

# Package ‘pdglasso’

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**Title** Graphical Lasso for Coloured Gaussian Graphical Models for Paired Data

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

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## R topics documented:

pdglasso-package . . . . .	2
admm.pdglasso . . . . .	4
compute.eBIC . . . . .	6
pdColG.get . . . . .	7
pdColG.summarize . . . . .	7
pdRCON.fit . . . . .	8
pdRCON.mle . . . . .	10
pdRCON.simulate . . . . .	11
toy_data . . . . .	13
<b>Index</b>	<b>14</b>

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pdglasso-package

*pdglasso: Graphical Lasso for Coloured Gaussian Graphical Models for Paired Data*

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## Description

This package deals with RCON models for paired data and implements an Alternating Directions Method of Multipliers (ADMM) algorithm to solve a penalized likelihood method. 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 uncoloured 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 group 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.

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**References**

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>

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admm.pdglasso

*ADMM graphical lasso algorithm for coloured GGMs for paired data.*

---

**Description**

By providing a covariance matrix  $S$  and values for  $\lambda_1$  and  $\lambda_2$ , this function estimates a concentration matrix  $X$  within the family of pdRCON submodel class identified by the arguments `type` and `force.symm`, 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 = 1000,
  eps.abs = 1e-12,
  eps.rel = 1e-12,
  verbose = FALSE,
  print.type = TRUE
)
```

**Arguments**

<code>S</code>	a sample covariance (or correlation) matrix with the block structure described in <a href="#">pdglasso-package</a> .
<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, force.symm</code>	two subvectors of <code>c("vertex", "inside.block.edge", "across.block.edge")</code> which identify the pdRCON submodel class of interest; see <a href="#">pdglasso-package</a> 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 <code>rho1</code> is updated iteratively to speed-up convergence.
<code>varying.rho2</code>	a logical; if TRUE the parameter <code>rho2</code> 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 pdRCON 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 pdRCON submodel class considered and the values of `lambda1` and `lambda2`.
- `acronyms` a vector of strings identifying the pdRCON 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.

## Examples

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

---

code compute.eBIC

Compute the extended Bayesian Information Criterion (eBIC).

---

## Description

The 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 = 1000)
```

## Arguments

S	a sample covariance (or correlation) matrix with the block structure described in <a href="#">pdglasso-package</a> .
mod	a list, the output object of a call to <a href="#">admm.pdglasso</a>
n	the sample size of the data used to compute the sample covariance matrix S.
gamma.eBIC	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.
max_iter	an integer; maximum number of iterations to be run in case the algorithm does not converge; passed to <a href="#">pdRCON.mle</a> .

## Value

A vector containing three elements:

- the value of the eBIC,
- the log-likelihood,
- and the estimated number of degrees of freedom.

## 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.pdglasso(S, lambda1=1, lambda2=0.5)
compute.eBIC(S,mod,n=60,gamma.eBIC=0.5)
```

---

pdColG.get	<i>Build a graph from the output of a call to <a href="#">admm.pdglasso</a>.</i>
------------	--

---

### 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

admm.out	An object of list type, that is the output of a call to the <a href="#">admm.pdglasso</a> function.
th1	(optional) A scalar, the threshold to identify edges in the graph; it must be non-negative.
th2	(optional) A scalar, the threshold to identify coloured edges in the graph; it must be non-negative.
print.summary	(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.
- dof the degrees of freedom of the pdRCON model represented by pdColg.

### Examples

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

---

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

### 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

- pdColG            a matrix representing a coloured graph for paired data; see [pdglasso-package](#) for details.
- print.summary    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)
```

---

pdRCON.fit	<i>Fit and select a coloured GGM for paired data according to eBIC criterion.</i>
------------	---

---

### Description

Performs a sequence of calls to [admm.pdglasso](#) 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 and corresponding graph.

