966) Estimation of principal components and related models by iterative least squares. In Multivariate Analysis (Ed., P.R. Krishnaiah), Academic Press, NY, 391-420.

Shigeyuki Oba, Masa-aki Sato, Ichiro Takemasa, Morito Monden, Ken-ichi Matsubara and Shin Ishii. A Bayesian missing value estimation method for gene expression profile data. *Bioinformatics, 19(16):2088-2096, Nov 2003*.

Troyanskaya O. and Cantor M. and Sherlock G. and Brown P. and Hastie T. and Tibshirani R. and Botstein D. and Altman RB. - Missing value estimation methods for DNA microarrays. *Bioinformatics. 2001 Jun;17(6):520-5*.

See Also

prcomp, princomp, nipalsPca, svdPca

Examples

```
data(iris)
##  Usually some kind of scaling is appropriate
pcIr <- pca(iris, method="svd", nPcs=2)
pcIr <- pca(iris, method="nipals", nPcs=3, cv="q2")
## Get a short summary on the calculated model
summary(pcIr)
plot(pcIr)
## Scores and loadings plot
slplot(pcIr, sl=as.character(iris[,5]))

## use an expressionset and ggplot
data(sample.ExpressionSet)
pc <- pca(sample.ExpressionSet)
df <- merge(scores(pc), pData(sample.ExpressionSet), by=0)
library(ggplot2)
ggplot(df, aes(PC1, PC2, shape=sex, color=type)) +
  geom_point() +
  xlab(paste("PC1", pc@R2[1] * 100, "% of the variance")) +
  ylab(paste("PC2", pc@R2[2] * 100, "% of the variance"))
```

---

pcaMethods *pcaMethods*

Description

Principal Component Analysis in R

Details

Package:	pcaMethods
Type:	Package
Developed since:	2006
License:	GPL (>=3)
LazyLoad:	yes

Provides Bayesian PCA, Probabilistic PCA, Nipals PCA, Inverse Non-Linear PCA and the conventional SVD PCA. A cluster based method for missing value estimation is included for comparison. BPCA, PPCA and NipalsPCA may be used to perform PCA on incomplete data as well as for accurate missing value estimation. A set of methods for printing and plotting the results is also provided. All PCA methods make use of the same data structure (pcaRes) to provide a unique interface to the PCA results. Developed at the Max-Planck Institute for Molecular Plant Physiology, Golm, Germany, RIKEN Plant Science Center Yokohama, Japan, and CAS-MPG Partner Institute for Computational Biology (PICB) Shanghai, P.R. China

Author(s)

Wolfram Stacklies, Henning Redestig

---

pcaMethods-deprecated *Deprecated methods for pcaMethods*

Description

plotR2 Lack of relevance for this plot and the fact that it can not show cross-validation based diagnostics in the same plot makes it redundant with the introduction of a dedicated `plot` function for `pcaRes`. The new plot only shows R2cum but the result is pretty much the same.

Author(s)

Henning Redestig

---

pcaNet *Class representation of the NLPCA neural net*

Description

This is a class representation of a non-linear PCA neural network. The `nlpcaNet` class is not meant for user-level usage.

Details

Creating Objects

`new("nlpcaNet", net=[the network structure],hierarchic=[hierarchic design],fct=[the functions at each layer], fkt=[the functions used for forward propagation], weightDecay=[incremental decrease of weight changes over iterations (between 0 and 1)], featureSorting=[sort features or not], dataDist=[represents the present values],inverse=[net is inverse mode or not], fCount=[amount of times features were sorted], componentLayer=[which layer is the 'bottleneck' (principal components)],erro=[the used error function], gradient=[the used gradient method],weights=[the present weights],maxIter=[the amount of iterations that was done], scalingFactor=[the scale of the original matrix])`

Slots

net "matrix", matrix showing the representation of the neural network, e.g. (2,4,6) for a network with two features, a hidden layer and six output neurons (original variables).

hierarchic "list", the hierarchic design of the network, holds 'idx' (), 'var' () and layer (which layer is the principal component layer).

fct "character", a vector naming the functions that will be applied on each layer. "linr" is linear (i.e.) standard matrix products and "tanh" means that the arcus tangens is applied on the result of the matrix product (for non-linearity).

fkt "character", same as fct but the functions used during back propagation.

weightDecay "numeric", the value that is used to incrementally decrease the weight changes to ensure convergence.

featureSorting "logical", indicates if features will be sorted or not. This is used to make the NLPCA assume properties closer to those of standard PCA were the first component is more important for reconstructing the data than the second component.

dataDist "matrix", a matrix of ones and zeroes indicating which values will add to the errror.

inverse "logical", network is inverse mode (currently only inverse is supported) or not. Eg. the case when we have truly missing values and wish to impute them.

fCount "integer", Counter for the amount of times features were really sorted.

componentLayer "numeric", the index of 'net' that is the component layer.

error "function", the used error function. Currently only one is provided `errorHierarchic`.

gradient "function", the used gradient function. Currently only one is provided `derrorHierarchic`

weights "list", A list holding managements of the weights. The list has two functions, weights$current() and weights$set() which access a matrix in the local environment of this object.

maxIter "integer", the amount of iterations used to train this network.

scalingFactor "numeric", training the network is best made with 'small' values so the original data is scaled down to a suitable range by division with this number.

Methods

vector2matrices Returns the weights in a matrix representation.

