

Package ‘pdglasso’

June 14, 2024

Type Package

Title Graphical Lasso for Coloured Gaussian Graphical Models for Paired Data

Version 1.1.0

Description This package deals with RCON models for paired data and implements an Alternating Directions Method of Multipliers (ADMM) algorithm to solve the penalized likelihood method introduced by Ranciati and Roverato (2023). Also functions for the computation of maximum likelihood estimates and for the generation of simulated pdRCON models and data are provided.

License GPL (>= 2)

Encoding UTF-8

LazyData true

RoxxygenNote 7.2.3

ByteCompile TRUE

Roxxygen list(markdown = TRUE)

Url <https://github.com/savranciati/pdglasso>

Depends R (>= 2.10)

Imports MASS

R topics documented:

pdglasso-package	2
admm.pdglasso	4
compute.eBIC	6
fMRI_parietal	7
GGM.simulate	7
lams.max	8
pdColG.get	9
pdColG.plot	10
pdColG.summarize	11
pdRCON.check	11
pdRCON.fit	12
pdRCON.mle	14
pdRCON.simulate	15
toy_data	17

Index

19

Description

This package deals with RCON models for paired data and implements an Alternating Directions Method of Multipliers (ADMM) algorithm to solve the penalized likelihood method introduced by Ranciati and Roverato (2023). Also functions for the computation of maximum likelihood estimates and for the generation of simulated pdRCON models and data are provided.

Details

An RCON model for paired data (pdRCON model) is a coloured Gaussian Graphical Model (GGM) where the p variables are partitioned into a Left block L and a Right block R . The two blocks are not independent, every variable in the left block has an homologous variable in the right block and certain types of equality Restrictions on the entries of the CONcentration matrix K are allowed. A pdRCON model is represented by a Coloured Graph for Paired Data (pdColG) with a vertex for every variable and where every vertex and edge is either *coloured* or *uncoloured*. More details on the equality constraints of pdRCON models, submodel classes of interest and on the usage of the package are given in the following.

pdRCON models - terminology and relevant submodel classes

A pdRCON model is a Gaussian Graphical Model with additional equality restrictions on the entries of the concentration matrix. In the paired data framework, there are three different types of equality restrictions of interest, identified with the names *vertex*, *inside-block edge* and *across-block edge*, respectively. Relevant submodel classes can be specified both by allowing different combinations of restriction types and by forcing different types of fully symmetric structures. In this package, different submodel classes are identified by the arguments *type* and *force.symm* and models are represented by coloured graphs for paired data encoded in the form of a pdColG matrix.

- Every variable in L has an homologous variable in R and the corresponding diagonal entries of K can be constrained to have equal value. Such entries of K are represented by *coloured vertices* of the independence graph whereas the unconstrained diagonal entries are represented by *uncoloured vertices*. Different types of submodel classes of interest may be obtained by (i) not allowing coloured vertices, (ii) allowing both coloured and uncoloured vertices and (iii) allowing only coloured vertices.
- For every pair of variables in L there exists an homologous pair of variables in R , thereby identifying a pair of homologous edges. If both edges are present in the graph the corresponding off-diagonal entries of K can be constrained to have equal value. These type of edges are referred to as *coloured symmetric inside-block edges*. Different types of submodel classes of interest may be obtained by (i) not allowing coloured inside-block edges, (ii) allowing both coloured and uncoloured inside-block edges and (iii) allowing only coloured inside-block edges.
- We say that two variables are *across-block* if one variable belongs to L and the other to R . For every pair of non-homologous across-block variables there exists an homologous pair across-block variables, thereby identifying a pair of homologous edges. If both edges are present in the graph the corresponding off-diagonal entries of K can be constrained to have equal value. These type of edges are referred to as *coloured symmetric across-block edges*. Different types of submodel classes of interest may be obtained by (i) not allowing coloured

across-block edges, (ii) allowing both coloured and uncoloured across block edges and (iii) allowing only coloured across-block edges, with the exception of edges joining a variable in L with its homologous in R .

