## Package 'BCDAG'

March 15, 2022

Title Bayesian Structure and Causal Learning of Gaussian Directed Graphs

Version 1.0.0

**Description** A collection of functions for structure learning of causal networks and estimation of joint causal effects from observational Gaussian data. Main algorithm consists of a Markov chain Monte Carlo

scheme for posterior inference of causal structures, parameters and causal effects between variables.

References:

F. Castelletti and A. Mascaro (2021) <doi:10.1007/s10260-021-00579-1>, F. Castelletti and A. Mascaro (2022) <arXiv:2201.12003>.

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Encoding UTF-8

LazyData true

RoxygenNote 7.1.1

biocViews

Imports graphics, gRbase, grDevices, lattice, methods, mvtnorm, stats,

utils

Suggests rmarkdown, knitr, testthat (>= 3.0.0)

Config/testthat/edition 3

VignetteBuilder knitr

**Depends** R (>= 2.10)

NeedsCompilation no

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acceptreject\_DAG

Accept/reject the proposed DAG given the current DAG (internal function)

## Description

This function computes the Metropolis Hastings acceptance rate for proposedDAG given currentDAG and the accepts/rejects proposedDAG based on the Metropolis Hastings acceptance probability. proposedDAG is a direct successor of currentDAG, which was obtained by applying an operator of type InsertD, DeleteD or ReverseD to currentDAG. The two DAGs only differ by one edge u - > v which has been inserted/deleted/reversed in currentDAG.

#### Usage

```
acceptreject_DAG(
    tXX,
    n,
    currentDAG,
    proposedDAG,
    node,
    op.type,
```

bd\_decode

```
a,
U,
w,
current.opcard,
proposed.opcard
)
```

## Arguments

tXX	(q,q) matrix $X'X$ with X the $(n,q)$ data matrix
n	number of observations (rows) in the data matrix $X$
currentDAG	(q,q) adjacency matrix of current DAG
proposedDAG	(q,q) adjacency matrix of proposed DAG
node	nodes $u$ and $v$ involved in the modified edge $u - > v$
op.type	the type of operator applied to $currentDAG$ to obtain proposedDAG
а	shape hyperparameter of the DAG Wishart prior
U	position hyperparameter of the DAG Wishart prior
W	prior probability of edge inclusion
current.opcard	number of direct successors of currentDAG
proposed.opcard	1
	number of direct successors of proposedDAG

## Value

A Boolean indicating whether proposedDAG has been accepted (TRUE) or not (FALSE)

bd\_decode

Convert strings into matrices (internal function)

## Description

This function restores matrices from string objects. It is implemented in several functions, such as get\_causal\_effect and get\_edge\_probs, when output of learn\_DAG was obtained with save.memory = TRUE

## Usage

bd\_decode(string, separator = ";")

## Arguments

string	a string to convert into matrix
separator	symbol used to separate elements in the input string

## Value

The (q,q) original matrix from which the string vector was created using the internal function bd\_encode

bd\_encode

Convert matrix into strings (internal function)

## Description

This function converts matrices into string objects. It is implemented in learn\_DAG when save.memory = TRUE

## Usage

```
bd_encode(matrix, separator = ";")
```

## Arguments

matrix	a matrix to convert into string
separator	symbol used to separate elements of the matrix in the string

causaleffect	Compute causal effects between variables	
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## Description

This function computes the total joint causal effect on variable response consequent to an intervention on variables targets for a given a DAG structure and parameters (D,L)

## Usage

```
causaleffect(targets, response, L, D)
```

## Arguments

targets	numerical vector with labels of target nodes
response	numerical label of response variable
L	(q,q) matrix of regression-coefficient parameters
D	(q,q) diagonal matrix of conditional-variance parameters

#### causaleffect

#### Details

We assume that the joint distribution of random variables  $X_1, \ldots, X_q$  is zero-mean Gaussian with covariance matrix Markov w.r.t. a Directed Acyclic Graph (DAG). In addition, the allied Structural Equation Model (SEM) representation of a Gaussian DAG-model allows to express the covariance matrix as a function of the (Cholesky) parameters (D,L), collecting the conditional variances and regression coefficients of the SEM.

