Package 'msma'

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Type Package

Title Multiblock Sparse Multivariable Analysis

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Depends mytnorm
Description Several functions can be used to analyze multiblock multivariable data. If the input is a single matrix, then principal components analysis (PCA) is implemented. If the input is a list of matrices, then multiblock PCA is implemented. If the input is two matrices, for exploratory and objective variables, then partial least squares (PLS) analysis is implemented. If the input is two lists of matrices, for exploratory and objective variables, then multiblock PLS analysis is implemented. Additionally, if an extra outcome variable is specified, then a supervised version of the methods above is implemented. For each method, sparse modeling is also incorporated. Functions for selecting the number of components and regularized parameters are also provided.
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Description

A Package for Implementation of the method

Author(s)

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References

Kawaguchi A, Yamashita F (2017). Supervised Multiblock Sparse Multivariable Analysis with Application to Multimodal Brain Imaging Genetics. Biostatistics, 18(4) 651-665.

See Also

msma

cvmsma Cross-Validation

Description

cross-validated method to evaluate the fit of "msma".

```
cvmsma(
   X,
   Y = NULL,
   Z = NULL,
   comp = 1,
   lambdaX,
   lambdaY = NULL,
   lambdaYsup = NULL,
   lambdaYsup = NULL,
   eta = 1,
```

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```
type = "lasso",
inX = NULL,
inY = NULL,
inXsup = NULL,
inYsup = NULL,
muX = 0,
muY = 0,
nfold = 5,
seed = 1,
intseed = 1
```

Arguments

X a (list of) matrix, explanatory variable(s).
 Y a (list of) matrix, objective variable(s).
 Z a (list of) matrix, response variable(s).

comp numeric scalar for the maximum number of componets to be considered.

lambdaX numeric vector of regularized parameters for X with length equal to the number

of blocks. If omitted, no regularization is conducted.

lambdaY numeric vector of regularized parameters for Y with length equal to the number

of blocks. If omitted, no regularization is conducted.

lambdaXsup numeric vector of regularized parameters for the super weight of X with length

equal to the number of blocks. If omitted, no regularization is conducted.

lambdaYsup numeric vector of regularized parameters for the super weight of Y with length

equal to the number of blocks. If omitted, no regularization is conducted.

eta numeric scalar the parameter indexing the penalty family.

type a character.

inX a (list of) numeric vector to specify the variables of X which are always in the

model.

inY a (list of) numeric vector to specify the variables of X which are always in the

model.

inXsup a (list of) numeric vector to specify the blocks of X which are always in the

model.

inYsup a (list of) numeric vector to specify the blocks of Y which are always in the

model.

muX a numeric scalar for the weight of X for the supervised.
muY a numeric scalar for the weight of Y for the supervised.

nfold number of folds - default is 5.

seed number of seed for the random number.

intseed seed number for the random number in the parameter estimation algorithm.

Details

k-fold cross-validation for msma

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Value

err

The mean cross-validated errors which has three elements consisting of the mean of errors for X and Y, the errors for X and for Y.

Examples

```
##### data #####
tmpdata = simdata(n = 50, rho = 0.8, Yps = c(10, 12, 15), Xps = 20, seed=1)
X = tmpdata$X; Y = tmpdata$Y

##### One Component CV #####
cv1 = cvmsma(X, Y, comp = 1, lambdaX=2, lambdaY=1:3, nfold=5, seed=1)
cv1

##### Two Component CV #####
cv2 = cvmsma(X, Y, comp = 2, lambdaX=2, lambdaY=1:3, nfold=5, seed=1)
cv2
```

msma

Multiblock Sparse Partial Least Squares

Description

This is a function for a matrix decomposition method incorporating sparse and supervised modeling for a multiblock multivariable data analysis