- We remark that every coloured edge belongs to a pair of coloured symmetric edges, either inside- or across- blocks. On the other hand, for an uncolored edge its homologous edge may or may not be present in the graph. In the case where an uncoloured edge and its homologous are both present we say that they form a pair of *uncoloured symmetric edges*, either inside- or across- blocks.

Use of the arguments type and force.symm to specify a submodel class

The functions of this package make it possible to specify different types of pdRCOn submodel classes of interest through the arguments `type` and `force.symm` which can both take as value any subvector of the character vector `c("vertex", "inside.block.edge", "across.block.edge")`; note that the names of the components can be abbreviated down, up to the first letter only, and are not case-sensitive. The argument `type` cannot be `NULL` and:

- If `type` contains the string "`vertex`" then coloured vertex symmetries are allowed and, if in addition also `force.symm` contains the string "`vertex`", then all vertices are coloured.
- If `type` contains the string "`inside.block.edge`" then coloured inside-block edge symmetries are allowed and, if in addition also `force.symm` contains the string "`inside.block.edge`", then only coloured edges are allowed inside blocks.
- If `type` contains the string "`across.block.edge`" then coloured across-block edge symmetries are allowed and, if in addition also `force.symm` contains the string "`across.block.edge`", then only coloured edges are allowed across blocks, with the exception of edges joining a variable in L with its homologous in R .

Note that `force.symm` is a, possibly `NULL`, subvector of `type`. Elements of `force.symm` which are not elements of `type` are ignored.

Variables position and block structure of sample covariance matrices

The functions of this package assume that the positions occupied by variables follow certain rules. More specifically, the positions from 1 to $q = p/2$ correspond to the first group of variables, say L , whereas the positions from $q + 1$ to p are associated with the second group of variables, R . Furthermore, the variables of the first group are ordered in the same way as those of the second group, in the sense that for every $i = 1, \dots, q$ the variable in position i is homologous to the variable in position $q + i$. Hence, for instance, the functions that receive in input a sample covariance matrix assume that the rows and columns of this matrix are ordered according to these rules, so that it can be partitioned into four $q \times q$ submatrices naturally associated with the inside- and across- block components.

Model representation through the pdColG matrix

Every pdRCOn model is uniquely represented by a Coloured Graph for Paired Data (pdColG) implemented in the form of a $p \times p$ symmetric matrix where every entry is one of the values 0, 1 or 2, as follows:

- The diagonal entries of the pdColG matrix are all equal to either 1, for uncoloured vertices, or 2, for coloured vertices.
- The off-diagonal entries of the pdColG matrix are equal to 0 for missing edges and either 1 or 2 for present edges, where the value 2 is used to encode coloured edges.

Author(s)

Saverio Ranciati (ORCID: 0000-0001-7880-9465) and Alberto Roverato (ORCID: 0000-0001-7984-3593)

Maintainer: Saverio Ranciati saverio.ranciati2@unibo.it

References

- Ranciati, S., Roverato, A., (2023). On the application of Gaussian graphical models to paired data problems. *arXiv pre-print*. <https://arxiv.org/abs/2307.14160>
- Ranciati, S., Roverato, A., Luati, A. (2021). Fused graphical lasso for brain networks with symmetries. *Journal of the Royal Statistical Society Series C: Applied Statistics*, 70(5), 1299-1322. <https://doi.org/10.1111/rssc.12514>
- Højsgaard, S., Lauritzen, S. L. (2008). Graphical Gaussian models with edge and vertex symmetries. *Journal of the Royal Statistical Society Series B: Statistical Methodology*, 70(5), 1005-1027 <https://doi.org/10.1111/j.1467-9868.2008.00666.x>

admm.pdglasso

ADMM graphical lasso algorithm for coloured GGMs for paired data.

Description

By providing a covariance matrix S and values for λ_1 and λ_2 , this function estimates a concentration matrix X within the pdRCOn submodel class, identified by the arguments `type` and `force.symm`, based on the pdglasso method (Ranciati & Roverato, 2023) using an (adaptive) ADMM algorithm. The output is the matrix and a list of internal parameters used by the function, together with the specific call with the relevant pdRCOn submodel class.

