Package 'singR'

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Type Package

Title Simultaneous Non-Gaussian Component Analysis

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Description Implementation of SING algorithm to extract joint and individual non-Gaussian components from two datasets. SING uses an objective function that maximizes the skewness and kurtosis of latent components with a penalty to enhance the similarity between subject scores. Unlike other existing methods, SING does not use PCA for dimension reduction, but rather uses non-Gaussianity, which can improve feature extraction. Benjamin B.Risk, Irina Gaynanova (2021) <doi:10.1214/21-AOAS1466>.

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LazyData true

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LinkingTo Rcpp, RcppArmadillo

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VignetteBuilder knitr

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R topics documented:

`angleMatchICA` *Match the colums of Mx and My*

Description

`angleMatchICA` match the colums of Mx and My, using the n x p parameterization of the JIN decomposition assumes

Usage

```
angleMatchICA(Mx, My, Sx = NULL, Sy = NULL)
```

Arguments

`Mx`	Subject score for X matrix of n x n.comp
`My`	Subject score for Y matrix of n x n.comp
`Sx`	Variable loadings for X matrix of n.comp x px
`Sy`	Variable loadings for Y matrix of n.comp x py

Value

a list of matrixes: ## Mx: ## My: ## matchedangles: ## allangles: ## perm: ## omangles:

`aveM` *Average Mj for Mx and My*

Description

Average Mj for Mx and My

Usage

```
aveM(mjX, mjY)
```

Arguments

`mjX`	n x rj
`mjY`	n x rj

Value

a new Mj

`calculateJB` *Calculates the sum of the JB scores across all components, useful for determining rho. The data has to be standardized and mean 0 and sd to 1.*

Description

Calculates the sum of the JB scores across all components, useful for determining rho. The data has to be standardized and mean 0 and sd to 1.

Usage

```
calculateJB(S = NULL, U = NULL, X = NULL, alpha = 0.8)
```

Arguments

`S`	the variable loadings r x px.
`U`	U matrix for matched columns rj x n
`X`	whitened data matrix n x px, data = whitenerXA %*% dXcentered
`alpha`	JB weighting of skewness and kurtosis. default = 0.8

Value

the sum of JB score across all components.

`covwhitener` *Returns square root of the precision matrix for whitening*

Description

Returns square root of the precision matrix for whitening

Usage

```
covwhitener(X, n.comp = ncol(X), center.row = FALSE)
```

Arguments

`X`	Matrix
`n.comp`	the number of components
`center.row`	whether to center

Value

square root of the precision matrix for whitening

`create.graph.long` *create graph dataset with netmat and mmp_order a data.frame called with vectorization of reordered netmat by mmp_order.*

Description

create graph dataset with netmat and mmp_order a data.frame called with vectorization of reordered netmat by mmp_order.

Usage

```
create.graph.long(gmatrix, sort_indices = NULL)
```

Arguments

`gmatrix`	netmat
`sort_indices`	mmp_order

Value

a data.frame with vectors: ## X1: vector of numerics. ## X2: vector of numerics. ## value: vectorization of reordered netmat by mmp_order.

curvilinear *Curvilinear algorithm with r0 joint components*

Description

Curvilinear algorithm with r0 joint components

Usage

```
curvilinear(
  Ux,
  Uy,
  xData,
  yData,
  invLx,
  invLy,
  rho,
  tau = 0.01,
  alpha = 0.8,
  maxiter = 1000,
  tol = 1e-06,
  rj
)
```

Arguments

Ux	Matrix with n.comp x n, initial value of Ux, comes from greedyMatch.
Uy	Matrix with n.comp x n, initial value of Uy, comes from greedyMatch.
xData	matrix with n x px, Xw = Lx %*% Xc.
yData	matrix with n x py, Yw = Ly %*% Yc.
invLx	Inverse matrix of Lx, matrix n x n.
invLy	Inverse matrix of Ly, matrix n x n.
rho	the weight parameter of matching relative to non-gaussianity.
tau	initial step size, default value is 0.01
alpha	controls weighting of skewness and kurtosis. Default value is 0.8, which corresponds to the Jarque-Bera test statistic with 0.8 weighting on squared skewness and 0.2 on squared kurtosis.
maxiter	default value is 1000
tol	the threshold of change in Ux and Uy to stop the curvlinear function
rj	the joint rank, comes from greedyMatch.

Value

a list of matrices:

`Ux` Optimized Ux with matrix n.comp x n.

`Uy` Optimized Uy with matrix n.comp x n.

`tau` step size

`iter` number of iterations.