The total causal effect on a given variable of interest (response) consequent to a joint intervention on a set of variables (targets) is defined according to Pearl's do-calculus theory and under the Gaussian assumption can be expressed as a function of parameters (D,L).

#### Value

The joint total causal effect, represented as a vector of same length of targets

#### Author(s)

Federico Castelletti and Alessandro Mascaro

## References

J. Pearl (2000). Causality: Models, Reasoning, and Inference. Cambridge University Press, Cambridge.

F. Castelletti and A. Mascaro (2021). Structural learning and estimation of joint causal effects among network-dependent variables. *Statistical Methods and Applications*, Advance publication.

P. Nandy, M.H. Maathuis and T. Richardson (2017). Estimating the effect of joint interventions from observational data in sparse high-dimensional settings. *Annals of Statistics* 45(2), 647-674.

## Examples

```
# Randomly generate a DAG and the DAG-parameters
q = 8
w = 0.2
set.seed(123)
DAG = rDAG(q = q, w = w)
outDL = rDAGWishart(n = 1, DAG = DAG, a = q, U = diag(1, q))
L = outDL$L; D = outDL$D
# Total causal effect on node 1 of an intervention on {5,6}
causaleffect(targets = c(6,7), response = 1, L = L, D = D)
# Total causal effect on node 1 of an intervention on {5,7}
causaleffect(targets = c(5,7), response = 1, L = L, D = D)
```

DW\_nodelml

## Description

This function computes the log-marginal likelihood of the conditional distribution of variable node given its parents in DAG under a DAG-Wishart prior on the DAG model-parameters

## Usage

DW\_nodelml(node, DAG, tXX, n, a, U)

## Arguments

numerical label of node in DAG
(q,q) adjacency matrix of DAG
$(q,q)$ matrix $X^\prime X$ with $X$ the $(n,q)$ data matrix
number of observations (rows) in the data matrix $\boldsymbol{X}$
shape hyperparameter of the DAG Wishart prior
position hyperparameter of the DAG Wishart prior

## Value

The logarithm of the marginal likelihood of node

fa

Find the family of a node in a DAG (internal function)

#### Description

This function finds the family (union of node and its parents) of node in DAG

## Usage

fa(node, DAG)

## Arguments

node	numerical label of the node in DAG
DAG	(q,q) adjacency matrix of the DAG

## Value

A numerical vector with the labels of the family of node in DAG

get\_causaleffect Estimate total causal effects from the MCMC output

#### Description

This function provides causal effect estimates from the output of learn\_DAG

#### Usage

```
get_causaleffect(
  learnDAG_output,
  targets,
  response,
  BMA = FALSE,
  verbose = TRUE
)
```

## Arguments

learnDAG\_output

	object of class bcdag
targets	numerical $(p, 1)$ vector with labels of target nodes
response	numerical label of response variable
BMA	boolean; if TRUE, the Bayesian model averaging (BMA) estimate of the total causal effect is returned; if FALSE, samples from the posterior distribution of causal effect coefficients are returned
verbose	if TRUE, progress bar of MCMC sampling is displayed

## Details

Output of learn\_dag function consists of S draws from the joint posterior of DAGs and DAGparameters in a zero-mean Gaussian DAG-model; see the documentation of learn\_DAG for more details.

The total causal effect on a given variable of interest (response) consequent to a joint intervention on a set of variables (targets) is defined according to Pearl's do-calculus theory and under the Gaussian assumption can be expressed as a function of parameters (D,L), representing a (Cholesky) reparameterization of the covariance matrix.

Specifically, to each intervened variable a causal effect coefficient is associated and the posterior distribution of the latter can be recovered from posterior draws of the DAG parameters returned by learn\_DAG. For each coefficient a sample of size S from its posterior is available. If required, the only Bayesian Model Average (BMA) estimate (obtained as the sample mean of the S draws) can be returned by setting BMA = TRUE.

Notice that, whenever implemented with collapse = FALSE, learn\_DAG returns the marginal posterior distribution of DAGs only. In this case, get\_causaleffect preliminarily performs posterior inference of DAG parameters by drawing samples from the posterior of (D,L).

