# Package 'CovTools'

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|--|
| Title Statistical Tools for Covariance Analysis  |
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| <b>Description</b> Covariance is of universal prevalence across various disciplines within statistics. We provide a rich collection of geometric and inferential tools for convenient analysis of covariance structures, topics including distance measures, mean covariance estimator, covariance hypothesis test for one-sample and two-sample cases, and covariance estimation. For an introduction to covariance in multivariate statistical analysis, see Schervish (1987) <doi:10.1214 1177013111="" ss="">.</doi:10.1214> |
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BCovTest1.mxPBF

One-Sample Covariance Test using Maximum Pairwise Bayes Factor

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#### Description

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It performs Bayesian version of 1-sample test for Covariance where the null hypothesis is

$$H_0: \Sigma_n = \Sigma_0$$

where  $\Sigma_n$  is the covariance of data model and  $\Sigma_0$  is a hypothesized covariance. Denote  $X_i$  be the *i*-th column of data matrix. Under the maximum pairwise Bayes Factor framework, we have following hypothesis,

$$H_0: a_{ij} = 0 \text{ and } \tau_{ij} = 1 \text{ versus. } H_1: \text{not } H_0.$$

The model is

$$X_i|X_j \sim N_n(a_{ij}X_j, \tau_{ij}^2 I_n)$$

and the prior is set, under  $H_1$ , as

$$a_{ij}|\tau_{ij}^2 \sim N(0, \tau_{ij}^2/(\gamma * ||X_j||^2))$$
  
$$\tau_{ij}^2 \sim IG(a0, b0).$$

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#### Usage

```
BCovTest1.mxPBF(data, Sigma0 = diag(ncol(data)), a0 = 2, b0 = 2, gamma = 1)
```

#### **Arguments**

data an  $(n \times p)$  data matrix where each row is an observation. Sigma0 a  $(p \times p)$  given covariance matrix.

a0 shape parameter for inverse-gamma prior.

b0 scale parameter for inverse-gamma prior.

gamma non-negative number. See the equation above.

#### Value

a named list containing:

**log.BF.mat** a  $(p \times p)$  matrix of pairwise log Bayes factors.

#### References

Lee K, Lin L, Dunson D (2018). "Maximum Pairwise Bayes Factors for Covariance Structure Testing." *arXiv preprint*. https://arxiv.org/abs/1809.03105.

```
## Not run:
## generate data from multivariate normal with trivial covariance.
pdim = 10
data = matrix(rnorm(100*pdim), nrow=100)

## run mxPBF-based test
out1 = BCovTest1.mxPBF(data)
out2 = BCovTest1.mxPBF(data, a0=5.0, b0=5.0) # change some params

## visualize two Bayes Factor matrices
opar <- par(no.readonly=TRUE)
par(mfrow=c(1,2), pty="s")
image(exp(out1$log.BF.mat)[,pdim:1], main="default")
image(exp(out2$log.BF.mat)[,pdim:1], main="a0=b0=5.0")
par(opar)

## End(Not run)</pre>
```

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BDiagTest1.mxPBF

One-Sample Diagonality Test by Maximum Pairwise Bayes Factor

#### **Description**

One-sample diagonality test can be stated with the null hypothesis

$$H_0: \sigma_{ij} = 0 \text{ for any } i \neq j$$

and alternative hypothesis  $H_1$ : not  $H_0$  with  $\Sigma_n = (\sigma_{ij})$ . Let  $X_i$  be the *i*-th column of data matrix. Under the maximum pairwise bayes factor framework, we have following hypothesis,

$$H_0: a_{ij} = 0$$
 versus.  $H_1: \text{not } H_0$ .

The model is

$$X_i|X_j \sim N_n(a_{ij}X_j, \tau_{ij}^2I_n).$$

Under  $H_0$ , the prior is set as

$$\tau_{ij}^2 \sim IG(a0, b0)$$

and under  $H_1$ , priors are

$$a_{ij}|\tau_{ij}^2 \sim N(0, \tau_{ij}^2/(\gamma * ||X_j||^2))$$
  
 $\tau_{ij}^2 \sim IG(a0, b0).$ 

#### Usage

#### **Arguments**

data an  $(n \times p)$  data matrix where each row is an observation.

shape parameter for inverse-gamma prior.scale parameter for inverse-gamma prior.

gamma non-negative number. See the equation above.

#### Value

a named list containing:

**log.BF.mat**  $(p \times p)$  matrix of pairwise log Bayes factors.

#### References

Lee K, Lin L, Dunson D (2018). "Maximum Pairwise Bayes Factors for Covariance Structure Testing." *arXiv preprint*. https://arxiv.org/abs/1809.03105.

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#### **Examples**

```
## Not run:
## generate data from multivariate normal with trivial covariance.
pdim = 10
data = matrix(rnorm(100*pdim), nrow=100)

## run test
## run mxPBF-based test
out1 = BDiagTest1.mxPBF(data)
out2 = BDiagTest1.mxPBF(data, a0=5.0, b0=5.0) # change some params

## visualize two Bayes Factor matrices
opar <- par(no.readonly=TRUE)
par(mfrow=c(1,2), pty="s")
image(exp(out1$log.BF.mat)[,pdim:1], main="default")
image(exp(out2$log.BF.mat)[,pdim:1], main="a0=b0=5.0")
par(opar)

## End(Not run)</pre>
```

CovDist

Compute Pairwise Distance for Symmetric Positive-Definite Matrices

#### **Description**

For a given 3-dimensional array where symmetric positive definite (SPD) matrices are stacked slice by slice, it computes pairwise distance using various popular measures. Some of measures are *metric* as they suffice 3 conditions in mathematical context; nonnegative definiteness, symmetry, and triangle inequalities. Other non-metric measures represent *dissimilarities* between two SPD objects.