Author(s)

Henning Redestig

See Also

nlpca

---

pcaRes *Class for representing a PCA result*

Description

This is a class representation of a PCA result

Details

Creating Objects

`new("pcaRes", scores=[the scores], loadings=[the loadings],nPcs=[amount of PCs], R2cum=[cumulative R2], nObs=[amount of observations], nVar=[amount of variables], R2=[R2 for each individual PC], sDev=[stdev for each individual PC],centered=[was data centered], center=[original means],varLimit=[what variance limit was exceeded], method=[method used to calculate PCA], missing=[amount of NAs],completeObs=[estimated complete observations])`

Slots

scores "matrix", the calculated scores

loadings "matrix", the calculated loadings

R2cum "numeric", the cumulative R2 values

sDev "numeric", the individual standard deviations of the score vectors

R2 "numeric", the individual R2 values

cvstat "numeric", cross-validation statistics

nObs "numeric", number of observations

nVar "numeric", number of variables

centered "logical", data was centered or not

center "numeric", the original variable centers

scaled "logical", data was scaled or not

scl "numeric", the original variable scales

varLimit "numeric", the exceeded variance limit

nPcs,nP "numeric", the number of calculated PCs

method "character", the method used to perform PCA

missing "numeric", the total amount of missing values in original data

completeObs "matrix", the estimated complete observations

network "nlpcaNet", the network used by non-linear PCA

Methods (not necessarily exhaustive)

print Print function

summary Extract information about PC relevance

screeplot Plot a barplot of standard deviations for PCs

slplot Make a side by side score and loadings plot

nPcs Get the number of PCs

nObs Get the number of observations

cvstat Cross-validation statistics

nVar Get the number of variables

loadings Get the loadings

scores Get the scores

dim Get the dimensions (number of observations, number of features)

centered Get a logical indicating if centering was done as part of the model

center Get the averages of the original variables.

completeObs Get the imputed data set

method Get a string naming the used PCA method

sDev Get the standard deviations of the PCs

scaled Get a logical indicating if scaling was done as part of the model

scl Get the scales of the original variablesb

R2cum Get the cumulative R2

Author(s)

Henning Redestig

`plot.pcaRes` *Plot diagnostics (screeplot)*

Description

Plot the computed diagnostics of PCA model to get an idea of their importance. Note though that the standard screeplot shows the standard deviations for the PCs this method shows the R2 values which empirically shows the importance of the P's and is thus applicable for any PCA method rather than just SVD based PCA.

Usage

```
## S3 method for class 'pcaRes'
plot(x, y = NULL, main = deparse(substitute(object)),
  col = gray(c(0.9, 0.5)), ...)
```

Arguments

x	pcaRes The pcaRes object.
y	not used
main	title of the plot
col	Colors of the bars
...	further arguments to barplot

Details

If cross-validation was done for the PCA the plot will also show the CV based statistics. A common rule-of-thumb for determining the optimal number of PCs is the PC where the CV diagnostic is at its maximum but not very far from R^2.

Value

None, used for side effect.

Author(s)

Henning Redestig

See Also

screeplot

Examples

```
data(metaboliteData)
pc <- pca(t(metaboliteData), nPcs=5, cv="q2", scale="uv")
plot(pc)
```

---

plotPcs *Plot many side by side scores XOR loadings plots*

Description

A function that can be used to visualise many PCs plotted against each other

Usage

```
plotPcs(object, pcs = 1:nP(object), type = c("scores", "loadings"),
  sl = NULL, hotelling = 0.95, ...)
```

Arguments

object	pcaRes a pcaRes object
pcs	numeric which pcs to plot
type	character Either "scores" or "loadings" for scores or loadings plot respectively
sl	character Text labels to plot instead of a point, if NULL points are plotted instead of text
hotelling	numeric Significance level for the confidence ellipse. NULL means that no ellipse is drawn.
...	Further arguments to pairs on which this function is based.

Details

Uses pairs to provide side-by-side plots. Note that this function only plots scores or loadings but not both in the same plot.

Value

None, used for side effect.

Author(s)

Henning Redestig

See Also

prcomp, pca, princomp, slplot

Examples

```
data(iris)
pcIr <- pca(iris[,1:4], nPcs=3,  method="svd")
plotPcs(pcIr, col=as.integer(iris[,4]) + 1)
```

---

ppca *Probabilistic PCA*

Description

Implementation of probabilistic PCA (PPCA). PPCA allows to perform PCA on incomplete data and may be used for missing value estimation. This script was implemented after the Matlab version provided by Jakob Verbeek (see http://lear.inrialpes.fr/~verbeek/) and the draft *"EM Algorithms for PCA and Sensible PCA"* written by Sam Roweis.

Usage

```
ppca(Matrix, nPcs = 2, seed = NA, threshold = 1e-05,
  maxIterations = 1000, ...)
```

Arguments

Matrix	matrix – Data containing the variables in columns and observations in rows. The data may contain missing values, denoted as NA.
nPcs	numeric – Number of components to estimate. The preciseness of the missing value estimation depends on the number of components, which should resemble the internal structure of the data.
seed	numeric Set the seed for the random number generator. PPCA creates fills the initial loading matrix with random numbers chosen from a normal distribution. Thus results may vary slightly. Set the seed for exact reproduction of your results.
threshold	Convergence threshold.
maxIterations	the maximum number of allowed iterations
...	Reserved for future use. Currently no further parameters are used.

Details

Probabilistic PCA combines an EM approach for PCA with a probabilistic model. The EM approach is based on the assumption that the latent variables as well as the noise are normal distributed.

In standard PCA data which is far from the training set but close to the principal subspace may have the same reconstruction error. PPCA defines a likelihood function such that the likelihood for data far from the training set is much lower, even if they are close to the principal subspace. This allows to improve the estimation accuracy.

A method called kEstimate is provided to estimate the optimal number of components via cross validation. In general few components are sufficient for reasonable estimation accuracy. See also the package documentation for further discussion on what kind of data PCA-based missing value estimation is advisable.

Complexity:
Runtime is linear in the number of data, number of data dimensions and number of principal components.