#### Value

Either a (p, 1) vector containing BMA causal effect estimates, or a (S, p) matrix collecting S draws from the posterior of the p causal effect coefficients.

#### Author(s)

Federico Castelletti and Alessandro Mascaro

#### References

J. Pearl (2000). *Causality: Models, Reasoning, and Inference*. Cambridge University Press, Cambridge.

F. Castelletti and A. Mascaro (2021) Structural learning and estimation of joint causal effects among network-dependent variables. *Statistical Methods and Applications*, Advance publication.

P. Nandy, M.H. Maathuis and T. Richardson (2017). Estimating the effect of joint interventions from observational data in sparse high-dimensional settings. *Annals of Statistics* 45(2), 647-674.

#### Examples

```
# Randomly generate a DAG and the DAG-parameters
q = 8
w = 0.2
set.seed(123)
DAG = rDAG(q = q, w = w)
outDL = rDAGWishart(n = 1, DAG = DAG, a = q, U = diag(1, q))
L = outDL$L; D = outDL$D
Sigma = solve(t(L))%*%D%*%solve(L)
n = 200
# Generate observations from a Gaussian DAG-model
X = mvtnorm::rmvnorm(n = n, sigma = Sigma)
# Run the MCMC (set S = 5000 and burn = 1000 for better results)
out_mcmc = learn_DAG(S = 500, burn = 100, a = q, U = diag(1,q)/n, data = X, w = w,
                     fast = TRUE, save.memory = FALSE)
head(out_mcmc$Graphs)
head(out_mcmc$L)
head(out_mcmc$D)
# Compute the BMA estimate of coefficients representing
# the causal effect on node 1 of an intervention on {3,4}
get_causaleffect(learnDAG_output = out_mcmc, targets = c(3,4), response = 1, BMA = TRUE)
```

get\_diagnostics MCMC diagnostics

#### Description

This function provides diagnostics of convergence for the MCMC output of learn\_DAG function.

#### get\_diagnostics

## Usage

get\_diagnostics(learnDAG\_output)

#### Arguments

learnDAG\_output

object of class bcdag

#### Details

Function learn\_DAG implements a Markov Chain Monte Carlo (MCMC) algorithm for structure learning and posterior inference of Gaussian DAGs. Output of the algorithm is a collection of S DAG structures (represented as (q, q) adjacency matrices) and DAG parameters (D, L) approximately drawn from the joint posterior. In addition, if learn\_DAG is implemented with collapse = TRUE, the only approximate marginal posterior of DAGs (represented by the collection of S DAG structures) is returned; see the documentation of learn\_DAG for more details.

Diagnostics of convergence for the MCMC output are conducted by monitoring across MCMC iterations: (1) the number of edges in the DAGs; (2) the posterior probability of edge inclusion for each possible edge u - > v. With regard to (1), a traceplot of the number of edges in the DAGs visited by the MCMC chain at each step s = 1, ..., S is first provided as the output of the function. The absence of trends in the plot can provide information on a genuine convergence of the MCMC chain. In addition, the traceplot of the average number of edges in the DAGs visited up to time s, for s = 1, ..., S, is also returned. The convergence of the curve around a "stable" average size generally suggests good convergence of the algorithm. With regard to (2), for each edge u - > v, the posterior probability at time s, for s = 1, ..., S, can be estimated as as the proportion of DAGs visited by the MCMC up to time s which contain the directed edge u - > v. Output is organized in q plots (one for each node v = 1, ..., q), each summarizing the posterior probabilities of edges u - > v, u = 1, ..., q. If the number of nodes is larger than 30 the traceplot of a random sample of 30 nodes is returned.

## Value

A collection of plots summarizing the behavior of the number of edges and the posterior probabilities of edge inclusion computed from the MCMC output.

## Author(s)

Federico Castelletti and Alessandro Mascaro

#### References

F. Castelletti and A. Mascaro (2021). Structural learning and estimation of joint causal effects among network-dependent variables. *Statistical Methods and Applications*, Advance publication.