Usage

```
admm.pdglasso(
  S,
  lambda1 = 1,
  lambda2 = 1e-04,
  type = c("vertex", "inside.block.edge", "across.block.edge"),
  force.symm = NULL,
  X.init = NULL,
  rho1 = 1,
  rho2 = 1,
  varying.rho1 = TRUE,
  varying.rho2 = TRUE,
  max_iter = 5000,
  eps.abs = 1e-06,
  eps.rel = 1e-06,
  verbose = FALSE,
  print.type = TRUE
)
```

Arguments

<code>S</code>	a sample covariance (or correlation) matrix with the block structure described in pdglasso-package .
<code>lambda1</code>	a non-negative scalar (or vector) penalty that encourages sparsity in the concentration matrix.
<code>lambda2</code>	a non-negative scalar (or vector) penalty that encourages equality constraints in the concentration matrix.
<code>type</code> , <code>force.symm</code>	two subvectors of <code>c("vertex", "inside.block.edge", "across.block.edge")</code> which identify the pdRCOM submodel class of interest; see pdglasso-package for details.
<code>X.init</code>	(optional) a $p \times p$ initial guess for the concentration matrix and/or starting solution for the ADMM algorithm.
<code>rho1</code>	a scalar; tuning parameter of the ADMM algorithm to be used for the outer loop. It must be strictly positive.
<code>rho2</code>	a scalar; tuning parameter of the ADMM algorithm to be used for the inner loop. It must be strictly positive.
<code>varying.rho1</code>	a logical; if TRUE the parameter rho1 is updated iteratively to speed-up convergence.
<code>varying.rho2</code>	a logical; if TRUE the parameter rho2 is updated iteratively to speed-up convergence.
<code>max_iter</code>	an integer; maximum number of iterations to be run in case the algorithm does not converge.
<code>eps.abs</code>	a scalar; the absolute precision required for the computation of primal and dual residuals of the ADMM algorithm.
<code>eps.rel</code>	a scalar; the relative precision required for the computation of primal and dual residuals of the ADMM algorithm.
<code>verbose</code>	a logical; if TRUE the progress (and internal convergence of inner loop) is shown in the console while the algorithm is running.
<code>print.type</code>	a logical; if TRUE the pdRCOM submodel class considered, as specified by the arguments <code>type</code> and <code>force.symm</code> - is returned as printed output in the console.

Value

A list with the following components:

- `X` the estimated concentration matrix under the pdRCOM submodel class considered and the values of `lambda1` and `lambda2`.
- `acronyms` a vector of strings identifying the pdRCOM submodel class considered as identified by the arguments `type` and `force.symm`.
- `internal.par` a list of internal parameters passed to the function at the call, as well as convergence information.

References

Ranciati, S., Roverato, A., (2023). On the application of Gaussian graphical models to paired data problems. *arXiv pre-print*. <https://arxiv.org/abs/2307.14160>

Examples

```
S <- cov(toy_data$sample.data)
admm.pdlasso(S)
```

`compute.eBIC`

Compute the extended Bayesian Information Criterion (eBIC).

Description

This function computes the value of the eBIC for a given model and gamma value, for the purpose of model selection (see Eq.1 of Feygel & Drton, 2010).

Usage

```
compute.eBIC(S, mod, n, gamma.eBIC = 0.5, max_iter = 5000)
```

Arguments

<code>S</code>	a sample covariance (or correlation) matrix with the block structure described in pdlasso-package .
<code>mod</code>	a list, the output object of a call to admm.pdlasso .
<code>n</code>	the sample size of the data used to compute the sample covariance matrix <code>S</code> .
<code>gamma.eBIC</code>	a parameter governing the magnitude of the penalization term inside the criterion; it ranges from 0 to 1, where 0 makes the eBIC equivalent to BIC, and 0.5 being the suggested default value.
<code>max_iter</code>	an integer; maximum number of iterations to be run in case the algorithm does not converge; passed to pdRCON.mle .

Value

A vector containing three elements:

- the value of the eBIC,
- the log-likelihood,
- and the number of parameters.