Convergence: The threshold indicating convergence was changed from 1e-3 in 1.2.x to 1e-5 in the current version leading to more stable results. For reproducability you can set the seed (parameter seed) of the random number generator. If used for missing value estimation, results may be checked by simply running the algorithm several times with changing seed, if the estimated values show little variance the algorithm converged well.

Value

Standard PCA result object used by all PCA-based methods of this package. Contains scores, loadings, data mean and more. See pcaRes for details.

Note

Requires MASS. It is not recommended to use this function directely but rather to use the pca() wrapper function.

Author(s)

Wolfram Stacklies

See Also

bpca, svdImpute, prcomp,nipalsPca, pca, pcaRes.

Examples

```
## Load a sample metabolite dataset with 5\% missing values (metaboliteData)
data(metaboliteData)
## Perform probabilistic PCA using the 3 largest components
result <- pca(t(metaboliteData), method="ppca", nPcs=3, seed=123)
## Get the estimated complete observations
cObs <- completeObs(result)
## Plot the scores
plotPcs(result, type = "scores")
```

---

predict-methods *Predict values from PCA.*

Description

Predict data using PCA model

Usage

```
## S3 method for class 'pcaRes'
predict(object, newdata, pcs = nP(object), pre = TRUE,
  post = TRUE, ...)

## S4 method for signature 'pcaRes'
predict(object, newdata, pcs = nP(object),
  pre = TRUE, post = TRUE, ...)
```

Arguments

object	pcaRes the pcaRes object of interest.
newdata	matrix new data with same number of columns as the used to compute object.
pcs	numeric The number of PC's to consider
pre	pre-process newdata based on the pre-processing chosen for the PCA model
post	unpre-process the final data (add the center back etc)
...	Not passed on anywhere, included for S3 consistency.

Details

This function extracts the predict values from a pcaRes object for the PCA methods SVD, Nipals, PPCA and BPCA. Newdata is first centered if the PCA model was and then scores (T) and data (X) is 'predicted' according to : $\hat{T} = X_{new}P$ $\hat{X}_{new} = \hat{T}P'$. Missing values are set to zero before matrix multiplication to achieve NIPALS like treatment of missing values.

Value

A list with the following components:

`scores`	The predicted scores
`x`	The predicted data

Author(s)

Henning Redestig

Examples

```
data(iris)
hidden <- sample(nrow(iris), 50)
pcIr <- pca(iris[-hidden,1:4])
pcFull <- pca(iris[,1:4])
irisHat <- predict(pcIr, iris[hidden,1:4])
cor(irisHat$scores[,1], scores(pcFull)[hidden,1])
```

---

prep *Pre-process a matrix for PCA*

Description

Scaling and centering a matrix.

Usage

```
prep(object, scale = c("none", "pareto", "vector", "uv"),
  center = TRUE, eps = 1e-12, simple = TRUE, reverse = FALSE, ...)
```

Arguments

`object`	Numerical matrix (or an object coercible to such) with samples in rows and variables as columns. Also takes `ExpressionSet` in which case the transposed expression matrix is used.
`scale`	One of "UV" (unit variance $a = a/\sigma_a$) "vector" (vector normalisation $b = b/\|\|b\|\|$), "pareto" (sqrt UV) or "none" to indicate which scaling should be used to scale the matrix with a variables and b samples. Can also be a vector of scales which should be used to scale the matrix. `NULL` value is interpreted as `"none"`.

center	Either a logical which indicates if the matrix should be mean centred or not, or a vector with averages which should be suntracted from the matrix. NULL value is interpreted as FALSE
eps	Minimum variance, variable with lower variance are not scaled and warning is issued instead.
simple	Logical indicating if only the data should be returned or a list with the pre-processing statistics as well.
reverse	Logical indicating if matrix should be 'post-processed' instead by multiplying each column with its scale and adding the center. In this case, center and scale should be vectors with the statistics (no warning is issued if not, instead output becomes the same as input).
...	Only used for passing through arguments.

Details

Does basically the same as scale but adds some alternative scaling options and functionality for treating pre-processing as part of a model.

Value

A pre-processed matrix or a list with

center	a vector with the estimated centers
scale	a vector with the estimated scales
data	the pre (or post) processed data

Author(s)

Henning Redestig

Examples

```
object <- matrix(rnorm(50), nrow=10)
res <- prep(object, scale="uv", center=TRUE, simple=FALSE)
obj <- prep(object, scale=res$scale, center=res$center)
## same as original
sum((object - prep(obj, scale=res$scale, center=res$center, rev=TRUE))^2)
```

Q2 *Cross-validation for PCA*

Description

Internal cross-validation can be used for estimating the level of structure in a data set and to optimise the choice of number of principal components.

Usage

```
Q2(object, originalData = completeObs(object), fold = 5, nruncv = 1,
  type = c("krzanowski", "impute"), verbose = interactive(),
  variables = 1:nVar(object), ...)
```

Arguments

object	A pcaRes object (result from previous PCA analysis.)
originalData	The matrix (or ExpressionSet) that used to obtain the pcaRes object.
fold	The number of groups to divide the data in.
nruncv	The number of times to repeat the whole cross-validation
type	krzanowski or imputation type cross-validation
verbose	boolean If TRUE Q2 outputs a primitive progress bar.
variables	indices of the variables to use during cross-validation calculation. Other variables are kept as they are and do not contribute to the total sum-of-squares.
...	Further arguments passed to the pca function called within Q2.