F. Castelletti (2020). Bayesian model selection of Gaussian Directed Acyclic Graph structures. *International Statistical Review* 88 752-775.

#### Examples

```
# Randomly generate a DAG and the DAG-parameters
q = 8
w = 0.2
set.seed(123)
DAG = rDAG(q = q, w = w)
outDL = rDAGWishart(n = 1, DAG = DAG, a = q, U = diag(1, q))
L = outDL$L; D = outDL$D
Sigma = solve(t(L))%*%D%*%solve(L)
n = 200
# Generate observations from a Gaussian DAG-model
X = mvtnorm::rmvnorm(n = n, sigma = Sigma)
# Run the MCMC for posterior inference of DAGs only (collapse = TRUE)
out_mcmc = learn_DAG(S = 5000, burn = 1000, a = q, U = diag(1,q)/n, data = X, w = 0.1,
                                   fast = TRUE, save.memory = FALSE, collapse = TRUE)
# Produce diagnostic plots
get_diagnostics(out_mcmc)
```

get_edgeprobs	Compute posterior probabilities of edge inclusion from the MCMC
	output

#### Description

This function computes the posterior probability of inclusion for each edge u - > v given the MCMC output of learn\_DAG;

#### Usage

```
get_edgeprobs(learnDAG_output)
```

#### Arguments

learnDAG\_output

object of class bcdag

#### Details

Output of learn\_dag function consists of S draws from the joint posterior of DAGs and DAGparameters in a zero-mean Gaussian DAG-model; see the documentation of learn\_DAG for more details.

The posterior probability of inclusion of u > v is estimated as the frequency of DAGs visited by the MCMC which contain the directed edge u > v. Posterior probabilities are collected in a (q, q)matrix with (u, v)-element representing the estimated posterior probability of edge u - > v.

## Value

A (q, q) matrix with posterior probabilities of edge inclusion

#### get\_MAPdag

## Author(s)

Federico Castelletti and Alessandro Mascaro

#### References

F. Castelletti and A. Mascaro (2021). Structural learning and estimation of joint causal effects among network-dependent variables. *Statistical Methods and Applications*, Advance publication.

#### Examples

```
# Randomly generate a DAG and the DAG-parameters
q = 8
w = 0.2
set.seed(123)
DAG = rDAG(q = q, w = w)
outDL = rDAGWishart(n = 1, DAG = DAG, a = q, U = diag(1, q))
L = outDL; D = outDL
Sigma = solve(t(L))%*%D%*%solve(L)
# Generate observations from a Gaussian DAG-model
n = 200
X = mvtnorm::rmvnorm(n = n, sigma = Sigma)
# Run the MCMC (Set S = 5000 and burn = 1000 for better results)
out_mcmc = learn_DAG(S = 500, burn = 100, a = q, U = diag(1,q)/n, data = X, w = 0.1,
                     fast = TRUE, save.memory = FALSE)
# Compute posterior probabilities of edge inclusion
get_edgeprobs(out_mcmc)
```

get\_MAPdag

*Compute the maximum a posteriori DAG model from the MCMC output* 

#### Description

This function computes the maximum a posteriori DAG model estimate (MAP) from the MCMC output of learn\_DAG

#### Usage

```
get_MAPdag(learnDAG_output)
```

#### Arguments

learnDAG\_output

object of class bcdag

## Details

Output of learn\_dag function consists of S draws from the joint posterior of DAGs and DAGparameters in a zero-mean Gaussian DAG-model; see the documentation of learn\_DAG for more details.

The Maximum A Posteriori (MAP) model estimate is defined as the DAG visited by the MCMC with the highest associated posterior probability. Each DAG posterior probability is estimated as the frequency of visits of the DAG in the MCMC chain. The MAP estimate is represented through its (q, q) adjacency matrix, with (u, v)-element equal to one whenever the MAP contains u - > v, zero otherwise.

## Value

The (q, q) adjacency matrix of the maximum a posteriori DAG model

## Author(s)

Federico Castelletti and Alessandro Mascaro

#### References

F. Castelletti and A. Mascaro (2021). Structural learning and estimation of joint causal effects among network-dependent variables. *Statistical Methods and Applications*, Advance publication.