References

Foygel, R., Drton, M. (2010). Extended Bayesian information criteria for Gaussian graphical models. *Advances in neural information processing systems*, 23. <https://proceedings.neurips.cc/paper/2010/file/072b030ba126b2f4b2374f342be9ed44-Paper.pdf>

Examples

```
S <- cov(toy_data$sample.data)
mod <- admm.pdlasso(S, lambda1=1, lambda2=0.5)
compute.eBIC(S,mod,n=60,gamma.eBIC=0.5)
```

<code>fMRI_parietal</code>	<i>fMRI Dataset</i>
----------------------------	---------------------

Description

Put reference here.

Usage

```
fMRI_parietal
```

Format

`fMRI_parietal`:
A 404×10 matrix.

<code>GGM.simulate</code>	<i>Random simulation of Gaussian graphical models (GGMs)</i>
---------------------------	--

Description

Randomly generates an undirected graph \mathcal{G} , a concentration matrix K adapted to \mathcal{G} and a random sample from a multivariate normal distribution with zero mean vector and covariance matrix $\Sigma = K^{-1}$.

Usage

```
GGM.simulate(  
  p,  
  concen.mat = TRUE,  
  sample = TRUE,  
  Sigma = NULL,  
  sample.size = NULL,  
  dens = 0.1  
)
```

Arguments

<code>p</code>	an even integer, that is the number of vertices of the generated undirected graph \mathcal{G} .
<code>concen.mat</code>	a logical (default TRUE) indicating whether a concentration matrix K adapted to \mathcal{G} should be generated.
<code>sample</code>	a logical (default TRUE) indicating whether a sample from a normal distribution with zero mean vector and concentration matrix K should be generated.
<code>Sigma</code>	a $p \times p$ positive definite matrix. This is the matrix argument of the rWishart function, which is used as starting point in the random generation of the concentration matrix, as described in the details section of the function pdRCON.simulate . The default <code>NULL</code> is equivalent to the identity matrix <code>Sigma=diag(p)</code> .
<code>sample.size</code>	size of the randomly generated sample. The default <code>NULL</code> is equivalent to <code>sample.size=3*p</code> .
<code>dens</code>	a value between zero and one used to specify the sparsity degree of the generated graph, as described in the details section of the function pdRCON.simulate .

Details

A GGM is a pdRCOM model with no parametric symmetries, and the purpose of this function is that of providing a simplified call to the function [pdRCOM.simulate](#), with the appropriate choice of arguments required to simulate from GGMs. Note, however, that pdRCOM models make sense only if the number of variables p is even, and this requirement is (unnecessarily) retained here.

Value

A list with the following components:

- G a randomly generated matrix encoding an undirected graph on p vertices. More specifically, G is a pdColG graph with no entry equal to 2, and it differs from the adjacency matrix of the undirected graph because its diagonal entries are equal to one.
- K a randomly generated concentration matrix adapted to G .
- sample.data a randomly generated sample form a multivariate normal distribution with mean vector zero and concentration matrix K .

Note that the variable are named V_1, \dots, V_p .

Examples

```
# generates distribution and data from a GGM on 20 variables and graph density equal to 0.2
p <- 20
n <- 100
set.seed(1234)
GenMod <- GGM.simulate(20, sample.size=n, dens=0.20)

# check graph sparsity degree
n.edges <- sum(GenMod$G[upper.tri(GenMod$G)])
n.edges/(p*(p-1)/2)

# check positive definiteness
min(eigen(GenMod$K)$values)

# computation of the partial correlation matrix
R <- -cov2cor(GenMod$K)
diag(R) <- 1
```

lams.max

Compute maximum theoretical values for lambda1 and lambda2.

Description

Computes the maximum values for λ_1 and λ_2 such that:

- if max of λ_1 is used, the estimated concentration matrix will be diagonal;
- if max of λ_2 is used, the estimated concentration matrix will be fully symmetric.

Usage

`lams.max(S)`

Arguments

`S` a covariance matrix.

Value

a vector of two elements.

Examples

```
S <- cov(toy_data$sample.data)
lams.max(S)
```

`pdColG.get`

Build a graph from the output of a call to [admm.pdglasso](#).

Description

This function returns a Coloured Graph for Paired Data (pdColG) from the output of a call to [admm.pdglasso](#). We refer to [pdglasso-package](#) both for the description of the matrix encoding a coloured graph for paired and the available submodel classes.