Details

This method calculates Q^2 for a PCA model. This is the cross-validated version of R^2 and can be interpreted as the ratio of variance that can be predicted independently by the PCA model. Poor (low) Q^2 indicates that the PCA model only describes noise and that the model is unrelated to the true data structure. The definition of Q^2 is:

$$Q^2 = 1 - \frac{\sum_i^k \sum_j^n (x - \hat{x})^2}{\sum_i^k \sum_j^n x^2}$$

for the matrix x which has n rows and k columns. For a given number of PC's x is estimated as $\hat{x} = TP'$ (T are scores and P are loadings). Although this defines the leave-one-out cross-validation this is not what is performed if fold is less than the number of rows and/or columns. In 'impute' type CV, diagonal rows of elements in the matrix are deleted and the re-estimated. In 'krzanowski' type CV, rows are sequentially left out to build fold PCA models which give the loadings. Then, columns are sequentially left out to build fold models for scores. By combining scores and loadings from different models, we can estimate completely left out values. The two types may seem similar but can give very different results, krzanowski typically yields more stable and reliable result for estimating data structure whereas impute is better for evaluating missing value imputation performance. Note that since Krzanowski CV operates on a reduced matrix, it is not possible estimate Q2 for all components and the result vector may therefore be shorter than `nPcs(object)`.

Value

A matrix or vector with Q^2 estimates.

Author(s)

Henning Redestig, Ondrej Mikula

References

Krzanowski, WJ. Cross-validation in principal component analysis. Biometrics. 1987(43):3,575-584

Examples

```
data(iris)
x <- iris[,1:4]
pcIr <- pca(x, nPcs=3)
q2 <- Q2(pcIr, x)
barplot(q2, main="Krzanowski CV", xlab="Number of PCs", ylab=expression(Q^2))
## q2 for a single variable
Q2(pcIr, x, variables=2)
pcIr <- pca(x, nPcs=3, method="nipals")
q2 <- Q2(pcIr, x, type="impute")
barplot(q2, main="Imputation CV", xlab="Number of PCs", ylab=expression(Q^2))
```

R2cum,pcaRes-method *Cumulative R2 is the total ratio of variance that is being explained by the model*

Description

Cumulative R2 is the total ratio of variance that is being explained by the model

Usage

```
## S4 method for signature 'pcaRes'
R2cum(object, ...)
```

Arguments

object	a pcaRes model
...	Not used

Value

Get the cumulative R2

Author(s)

Henning Redestig

R2VX,pcaRes-method *R2 goodness of fit*

Description

Flexible calculation of R2 goodness of fit.

Usage

```
## S4 method for signature 'pcaRes'
R2VX(object, direction = c("variables",
  "observations", "complete"), data = completeObs(object),
  pcs = nP(object))
```

Arguments

object	a PCA model object
direction	choose between calculating R2 per variable, per observation or for the entire data with 'variables', 'observations' or 'complete'.
data	the data used to fit the model
pcs	the number of PCs to use to calculate R2

Value

A vector with R2 values

Author(s)

Henning Redestig

Examples

```
R2VX(pca(iris))
```

rediduals-methods *Residuals values from a PCA model.*

Description

This function extracts the residuals values from a pcaRes object for the PCA methods SVD, Nipals, PPCA and BPCA

Usage

```
## S3 method for class 'pcaRes'
residuals(object, data = completeObs(object), ...)

## S4 method for signature 'pcaRes'
residuals(object, data = completeObs(object), ...)

## S4 method for signature 'pcaRes'
resid(object, data = completeObs(object), ...)
```

Arguments

object	pcaRes the pcaRes object of interest.
data	matrix The data that was used to calculate the PCA model (or a different dataset to e.g. adress its proximity to the model).
...	Passed on to predict.pcaRes. E.g. setting the number of used components.

Value

A matrix with the residuals

Author(s)

Henning Redestig

Examples

```
data(iris)
pcIr <- pca(iris[,1:4])
head(residuals(pcIr, iris[,1:4]))
```

---

repmat *Replicate and tile an array.*

Description

Creates a large matrix B consisting of an M-by-N tiling of copies of A

Usage

```
repmat(mat, M, N)
```

Arguments

mat	numeric matrix
M	number of copies in vertical direction
N	number of copies in horizontal direction

Value

Matrix consiting of M-by-N tiling copies of input matrix

Author(s)

Wolfram Stacklies

`RnipalsPca` *NIPALS PCA implemented in R*

Description

PCA by non-linear iterative partial least squares

Usage

```
RnipalsPca(Matrix, nPcs = 2, varLimit = 1, maxSteps = 5000,
  threshold = 1e-06, verbose = interactive(), ...)
```

Arguments

`Matrix`	Pre-processed (centered, scaled) numerical matrix samples in rows and variables as columns.
`nPcs`	Number of components that should be extracted.
`varLimit`	Optionally the ratio of variance that should be explained. `nPcs` is ignored if varLimit < 1
`maxSteps`	Defines how many iterations can be done before algorithm should abort (happens almost exclusively when there were some wrong in the input data).
`threshold`	The limit condition for judging if the algorithm has converged or not, specifically if a new iteration is done if $(T_{old} - T)^T (T_{old} - T) >$ `limit`.
`verbose`	Show simple progress information.
`...`	Only used for passing through arguments.

Details

Can be used for computing PCA on a numeric matrix using either the NIPALS algorithm which is an iterative approach for estimating the principal components extracting them one at a time. NIPALS can handle a small amount of missing values. It is not recommended to use this function directely but rather to use the pca() wrapper function. There is a C++ implementation given as `nipalsPca` which is faster.

Value

A `pcaRes` object.

Author(s)

Henning Redestig

References

Wold, H. (1966) Estimation of principal components and related models by iterative least squares. In Multivariate Analysis (Ed., P.R. Krishnaiah), Academic Press, NY, 391-420.