```
msma(X, ...)
## Default S3 method:
msma(
 Χ,
  Y = NULL,
  Z = NULL
  comp = 2,
  lambdaX = NULL,
  lambdaY = NULL,
  lambdaXsup = NULL,
  lambdaYsup = NULL,
  eta = 1,
  type = "lasso",
  inX = NULL,
  inY = NULL,
  inXsup = NULL,
  inYsup = NULL,
 muX = 0,
```

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```
muY = 0,
  defmethod = "canonical",
  scaling = TRUE,
  verbose = FALSE,
  intseed = 1,
   ...
)

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

Arguments

١	•	
	Χ	a matrix or list of matrices indicating the explanatory variable(s). This parameter is required.
		further arguments passed to or from other methods.
	Υ	a matrix or list of matrices indicating objective variable(s). This is optional. If there is no input for Y, then PCA is implemented.
	Z	a vector, response variable(s) for implementing the supervised version of (multiblock) PCA or PLS. This is optional. The length of Z is the number of subjects. If there is no input for Z , then unsupervised PLS/PCA is implemented.
	comp	numeric scalar for the maximum number of componets to be considered.
	lambdaX	numeric vector of regularized parameters for X, with a length equal to the number of blocks. If lambdaX is omitted, no regularization is conducted.
	lambdaY	numeric vector of regularized parameters for Y, with a length equal to the number of blocks. If lambdaY is omitted, no regularization is conducted.
	lambdaXsup	numeric vector of regularized parameters for the super weight of \boldsymbol{X} with length equal to the number of blocks. If omitted, no regularization is conducted.
	lambdaYsup	numeric vector of regularized parameters for the super weight of Y with length equal to the number of blocks. If omitted, no regularization is conducted.
	eta	numeric scalar indicating the parameter indexing the penalty family. This version contains only choice $1.$
	type	a character, indicating the penalty family. In this version, only one choice is available: "lasso."
	inX	a vector or list of numeric vectors specifying the variables in X, always included in the model
	inY	a vector or list of numeric vectors specifying the variables in Y, always included in the model
	inXsup	a (list of) numeric vector to specify the blocks of X which are always in the model.
	inYsup	a (list of) numeric vector to specify the blocks of Y which are always in the model.
	muX	a numeric scalar for the weight of X for the supervised case. $0 \le muX \le 1$.
	muY	a numeric scalar for the weight of Y for the supervised case. $0 \le muY \le 1$.

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defmethod a character representing the deflation method. This version has only the choice

"canonical."

scaling a logical, indicating whether or not data scaling is performed. The default is

TRUE.

verbose information

intseed seed number for the random number in the parameter estimation algorithm.

x an object of class "msma", usually, a result of a call to msma

Details

msma requires at least one input X (a matrix or list). In this case, (multiblock) PCA is conducted. If Y is also specified, then a PLS is conducted using X as explanatory variables and Y as objective variables. This function scales each data matrix to a mean of 0 and variance of 1 in the default. The block structure can be represented as a list. If Z is also specified, a supervised version is implemented, and the degree is controlled by muX or muY, where $0 \le \max \le 1, 0 \le \max Y \le 1$, and $0 \le \max Y \le 1$. If a positive lambdaX or lambdaY is specified, then a sparse estimation based on the L1 penalty is implemented.

Value

wsY

dmode Which modes "PLS" or "PCA"

X Scaled X which has a list form.

Y Scaled Y which has a list form.

Xscale Scaling information for X. The means and standard deviations for each block of

X are returned.

Yscale Scaling information for Y. The means and standard deviations for each block of

Y are returned.

comp the number of componets wbX block loading for X sbX block score for X wbY block loading for Y block score for Y sbY ssX super score for X super loading for X wsX super score for Y ssY

nzwbX number of nonzeros in block loading for X
nzwbY number of nonzeros in block loading for Y
nzwsX number of nonzeros in super loading for X
nzwsY number of nonzeros in super loading for Y

super loading for Y

selectXnames names of selected variables for X selectYnames names of selected variables for Y

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Examples

```
##### data #####
tmpdata = simdata(n = 50, rho = 0.8, Yps = c(10, 12, 15), Xps = 20, seed=1)
X = tmpdata$X; Y = tmpdata$Y
##### One Component #####
fit1 = msma(X, Y, comp=1, lambdaX=2, lambdaY=1:3)
fit1
##### Two Component #####
fit2 = msma(X, Y, comp=2, lambdaX=2, lambdaY=1:3)
fit2
##### Matrix data #####
sigma = matrix(0.8, 10, 10)
diag(sigma) = 1
X2 = rmvnorm(50, rep(0, 10), sigma)
Y2 = rmvnorm(50, rep(0, 10), sigma)
fit3 = msma(X2, Y2, comp=1, lambdaX=2, lambdaY=2)
fit3
##### Sparse Principal Component Analysis #####
fit5 = msma(X2, comp=5, lambdaX=2.5)
summary(fit5)
```

ncompsearch

Search for Number of Components

Description

Determination of the number of components based on cross-validated method or Bayesian information criterion (BIC)