Usage

```
pdColG.get(admm.out, th1 = NULL, th2 = NULL, print.summary = FALSE)
```

Arguments

<code>admm.out</code>	An object of list type, that is the output of a call to the admm.pdglasso function.
<code>th1</code>	(optional) A scalar, the threshold to identify edges in the graph; it must be non-negative.
<code>th2</code>	(optional) A scalar, the threshold to identify coloured edges in the graph; it must be non-negative.
<code>print.summary</code>	(optional) if TRUE provides summary statistics of the graph.

Value

a list with the following components:

- `pdColG` a matrix representing a coloured graph for paired data; see [pdglasso-package](#) for details.
- `n.par` the number of parameters of the pdRCON model represented by `pdColG`.

Examples

```
S <- cov(toy_data$sample.data)
mod.out <- admm.pdglasso(S)
pdColG.get(mod.out)
```

pdColG.plot*Visualize a coloured graph for paired data***Description**

This functions produces a heatmap-style graphical representation of a graph object produced by a call to [pdColG.get](#), or a matrix compatible with the coloured graph specification used in this package.

Usage

```
pdColG.plot(
  G,
  block = "everything",
  which.sym = c("structural", "parametric"),
  asym.edges = TRUE,
  export.plot = FALSE,
  fancy = TRUE
)
```

Arguments

block	a string; allows the user to specify which portion of the graph (a block) is to be plotted: possible mutually exclusive options are "left", "right", "across", "everything"; default is "everything", which means the entire graph is plotted.
which.sym	a string or a vector of strings; specifies which kind of symmetries are plotted (structural, parametric or both).
asym.edges	a logical value; if TRUE, Asymmetric edges are plotted otherwise their symbol is suppressed
export.plot	a logical value; if TRUE, a .pdf file is produced in the working director instead of plotting the graph as a new panel/window.
fancy	a logical value; if TRUE, symbols in the plot are used from the Latin1 encoding for characters; set to FALSE if characters are not properly displayed, so symbols are reverted to latin letters.
g	a symmetric $p \times p$ matrix coding a coloured graphical model; only values allowed are the integers $\{0, 1, 2\}$; usually, an object produced by a call to the function pdColG.get

Value

either a plot within the running R session or a .pdf file saved in the working directory if the option `export.plot` is set to TRUE.

Examples

```
pdColG.plot(toy_data$pdColG)
```

<code>pdColG.summarize</code>	<i>Structural properties of a coloured graph for paired data</i>
-------------------------------	--

Description

This function returns some summary statistics relative to the structural properties of a coloured graph for paired data \mathcal{G} . We refer to [pdglasso-package](#) both for the description of the matrix encoding a coloured graph for paired and details on how the structural quantities are defined and computed.

Usage

```
pdColG.summarize(pdColG, print.summary = TRUE)
```

Arguments

- | | |
|----------------------------|---|
| <code>pdColG</code> | a matrix representing a coloured graph for paired data; see pdglasso-package for details. |
| <code>print.summary</code> | a logical (default TRUE) indicating whether a summary should be printed. |

Value

An invisible list with the following components:

- `overall` a list with the number of vertices and edges of \mathcal{G} .
- `vertex` a list with the number of coloured vertices of \mathcal{G} .
- `inside` a list with the number of inside-block edges, the number of uncolored symmetric and coloured inside block edges of \mathcal{G} .
- `across` a list with the number of across-block edges, the number of uncolored symmetric and coloured across block edges of \mathcal{G} .

If `print.summary=TRUE` some summary statistics are also printed on the console

Examples

```
pdColG.summarize(toy_data$pdColG)
```

<code>pdRCON.check</code>	<i>Check orders of magnitude of entries of the estimated concentration matrix X under the pdRCON submodel class considered.</i>
---------------------------	---

Description

This function produces different plots of values of X in [log10](#) scale, depending on the submodel class identified by the acronym stored in the input object `mod.out`. The user might want to call this function to identify what values to pass as arguments `th1` and `th2` to a call to the function [pdColGet](#).