See Also

`prcomp`, `princomp`, `pca`

Examples

```
data(metaboliteData)
mat <- prep(t(metaboliteData))
## c++ version is faster
system.time(pc <- RnipalsPca(mat, method="rnipals", nPcs=2))
system.time(pc <- nipalsPca(mat, nPcs=2))
## better use pca()
pc <- pca(t(metaboliteData), method="rnipals", nPcs=2)
```

---

robustPca *PCA implementation based on robustSvd*

Description

This is a PCA implementation robust to outliers in a data set. It can also handle missing values, it is however NOT intended to be used for missing value estimation. As it is based on robustSVD we will get an accurate estimation for the loadings also for incomplete data or for data with outliers. The returned scores are, however, affected by the outliers as they are calculated inputData X loadings. This also implies that you should look at the returned R2/R2cum values with caution. If the data show missing values, scores are caluclated by just setting all NA - values to zero. This is not expected to produce accurate results. Please have also a look at the manual page for `robustSvd`. Thus this method should mainly be seen as an attempt to integrate `robustSvd()` into the framework of this package. Use one of the other methods coming with this package (like PPCA or BPCA) if you want to do missing value estimation. It is not recommended to use this function directely but rather to use the pca() wrapper function.

Usage

```
robustPca(Matrix, nPcs = 2, verbose = interactive(), ...)
```

Arguments

Matrix	matrix – Data containing the variables in columns and observations in rows. The data may contain missing values, denoted as NA.
nPcs	numeric – Number of components to estimate. The preciseness of the missing value estimation depends on the number of components, which should resemble the internal structure of the data.
verbose	boolean Print some output to the command line if TRUE
...	Reserved for future use. Currently no further parameters are used

Details

The method is very similar to the standard prcomp() function. The main difference is that robustSvd() is used instead of the conventional svd() method.

Value

Standard PCA result object used by all PCA-based methods of this package. Contains scores, loadings, data mean and more. See pcaRes for details. are used.

Author(s)

Wolfram Stacklies

See Also

robustSvd, svd, prcomp, pcaRes.

Examples

```
## Load a complete sample metabolite data set and mean center the data
data(metaboliteDataComplete)
mdc <- scale(metaboliteDataComplete, center=TRUE, scale=FALSE)
## Now create 5\% of outliers.
cond   <- runif(length(mdc)) < 0.05;
mdcOut <- mdc
mdcOut[cond] <- 10
## Now we do a conventional PCA and robustPca on the original and the data
## with outliers.
## We use center=FALSE here because the large artificial outliers would
## affect the means and not allow to objectively compare the results.
resSvd    <- pca(mdc, method="svd", nPcs=10, center=FALSE)
resSvdOut <- pca(mdcOut, method="svd", nPcs=10, center=FALSE)
resRobPca <- pca(mdcOut, method="robustPca", nPcs=10, center=FALSE)
## Now we plot the results for the original data against those with outliers
## We can see that robustPca is hardly effected by the outliers.
plot(loadings(resSvd)[,1], loadings(resSvdOut)[,1])
plot(loadings(resSvd)[,1], loadings(resRobPca)[,1])
```

`robustSvd` *Alternating L1 Singular Value Decomposition*

Description

A robust approximation to the singular value decomposition of a rectangular matrix is computed using an alternating L1 norm (instead of the more usual least squares L2 norm). As the SVD is a least-squares procedure, it is highly susceptible to outliers and in the extreme case, an individual cell (if sufficiently outlying) can draw even the leading principal component toward itself.

Usage

```
robustSvd(x)
```

Arguments

`x`	A matrix whose SVD decomposition is to be computed. Missing values are allowed.

Details

See Hawkins et al (2001) for details on the robust SVD algorithm. Briefly, the idea is to sequentially estimate the left and right eigenvectors using an L1 (absolute value) norm minimization.

Note that the robust SVD is able to accomodate missing values in the matrix `x`, unlike the usual `svd` function.

Also note that the eigenvectors returned by the robust SVD algorithm are NOT (in general) orthogonal and the eigenvalues need not be descending in order.

Value

The robust SVD of the matrix is x=u d v'.

`d`	A vector containing the singular values of `x`.
`u`	A matrix whose columns are the left singular vectors of `x`.
`v`	A matrix whose columns are the right singular vectors of `x`.

Note

Two differences from the usual SVD may be noted. One relates to orthogonality. In the conventional SVD, all the eigenvectors are orthogonal even if not explicitly imposed. Those returned by the AL1 algorithm (used here) are (in general) not orthogonal. Another difference is that, in the L2 analysis of the conventional SVD, the successive eigen triples (eigenvalue, left eigenvector, right eigenvector) are found in descending order of eigenvalue. This is not necessarily the case with the AL1 algorithm. Hawkins et al (2001) note that a larger eigen value may follow a smaller one.

Author(s)

Kevin Wright, modifications by Wolfram Stacklies

References

Hawkins, Douglas M, Li Liu, and S Stanley Young (2001) Robust Singular Value Decomposition, National Institute of Statistical Sciences, Technical Report Number 122. http://www.niss.org/technicalreports/tr122.pdf

See Also

svd, nipals for an alternating L2 norm method that also accommodates missing data.