G. Garcia-Donato and M.A. Martinez-Beneito (2013). On sampling strategies in Bayesian variable selection problems with large model spaces. *Journal of the American Statistical Association* 108 340-352.

#### Examples

```
# Randomly generate a DAG and the DAG-parameters
q = 8
w = 0.2
set.seed(123)
DAG = rDAG(q = q, w = w)
outDL = rDAGWishart(n = 1, DAG = DAG, a = q, U = diag(1, q))
L = outDL$L; D = outDL$D
Sigma = solve(t(L))%*%D%*%solve(L)
# Generate observations from a Gaussian DAG-model
n = 200
X = mvtnorm::rmvnorm(n = n, sigma = Sigma)
# Run the MCMC (Set S = 5000 and burn = 1000 for better results)
out_mcmc = learn_DAG(S = 500, burn = 100, a = q, U = diag(1,q)/n, data = X, w = 0.1,
                     fast = TRUE, save.memory = FALSE)
# Produce the MAP DAG estimate
get_MAPdag(out_mcmc)
```

get\_MPMdag

#### Description

This function computes the Median Probability DAG Model estimate (MPM) from the MCMC output of learn\_DAG

#### Usage

get\_MPMdag(learnDAG\_output)

## Arguments

learnDAG\_output

object of class bcdag

#### Details

Output of learn\_dag function consists of S draws from the joint posterior of DAGs and DAGparameters in a zero-mean Gaussian DAG-model; see the documentation of learn\_DAG for more details.

The Median Probability DAG Model estimate (MPM) is obtained by including all edges whose posterior probability exceeds 0.5. The posterior probability of inclusion of u - > v is estimated as the frequency of DAGs visited by the MCMC which contain the directed edge u - > v; see also function get\_edgeprobs and the corresponding documentation.

#### Value

The (q, q) adjacency matrix of the median probability DAG model

## Author(s)

Federico Castelletti and Alessandro Mascaro

#### References

F. Castelletti and A. Mascaro (2021). Structural learning and estimation of joint causal effects among network-dependent variables. *Statistical Methods and Applications*, Advance publication

M.M. Barbieri and J.O. Berger (2004). Optimal predictive model selection. *The Annals of Statistics* 32 870-897

## Examples

```
# Randomly generate a DAG and the DAG-parameters
q = 8
w = 0.2
set.seed(123)
DAG = rDAG(q = q, w = w)
outDL = rDAGWishart(n = 1, DAG = DAG, a = q, U = diag(1, q))
L = outDL$L; D = outDL$D
Sigma = solve(t(L))%*%D%*%solve(L)
# Generate observations from a Gaussian DAG-model
n = 200
X = mvtnorm::rmvnorm(n = n, sigma = Sigma)
# Run the MCMC (Set S = 5000 and burn = 1000 for better results)
out_mcmc = learn_DAG(S = 500, burn = 100, a = q, U = diag(1,q)/n, data = X, w = 0.1,
                     fast = TRUE, save.memory = FALSE)
# Produce the MPM DAG estimate
get_MPMdag(out_mcmc)
```

```
get_opcard
```

Find the direct successors DAGs of an input DAG (internal function)

## Description

Find the direct successors DAGs of an input DAG (internal function)

## Usage

```
get_opcard(DAG)
```

## Arguments

DAG The input DAG

```
learn_DAG
```

MCMC scheme for Gaussian DAG posterior inference

## Description

This function implements a Markov Chain Monte Carlo (MCMC) algorithm for structure learning of Gaussian DAGs and posterior inference of DAG model parameters

## learn\_DAG

## Usage

```
learn_DAG(
   S,
   burn,
   data,
   a,
   U,
   w,
   fast = FALSE,
   save.memory = FALSE,
   collapse = FALSE,
   verbose = TRUE
)
```