```
ncompsearch(
   X,
   Y = NULL,
   Z = NULL,
   comps = 1:3,
   lambdaX = NULL,
   lambdaY = NULL,
   lambdaYsup = NULL,
   lambdaYsup = NULL,
   eta = 1,
   type = "lasso",
```

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```
inX = NULL,
  inY = NULL,
  inXsup = NULL,
  inYsup = NULL,
 muX = 0,
 muY = 0,
 nfold = 5,
 regpara = FALSE,
 maxrep = 3,
 minpct = 0,
 maxpct = 1,
 criterion = c("CV", "BIC")[1],
 whichselect = NULL,
 intseed = 1
)
## S3 method for class 'ncompsearch'
print(x, ...)
## S3 method for class 'ncompsearch'
plot(x, ...)
```

Arguments

X	a matrix or list of matrices indicating the explanatory variable(s). This parameter is required.
Υ	a matrix or list of matrices indicating objective variable(s). This is optional. If there is no input for Y, then PCA is implemented.
Z	a vector, response variable(s) for implementing the supervised version of (multiblock) PCA or PLS. This is optional. The length of Z is the number of subjects. If there is no input for Z, then unsupervised PLS/PCA is implemented.
comps	numeric vector for the maximum numbers of componets to be considered.
lambdaX	numeric vector of regularized parameters for X, with a length equal to the number of blocks. If lambdaX is omitted, no regularization is conducted.
lambdaY	numeric vector of regularized parameters for Y, with a length equal to the number of blocks. If lambdaY is omitted, no regularization is conducted.
lambdaXsup	numeric vector of regularized parameters for the super weight of X with length equal to the number of blocks. If omitted, no regularization is conducted.
lambdaYsup	numeric vector of regularized parameters for the super weight of Y with length equal to the number of blocks. If omitted, no regularization is conducted.
eta	numeric scalar indicating the parameter indexing the penalty family. This version contains only choice 1.
type	a character, indicating the penalty family. In this version, only one choice is available: "lasso."
inX	a (list of) numeric vector to specify the variables of X which are always in the model.

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inY	a (list of) numeric vector to specify the variables of X which are always in the model.
inXsup	a (list of) numeric vector to specify the blocks of X which are always in the model.
inYsup	a (list of) numeric vector to specify the blocks of Y which are always in the model.
muX	a numeric scalar for the weight of X for the supervised case. $0 \le muX \le 1$.
muY	a numeric scalar for the weight of Y for the supervised case. $0 \le muY \le 1$.
nfold	number of folds - default is 5.
regpara	logical, If TRUE, the regularized parameters search is also conducted simultaneously.
maxrep	numeric scalar for the number of iteration.
minpct	minimum candidate parameters defined as a percentile of automatically determined (possible) candidates.
maxpct	maximum candidate parameters defined as a percentile of automatically determined (possible) candidates.
criterion	a character, the evaluation criterion, "CV" for cross-validation, based on a matrix element-wise error, and "BIC" for Bayesian information criteria. The "BIC" is the default.
whichselect	which blocks selected.
intseed	seed number for the random number in the parameter estimation algorithm.
X	an object of class "ncompsearch", usually, a result of a call to ncompsearch
	further arguments passed to or from other methods.

Details

This function searches for the optimal number of components.

Value

comps numbers of components
mincriterion minimum criterion values

criterions criterion values

optncomp optimal number of components based on minimum cross-validation error

Examples

```
##### data #####
tmpdata = simdata(n = 50, rho = 0.8, Yps = c(10, 12, 15), Xps = 20, seed=1)
X = tmpdata$X; Y = tmpdata$Y

##### number of components search #####
ncomp1 = ncompsearch(X, Y, comps = c(1, 5, 10*(1:2)), nfold=5)
plot(ncomp1)
```

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optparasearch

Parameters Search

Description

Combined method for optimizing the number of components and regularized parameters for "msma".