Examples

```
## Load a complete sample metabolite data set and mean center the data
data(metaboliteDataComplete)
mdc <- prep(metaboliteDataComplete, center=TRUE, scale="none")
## Now create 5% of outliers.
cond   <- runif(length(mdc)) < 0.05;
mdcOut <- mdc
mdcOut[cond] <- 10
## Now we do a conventional SVD and a robustSvd on both, the original and the
## data with outliers.
resSvd <- svd(mdc)
resSvdOut <- svd(mdcOut)
resRobSvd <- robustSvd(mdc)
resRobSvdOut <- robustSvd(mdcOut)
## Now we plot the results for the original data against those with outliers
## We can see that robustSvd is hardly affected by the outliers.
plot(resSvd$v[,1], resSvdOut$v[,1])
plot(resRobSvd$v[,1], resRobSvdOut$v[,1])
```

---

scaled,pcaRes-method *Check if scaling was part of the PCA model*

Description

Check if scaling was part of the PCA model

Usage

```
scaled(object, ...)
```

Arguments

object	pcaRes object
...	Not used

Value

TRUE if scaling was part of the PCA model

Author(s)

Henning Redestig

`scl,pcaRes-method` *Get the scales (e.g. standard deviations) of the original variables*

Description

Get the scales (e.g. standard deviations) of the original variables

Usage

```
scl(object, ...)
```

Arguments

`object`	pcaRes object
`...`	Not used

Value

Vector with the scales

Author(s)

Henning Redestig

See Also

`prep`

`scores,pcaRes-method` *Get scores from a pcaRes object*

Description

Get scores from a pcaRes object

Usage

```
## S4 method for signature 'pcaRes'
scores(object, ...)
```

Arguments

object	a pcaRes object
...	not used

Value

The scores as a matrix

Author(s)

Henning Redestig

See Also

scores.pcaRes

---

scores.pcaRes *Get scores from a pcaRes object*

Description

Get scores from a pcaRes object

Usage

```
## S3 method for class 'pcaRes'
scores(object, ...)
```

Arguments

object	a pcaRes object
...	not used

Value

The scores as a matrix

Author(s)

Henning Redestig

sDev,pcaRes-method *Get the standard deviations of the scores (indicates their relevance)*

Description

Get the standard deviations of the scores (indicates their relevance)

Usage

```
sDev(object, ...)
```

Arguments

object	pcaRes object
...	Not used

Value

Standard devations of the scores

Author(s)

Henning Redestig

show-methods *Print/Show for pcaRes*

Description

Print basic information about pcaRes object

Usage

```
showPcaRes(x, ...)

## S4 method for signature 'pcaRes'
print(x, ...)

## S4 method for signature 'pcaRes'
show(object)
```

Arguments

x	a pcaRes object
...	not used
object	the object to print information about

Value

nothing, used for its side effect

Author(s)

Henning Redestig

---

showNniRes *Print a nniRes model*

Description

Print a brief description of nniRes model

Usage

```
showNniRes(x, ...)
```

Arguments

x	An nniRes object
...	Not used

Value

Nothing, used for side-effect

Author(s)

Henning Redestig

---

simpleEllipse *Hotelling's T^2 Ellipse*

Description

Get a confidence ellipse for uncorrelated bivariate data

Usage

```
simpleEllipse(x, y, alfa = 0.95, len = 200)
```

Arguments

x	first variable
y	second variable
alfa	confidence level of the circle
len	Number of points in the circle

Details

As described in 'Introduction to multi and megavariate data analysis using PCA and PLS' by Eriksson et al. This produces very similar ellipse as compared to the ellipse function the ellipse package except that this function assumes that and y are uncorrelated (which they of are if they are scores or loadings from a PCA).

Value

A matrix with X and Y coordinates for the circle

Author(s)

Henning Redestig

See Also

ellipse

---

slplot,pcaRes-method *Side by side scores and loadings plot*

Description

A common way of visualizing two principal components

Usage

```
slplot(object, pcs=c(1,2), scoresLoadings=c(TRUE, TRUE),
sl="def", ll="def", hotelling=0.95, rug=TRUE, sub=NULL,...)
```

Arguments

object	a pcaRes object
pcs	which two pcs to plot
scoresLoadings	Which should be shown scores and or loadings
sl	labels to plot in the scores plot
ll	labels to plot in the loadings plot
hotelling	confidence interval for ellipse in the score plot

rug	logical, rug x axis in score plot or not
sub	Subtitle, defaults to annotate with amount of explained variance.
...	Further arguments to plot functions. Prefix arguments to par() with 's' for the scores plot and 'l' for the loadings plot. I.e. cex become scex for setting character expansion in the score plot and lcex for the loadings plot.

Details

This method is meant to be used as a quick way to visualize results, if you want a more specific plot you probably want to get the scores, loadings with scores(object), loadings(object) and then design your own plotting method.

Value

None, used for side effect.

Note

Uses layout instead of par to provide side-by-side so it works with Sweave (but can not be combined with par(mfrow=..))

Author(s)

Henning Redestig

See Also

pca, biplot

Examples

```
data(iris)
pcIr <- pca(iris[,1:4], scale="uv")
slplot(pcIr, sl=NULL, spch=5)
slplot(pcIr, sl=NULL, lcex=1.3, scol=as.integer(iris[,5]))
```

---

sortFeatures *Sort the features of NLPCA object*

Description

Sort the features of NLPCA object

Usage

```
sortFeatures(nlnet, trainIn, trainOut)
```

Arguments

nlnet	The nlnet
trainIn	Training data in
trainOut	Training data after it passed through the net

Value

...

Author(s)

Henning Redestig

---

summary *Summary of PCA model*

Description

Print a brief description of the PCA model

Usage

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

Arguments

object	a pcaRes object
...	Not used

Value

Nothing, used for side-effect

Author(s)

Henning Redestig

svdImpute *SVDimpute algorithm*

Description

This implements the SVDimpute algorithm as proposed by Troyanskaya et al, 2001. The idea behind the algorithm is to estimate the missing values as a linear combination of the k most significant eigengenes.