`error` PMSE(Ux,Uxnew)+PMSE(Uy,Uynew)

`obj` Objective Function value

`curvilinear_c` *Curvilinear algorithm based on C code with r0 joint components*

Description

Curvilinear algorithm based on C code with r0 joint components

Usage

```
curvilinear_c(
  Ux,
  Uy,
  xData,
  yData,
  invLx,
  invLy,
  rho,
  tau = 0.01,
  alpha = 0.8,
  maxiter = 1000,
  tol = 1e-06,
  rj
)
```

Arguments

`Ux`	Matrix with n.comp x n, initial value of Ux, comes from greedyMatch.
`Uy`	Matrix with n.comp x n, initial value of Uy, comes from greedyMatch.
`xData`	matrix with n x px, Xw = Lx %*% Xc.
`yData`	matrix with n x py, Yw = Ly %*% Yc.
`invLx`	Inverse matrix of Lx, matrix n x n.
`invLy`	Inverse matrix of Ly, matrix n x n.
`rho`	the weight parameter of matching relative to non-gaussianity.

tau	initial step size, default value is 0.01
alpha	controls weighting of skewness and kurtosis. Default value is 0.8, which corresponds to the Jarque-Bera test statistic with 0.8 weighting on squared skewness and 0.2 on squared kurtosis.
maxiter	default value is 1000
tol	the threshold of change in Ux and Uy to stop the curvilinear function
rj	the joint rank, comes from greedyMatch.

Value

a list of matrices:

Ux Optimized Ux with matrix n.comp x n.

Uy Optimized Uy with matrix n.comp x n.

tau step size

iter number of iterations.

error PMSE(Ux,Uxnew)+PMSE(Uy,Uynew)

obj Objective Function value

---

est.M.ols *Estimate mixing matrix from estimates of components*

Description

Estimate mixing matrix from estimates of components

Usage

```
est.M.ols(sData, xData, intercept = TRUE)
```

Arguments

sData	S rx x px
xData	dX n x px
intercept	default = TRUE

Value

a matrix Mx, dimension n x rx.

exampledata *Data for simulation example 1*

Description

Data for simulation example 1

Usage

```
exampledata
```

Format

A data list with 10 subsets:

dX original data matrix for X with n x px, 48x3602

dY original data matrix for Y with n x py, 48x4950

mj true mj matrix, n x rj, 48x2

sIx true S matrix of independent non-Gaussian components in X, ri_x x px, 2x3602

sIy true S matrix of independent non-Gaussian components in Y, ri_y x py, 2x4950

sjx true S matrix of joint non-Gaussian components in X, rj x px, 2x3602

sjy true S matrix of joint non-Gaussian components in Y, rj x py, 2x4950

snr signal to noise ratio

R2x R2 for x data

R2y R2 for y data

gen.inits *Generate initialization from specific space*

Description

Generate initialization from specific space

Usage

```
gen.inits(p, d, runs, orth.method = c("svd", "givens"))
```

Arguments

p	p*p orthodox matrix
d	p*d orthodox matrix
runs	the number of orthodox matrix
orth.method	orthodox method

Value

a list of initialization of mixing matrices.

Examples

```
gen.inits(2,3,3,'svd')
```

`greedymatch` *Greedy Match*

Description

`Greedy Match` matches a column of Mx and My by minimizing chordal distance between vectors, removes the matched columns and then finds the next pair. This equivalent to maximizing absolute correlation for data in which each column has mean equal to zero. Returns permuted columns of Mx and My. This function does not do any scaling or sign flipping. For this matching to coincide with angle matching, the columns must have zero mean.

Usage

```
greedymatch(Mx, My, Ux, Uy)
```

Arguments

`Mx`	Subject Score for X with n x n.comp.X matrix
`My`	Subject Score for Y with n x n.comp.Y matrix
`Ux`	Matrix with n.comp x n, Mx = Lx^-1 %*% t Ux, Lx is the whitener matrix of dX.
`Uy`	Matrix with n.comp x n, My = Ly^-1 %*% t Uy, Ly is the whitener matrix of dY.

Value

a list of matrices:

`Mx` Columns of original Mx reordered from highest to lowest correlation with matched component in My

`My` Columns of original My reordered from highest to lowest correlation with matched component in Mx

`Ux` Permuted rows of original Ux corresponds to MapX

`Uy` Permuted rows of original Uy corresponds to MapY

`correlations` a vector of correlations for each pair of columns in permuted Mx and M

`mapX` the sequence of the columns in original Mx.

`mapY` the sequence of the columns in original MY.