Usage

```
optparasearch(
 Χ,
 Y = NULL
  Z = NULL
 search.method = c("simultaneous", "regpara1st", "ncomp1st", "regparaonly")[1],
 eta = 1,
  type = "lasso",
  inX = NULL,
  inY = NULL,
 muX = 0,
 muY = 0,
  comp = 1,
  nfold = 5,
 maxrep = 3,
 minpct = 0,
 maxpct = 1,
 maxpct4ncomp = NULL,
  criterion = c("BIC", "CV")[1],
  whichselect = NULL,
  homo = NULL,
  intseed = 1
)
## S3 method for class 'optparasearch'
print(x, ...)
```

Arguments

X	a matrix or list of matrices indicating the explanatory variable(s). This parameter is required.
Υ	a matrix or list of matrices indicating objective variable(s). This is optional. If there is no input for Y, then PCA is implemented.
Z	a vector, response variable(s) for implementing the supervised version of (multiblock) PCA or PLS. This is optional. The length of Z is the number of subjects. If there is no input for Z, then unsupervised PLS/PCA is implemented.

search.method a character indicationg search methods, see Details. Default is "simultaneous".

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eta	numeric scalar indicating the parameter indexing the penalty family. This version contains only choice $1.$
type	a character, indicating the penalty family. In this version, only one choice is available: "lasso."
inX	a vector or list of numeric vectors specifying the variables in \boldsymbol{X} , always included in the model
inY	a vector or list of numeric vectors specifying the variables in Y, always included in the model
muX	a numeric scalar for the weight of X for the supervised case. $0 \le muX \le 1$.
muY	a numeric scalar for the weight of Y for the supervised case. $0 \le muY \le 1$.
comp	numeric scalar for the number of components to be considered or the maximum canditate number of components.
nfold	number of folds - default is 5.
maxrep	numeric scalar for the number of iteration.
minpct	minimum candidate parameters defined as a percentile of automatically determined (possible) candidates.
maxpct	maximum candidate parameters defined as a percentile of automatically determined (possible) candidates.
maxpct4ncomp	maximum candidate parameters defined as a percentile of automatically determined (possible) candidates.
criterion	a character, the evaluation criterion, "CV" for cross-validation, based on a matrix element-wise error, and "BIC" for Bayesian information criteria. The "BIC" is the default.
whichselect	which blocks selected.
homo	same parameters.
intseed	seed number for the random number in the parameter estimation algorithm.
X	an object of class "optparasearch", usually, a result of a call to optparasearch
	further arguments passed to or from other methods.

Details

A function for identifying the regularized sparseness parameters lambdaX and lambdaY and the number of components for msma. Four search methods are available. The "simultaneous" method identifies the number of components by searching the regularized parameters in each component. The "regpara1st" identifies the regularized parameters by fixing the number of components, then searching for the number of components with the selected regularized parameters. The "ncomp1st" method identifies the number of components with a regularized parameter of 0, then searches for the regularized parameters with the selected number of components. The "regparaonly" method searches for the regularized parameters with a fixed number of components.

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Value

optncomp Optimal number of components

optlambdaX Optimal parameters for X

optlambdaY Optimal parameters for Y

mincriterion Minimum criterion value

criteria All resulting criterion values in the process

pararange Range of candidates parameters

Examples

```
##### data #####
tmpdata = simdata(n = 50, rho = 0.8, Yps = c(10, 12, 15), Xps = 20, seed=1)
X = tmpdata$X; Y = tmpdata$Y

##### Regularized parameters search #####
opt1 = optparasearch(X, Y, search.method = "regparaonly", comp=1, nfold=5, maxrep=2)
opt1
fit4 = msma(X, Y, comp=opt1$optncomp, lambdaX=opt1$optlambdaX, lambdaY=opt1$optlambdaY)
fit4
summary(fit4)

##### Restrict search range #####
opt2 = optparasearch(X, Y, comp=3, nfold=5, maxrep=2, minpct=0.5)
opt2
```

plot.msma

Plot msma

Description

plot method for class "msma".

```
## S3 method for class 'msma'
plot(
    x,
    v = c("weight", "score", "cpev")[1],
    axes = 1,
    block = c("block", "super")[1],
    plottype = c("bar", "scatter")[1],
    XY = c("X", "Y", "XY")[1],
    col = NULL,
    signflip = FALSE,
    ...
)
```