#### Usage

```
CovDist(
   A,
   method = c("AIRM", "Bhattacharyya", "Cholesky", "Euclidean", "Hellinger", "JBLD",
        "KLDM", "LERM", "Procrustes.SS", "Procrustes.Full", "PowerEuclidean",
        "RootEuclidean"),
   power = 1
)
```

#### **Arguments**

Α

a  $(p \times p \times N)$  3d array of N SPD matrices.

method

the type of distance measures to be used; "AIRM" for Affine Invariant Riemannian Metric, "Bhattacharyya" for Bhattacharyya distance based on normal model, "Cholesky" for Cholesky difference in Frobenius norm, "Euclidean"

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for naive Frobenius norm as distance, "Hellinger" for Hellinger distance based on normal model, "JBLD" for Jensen-Bregman Log Determinant Distance, "KLDM" for symmetrized Kullback-Leibler Distance Measure, "LERM" for Log Euclidean Riemannian Metric, "Procrustes.SS" for Procrustes Size and Shape measure, "Procrustes.Full" for Procrustes analysis with scale, "PowerEuclidean" for weighted eigenvalues by some exponent, and "RootEuclidean" for matrix square root.

power

a non-zero number for PowerEuclidean distance.

#### Value

an  $(N \times N)$  symmetric matrix of pairwise distances.

#### References

Arsigny V, Fillard P, Pennec X, Ayache N (2006). "Log-Euclidean metrics for fast and simple calculus on diffusion tensors." *Magnetic Resonance in Medicine*, **56**(2), 411–421. ISSN 0740-3194, 1522-2594.

Dryden IL, Koloydenko A, Zhou D (2009). "Non-Euclidean statistics for covariance matrices, with applications to diffusion tensor imaging." *The Annals of Applied Statistics*, **3**(3), 1102–1123. ISSN 1932-6157.

#### **Examples**

```
## generate 100 SPD matrices of size (5-by-5)
samples = samplecovs(100,5)

## get pairwise distance for "AIRM"
distAIRM = CovDist(samples, method="AIRM")

## dimension reduction using MDS
ss = cmdscale(distAIRM)

## visualize
opar <- par(no.readonly=TRUE)
plot(ss[,1],ss[,2],main="2d projection")
par(opar)</pre>
```

CovEst.2003LW

Covariance Estimation with Linear Shrinkage

#### **Description**

Ledoit and Wolf (2003, 2004) proposed a linear shrinkage strategy to estimate covariance matrix with an application to portfolio optimization. An optimal covariance is written as a convex combination as follows,

$$\hat{\Sigma} = \delta \hat{F} + (1 - \delta)\hat{S}$$

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where  $\delta \in (0,1)$  a control parameter/weight,  $\hat{S}$  an empirical covariance matrix, and  $\hat{F}$  a target matrix. Although authors used F a highly structured estimator, we also enabled an arbitrary target matrix to be used as long as it's symmetric and positive definite of corresponding size.

#### Usage

```
CovEst.2003LW(X, target = NULL)
```

#### **Arguments**

X an  $(n \times p)$  matrix where each row is an observation.

target matrix F. If target=NULL,  $constant\ correlation\ model$  estimator is used.

If target is specified as a qualified matrix, it is used instead.

#### Value

a named list containing:

**S** a  $(p \times p)$  covariance matrix estimate.

**delta** an estimate for convex combination weight according to the relevant theory.

#### References

Ledoit O, Wolf M (2003). "Improved estimation of the covariance matrix of stock returns with an application to portfolio selection." *Journal of Empirical Finance*, **10**(5), 603–621. ISSN 09275398.

Ledoit O, Wolf M (2004). "A well-conditioned estimator for large-dimensional covariance matrices." *Journal of Multivariate Analysis*, **88**(2), 365–411. ISSN 0047259X.

Ledoit O, Wolf M (2004). "Honey, I Shrunk the Sample Covariance Matrix." *The Journal of Portfolio Management*, **30**(4), 110–119. ISSN 0095-4918.

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```
## Not run:
## want to see how delta is determined according to
# the number of observations we have.
nsamples = seq(from=5, to=200, by=5)
nnsample = length(nsamples)
# we will record two values; delta and norm difference
vec.delta = rep(0, nnsample)
vec.normd = rep(0, nnsample)
for (i in 1:nnsample){
  dat.norun <- matrix(rnorm(nsamples[i]*pdim), ncol=pdim) # sample in R^5</pre>
  out.norun <- CovEst.2003LW(dat.norun)</pre>
                                                            # run with default
  vec.delta[i] = out.norun$delta
  vec.normd[i] = norm(out.norun$S - diag(pdim),"f")
                                                            # Frobenius norm
}
# let's visualize the results
opar <- par(no.readonly=TRUE)</pre>
par(mfrow=c(1,2))
plot(nsamples, vec.delta, 1wd=2, type="b", col="red", main="estimated deltas")
plot(nsamples, vec.normd, lwd=2, type="b", col="blue",main="Frobenius error")
par(opar)
## End(Not run)
```

CovEst.20100AS

Oracle Approximating Shrinkage Estimator

#### Description

Authors propose to estimate covariance matrix by iteratively approximating the shrinkage with

$$\hat{\Sigma} = \rho \hat{F} + (1 - \rho)\hat{S}$$

where  $\rho \in (0,1)$  a control parameter/weight,  $\hat{S}$  an empirical covariance matrix, and  $\hat{F}$  a target matrix. It is proposed to use a structured estimate  $\hat{F} = \text{Tr}(\hat{S}/p) \cdot I_{p \times p}$  where  $I_{p \times p}$  is an identity matrix of dimension p.

#### Usage

```
CovEst.20100AS(X)
```

#### **Arguments**

Χ

an  $(n \times p)$  matrix where each row is an observation.

CovEst.2010OAS

#### Value

```
a named list containing:
```

**S** a  $(p \times p)$  covariance matrix estimate.

rho an estimate for convex combination weight.

#### References

Chen Y, Wiesel A, Eldar YC, Hero AO (2010). "Shrinkage Algorithms for MMSE Covariance Estimation." *IEEE Transactions on Signal Processing*, **58**(10), 5016–5029. ISSN 1053-587X, 1941-0476.