`lngca` *Decompose the original data through LNGCA method.*

Description

Implements the methods of linear non-Gaussian component analysis (LNGCA) and likelihood component analysis (when using a density, e.g., tilted Gaussian) from the LNGCA paper

Usage

```
lngca(
  xData,
  n.comp = NULL,
  Ux.list = NULL,
  whiten = c("sqrtprec", "eigenvec", "none"),
  maxit = 1000,
  eps = 1e-06,
  verbose = FALSE,
  restarts.pbyd = 0,
  restarts.dbyd = 0,
  distribution = c("JB", "tiltedgaussian", "logistic"),
  density = FALSE,
  out.all = FALSE,
  orth.method = c("svd", "givens"),
  df = 0,
  stand = FALSE,
  ...
)
```

Arguments

`xData`	the original dataset for decomposition, matrix of n x px.
`n.comp`	the number of components to be estimated.
`Ux.list`	list of user specified initial values for Ux. If null, will generate random orthogonal matrices. See restarts.pbyd and restarts.dbyd
`whiten`	whitening method. Defaults to "svd" which uses the n left eigenvectors divided by sqrt(px-1). Optionally uses the square root of the n x n "precision" matrix.
`maxit`	max iteration, defalut = 1000
`eps`	default = 1e-06
`verbose`	default = FALSE
`restarts.pbyd`	default = 0. Generates p x d random orthogonal matrices. Use a large number for large datasets. Note: it is recommended that you run lngca twice with different seeds and compare the results, which should be similar when a sufficient number of restarts is used. In practice, stability with large datasets and a large number of components can be challenging.

restarts.dbyd	default = 0. These are d x d initial matrices padded with zeros, which results in initializations from the principal subspace. Can speed up convergence but may miss low variance non-Gaussian components.
distribution	distribution methods with default to tilted Gaussian. "logistic" is similar to infomax ICA, JB is capable of capture super and sub Gaussian distribution while being faster than tilted Gaussian. (tilted Gaussian tends to be most accurate, but computationally much slower.)
density	return the estimated tilted Gaussian density? default = FALSE
out.all	default = FALSE
orth.method	default = 'svd'. Method to generate random initial matrices. See [gen.inits()]
df	default = 0, df of the spline used in fitting the non-parametric density. use df=8 or so for tilted gaussian. set df=0 for JB and logistic.
stand	whether to standardize the data to have row and column means equal to 0 and the row standard deviation equal to 1 (i.e., all variables on same scale). Often used when combined with singR for data integration.
...	other arguments to tiltedgaussian estimation

Value

Function outputs a list including the following:

U matrix rx x n, part of the expression that Ax = Ux x Lx and Ax x Xc = Sx, where Lx is the whitener matrix.

loglik the value of log-likelihood in the lngca method.

S the variable loading matrix r x px, each row is a component, which can be used to measure nongaussianity

df egree of freedom.

distribution the method used for data decomposition.

whitener A symmetric whitening matrix n x n from dX, the same with whitenerXA = est.sigmaXA %^% -0.5

M Mx Mtrix with n x rx.

nongaussianity the nongaussianity score for each component saved in S matrix.

Examples

```
#get simulation data
data(exampledata)
data=exampledata

# To get n.comp value, we can use NG_number function.

# use JB statistic as the measure of nongaussianity to run lngca with df=0
estX_JB = lngca(xData = data$dX, n.comp = 4,
 whiten = 'sqrtprec', restarts.pbyd = 20, distribution='JB',df=0)
```

```
# use the tiltedgaussian distribution to run lngca with df=8. This takes a long time:
estX_tilt = lngca(xData = data$dX, n.comp = 4,
 whiten = 'sqrtprec', restarts.pbyd = 20, distribution='tiltedgaussian',df=8)

# true non-gaussian component of Sx, include individual and joint components
trueSx = rbind(data$sjX,data$siX)

# use pmse to compare the difference of the two methods
pmse(S1 = t(trueSx),S2=t(estX_JB$S),standardize = TRUE)
pmse(S1 = t(trueSx),S2=t(estX_tilt$S),standardize = TRUE)

# the lngca using tiltedgaussian tends to be more accurate
# with smaller pmse value, but takes longer to run.
```

`matchICA` *match ICA*

Description

match ICA

Usage

```
matchICA(S, template, M = NULL)
```

Arguments

`S`	loading variable matrix
`template`	template for match
`M`	subject score matrix

Value

the match result

`NG_number` *find the number of non-Gaussian components in the data.*

Description

find the number of non-Gaussian components in the data.