Usage

```
pdRCON.check(mod.out)
```

Arguments

mod.out	An object of list type, that is the output of a call to the admm.pdlasso function. This can also be the output of a call to pdRCON.fit .
---------	---

Value

Depending on the acronym stored inside the input object, one or more plots depicting:

- off-diagonal elements,
- vertices,
- inside-block,
- across-block.

Examples

```
S <- cov(toy_data$sample.data)
mod.out <- pdRCON.fit(S,n=60)
pdRCON.check(mod.out)
```

pdRCON.fit

Fit and select a coloured GGM for paired data according to eBIC criterion.

Description

Performs a sequence of calls to [admm.pdlasso](#) providing two grids of values for lambda1 and lambda2. First, a grid search conditional on lambda2=0 is run to select the best lambda1 value among the candidates (according to eBIC); conditional on the best lambda1, a similar search is performed for lambda2. The output is the select model, given by the estimated concentration matrix. The user may call [pdColG.get](#) to obtain the corresponding Coloured Graph for Paired Data (pdColG) from the selected model.

Usage

```
pdRCON.fit(
  S,
  n,
  lams = NULL,
  gamma.eBIC = 0.5,
  type = c("vertex", "inside.block.edge", "across.block.edge"),
  force.symm = NULL,
  X.init = NULL,
  rho1 = 1,
  rho2 = 1,
  varying.rho1 = TRUE,
  varying.rho2 = TRUE,
```

```

max_iter = 5000,
eps.abs = 1e-08,
eps.rel = 1e-08,
verbose = FALSE,
progress = TRUE,
print.type = TRUE
)

```

Arguments

S	a sample covariance (or correlation) matrix with the block structure described in pdlasso-package .
n	the sample size of the data used to compute the sample covariance matrix S.
lams	a 2x4 matrix; first row refers to lambda1 and second row to lambda2; for each row, values are (i) minimum value for the grid; (ii) maximum value for the grid; (iii) number of points in the grid; (iv) if a logarithmic spacing (TRUE) is desired for the grid or not (FALSE); if NULL default values are used, i.e. from max.lams to max.lams/20, and 20 grid points, log spacing for both.
gamma.eBIC	the parameter for the eBIC computation. gamma=0 is equivalent to BIC.
type, force.symm	two subvectors of c("vertex", "inside.block.edge", "across.block.edge") which identify the pdRCON submodel class of interest; see pdlasso-package for details.
X.init	(optional) a $p \times p$ initial guess for the concentration matrix and/or starting solution for the ADMM algorithm.
rho1	a scalar; tuning parameter of the ADMM algorithm to be used for the outer loop. It must be strictly positive.
rho2	a scalar; tuning parameter of the ADMM algorithm to be used for the inner loop. It must be strictly positive.
varying.rho1	a logical; if TRUE the parameter rho1 is updated iteratively to speed-up convergence.
varying.rho2	a logical; if TRUE the parameter rho2 is updated iteratively to speed-up convergence.
max_iter	an integer; maximum number of iterations to be run in case the algorithm does not converge.
eps.abs	a scalar; the absolute precision required for the computation of primal and dual residuals of the ADMM algorithm.
eps.rel	a scalar; the relative precision required for the computation of primal and dual residuals of the ADMM algorithm.
verbose	a logical; if TRUE the progress (and internal convergence of inner loop) is shown in the console while the algorithm is running.
progress	a logical value; if TRUE provides a visual update in the console about the grid search over lambda1 and lambda2
print.type	a logical; if TRUE the pdRCON submodel class considered, as specified by the arguments type and force.symm - is returned as printed output in the console.

Value

A list with the following components:

- `model` selected model; object resulting from the function `admm.pdlasso` with `best.lambdas`.
- `lambda.grid` the grid of values used for `lambda1` and `lambda2`.
- `best.lambdas` the selected values of `lambda1` and `lambda2` according to eBIC criterion.
- `11.path` a matrix containing the grid values for `lambda1` as well as quantities used in eBIC computation.
- `12.path` a matrix containing the grid values for `lambda2` as well as quantities used in eBIC computation.
- `time.exec` total execution time for the called function.