```
## CRAN-purpose small computation
# set a seed for reproducibility
set.seed(11)
# small data with identity covariance
         <- 5
dat.small <- matrix(rnorm(10*pdim), ncol=pdim)</pre>
# run the code
out.small <- CovEst.20100AS(dat.small)
# visualize
opar <- par(no.readonly=TRUE)</pre>
par(mfrow=c(1,3), pty="s")
image(diag(pdim)[,pdim:1], main="true cov")
image(cov(dat.small)[,pdim:1], main="sample cov")
image(out.small$S[,pdim:1], main="estimated cov")
par(opar)
## Not run:
## want to see how delta is determined according to
# the number of observations we have.
nsamples = seq(from=5, to=200, by=5)
nnsample = length(nsamples)
# we will record two values; rho and norm difference
vec.rho = rep(0, nnsample)
vec.normd = rep(0, nnsample)
for (i in 1:nnsample){
  dat.norun <- matrix(rnorm(nsamples[i]*pdim), ncol=pdim) # sample in R^5</pre>
                                                          # run with default
  out.norun <- CovEst.20100AS(dat.norun)</pre>
  vec.rho[i] = out.norun$rho
  vec.normd[i] = norm(out.norun$S - diag(pdim), "f")
                                                          # Frobenius norm
}
# let's visualize the results
opar <- par(no.readonly=TRUE)</pre>
```

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```
par(mfrow=c(1,2))
plot(nsamples, vec.rho, lwd=2, type="b", col="red", main="estimated rhos")
plot(nsamples, vec.normd, lwd=2, type="b", col="blue", main="Frobenius error")
par(opar)
## End(Not run)
```

CovEst.2010RBLW

Rao-Blackwell Ledoit-Wolf Estimator

#### **Description**

Authors propose to estimate covariance matrix by minimizing mean squared error with the following formula,

$$\hat{\Sigma} = \rho \hat{F} + (1 - \rho)\hat{S}$$

where  $\rho \in (0,1)$  a control parameter/weight,  $\hat{S}$  an empirical covariance matrix, and  $\hat{F}$  a target matrix. It is proposed to use a structured estimate  $\hat{F} = \text{Tr}(\hat{S}/p) \cdot I_{p \times p}$  where  $I_{p \times p}$  is an identity matrix of dimension p.

#### Usage

```
CovEst.2010RBLW(X)
```

#### **Arguments**

Χ

an  $(n \times p)$  matrix where each row is an observation.

#### Value

a named list containing:

**S** a  $(p \times p)$  covariance matrix estimate.

rho an estimate for convex combination weight.

#### References

Chen Y, Wiesel A, Eldar YC, Hero AO (2010). "Shrinkage Algorithms for MMSE Covariance Estimation." *IEEE Transactions on Signal Processing*, **58**(10), 5016–5029. ISSN 1053-587X, 1941-0476.

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```
## CRAN-purpose small computation
# set a seed for reproducibility
set.seed(11)
# small data with identity covariance
         <- 10
dat.small <- matrix(rnorm(5*pdim), ncol=pdim)</pre>
# run the code
out.small <- CovEst.2010RBLW(dat.small)</pre>
# visualize
opar <- par(no.readonly=TRUE)</pre>
par(mfrow=c(1,3), pty="s")
image(diag(pdim)[,pdim:1], main="true cov")
image(cov(dat.small)[,pdim:1], main="sample cov")
image(out.small$S[,pdim:1], main="estimated cov")
par(opar)
## Not run:
## want to see how delta is determined according to
# the number of observations we have.
nsamples = seq(from=5, to=200, by=5)
nnsample = length(nsamples)
# we will record two values; rho and norm difference
vec.rho = rep(0, nnsample)
vec.normd = rep(0, nnsample)
for (i in 1:nnsample){
  dat.norun <- matrix(rnorm(nsamples[i]*pdim), ncol=pdim) # sample in R^5</pre>
  out.norun <- CovEst.2010RBLW(dat.norun)</pre>
                                                          # run with default
  vec.rho[i] = out.norun$rho
  vec.normd[i] = norm(out.norun$S - diag(5),"f")
                                                        # Frobenius norm
}
# let's visualize the results
opar <- par(mfrow=c(1,2))</pre>
plot(nsamples, vec.rho, lwd=2, type="b", col="red", main="estimated rhos")
plot(nsamples, vec.normd, lwd=2, type="b", col="blue",main="Frobenius error")
par(opar)
## End(Not run)
```

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#### **Description**

Cai and Liu (2011) proposed an adaptive variant of Bickel and Levina (2008) - CovEst.hard. The idea of *adaptive thresholding* is to apply thresholding technique on correlation matrix in that it becomes *adaptive* in terms of each variable.

#### Usage

```
CovEst.adaptive(X, thr = 0.5, nCV = 10, parallel = FALSE)
```

#### **Arguments**

X an  $(n \times p)$  matrix where each row is an observation.

thr user-defined threshold value. If it is a vector of regularization values, it auto-

matically selects one that minimizes cross validation risk.

nCV the number of repetitions for 2-fold random cross validations for each threshold

value.

parallel a logical; TRUE to use half of available cores, FALSE to do every computation

sequentially.

#### Value

a named list containing:

**S** a  $(p \times p)$  covariance matrix estimate.

**CV** a dataframe containing vector of tested threshold values(thr) and corresponding cross validation scores(CVscore).

#### References

Cai T, Liu W (2011). "Adaptive Thresholding for Sparse Covariance Matrix Estimation." *Journal of the American Statistical Association*, **106**(494), 672–684. ISSN 0162-1459, 1537-274X.

```
## generate data from multivariate normal with Identity covariance.
pdim <- 5
data <- matrix(rnorm(10*pdim), ncol=pdim)

## apply 4 different schemes
# mthr is a vector of regularization parameters to be tested
mthr <- seq(from=0.01,to=0.99,length.out=10)

out1 <- CovEst.adaptive(data, thr=0.1) # threshold value 0.1
out2 <- CovEst.adaptive(data, thr=0.5) # threshold value 0.5
out3 <- CovEst.adaptive(data, thr=0.1) # threshold value 0.9
out4 <- CovEst.adaptive(data, thr=mthr) # automatic threshold checking

## visualize 4 estimated matrices
opar <- par(no.readonly=TRUE)</pre>
```

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```
par(mfrow=c(2,2), pty="s")
image(out1$S[,pdim:1], col=gray((0:100)/100), main="thr=0.1")
image(out2$S[,pdim:1], col=gray((0:100)/100), main="thr=0.5")
image(out3$S[,pdim:1], col=gray((0:100)/100), main="thr=0.9")
image(out4$S[,pdim:1], col=gray((0:100)/100), main="automatic")
par(opar)
```

CovEst.hard

Covariance Estimation via Hard Thresholding

#### **Description**

Bickel and Levina (2008) proposed a sparse covariance estimation technique to apply thresholding on off-diagonal elements of the sample covariance matrix. The entry of sample covariance matrix  $S_{i,j}=0$  if  $|S_{i,j}|<=\tau$  where  $\tau$  is a thresholding value (thr). If thr is rather a vector of regularization parameters, it applies cross-validation scheme to select an optimal value.