Usage

```
NG_number(data, type = "S3")
```

Arguments

data	original matrix with n x p.
type	'S1', 'S2' or 'S3'

Value

the number of non-Gaussian components in the data.

Examples

```
library(singR)
data("exampledata")
data=exampledata
NG_number(data$dX)
```

---

orthogonalize *Orthogonalization of matrix*

Description

Orthogonalization of matrix

Usage

```
orthogonalize(W)
```

Arguments

W	arbitrary matrix

Value

orthogonalized matrix

permmatRank_joint *Permutation test to get joint components ranks*

Description

Permutation test to get joint components ranks

Usage

```
permmatRank_joint(matchedResults, nperms = 100)
```

Arguments

matchedResults	results generated by angleMatchICA
nperms	the number of permutation

Value

a list of matrixes ## pvalues: pvalues for the matched colunmns don't have correlation. ## corrperm: correlation value for original Mx with each random permutation of My. ## corrmatched: the correlation for each pair of matched columns.

permTestJointRank *Permutation test with Greedymatch*

Description

Permutation test with Greedymatch

Usage

```
permTestJointRank(
  MatchedMx,
  MatchedMy,
  nperm = 1000,
  alpha = 0.01,
  multicore = 0
)
```

Arguments

MatchedMx	matrix with nsubject x n.comp.X, comes from greedymatch
MatchedMy	matrix with nsubject2 x n.comp.Y, comes from greedymatch
nperm	default value = 1000
alpha	default value = 0.01
multicore	default value = 0

Value

a list of matrixes ## rj: joint component rank ## pvalues: pvalue for the components(columns) not matched ## fwer_alpha: quantile of corr permutation with 1- alpha

---

pmse *Permutation invariant mean squared error*

Description

Permutation invariant mean squared error

Usage

```
pmse(M1 = NULL, M2 = NULL, S1 = NULL, S2 = NULL, standardize = FALSE)
```

Arguments

M1	Subject score 1 matrix r x n.
M2	Subject score 2 matrix r x n.
S1	Loading 1 with matrix p x r.
S2	Loading 2 with matrix p x r.
standardize	whether to standardize

Value

permutation invariant mean squared error

---

signchange *Sign change for S matrix to image*

Description

Sign change for S matrix to image

Usage

```
signchange(S, M = NULL)
```

Arguments

S	S, r x px.
M	Mx, n x r.

Value

a list of positive S and positive Mx.

singR *SImultaneous Non-Gaussian Component analysis for data integration.*

Description

This function combines all steps from the SING paper

Usage

```
singR(
  dX,
  dY,
  n.comp.X = NULL,
  n.comp.Y = NULL,
  df = 0,
  rho_extent = c("small", "medium", "large"),
  Cplus = TRUE,
  tol = 1e-10,
  stand = FALSE,
  distribution = "JB",
  maxiter = 1500,
  individual = FALSE,
  whiten = c("sqrtprec", "eigenvec", "none"),
  restarts.dbyd = 0,
  restarts.pbyd = 20
)
```

Arguments

dX	original dataset for decomposition, matrix of n x px.
dY	original dataset for decomposition, matrix of n x py.
n.comp.X	the number of non-Gaussian components in dataset X. If null, will estimate the number using ICtest::FOBIasymp.
n.comp.Y	the number of non-Gaussian components in dataset Y. If null, will estimate the number using ICtest::FOBIasymp.
df	default value=0 when use JB, if df>0, estimates a density for the loadings using a tilted Gaussian (non-parametric density estimate).
rho_extent	Controls similarity of the scores in the two datasets. Numerical value and three options in character are acceptable. small, medium or large is defined from the JB statistic. Try "small" and see if the loadings are equal, then try others if needed. If numeric input, it will multiply the input by JBall to get the rho.
Cplus	whether to use C code (faster) in curvilinear search.
tol	difference tolerance in curvilinear search.
stand	whether to use standardization, if true, it will make the column and row means to 0 and columns sd to 1. If false, it will only make the row means to 0.

distribution	"JB" or "tiltedgaussian"; "JB" is much faster. In SING, this refers to the "density" formed from the vector of loadings. "tiltedgaussian" with large df can potentially model more complicated patterns.
maxiter	the max iteration number for the curvilinear search.
individual	whether to return the individual non-Gaussian components, default value = F.
whiten	whitening method used in lngca. Defaults to "svd" which uses the n left eigenvectors divided by sqrt(px-1). Optionally uses the square root of the n x n "precision" matrix.
restarts.dbyd	default = 0. These are d x d initial matrices padded with zeros, which results in initializations from the principal subspace. Can speed up convergence but may miss low variance non-Gaussian components.
restarts.pbyd	default = 20. Generates p x d random orthogonal matrices. Use a large number for large datasets. Note: it is recommended that you run lngca twice with different seeds and compare the results, which should be similar when a sufficient number of restarts is used. In practice, stability with large datasets and a large number of components can be challenging.