Usage

```
svdImpute(Matrix, nPcs = 2, threshold = 0.01, maxSteps = 100,
  verbose = interactive(), ...)
```

Arguments

Matrix	matrix – Pre-processed (centered, scaled) data with variables in columns and observations in rows. The data may contain missing values, denoted as NA.
nPcs	numeric – Number of components to estimate. The preciseness of the missing value estimation depends on the number of components, which should resemble the internal structure of the data.
threshold	The iteration stops if the change in the matrix falls below this threshold.
maxSteps	Maximum number of iteration steps.
verbose	Print some output if TRUE.
...	Reserved for parameters used in future version of the algorithm

Details

Missing values are denoted as NA. It is not recommended to use this function directely but rather to use the pca() wrapper function.

As SVD can only be performed on complete matrices, all missing values are initially replaced by 0 (what is in fact the mean on centred data). The algorithm works iteratively until the change in the estimated solution falls below a certain threshold. Each step the eigengenes of the current estimate are calculated and used to determine a new estimate. Eigengenes denote the loadings if pca is performed considering variable (for Microarray data genes) as observations.

An optimal linear combination is found by regressing the incomplete variable against the k most significant eigengenes. If the value at position j is missing, the j^th value of the eigengenes is not used when determining the regression coefficients.

Value

Standard PCA result object used by all PCA-based methods of this package. Contains scores, loadings, data mean and more. See pcaRes for details.

Note

Each iteration, standard PCA (prcomp) needs to be done for each incomplete variable to get the eigengenes. This is usually fast for small data sets, but complexity may rise if the data sets become very large.

Author(s)

Wolfram Stacklies

References

Troyanskaya O. and Cantor M. and Sherlock G. and Brown P. and Hastie T. and Tibshirani R. and Botstein D. and Altman RB. - Missing value estimation methods for DNA microarrays. *Bioinformatics. 2001 Jun;17(6):520-5.*

Examples

```
## Load a sample metabolite dataset with 5\% missing values
data(metaboliteData)
## Perform svdImpute using the 3 largest components
result <- pca(metaboliteData, method="svdImpute", nPcs=3, center = TRUE)
## Get the estimated complete observations
cObs <- completeObs(result)
## Now plot the scores
plotPcs(result, type = "scores")
```

---

svdPca *Perform principal component analysis using singular value decomposition*

Description

A wrapper function for prcomp to deliver the result as a pcaRes method. Supplied for compatibility with the rest of the pcaMethods package. It is not recommended to use this function directely but rather to use the pca() wrapper function.

Usage

```
svdPca(Matrix, nPcs = 2, varLimit = 1, verbose = interactive(), ...)
```

Arguments

Matrix	Pre-processed (centered and possibly scaled) numerical matrix samples in rows and variables as columns. No missing values allowed.
nPcs	Number of components that should be extracted.
varLimit	Optionally the ratio of variance that should be explained. nPcs is ignored if varLimit < 1
verbose	Verbose complaints to matrix structure
...	Only used for passing through arguments.

Value

A pcaRes object.

Author(s)

Henning Redestig

See Also

prcomp, princomp, pca

Examples

```
data(metaboliteDataComplete)
mat <- prep(t(metaboliteDataComplete))
pc <- svdPca(mat, nPcs=2)
## better use pca()
pc <- pca(t(metaboliteDataComplete), method="svd", nPcs=2)
```

---

tempFixNas *Temporary fix for missing values*

Description

Simply replace completely missing rows or cols with zeroes.

Usage

```
tempFixNas(mat)
```

Arguments

mat	a matrix

Value

The original matrix with completely missing rows/cols filled with zeroes.

Author(s)

Henning Redestig

`vector2matrices,matrix-method`

Tranform the vectors of weights to matrix structure

Description

Tranform the vectors of weights to matrix structure

Usage

```
## S4 method for signature 'matrix'
vector2matrices(object, net)
```

Arguments

`object`	an nlpcaNet
`net`	the neural network

Value

weights in matrix structure

Author(s)

Henning Redestig

`vector2matrices,nlpcaNet-method`

Tranform the vectors of weights to matrix structure

Description

Tranform the vectors of weights to matrix structure

Usage

```
## S4 method for signature 'nlpcaNet'
vector2matrices(object)
```

Arguments

`object`	an nlpcaNet

Value

weights in matrix structure

Author(s)

Henning Redestig

`wasna,pcaRes-method` *Get a matrix with indicating the elements that were missing in the input data. Convenient for estimating imputation performance.*

Description

Get a matrix with indicating the elements that were missing in the input data. Convenient for estimating imputation performance.

Usage

```
wasna(object, ...)
```

Arguments

`object`	pcaRes object
`...`	Not used

Value

A matrix with logicals

Author(s)

Henning Redestig

Examples

```
data(metaboliteData)
data(metaboliteDataComplete)
result <- pca(metaboliteData, nPcs=2)
plot(completeObs(result)[wasna(result)], metaboliteDataComplete[wasna(result)])
```

`weightsAccount` *Create an object that holds the weights for nlpcaNet. Holds and sets weights in using an environment object.*

Description

Create an object that holds the weights for nlpcaNet. Holds and sets weights in using an environment object.

Usage

```
weightsAccount(w)
```

Arguments

`w`	`matrix` – New weights

Value

A weightsAccound with `set` and `current` functions.