## Arguments

S	integer final number of MCMC draws from the posterior of DAGs and parameters
burn	integer initial number of burn-in iterations, needed by the MCMC chain to reach its stationary distribution and not included in the final output
data	(n,q) data matrix
а	common shape hyperparameter of the compatible DAG-Wishart prior, $a>q-1$
U	position hyperparameter of the compatible DAG-Wishart prior, a $(q,q)$ s.p.d. matrix
W	edge inclusion probability hyperparameter of the DAG prior in $[0, 1]$
fast	boolean, if TRUE an approximate proposal for the MCMC moves is implemented
save.memory	boolean, if TRUE MCMC draws are stored as strings, instead of arrays
collapse	boolean, if TRUE only structure learning of DAGs is performed
verbose	If TRUE, progress bars are displayed

## Details

Consider a collection of random variables  $X_1, \ldots, X_q$  whose distribution is zero-mean multivariate Gaussian with covariance matrix Markov w.r.t. a Directed Acyclic Graph (DAG). Assuming the underlying DAG is unknown (model uncertainty), a Bayesian method for posterior inference on the joint space of DAG structures and parameters can be implemented. The proposed method assigns a prior on each DAG structure through independent Bernoulli distributions, Ber(w), on the 0-1 elements of the DAG adjacency matrix. Conditionally on a given DAG, a prior on DAG parameters (D, L) (representing a Cholesky-type reparameterization of the covariance matrix) is assigned through a compatible DAG-Wishart prior; see also function rDAGWishart for more details.

Posterior inference on the joint space of DAGs and DAG parameters is carried out through a Partial Analytic Structure (PAS) algorithm. Two steps are iteratively performed for s = 1, 2, ...: (1) update of the DAG through a Metropolis Hastings (MH) scheme; (2) sampling from the posterior distribution of the (updated DAG) parameters. In step (1) the update of the (current) DAG is performed by drawing a new (direct successor) DAG from a suitable proposal distribution. The proposed DAG

is obtained by applying a local move (insertion, deletion or edge reversal) to the current DAG and is accepted with probability given by the MH acceptance rate. The latter requires to evaluate the proposal distribution at both the current and proposed DAGs, which in turn involves the enumeration of all DAGs that can be obtained from local moves from respectively the current and proposed DAG. Because the ratio of the two proposals is approximately equal to one, and the approximation becomes as precise as q grows, a faster strategy implementing such an approximation is provided with fast = TRUE. The latter choice is especially recommended for moderate-to-large number of nodes q.

Output of the algorithm is a collection of S DAG structures (represented as (q, q) adjacency matrices) and DAG parameters (D, L) approximately drawn from the joint posterior. The various outputs are organized in (q, q, S) arrays; see also the example below. If the target is DAG learning only, a collapsed sampler implementing the only step (1) of the MCMC scheme can be obtained by setting collapse = TRUE. In this case, the algorithm outputs a collection of S DAG structures only. See also functions get\_edgeprobs, get\_MAPdag, get\_MPMdag for posterior summaries of the MCMC output.

#### Value

An S3 object of class bcdag containing S draws from the posterior of DAGs and (if collapse = FALSE) of DAG parameters D and L. If save.memory = FALSE, these are stored in three arrays of dimension (q, q, S). Otherwise, they are stored as strings.

#### Author(s)

Federico Castelletti and Alessandro Mascaro

## References

F. Castelletti and A. Mascaro (2021). Structural learning and estimation of joint causal effects among network-dependent variables. *Statistical Methods and Applications*, Advance publication.

F. Castelletti and A. Mascaro (2022). BCDAG: An R package for Bayesian structural and Causal learning of Gaussian DAGs. *arXiv pre-print*, url: https://arxiv.org/abs/2201.12003

F. Castelletti (2020). Bayesian model selection of Gaussian Directed Acyclic Graph structures. *International Statistical Review* 88 752-775.