#### Usage

```
CovEst.hard(X, thr = sqrt(log(ncol(X))/nrow(X)), nCV = 10, parallel = FALSE)
```

#### **Arguments**

X an  $(n \times p)$  matrix where each row is an observation.

thr user-defined threshold value. If it is a vector of regularization values, it automatically selects one that minimizes cross validation risk.

nCV the number of repetitions for 2-fold random cross validations for each threshold value.

parallel a logical; TRUE to use half of available cores, FALSE to do every computation sequentially.

Sequentia

#### Value

a named list containing:

**S** a  $(p \times p)$  covariance matrix estimate.

**CV** a dataframe containing vector of tested threshold values(thr) and corresponding cross validation scores(CVscore).

#### References

Bickel PJ, Levina E (2008). "Covariance regularization by thresholding." *The Annals of Statistics*, **36**(6), 2577–2604. ISSN 0090-5364.

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#### **Examples**

```
## generate data from multivariate normal with Identity covariance.
pdim <- 5
data <- matrix(rnorm(10*pdim), ncol=pdim)</pre>
## apply 4 different schemes
# mthr is a vector of regularization parameters to be tested
mthr <- exp(seq(from=log(0.1),to=log(10),length.out=10))</pre>
out1 <- CovEst.hard(data, thr=0.1) # threshold value 0.1
out2 <- CovEst.hard(data, thr=1)
                                    # threshold value 1
out3 <- CovEst.hard(data, thr=10) # threshold value 10
out4 <- CovEst.hard(data, thr=mthr) # automatic threshold checking
## visualize 4 estimated matrices
gcol <- gray((0:100)/100)
opar <- par(no.readonly=TRUE)</pre>
par(mfrow=c(2,2), pty="s")
image(out1$S[,pdim:1], col=gcol, main="thr=0.1")
image(out2$S[,pdim:1], col=gcol, main="thr=1")
image(out3$S[,pdim:1], col=gcol, main="thr=10")
image(out4$S[,pdim:1], col=gcol, main="automatic")
par(opar)
```

CovEst.hardPD

Covariance Estimation via Hard Thresholding under Positive-Definiteness Constraint

#### **Description**

Sparse covariance estimation does not necessarily guarantee positive definiteness of an estimated covariance matrix. Fan et al. (2013) proposed to solve this issue by taking an iterative procedure to take an incremental decrease of threshold value until positive definiteness is preserved.

#### Usage

```
CovEst.hardPD(X)
```

## **Arguments** Χ

an  $(n \times p)$  matrix where each row is an observation.

#### Value

a named list containing:

```
S a (p \times p) covariance matrix estimate.
```

**optC** an optimal threshold value  $C_{min}$  that guarantees positive definiteness after thresholding.

CovEst.nearPD 15

#### References

Fan J, Liao Y, Mincheva M (2013). "Large covariance estimation by thresholding principal orthogonal complements." *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, **75**(4), 603–680. ISSN 13697412.

#### **Examples**

```
## generate data from multivariate normal with Identity covariance.
pdim <- 5
data <- matrix(rnorm(10*pdim), ncol=pdim)</pre>
## apply 4 different schemes
out1 <- CovEst.hard(data, thr=0.1) # threshold value 0.1
out2 <- CovEst.hard(data, thr=1)
                                    # threshold value 1
out3 <- CovEst.hard(data, thr=10) # threshold value 10
out4 <- CovEst.hardPD(data) # automatic threshold checking</pre>
## visualize 4 estimated matrices
mmessage <- paste("hardPD::optimal thr=",sprintf("%.2f",out4$optC),sep="")</pre>
         <- gray((0:100)/100)
opar <- par(no.readonly=TRUE)</pre>
par(mfrow=c(2,2), pty="s")
image(out1$S[,pdim:1], col=gcol, main="thr=0.1")
image(out2$S[,pdim:1], col=gcol, main="thr=1")
image(out3$S[,pdim:1], col=gcol, main="thr=10")
image(out4$S[,pdim:1], col=gcol, main=mmessage)
par(opar)
```

CovEst.nearPD

Covariance Estimation via Nearest Positive-Definite Matrix Projection

#### **Description**

Qi and Sun (2006) proposed an algorithm for computing the positive correlation matrix with Positive Definiteness and transforming it back in order to estimate covariance matrix. This algorithm does not depend on any parameters.

#### Usage

```
CovEst.nearPD(X)
```

#### **Arguments**

Χ

an  $(n \times p)$  matrix where each row is an observation.

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#### Value

a named list containing:

**S** a  $(p \times p)$  covariance matrix estimate.

#### References

Qi H, Sun D (2006). "A Quadratically Convergent Newton Method for Computing the Nearest Correlation Matrix." *SIAM Journal on Matrix Analysis and Applications*, **28**(2), 360–385. ISSN 0895-4798, 1095-7162.

#### **Examples**

```
## generate data from multivariate normal with Identity covariance.
pdim <- 5
data <- matrix(rnorm(10*pdim), ncol=pdim)

## compare against sample covariance
out1 <- cov(data)
out2 <- CovEst.nearPD(data) # apply nearPD

## visualize 2 estimated matrices
gcol <- gray((0:100)/100)
opar <- par(no.readonly=TRUE)
par(mfrow=c(1,2), pty="s")
image(out1[,pdim:1], col=gcol, main="sample covariance")
image(out2$S[,pdim:1], col=gcol, main="SPD Projection")
par(opar)</pre>
```

CovEst.soft

Covariance Estimation via Soft Thresholding

#### **Description**

Soft Thresholding method for covariance estimation takes off-diagonal elements z of sample covariance matrix and applies

$$h_{\tau}(z) = \operatorname{sgn}(z)(|z| - \tau)_{+}$$

where sgn(z) is a sign of the value z, and  $(x)_+ = max(x,0)$ . If thr is rather a vector of regularization parameters, it applies cross-validation scheme to select an optimal value.