Author(s)

Henning Redestig

Index

∗ **algebra**
  robustSvd, 60
∗ **classes**
  nniRes, 36
  pcaNet, 43
  pcaRes, 45
∗ **datasets**
  helix, 19
  metaboliteData, 29
  metaboliteDataComplete, 30
∗ **multivariate**
  asExprSet, 4
  biplot-methods, 4
  bpca, 5
  checkData, 10
  fitted-methods, 17
  kEstimate, 19
  kEstimateFast, 22
  leverage,pcaRes-method, 23
  llsImpute, 26
  nipalsPca, 31
  nni, 35
  pca, 40
  plotPcs, 47
  ppca, 48
  predict-methods, 50
  Q2, 52
  rediduals-methods, 55
  RnipalsPca, 57
  robustPca, 58
  slplot,pcaRes-method, 66
  svdImpute, 69
  svdPca, 70

asExprSet, 4

biplot, *67*
biplot,pcaRes-method *(*biplot-methods*)*, 4
biplot-methods, 4
biplot.pcaRes *(*biplot-methods*)*, 4

bpca, 5, *41*, *50*
BPCA_dostep, 8
BPCA_initmodel, 8

center *(*center,pcaRes-method*)*, 9
center,pcaRes-method, 9
centered *(*centered,pcaRes-method*)*, 10
centered,pcaRes-method, 10
checkData, 10
completeObs
        *(*completeObs,nniRes-method*)*, 11
completeObs,nniRes-method, 11
completeObs,pcaRes-method
        *(*completeObs,nniRes-method*)*, 11
cvseg, 12
cvstat *(*cvstat,pcaRes-method*)*, 13
cvstat,pcaRes-method, 13

deletediagonals, 13
derrorHierarchic, 14
dim.pcaRes, 14
DModX *(*DModX,pcaRes-method*)*, 15
DModX,pcaRes-method, 15

errorHierarchic, 16

fitted,pcaRes-method *(*fitted-methods*)*,
        17
fitted-methods, 17
fitted.pcaRes *(*fitted-methods*)*, 17
forkNlpcaNet, 18

getHierarchicIdx, 18

helix, 19

kEstimate, *7*, 19, *23*
kEstimateFast, *21*, 22

leverage *(*leverage,pcaRes-method*)*, 23
leverage,pcaRes-method, 23

lineSearch, 24
linr, 25
listPcaMethods, 25
llsImpute, 26, *35*
loadings *(*loadings,ANY-method*)*, 28
loadings,ANY-method, 28
loadings,pcaRes-method, 28
loadings.pcaRes, 29, *29*

metaboliteData, 29, *30*
metaboliteDataComplete, 30, *30*
method *(*method,pcaRes-method*)*, 31
method,pcaRes-method, 31

nipals, *61*
nipalsPca, *7*, 31, *41*, *42*, *50*
nlpca, 32, *45*
nlpcaNet *(*pcaNet*)*, 43
nlpcaNet-class *(*pcaNet*)*, 43
nmissing *(*nmissing,pcaRes-method*)*, 34
nmissing,nniRes-method
*(*nmissing,pcaRes-method*)*, 34
nmissing,pcaRes-method, 34
nni, *21*, *27*, 35
nniRes, *27*, 36
nniRes-class *(*nniRes*)*, 36
nObs *(*nObs,pcaRes-method*)*, 37
nObs,pcaRes-method, 37
nP *(*nP,pcaRes-method*)*, 37
nP,pcaRes-method, 37
nPcs *(*nPcs,pcaRes-method*)*, 38
nPcs,pcaRes-method, 38
nVar *(*nVar,pcaRes-method*)*, 38
nVar,pcaRes-method, 38

optiAlgCgd, 39
orth, 40

pairs, *48*
pca, *7*, *21*, *22*, *27*, *35*, 40, *50*, *53*, *67*
pcaMethods, 42
pcaMethods-deprecated, 43
pcaMethods-package *(*pcaMethods*)*, 42
pcaNet, 43
pcaRes, *7*, *33*, 45, *49*, *50*, *59*, *69*
pcaRes-class *(*pcaRes*)*, 45
plot,pcaRes-method *(*plot.pcaRes*)*, 46
plot.pcaRes, 46
plotPcs, 47

ppca, *7*, *41*, 48
prcomp, *7*, *42*, *50*, *59*
predict,pcaRes-method
*(*predict-methods*)*, 50
predict-methods, 50
predict.pcaRes, *56*
predict.pcaRes *(*predict-methods*)*, 50
prep, *41*, 51, *62*
princomp, *42*
print,nniRes-method *(*show-methods*)*, 64
print,pcaRes-method *(*show-methods*)*, 64

Q2, *21*, *41*, 52

R2cum *(*R2cum,pcaRes-method*)*, 54
R2cum,pcaRes-method, 54
R2VX *(*R2VX,pcaRes-method*)*, 55
R2VX,pcaRes-method, 55
rediduals-methods, 55
repmat, 56
resid,pcaRes-method
*(*rediduals-methods*)*, 55
residuals,pcaRes-method
*(*rediduals-methods*)*, 55
residuals.pcaRes *(*rediduals-methods*)*, 55
RnipalsPca, 57
robustPca, 58
robustSvd, *59*, 60

scale, *52*
scaled *(*scaled,pcaRes-method*)*, 61
scaled,pcaRes-method, 61
scl *(*scl,pcaRes-method*)*, 62
scl,pcaRes-method, 62
scores *(*scores,pcaRes-method*)*, 62
scores,pcaRes-method, 62
scores.pcaRes, 63, *63*
screeplot, *47*
sDev *(*sDev,pcaRes-method*)*, 64
sDev,pcaRes-method, 64
show,nniRes-method *(*show-methods*)*, 64
show,pcaRes-method *(*show-methods*)*, 64
show-methods, 64
showNniRes, 65
showPcaRes *(*show-methods*)*, 64
simpleEllipse, 65
slplot *(*slplot,pcaRes-method*)*, 66
slplot,pcaRes-method, 66
sortFeatures, 67

summary, 68
summary,pcaRes-method *(summary)*, 68
summary.pcaRes *(summary)*, 68
svd, *59*, *61*
svdImpute, *7*, *41*, *50*, 69
svdPca, *41*, *42*, 70

tempFixNas, 71

vector2matrices,matrix-method, 72
vector2matrices,nlpcaNet-method, 72

wasna *(wasna,pcaRes-method)*, 73
wasna,pcaRes-method, 73
weightsAccount, 74