A warning is produced if at least one run of the algorithm for the grid searches has resulted in non-convergence (status can be checked by inspecting `11.path` and `12.path`).

Examples

```
S <- cov(toy_data$sample.data)
sel.mod <- pdRCON.fit(S, n=60)
sel.mod$11.path
sel.mod$12.path
pdRCON.check(sel.mod$model)
pdColG.get(sel.mod$model)
```

`pdRCON.mle`

Maximum likelihood estimation

Description

Computes the maximum likelihood estimate of the concentration matrix of a pdRCON model.

Usage

```
pdRCON.mle(S, pdColG, eps.rel = 1e-06, eps.abs = 1e-06, max_iter = 5000)
```

Arguments

<code>S</code>	a sample covariance matrix with the block structure described in pdlasso-package .
<code>pdColG</code>	<code>pdColG</code> a matrix representing a coloured graph for paired data; see pdlasso-package for details.
<code>eps.rel</code>	a scalar; the relative precision required for the computation of primal and dual residuals of the ADMM algorithm.
<code>eps.abs</code>	a scalar; the absolute precision required for the computation of primal and dual residuals of the ADMM algorithm.
<code>max_iter</code>	an integer; maximum number of iterations to be run in case the algorithm does not converge.

Details

If the sample covariance matrix is not full-rank, then it is possible that the maximum likelihood estimate does not exist. The maximum likelihood estimate is computed by running the function [admm.pdglasso](#) with suitable penalties and, if it does not exist, then the ADMM algorithm fails to converge, a warning is produced and a NULL is returned.

Value

Either a matrix, that is the maximum likelihood estimate of $K = \Sigma^{-1}$ under the pdRCON model represented by pdColG, or NULL if the maximum likelihood estimate does not exist.

Examples

```
S <- var(toy_data$sample.data)
K.hat <- pdRCON.mle(S, toy_data$pdColG)
```

pdRCON.simulate *Random simulation of pdRCON models*

Description

Randomly generates a coloured graph for paired data \mathcal{G} , a concentration matrix K that both is adapted to \mathcal{G} and satisfies the equality constraints implied by \mathcal{G} , and a random sample from a multivariate normal distribution with zero mean vector and covariance matrix $\Sigma = K^{-1}$.

Usage

```
pdRCON.simulate(
  p,
  concent.mat = TRUE,
  sample = TRUE,
  Sigma = NULL,
  sample.size = NULL,
  type = c("vertex", "inside.block.edge", "across.block.edge"),
  force.symm = NULL,
  dens = 0.1,
  dens.vertex = NULL,
  dens.inside = NULL,
  dens.across = NULL,
  print.type = TRUE
)
```

Arguments

- | | |
|--------------------------|---|
| <code>p</code> | an even integer, that is the number of vertices of the generated coloured graph for paired data pdColG. |
| <code>concent.mat</code> | a logical (default TRUE) indicating whether a concentration matrix K adapted to pdColG should be generated. |

sample	a logical (default TRUE) indicating whether a sample from a normal distribution with zero mean vector and concentration matrix K should be generated.
Sigma	a $p \times p$ positive definite matrix. This is the matrix argument of the rWishart function, which is used as starting point in the random generation of the concentration matrix, as described in the details section below. The default NULL is equivalent to the identity matrix Sigma=diag(p).
sample.size type, force.symm	size of the randomly generated sample. The default NULL is equivalent to sample.size=3*p. two subvectors of c("vertex", "inside.block.edge", "across.block.edge") which identify the pdRCON submodel class of interest; see pdglasso-package for details.
dens, dens.vertex, dens.inside, dens.across	four values between zero and one used to specify the sparsity degree of the generated graph, as described in the details section below. The default dens.vertex=NULL is equivalent to dens.vertex=dens, and similarly for dens.inside and dens.across.
print.type	a logical; if TRUE the pdRCON submodel class considered, as specified by the arguments type and force.symm - is returned as printed output in the console.

Details

Details on the sparsity degree of the generated graph

The argument dens.vertex specifies the proportion of coloured vertices among the p vertices. This is used if the string "vertex" is a component of type but not of force.symm. The string "vertex" not being a component of type is equivalent to dens.vertex=0 whereas the string "vertex" being a component of both type and force.symm is equivalent to dens.vertex=1.