#### Usage

```
CovEst.soft(X, thr = 0.5, nCV = 10, parallel = FALSE)
```

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#### **Arguments**

| Χ        | an $(n \times p)$ matrix where each row is an observation.   |
|----------|--|
| thr      | user-defined threshold value. If it is a vector of regularization values, it automatically selects one that minimizes cross validation risk. |
| nCV      | the number of repetitions for 2-fold random cross validations for each threshold value.  |
| parallel | a logical; TRUE to use half of available cores, FALSE to do every computation sequentially.  |

#### Value

a named list containing:

**S** a  $(p \times p)$  covariance matrix estimate.

**CV** a dataframe containing vector of tested threshold values(thr) and corresponding cross validation scores(CVscore).

#### References

Antoniadis A, Fan J (2001). "Regularization of Wavelet Approximations." *Journal of the American Statistical Association*, **96**(455), 939–967. ISSN 0162-1459, 1537-274X.

Donoho DL, Johnstone IM, Kerkyacharian G, Picard D (1995). "Wavelet Shrinkage: Asymptopia?" *Journal of the Royal Statistical Society. Series B (Methodological)*, **57**(2), 301–369. ISSN 00359246.

```
## generate data from multivariate normal with Identity covariance.
pdim <- 5
data <- matrix(rnorm(10*pdim), ncol=pdim)</pre>
## apply 4 different schemes
# mthr is a vector of regularization parameters to be tested
mthr \leftarrow exp(seq(from=log(0.1), to=log(10), length.out=10))
out1 <- CovEst.soft(data, thr=0.1) # threshold value 0.1
out2 <- CovEst.soft(data, thr=1) # threshold value 1</pre>
out3 <- CovEst.soft(data, thr=10) # threshold value 10
out4 <- CovEst.soft(data, thr=mthr) # automatic threshold checking
## visualize 4 estimated matrices
gcol <- gray((0:100)/100)
opar <- par(no.readonly=TRUE)</pre>
par(mfrow=c(2,2), pty="s")
image(out1$S[,pdim:1], col=gcol, main="thr=0.1")
image(out2$S[,pdim:1], col=gcol, main="thr=1")
image(out3$S[,pdim:1], col=gcol, main="thr=10")
image(out4$S[,pdim:1], col=gcol, main="automatic")
par(opar)
```

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CovMean

Estimate Mean Covariance Matrix

#### **Description**

For a given 3-dimensional array where symmetric positive definite (SPD) matrices are stacked slice by slice, it estimates Frechet mean on an open cone of SPD matrices under corresponding metric/distance measure.

#### Usage

```
CovMean(
   A,
   method = c("AIRM", "Cholesky", "Euclidean", "LERM", "Procrustes.SS",
        "Procrustes.Full", "PowerEuclidean", "RootEuclidean"),
   power = 1
)
```

#### **Arguments**

A a  $(p \times p \times N)$  3d array of N SPD matrices.

method the type of distance measures to be used; "AIRM" for Affine Invariant Rieman-

nian Metric, "Cholesky" for Cholesky difference in Frobenius norm, "Euclidean" for naive Frobenius norm as distance, "LERM" for Log Euclidean Riemannian Metric, "Procrustes.SS" for Procrustes Size and Shape measure, "Procrustes.Full"

for Procrustes analysis with scale, "PowerEuclidean" for weighted eigenvalues

by some exponent, and "RootEuclidean" for matrix square root.

power a non-zero number for PowerEuclidean distance.

#### Value

a  $(p \times p)$  mean covariance matrix estimated.

#### References

Dryden IL, Koloydenko A, Zhou D (2009). "Non-Euclidean statistics for covariance matrices, with applications to diffusion tensor imaging." *The Annals of Applied Statistics*, **3**(3), 1102–1123. ISSN 1932-6157.

```
## Not run:
## generate 100 sample covariances of size (5-by-5).
pdim = 5
samples = samplecovs(100,pdim)

## compute mean of first 50 sample covariances from data under Normal(0,Identity).
mLERM = CovMean(samples[,,1:50], method="LERM")
```

CovTest1.2013Cai 19

```
mAIRM = CovMean(samples[,,1:50], method="AIRM")
mChol = CovMean(samples[,,1:50], method="Cholesky")
mRoot = CovMean(samples[,,1:50], method="RootEuclidean")

## visualize
opar <- par(no.readonly=TRUE)
par(mfrow=c(2,2), pty="s")
image(mLERM[,pdim:1], main="LERM mean")
image(mAIRM[,pdim:1], main="AIRM mean")
image(mChol[,pdim:1], main="Cholesky mean")
image(mRoot[,pdim:1], main="RootEuclidean mean")
par(opar)

## End(Not run)</pre>
```

CovTest1.2013Cai

One-Sample Covariance Test by Cai and Ma (2013)

#### **Description**

Given data, it performs 1-sample test for Covariance where the null hypothesis is

$$H_0: \Sigma_n = \Sigma_0$$

where  $\Sigma_n$  is the covariance of data model and  $\Sigma_0$  is a hypothesized covariance based on a procedure proposed by Cai and Ma (2013).

#### Usage

```
CovTest1.2013Cai(data, Sigma0 = diag(ncol(data)), alpha = 0.05)
```

#### **Arguments**

data an  $(n \times p)$  data matrix where each row is an observation.

Sigma0 a  $(p \times p)$  given covariance matrix.

alpha level of significance.

#### Value

a named list containing:

statistic a test statistic value.

threshold rejection criterion to be compared against test statistic.

reject a logical; TRUE to reject null hypothesis, FALSE otherwise.

#### References

Cai TT, Ma Z (2013). "Optimal hypothesis testing for high dimensional covariance matrices." *Bernoulli*, **19**(5B), 2359–2388. ISSN 1350-7265.