#### Examples

```
# Randomly generate a DAG and the DAG-parameters
q = 8
w = 0.2
set.seed(123)
DAG = rDAG(q = q, w = w)
outDL = rDAGWishart(n = 1, DAG = DAG, a = q, U = diag(1, q))
L = outDL$L; D = outDL$D
Sigma = solve(t(L))%*%D%*%solve(L)
# Generate observations from a Gaussian DAG-model
n = 200
X = mvtnorm::rmvnorm(n = n, sigma = Sigma)
```

## leukemia

```
## Set S = 5000 and burn = 1000 for better results
# [1] Run the MCMC for posterior inference of DAGs and parameters (collapse = FALSE)
out_mcmc = learn_DAG(S = 50, burn = 10, a = q, U = diag(1,q)/n, data = X, w = 0.1,
                     fast = FALSE, save.memory = FALSE, collapse = FALSE)
# [2] Run the MCMC for posterior inference of DAGs only (collapse = TRUE)
out_mcmc_collapse = learn_DAG(S = 50, burn = 10, a = q, U = diag(1,q)/n, data = X, w = 0.1,
                              fast = FALSE, save.memory = FALSE, collapse = TRUE)
# [3] Run the MCMC for posterior inference of DAGs only with approximate proposal
# distribution (fast = TRUE)
# out_mcmc_collapse_fast = learn_DAG(S = 50, burn = 10, a = q, U = diag(1,q)/n, data = X, w = 0.1,
                                     fast = FALSE, save.memory = FALSE, collapse = TRUE)
# Compute posterior probabilities of edge inclusion and Median Probability DAG Model
# from the MCMC outputs [2] and [3]
get_edgeprobs(out_mcmc_collapse)
# get_edgeprobs(out_mcmc_collapse_fast)
get_MPMdag(out_mcmc_collapse)
# get_MPMdag(out_mcmc_collapse_fast)
```

leukemia

Protein levels for 68 diagnosed AML patients of subtype M2

## Description

A dataset containing the protein expression levels of 18 proteins for 68 AML patients of subtype M2 (according to French-American-British (FAB) classification system). The 18 proteins selected are known to be involved in apoptosis and cell cycle regulation according to the KEGG database (Kanehisa et al. 2012). This is a subset of the dataset presented in Kornblau et al. (2009).

## Usage

leukemia

#### Format

A data frame with 68 rows and 18 variables:

**AKT** AKT protein, expression level

AKT.p308 AKT.p308 protein, expression level

AKT.p473 AKT.p473 protein, expression level

BAD BAD protein, expression level

BAD.p112 BAD.p112 protein, expression level

BAD.p136 BAD.p136 protein, expression level

BAD.p155 BAD.p155 protein, expression level

**BAX** BAX protein, expression level

BCL2 BCL2 protein, expression level

BCLXL BCLXL protein, expression level
CCND1 CCND1 protein, expression level
GSK3 GSK3 protein, expression level
GSK3.p GSK3.p protein, expression level
MYC MYC protein, expression level
PTEN PTEN protein, expression level
PTEN.p PTEN.p protein, expression level
TP53 TP53 protein, expression level
XIAP XIAP protein, expression level ...

#### Source

http://bioinformatics.mdanderson.org/Supplements/Kornblau-AML-RPPA/aml-rppa.xls

#### References

Kornblau, S. M., Tibes, R., Qiu, Y. H., Chen, W., Kantarjian, H. M., Andreeff, M., ... & Mills, G. B. (2009). Functional proteomic profiling of AML predicts response and survival. Blood, The Journal of the American Society of Hematology, 113(1), 154-164.

Kanehisa, M., Goto, S., Sato, Y., Furumichi, M., & Tanabe, M. (2012). KEGG for integration and interpretation of large-scale molecular data sets. Nucleic acids research, 40(D1), D109-D114.

new\_bcdag

*Create new bcdag objects* 

## Description

Internal function used as constructor for S3 objects of class bcdag, which constitute the output of function learn\_DAG() and the input of functions belonging to the get\_ family such as get\_causaleffect().