Value

Function outputs a list including the following:

`Sjx` variable loadings for joint NG components in dataset X with matrix rj x px.

`Sjy` variable loadings for joint NG components in dataset Y with matrix rj x py.

`Six` variable loadings for individual NG components in dataset X with matrix riX x px.

`Siy` variable loadings for individual NG components in dataset Y with matrix riX x py.

`Mix` scores of individual NG components in X with matrix n x riX.

`Miy` scores of individual NG components in Y with matrix n x riY.

`est.Mjx` Estimated subject scores for joint components in dataset X with matrix n x rj.

`est.Mjy` Estimated subject scores for joint components in dataset Y with matrix n x rj.

`est.Mj` Average of est.Mjx and est.Mjy as the subject scores for joint components in both datasets with matrix n x rj.

`C_plus` whether to use C version of curvilinear search.

`rho_extent` the weight of rho in search

`df` degree of freedom, = 0 when use JB, >0 when use tiltedgaussian.

Examples

```
#get simulation data
library(singR)
data(exampledata)

# use JB stat to compute with singR
output_JB=singR(dX=exampledata$dX,dY=exampledata$dY,
df=0,rho_extent="small",distribution="JB",individual=TRUE)
```

```
# use tiltedgaussian distribution to compute with singR.
# tiltedgaussian may be more accurate but is considerably slower,
# and is not recommended for large datasets.
output_tilted=singR(dX=expampledata$dX,dY=expampledata$dY,
df=5,rho_extent="small",distribution="tiltedgaussian",individual=TRUE)

# use pmse to measure difference from the truth
pmse(M1 = t(output_JB$est.Mj),M2 = t(expampledata$mj),standardize = TRUE)

pmse(M1 = t(output_tilted$est.Mj),M2 = t(expampledata$mj),standardize = TRUE)
```

`standard` *Standardization with double centered and column scaling*

Description

Standardization with double centered and column scaling

Usage

```
standard(data, dif.tol = 0.001, max.iter = 10)
```

Arguments

`data`	input matrix with n x px.
`dif.tol`	the value for the threshold of scaling
`max.iter`	default value = 10

Value

standardized matrix with n x px.

Examples

```
spmwm = 3*matrix(rnorm(100000),nrow=100)+1
dim(spmwm)
apply(spmwm,1,mean) # we want these to be 0
apply(spmwm,2,mean) # we want these to be 0
apply(spmwm,2,sd) # we want each of these variances to be 1

spmwm_cp=standard(spmwm)
max(abs(apply(spmwm_cp,1,mean)))
max(abs(apply(spmwm_cp,2,mean)))
max(abs(apply(spmwm_cp,2,sd)-1))
```

theta2W *Convert angle vector into orthodox matrix*

Description

Convert angle vector into orthodox matrix

Usage

```
theta2W(theta)
```

Arguments

theta	vector of angles theta

Value

an orthodox matrix

tiltedgaussian *tiltedgaussian*

Description

tiltedgaussian

Usage

```
tiltedgaussian(xData, df = 8, B = 100, ...)
```

Arguments

xData	input data
df	degree freedom
B	default value=100
...	ellipsis

vec2net *Create network matrices from vectorized lower diagonals* vec2net *transfer the matrix vectorized lower diagonals into net to show the component image.*

Description

Create network matrices from vectorized lower diagonals vec2net transfer the matrix vectorized lower diagonals into net to show the component image.

Usage

```
vec2net(invector, make.diag = 1)
```

Arguments

invector	vectorized lower diagonals.
make.diag	default value = 1.

Value

a net matrx

Examples

```
net = vec2net(1:10)
```

whitener *Whitening Function*

Description

Whitening Function

Usage

```
whitener(X, n.comp = ncol(X), center.row = FALSE)
```

Arguments

X	dataset p x n.
n.comp	the number of components
center.row	whether center the row of data

Value

a whitener matrix

`%^%` *Calculate the power of a square matrix*

Description

returns a matrix composed of eigenvector x diag(eigenvalue ^ power) x eigenvector'

Usage

```
S %^% power
```

Arguments

`S`	a square matrix
`power`	the times of power

Value

a matrix after power calculation that eigenvector x diag(eigenvalue ^ power) x eigenvector'

Examples

```
a <- matrix(1:9,3,3)
a %^% 2
```

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