The argument dens.inside specifies the proportion of coloured symmetric inside block edges among the $q(q-1)$, with $q = p/2$, inside block edges. This is used if the string "inside.block.edge" is a component of type, otherwise it is equivalent to dens.inside=0. The overall density of inside block edges is obtained by the sum of the densities of coloured and uncoloured inside block edges. This is a value between dens.inside and dens.inside+dens. Furthermore, it is exactly equal to dens if "inside.block.edge" is not a component of type and to dens.inside if "inside.block.edge" is a component of both type and force.symm.

The argument dens.across specifies the proportion of coloured symmetric across block edges among the potentially coloured $q(q-1)$ across block edges. This is used if the string "across.block.edge" is a component of type, otherwise it is equivalent to dens.across=0. The overall density of across block edges is obtained by the sum of the densities of coloured and uncoloured across block edges. This is a value between dens.across and dens.across+dens. Furthermore, it is exactly equal to dens if "across.block.edge" is not a component of type.

The argument dens specifies the density of uncoloured edges. Note that the algorithm generates uncoloured edges first, which may be overwritten by coloured edges. For this reason the actual density of uncoloured edges is typically smaller than dens.

Details on the generating process of the concentration matrix

The concentration matrix is obtained by first generating a random Wishart matrix with matrix parameter Sigma and p degrees of freedom, which represents an initial unconstrained covariance matrix. This is inverted and adapted to a suitable coloured graph for paired data with sparsity degree according to the dens.xxx arguments.

Value

A list with the following components:

- pdColG a randomly generated a matrix representing a coloured graph for paired data on p vertices; see [pdlasso-package](#) for details.
- K a randomly generated concentration matrix adapted to pdColG.
- sample.data a randomly generated sample form a multivariate normal distribution with mean vector zero and concentration matrix K.

Note that the variable in L are named L_1, \dots, L_q and variables in R are are named R_1, \dots, R_q where L_i is homologous to R_i for every $i=1, \dots, q$.

Examples

```
# generates a pdRCON model on 10 variables in the form of a pdColG matrix

set.seed(123)
pdRCON.model <- pdRCON.simulate(10, concent=FALSE, sample=FALSE, dens=0.25)$pdColG

# generates a distribution from a pdRCON model on 20 variables, a concentration matrix
# for this model and a sample of size 50
# all vertices are coloured and no coloured across block edge is allowed

set.seed(123)
GenMod <- pdRCON.simulate(20, type=c("v", "i"), force.symm=c("v"), sample.size=50, dens=0.20)

pdColG.summarize(GenMod$pdColG)

# computation of the partial correlation matrix
R <- -cov2cor(GenMod$K)
diag(R) <- 1
```

toy_data

Toy dataset generated through [pdRCON.simulate](#) function

Description

Data simulated by the function [pdRCON.simulate](#) with parameters:

- p=20
- type=c("v", "i", "a")
- force.symm=NULL
- dens=0.5
- Sigma a $p \times p$ matrix with unitary diagonal and 0.5 on off-diagonal elements.

Usage

toy_data

Format

`toy_data`:

A list with the following components:

- `pdColG` a matrix representing a coloured graph for paired data; see [pdglasso-package](#) for details.
- `K`, a concentration matrix adapted to `pdColG`.
- `sample.data`, a data frame with 250 rows and 20 columns from a multivariate normal distribution with zero mean vector and concentration matrix `K`.

Index

* datasets

fMRI_parietal, 7
toy_data, 17

admm.pdglasso, 4, 6, 9, 12, 14, 15

compute.eBIC, 6

fMRI_parietal, 7

GGM.simulate, 7

lams.max, 8

log10, 11

pdColG.get, 9, 10, 12

pdColG.plot, 10

pdColG.summarize, 11

pdColGet, 11

pdglasso-package, 2

pdRCOn.check, 11

pdRCOn.fit, 12, 12

pdRCOn.mle, 6, 14

pdRCOn.simulate, 7, 8, 15, 17

rWishart, 7, 16

toy_data, 17