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Arguments

Х		an object of class "msma." Usually, a result of a call to msma
V		a character, "weight" for the weight, "score" for the score, and "cpev" for the cumulative percentage of explained variance $(CPEV)$.
axe	S	a numeric (or vector), specifying the component(s) to plot.
blo	ck	a character, indicating which the "block" or "super" is used.
plo	ttype	a character, indicating the plot type. "bar" for the bar plot, "scatter" for the scatter plot.
XY		a character, indicating "X" or "Y". "XY" for the scatter plots using X and Y scores from PLS.
col		a color vector.
sig	nflip	a logical if the sign in the block is flipped to pose the super as possitive.
		further arguments passed to or from other methods.

Details

This function provides a plot of results.

Examples

```
tmpdata = simdata(n = 50, rho = 0.8, Yps = c(10, 12, 15), Xps = 20, seed=1)
X = tmpdata$X; Y = tmpdata$Y

fit1 = msma(X, Y, comp=1, lambdaX=2, lambdaY=1:3)
plot(fit1)
```

predict.msma

Prediction

Description

predict method for class "msma".

Usage

```
## S3 method for class 'msma'
predict(object, newX, newY = NULL, ...)
```

Arguments

object an object of class "msma", usually, a result of a call to msma

newX a matrix in which to look for variables with which to predict X.

newY a matrix in which to look for variables with which to predict Y.

further arguments passed to or from other methods.

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Details

This function produces a prediction from new data based on msma fit. It is mainly used in cross-validation

Value

```
X predicted X
sbX block score for X
Y predicted Y
sbY block score for Y
```

Examples

```
##### data #####
tmpdata = simdata(n = 50, rho = 0.8, Yps = c(10, 12, 15), Xps = 20, seed=1)
X = tmpdata$X; Y = tmpdata$Y

##### Two Component #####
fit2 = msma(X, Y, comp=2, lambdaX=2, lambdaY=1:3)
summary(fit2)

##### Predict #####
test = predict(fit2, newX=X, newY=Y)
```

regparasearch

Regularized Parameters Search

Description

Regularized parameters search method for "msma".

```
regparasearch(
   X,
   Y = NULL,
   Z = NULL,
   eta = 1,
   type = "lasso",
   inX = NULL,
   inY = NULL,
   inYsup = NULL,
   inYsup = NULL,
   muX = 0,
   muY = 0,
   comp = 1,
```

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```
nfold = 5,
maxrep = 3,
minpct = 0,
maxpct = 1,
criterion = c("CV", "BIC")[1],
whichselect = NULL,
homo = NULL,
intseed = 1
)

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

the default.

Arguments

X	a matrix or list of matrices indicating the explanatory variable(s). This parameter is required.
Υ	a matrix or list of matrices indicating objective variable(s). This is optional. If there is no input for Y, then PCA is implemented.
Z	a vector, response variable(s) for implementing the supervised version of (multiblock) PCA or PLS. This is optional. The length of Z is the number of subjects. If there is no input for Z, then unsupervised PLS/PCA is implemented.
eta	numeric scalar indicating the parameter indexing the penalty family. This version contains only choice 1.
type	a character, indicating the penalty family. In this version, only one choice is available: "lasso."
inX	a (list of) numeric vector to specify the variables of X which are always in the model.
inY	a (list of) numeric vector to specify the variables of X which are always in the model.
inXsup	a (list of) numeric vector to specify the blocks of X which are always in the model.
inYsup	a (list of) numeric vector to specify the blocks of Y which are always in the model.
muX	a numeric scalar for the weight of X for the supervised case. $0 \le muX \le 1$.
muY	a numeric scalar for the weight of Y for the supervised case. $0 \le \text{muY} \le 1$.
comp	numeric scalar for the maximum number of componets to be considered.
nfold	number of folds. Default is 5.
maxrep	numeric scalar for the number of iteration.
minpct	percent of minimum candidate parameters.
maxpct	percent of maximum candidate parameters.
criterion	a character, the evaluation criterion, "CV" for cross-validation, based on a matrix element-wise error, and "BIC" for Bayesian information criteria. The "BIC" is

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which select which blocks selected.

homo same parameters.

intseed seed number for the random number in the parameter estimation algorithm.

x an object of class "regparasearch", usually, a result of a call to regparasearch further arguments passed to or from other methods.