CovTest1.2014Srivastava

#### **Examples**

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```
## Not run:
## generate data from multivariate normal with trivial covariance.
pdim = 5
data = matrix(rnorm(10*pdim), ncol=pdim)

## run the test
CovTest1.2013Cai(data)

## End(Not run)
```

CovTest1.2014Srivastava

One-Sample Covariance Test by Srivastava, Yanagihara, and Kubokawa (2014)

#### **Description**

Given data, it performs 1-sample test for Covariance where the null hypothesis is

$$H_0: \Sigma_n = \Sigma_0$$

where  $\Sigma_n$  is the covariance of data model and  $\Sigma_0$  is a hypothesized covariance based on a procedure proposed by Srivastava, Yanagihara, and Kubokawa (2014).

#### Usage

```
CovTest1.2014Srivastava(data, Sigma0 = diag(ncol(data)), alpha = 0.05)
```

#### **Arguments**

data an  $(n \times p)$  data matrix where each row is an observation.

Sigma0 a  $(p \times p)$  given covariance matrix.

alpha level of significance.

#### Value

a named list containing

statistic a test statistic value.

threshold rejection criterion to be compared against test statistic.

reject a logical; TRUE to reject null hypothesis, FALSE otherwise.

#### References

Srivastava MS, Yanagihara H, Kubokawa T (2014). "Tests for covariance matrices in high dimension with less sample size." *Journal of Multivariate Analysis*, **130**, 289–309. ISSN 0047259X.

CovTest2.2013Cai 21

#### **Examples**

```
## Not run:
## generate data from multivariate normal with trivial covariance.
pdim = 5
data = matrix(rnorm(10*pdim), ncol=pdim)

## run the test
CovTest1.2014Srivastava(data)

## End(Not run)
```

CovTest2.2013Cai

Two-Sample Covariance Test by Cai and Ma (2013)

#### **Description**

Given two sets of data, it performs 2-sample test for equality of covariance matrices where the null hypothesis is

$$H_0: \Sigma_1 = \Sigma_2$$

where  $\Sigma_1$  and  $\Sigma_2$  represent true (unknown) covariance for each dataset based on a procedure proposed by Cai and Ma (2013). If statistic > threshold, it rejects null hypothesis.

#### Usage

```
CovTest2.2013Cai(X, Y, alpha = 0.05)
```

#### **Arguments**

X an  $(m \times p)$  matrix where each row is an observation from the first dataset. Y an  $(n \times p)$  matrix where each row is an observation from the second dataset.

alpha level of significance.

#### Value

a named list containing

statistic a test statistic value.

threshold rejection criterion to be compared against test statistic.

reject a logical; TRUE to reject null hypothesis, FALSE otherwise.

#### References

Cai TT, Ma Z (2013). "Optimal hypothesis testing for high dimensional covariance matrices." *Bernoulli*, **19**(5B), 2359–2388. ISSN 1350-7265.

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#### **Examples**

```
## generate 2 datasets from multivariate normal with identical covariance.
pdim = 5
data1 = matrix(rnorm(100*pdim), ncol=pdim)
data2 = matrix(rnorm(150*pdim), ncol=pdim)
## run test
CovTest2.2013Cai(data1, data2)
```

DiagTest1.2011Cai

One-Sample Diagonality Test by Cai and Jiang (2011)

#### **Description**

Given data, it performs 1-sample test for diagonal entries of a Covariance matrix where the null hypothesis is

$$H_0: \sigma_{ij} = 0 \text{ for any } i \neq j$$

and alternative hypothesis is  $H_1$ : not  $H_0$  with  $\Sigma_n = (\sigma_{ij})$  based on a procedure proposed by Cai and Jiang (2011).

#### Usage

```
DiagTest1.2011Cai(data, alpha = 0.05)
```

#### **Arguments**

data an  $(n \times p)$  data matrix where each row is an observation.

alpha level of significance.

#### Value

a named list containing:

statistic a test statistic value.

threshold rejection criterion to be compared against test statistic.

reject a logical; TRUE to reject null hypothesis, FALSE otherwise.

#### References

Cai TT, Jiang T (2011). "Limiting laws of coherence of random matrices with applications to testing covariance structure and construction of compressed sensing matrices." *The Annals of Statistics*, **39**(3), 1496–1525. ISSN 0090-5364.

DiagTest1.2015Lan 23

#### **Examples**

```
## Not run:
## generate data from multivariate normal with trivial covariance.
pdim = 5
data = matrix(rnorm(100*pdim), ncol=pdim)

## run test with different alpha values
DiagTest1.2011Cai(data, alpha=0.01)
DiagTest1.2011Cai(data, alpha=0.05)
DiagTest1.2011Cai(data, alpha=0.10)

## End(Not run)
```

DiagTest1.2015Lan

One-Sample Diagonality Test by Lan et al. (2015)

#### Description

Given data, it performs 1-sample test for diagonal entries of a Covariance matrix where the null hypothesis is

$$H_0: \sigma_{ij} = 0 \text{ for any } i \neq j$$

and alternative hypothesis is  $H_1$ : not  $H_0$  with  $\Sigma_n = (\sigma_{ij})$  based on a procedure proposed by Lan et al. (2015).

#### Usage

```
DiagTest1.2015Lan(data, alpha = 0.05)
```

#### **Arguments**

data an  $(n \times p)$  data matrix where each row is an observation.

alpha level of significance.

#### Value

a named list containing:

statistic a test statistic value.

threshold rejection criterion to be compared against test statistic.

reject a logical; TRUE to reject null hypothesis, FALSE otherwise.

#### References

Lan W, Luo R, Tsai C, Wang H, Yang Y (2015). "Testing the Diagonality of a Large Covariance Matrix in a Regression Setting." *Journal of Business* & *Economic Statistics*, **33**(1), 76–86. ISSN 0735-0015, 1537-2707.

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#### **Examples**

```
## Not run:
## generate data from multivariate normal with trivial covariance.
pdim = 5
data = matrix(rnorm(100*pdim), ncol=pdim)