### Usage

```
pdRCON.fit(
  S,
  n,
  n.l1 = 10,
  n.l2 = 10,
  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 = 500,
    eps.abs = 1e-08,
    eps.rel = 1e-08,
    verbose = FALSE,
    print.type = TRUE
  )

```

## Arguments

<code>S</code>	a sample covariance (or correlation) matrix with the block structure described in <a href="#">pdglasso-package</a> .
<code>n</code>	the sample size of the data used to compute the sample covariance matrix <code>S</code> .
<code>n.l1</code>	the number of values in the grid of candidates for <code>lambda1</code> .
<code>n.l2</code>	the number of values in the grid of candidates for <code>lambda2</code> .
<code>gamma.eBIC</code>	the parameter for the eBIC computation. <code>gamma=0</code> is equivalent to BIC.
<code>type, force.symm</code>	two subvectors of <code>c("vertex", "inside.block.edge", "across.block.edge")</code> which identify the pdRCON submodel class of interest; see <a href="#">pdglasso-package</a> 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 <code>rho1</code> is updated iteratively to speed-up convergence.
<code>varying.rho2</code>	a logical; if TRUE the parameter <code>rho2</code> 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 pdRCON 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:

- `model` the final model.
- `pdColG` the associated coloured graph.
- `best.lambdas` the selected values of `lambda1` and `lambda2` according to eBIC criterion.

- `l1.path` a matrix containing the grid values for `lambda1` as well as quantities used in eBIC computation.
- `l2.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.

### Examples

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

---

pdRCON.mle	<i>Maximum likelihood estimation</i>
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---

### Description

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

### Usage

```
pdRCON.mle(S, pdColG, max_iter = 1000, verbose = FALSE)
```

### Arguments

<code>S</code>	a sample covariance matrix with the block structure described in <a href="#">pdglasso-package</a> .
<code>pdColG</code>	<code>pdColG</code> a matrix representing a coloured graph for paired data; see <a href="#">pdglasso-package</a> for details.
<code>max_iter</code>	an integer; maximum number of iterations to be run in case the algorithm does not converge.
<code>verbose</code>	a logical (default FALSE) that is passed to the function <a href="#">admm.pdglasso</a> .

### 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  $K$  adapted to  $\mathcal{G}$  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
)
```

**Arguments**

- |   |  |
|---|--|
| p   | an even integer, that is the number of vertices of the generated coloured graph for paired data pdColG.  |
| concent.mat                                 | 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 the matrix argument of the <a href="#">rWishart</a> 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 $\text{Sigma}=\text{diag}(p)$ . |
| sample.size                                 | size of the randomly generated sample. The default NULL is equivalent to <code>sample.size=3*p</code> .  |
| type, force.symm                            | two subvectors of <code>c("vertex", "inside.block.edge", "across.block.edge")</code> which identify the pdRCON submodel class of interest; see <a href="#">pdglasso-package</a> 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 <code>dens.vertex=NULL</code> is equivalent to <code>dens.vertex=dens</code> , and similarly for <code>dens.inside</code> and <code>dens.across</code> .                       |

## 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  $q(q-1)/2$ , 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  $q(q-1)/2$  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 [pdglasso-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 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 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)
```

---

toy\_data

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

---

## Description

Data simulated by the function [pdRCON.simulate](#) with a call: `toy_data <- pdRCON.simulate(20, type=c("v", "i"),`

## 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 60 rows and 20 columns from a multivariate normal distribution with zero mean vector and concentration matrix `K`.

# Index

## \* datasets

toy\_data, [13](#)

admm.pdglasso, [4](#), [6–8](#), [10](#)

compute.eBIC, [6](#)

pdColG.get, [7](#)

pdColG.summarize, [7](#)

pdglasso-package, [2](#)

pdRCON.fit, [8](#)

pdRCON.mle, [6](#), [10](#)

pdRCON.simulate, [11](#), [13](#)

rWishart, [11](#)

toy\_data, [13](#)