Details

This is a function for identifying the regularized parameters of sparseness lambdaX and lambdaY for msma. The initial range of candidates is computed based on fit, with regularized parameter values of 0. A binary search is conducted for dividing the parameter range into two regions. The representative value for the region is a median value, and the optimal region is selected using the minimum criteria obtained from the fit with that median value. The CV error or BIC can be used as criteria. The selected region is also divided into two region and the same process is iterated by maxrep times. Thus, the final median value in the selected region is set to be the optimal regularized parameter. The search is conducted with combinations of parameters for X and Y. The range of candidates for regularized parameters can be restricted, with a percentile of the limit (minimum or maximum) for the range.

Value

optlambdaX Optimal parameters for X
optlambdaY Optimal parameters for Y
mincriterion Minimum of criterion values
criterions Resulting criterion value
pararange Range of candidates parameters

Examples

```
##### data #####
tmpdata = simdata(n = 50, rho = 0.8, Yps = c(10, 12, 15), Xps = c(20, 15), seed=1)
X = tmpdata$X; Y = tmpdata$Y

##### Regularized parameters search #####
opt1 = regparasearch(X, Y, comp=1, criterion="BIC", maxrep=2,
whichselect=c("X", "Y", "Xsup", "Ysup"))
opt1
fit4 = msma(X, Y, comp=1, lambdaX=opt1$optlambdaX, lambdaY=opt1$optlambdaY,
lambdaXsup=opt1$optlambdaXsup, lambdaYsup=opt1$optlambdaYsup)
fit4
summary(fit4)
```

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simdata	Simulate Data sets	

Description

This is a function for generating multiblock data based on the multivariable normal distribusion

Usage

```
simdata(n = 100, rho = 0.8, Yps = c(100, 120, 150), Xps = 500, seed = 1)
```

Arguments

n	a numeric scalar, sample size.
rho	a numeric scalar, correlation coefficient.
Yps	a numeric vector, numbers of columns for Y. The length of vector corresponds to the number of blocks.
Xps	a numeric vector, numbers of columns for X. The length of vector corresponds to the number of blocks.
seed	a seed number for generating random numbers.

Details

The output is a list of matrics.

Value

Χ	Simulated X which has a list form
Υ	Simulated Y which has a list form

strsimdata Structured Simulate Data sets
Structured Simulate Data sets

Description

This is a function for generating multiblock data based on the multivariable normal distribusion

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Usage

```
strsimdata(
    n = 100,
    ncomp = 5,
    WX = NULL,
    Xps = 10,
    Yps = FALSE,
    rho = 0.8,
    Z = FALSE,
    seed = 1,
    minpct = 0.25,
    maxpct = 0.75
)
```

Arguments

	•	1	1 .	
n	a numeric so	calar	cample cize	
11	a mumeric sv	carar,	sample size.	

ncomp number of components

WX a matrix or a list, weights.

Xps a numeric vector, numbers of columns for X. The length of vector corresponds

to the number of blocks.

Yps a numeric vector, numbers of columns for Y. The length of vector corresponds

to the number of blocks.

rho a numeric, correlation

Z outcome

seed a seed number for generating random numbers.

minpct minimum percent of nonzero
maxpct maximum percent of nonzero

Details

The output is a list of matrics.

Value

X Simulated X which has a list form

Y Simulated Y which has a list form

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summary.msma

Summarizing Fits

Description

```
summary method for class "msma".
```

Usage

```
## $3 method for class 'msma'
summary(object, ...)
## $3 method for class 'summary.msma'
print(x, ...)
```

Arguments

```
object, x an object of class "msma", usually, a result of a call to msma ... further arguments passed to or from other methods.
```

Details

This function provide the summary of results .

Examples

```
##### data #####
tmpdata = simdata(n = 50, rho = 0.8, Yps = c(10, 12, 15), Xps = 20, seed=1)
X = tmpdata$X; Y = tmpdata$Y

##### One Component #####
fit1 = msma(X, Y, comp=1, lambdaX=2, lambdaY=1:3)
summary(fit1)
```

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