## run test with different alpha values
DiagTest1.2015Lan(data, alpha=0.01)
DiagTest1.2015Lan(data, alpha=0.05)
DiagTest1.2015Lan(data, alpha=0.10)

## End(Not run)
```

package-CovTools

A Collection of Geometric and Statistical Tools for Covariance (and Precision) Analysis

#### **Description**

Covariance is of universal prevalence across various disciplines within statistics. **CovTools** package aims at providing a rich collection of geometric and statistical tools for a variety of inferences on covariance structures as well as its inverse called precision matrix. See the sections below for a comprehensive list of functions provided from the package.

#### **Geometric Methods**

From inference on manifolds perspective, we have following functions,

name of a function description

CovDist compute pairwise distance of covariance matrices

CovMean compute mean covariance matrix

PreEst.2014An

Banded Precision Matrix Estimation via Bandwidth Test

#### **Description**

PreEst. 2014An returns an estimator of the banded precision matrix using the modified Cholesky decomposition. It uses the estimator defined in Bickel and Levina (2008). The bandwidth is determined by the bandwidth test suggested by An, Guo and Liu (2014).

#### Usage

PreEst.2014An(

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```
X,
upperK = floor(ncol(X)/2),
algorithm = c("Bonferroni", "Holm"),
alpha = 0.01
)
```

#### **Arguments**

```
X an (n \times p) data matrix where each row is an observation. upper K upper bound of bandwidth k. algorithm bandwidth test algorithm to be used. alpha significance level for the bandwidth test.
```

#### Value

a named list containing:

 $\mathbf{C}$  a  $(p \times p)$  estimated banded precision matrix.

optk an estimated optimal bandwidth acquired from the test procedure.

#### References

An B, Guo J, Liu Y (2014). "Hypothesis testing for band size detection of high-dimensional banded precision matrices." *Biometrika*, **101**(2), 477–483. ISSN 0006-3444, 1464-3510.

Bickel PJ, Levina E (2008). "Regularized estimation of large covariance matrices." *The Annals of Statistics*, **36**(1), 199–227. ISSN 0090-5364.

```
## Not run:
## parameter setting
p = 200; n = 100
k0 = 5; A0min=0.1; A0max=0.2; D0min=2; D0max=5
set.seed(123)
A0 = matrix(0, p,p)
for(i in 2:p){
  term1 = runif(n=min(k0,i-1),min=A0min, max=A0max)
  term2 = sample(c(1,-1), size=min(k0, i-1), replace=TRUE)
  vals = term1*term2
  vals = vals[ order(abs(vals)) ]
  A0[i, max(1, i-k0):(i-1)] = vals
D0 = diag(runif(n = p, min = D0min, max = D0max))
Omega0 = t(diag(p) - A0)%*%diag(1/diag(D0))%*%(diag(p) - A0)
## data generation (based on AR representation)
## it is same with generating n random samples from N_p(0, Omega0^{-1})
X = matrix(0, nrow=n, ncol=p)
```

PreEst.2014Banerjee

```
X[,1] = rnorm(n, sd = sqrt(D0[1,1]))
for(j in 2:p){
  mean.vec.j = X[, 1:(j-1)]%*%as.matrix(A0[j, 1:(j-1)])
  X[,j] = rnorm(n, mean = mean.vec.j, sd = sqrt(D0[j,j]))
}
## banded estimation using two different schemes
Omega1 <- PreEst.2014An(X, upperK=20, algorithm="Bonferroni")</pre>
Omega2 <- PreEst.2014An(X, upperK=20, algorithm="Holm")</pre>
## visualize true and estimated precision matrices
opar <- par(no.readonly=TRUE)</pre>
par(mfrow=c(1,3), pty="s")
image(Omega0[,p:1], main="Original Precision")
image(Omega1$C[,p:1], main="banded3::Bonferroni")
image(Omega2$C[,p:1], main="banded3::Holm")
par(opar)
## End(Not run)
```

PreEst.2014Banerjee

Bayesian Estimation of a Banded Precision Matrix (Banerjee 2014)

#### **Description**

PreEst.2014Banerjee returns a Bayes estimator of the banded precision matrix using G-Wishart prior. Stein's loss or squared error loss function is used depending on the "loss" argument in the function. The bandwidth is set at the mode of marginal posterior for the bandwidth parameter.

#### Usage

```
PreEst.2014Banerjee(
   X,
   upperK = floor(ncol(X)/2),
   delta = 10,
   logpi = function(k) {     -k^4 }
   loss = c("Stein", "Squared")
)
```

#### **Arguments**

X an  $(n \times p)$  data matrix where each row is an observation. upper K upper bound of bandwidth k. delta hyperparameter for G-Wishart prior. Default value is 10. It has to be larger than 2. log of prior distribution for bandwidth k. Default is a function proportional to  $-k^4$ . loss type of loss; either "Stein" or "Squared".

PreEst.2017Lee 27

#### Value

a named list containing:

 $\mathbf{C}$  a  $(p \times p)$  MAP estimate for precision matrix.

#### References

Banerjee S, Ghosal S (2014). "Posterior convergence rates for estimating large precision matrices using graphical models." *Electronic Journal of Statistics*, **8**(2), 2111–2137. ISSN 1935-7524.

#### **Examples**

```
## generate data from multivariate normal with Identity precision.
pdim = 10
data = matrix(rnorm(50*pdim), ncol=pdim)

## compare different K
out1 <- PreEst.2014Banerjee(data, upperK=1)
out2 <- PreEst.2014Banerjee(data, upperK=3)
out3 <- PreEst.2014Banerjee(data, upperK=5)

## visualize
opar <- par(no.readonly=TRUE)
par(mfrow=c(2,2), pty="s")
image(diag(pdim)[,pdim:1],main="Original Precision")
image(out1$C[,pdim:1], main="banded1::upperK=1")
image(out2$C[,pdim:1], main="banded1::upperK=3")
image(out3$C[,pdim:1], main="banded1::upperK=5")
par(opar)</pre>
```

PreEst.2017Lee

Bayesian Estimation of a Banded Precision Matrix (Lee 2017)

#### **Description**

PreEst.2017Lee returns a Bayes estimator of the banded precision matrix, which is defined in subsection 3.3 of Lee and Lee (2017), using the k-BC prior. The bandwidth is set at the mode of marginal posterior for the bandwidth parameter.

#### Usage

```
PreEst.2017Lee(X, upperK = floor(ncol(X)/2), logpi = function(k) {
    -k^4
})
```

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#### **Arguments**

X an  $(n \times p)$  data matrix where each row is an observation. upper K upper bound of bandwidth k. log of prior distribution for bandwidth k. Default is a function proportional to  $-k^4$ .

#### Value

a named list containing:

 $\mathbf{C}$  a  $(p \times p)$  MAP estimate for precision matrix.

#### References

Lee K, Lee J (2017). "Estimating Large Precision Matrices via Modified Cholesky Decomposition." *ArXiv e-prints*.

#### **Examples**

```
## generate data from multivariate normal with Identity precision.
pdim = 5
data = matrix(rnorm(100*pdim), ncol=pdim)
## compare different K
out1 <- PreEst.2017Lee(data, upperK=1)
out2 <- PreEst.2017Lee(data, upperK=3)
out3 <- PreEst.2017Lee(data, upperK=5)
## visualize
opar <- par(no.readonly=TRUE)</pre>
par(mfrow=c(2,2), pty="s")
image(diag(pdim)[,pdim:1], main="Original Precision")
image(out1$C[,pdim:1], main="banded2::upperK=1")
image(out2$C[,pdim:1],
                          main="banded2::upperK=3")
image(out3$C[,pdim:1],
                          main="banded2::upperK=5")
par(opar)
```

PreEst.glasso

Precision Matrix Estimation via Graphical Lasso

#### **Description**

Given a sample covariance matrix S, graphical lasso aims at estimating sparse precision matrix X - inverse of covariance. It solves a following optimization problem,

$$\max_X \log \det\! X - < S, X > -\lambda \|X\|_1$$
 such that  $X \succ 0$ 

where  $\lambda$  a regularization parameter,  $\langle S, X \rangle = tr(S^TX)$ ,  $\|X\|_1 = \sum X_{ij}$  and  $X \succ 0$  indicates positive definiteness. We provide three modes of computations, 'fixed', 'confidence', or 'BIC' with respect to  $\lambda$ . Please see the section below for more details.

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#### Usage

PreEst.glasso(X, method = list(type = "fixed", param = 1), parallel = FALSE)

#### **Arguments**

X an  $(n \times p)$  data matrix where each row is an observation.

method a list containing following parameters,

**type** one of 'fixed','confidence', or 'BIC'. **param** either a numeric value or vector of values.

parallel a logical; TRUE for using half the cores available, FALSE otherwise.

#### Value

a named list containing:

 $\mathbf{C}$  a  $(p \times p)$  estimated precision matrix.

**BIC** a dataframe containing  $\lambda$  values and corresponding BIC scores with type='BIC' method.

#### regularization parameters

We currently provide three options for solving the problem, 'fixed','confidence', or 'BIC' with respect to  $\lambda$ . When the method type is 'fixed', the parameter should be a single numeric value as a user-defined  $\lambda$  value. Likewise, method type of 'confidence' requires a singule numeric value in (0,1), where the value is set heuristically according to

$$\rho = \frac{t_{n-2}(\gamma) \max S_{ii} S_{jj}}{\sqrt{n - 2 + t_{n-2}^2(\gamma)}}$$

for a given confidence level  $\gamma \in (0,1)$  as proposed by Banerjee et al. (2006). Finally, 'BIC' type requires a vector of  $\lambda$  values and opts for a lambda value with the lowest BIC values as proposed by Yuan and Lin (2007).

#### References

Banerjee O, Ghaoui LE, d'Aspremont A, Natsoulis G (2006). "Convex optimization techniques for fitting sparse Gaussian graphical models." In *Proceedings of the 23rd international conference on Machine learning*, 89–96. ISBN 978-1-59593-383-6.

Yuan M, Lin Y (2007). "Model Selection and Estimation in the Gaussian Graphical Model." *Biometrika*, **94**(1), 19–35. ISSN 00063444.

Friedman J, Hastie T, Tibshirani R (2008). "Sparse inverse covariance estimation with the graphical lasso." *Biostatistics*, **9**(3), 432–441. ISSN 1465-4644, 1468-4357.

30 samplecovs

#### **Examples**

```
## generate data from multivariate normal with Identity precision.
data = matrix(rnorm(100*pdim), ncol=pdim)
## prepare input arguments for diefferent scenarios
lbdvec <- c(0.01, 0.1, 1, 10, 100)
                                              # a vector of regularization parameters
list1 <- list(type="fixed",param=1.0)</pre>
                                             # single regularization parameter case
list2 <- list(type="confidence",param=0.95) # single confidence level case
list3 <- list(type="BIC",param=lbdvec)</pre>
                                             # multiple regularizers with BIC selection
## compute with different scenarios
out1 <- PreEst.glasso(data, method=list1)</pre>
out2 <- PreEst.glasso(data, method=list2)</pre>
out3 <- PreEst.glasso(data, method=list3)</pre>
## visualize
opar <- par(no.readonly=TRUE)</pre>
par(mfrow=c(2,2), pty="s")
image(diag(pdim)[,pdim:1], main="Original Precision")
image(out1$C[,pdim:1], main="glasso::lambda=1.0")
image(out2$C[,pdim:1],
                           main="glasso::Confidence=0.95")
image(out3$C[,pdim:1],
                           main="glasso::BIC selection")
par(opar)
```

samplecovs

Generate Sample Covariances of 2 groups

#### **Description**

For visualization purpose, samplecovs generates a 3d array of stacked sample covariances where - in 3rd dimension, the first half are sample covariances of samples generated independently from normal distribution with identity covariance, where the latter half consists of samples covariances from dense random population covariance.

#### Usage

```
samplecovs(ncopy, size)
```

#### **Arguments**

ncopy the total number of sample covariances to be generated. size dimension p.

#### Value

```
a (p \times p \times ncopy) array of strictly positive definite sample covariances.
```

samplecovs 31

```
## generate total of 20 samples covariances of size 5-by-5.
samples <- samplecovs(20,5)</pre>
```

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