#### Usage

```
new_bcdag(x = list(), input = list(), type = "complete")
```

#### Arguments

х	A list
input	A list containing the inputs given to learn_DAG()
type	A string indicating whether the output produced by learn_DAG() should be of
	type "complete", "compressed", "collapsed" or "compressed and collapsed"

#### Value

An S3 object of class bcdag

## operation

## Author(s)

Federico Castelletti and Alessandro Mascaro

#### References

F. Castelletti and A. Mascaro (2022). BCDAG: An R package for Bayesian structural and Causal learning of Gaussian DAGs. *arXiv pre-print*, url: https://arxiv.org/abs/2201.12003

operation

Perform local moves given a DAG (internal function)

## Description

This function locally modifies a DAG by inserting (op = 1), deleting (op = 2) or reversing (op = 3) an edge between two nodes

#### Usage

operation(op, A, nodes)

## Arguments

ор	numerical type in $1, 2, 3$ of the operator applied to DAG
A	$\left( q,q ight)$ adjacency matrix of the input DAG
nodes	numerical labels of nodes on which the operator is applied, a $\left(2,1\right)$ vector

## Value

The (q, q) adjacency matrix of the modified DAG

Find the parents of a node in a DAG (internal function)

## Description

This function finds the set of parents of node in DAG

## Usage

```
pa(node, DAG)
```

## Arguments

node	numerical label of the node in DAG
DAG	(q,q) adjacency matrix of the DAG

#### Value

A numerical vector with the labels of the parents of node in DAG

propose\_DAG MCMC proposal distribution (internal function)

#### Description

This function implements a proposal distribution for the MCMC scheme of learn\_DAG. Given an input DAG, it first builds the set of all DAGs which can be obtained by applying a local move (insertion, deletion or reversal of one edge) to DAG, that is the set of direct successors of DAG; next, it randomly draws one candidate (proposed) DAG from the so-obtained set. Finally, the set of direct successors of the proposed DAG is constructed. The function returns: the proposed DAG, the type of operator applied to DAG to obtain the proposed DAG (with value 1 if insertion, 2 if deletion, 3 if reversal), the nodes involved in the local move, the number of direct successors of DAG and of the proposed DAG. If fast = TRUE the two numbers of direct successors are approximated by the number of possible operators that can be applied to the DAGs (equal for the two graphs)

## Usage

propose\_DAG(DAG, fast)

#### Arguments

DAG	Adjacency matrix of the current DAG
fast	boolean, if TRUE an approximate proposal is implemented

#### Value

A list containing the (q,q) adjacency matrix of the proposed DAG, the type of applied operator (with values in 1, 2, 3), the numerical labels of the nodes involved in the move, the integer number of direct successors of DAG and of the proposed DAG

Generate a Directed Acyclic Graph (DAG) randomly

## Description

This function randomly generates a Directed Acyclic Graph (DAG) with q nodes and probability of edge inclusion w.

#### Usage

rDAG(q, w)

rDAG

## rDAGWishart

#### Arguments

q	number of nodes
W	probability of edge inclusion in $[0, 1]$

## Details

The 0-1 adjacency matrix of the DAG is generated by drawing each element in the lower triangular part in 0, 1 with probability 1 - w, w. Accordingly, the DAG has lower-triangular adjacency matrix and nodes are numerically labeled according to a topological ordering implying u > v whenever u - > v.

## Value

DAG (q, q) adjacency matrix of the generated DAG

## Examples

```
# Randomly generate a DAG on q = 8 nodes with probability of edge inclusion w = 0.2
q = 8
w = 0.2
set.seed(123)
rDAG(q = q, w = w)
```

rDAGWis	hart
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#### Random samples from a compatible DAG-Wishart distribution

## Description

This function implements a direct sampling from a compatible DAG-Wishart distribution with parameters a and U.

#### Usage

rDAGWishart(n, DAG, a, U)

#### Arguments

n	number of samples
DAG	(q,q) adjacency matrix of the DAG
а	common shape hyperparameter of the compatible DAG-Wishart, $a > q - 1$
U	position hyperparameter of the compatible DAG-Wishart, a $(q,q)$ s.p.d. matrix

## Details

Assume the joint distribution of random variables  $X_1, \ldots, X_q$  is zero-mean Gaussian with covariance matrix Markov w.r.t. a Directed Acyclic Graph (DAG). The allied Structural Equation Model (SEM) representation of a Gaussian DAG-model allows to express the covariance matrix as a function of the (Cholesky) parameters (D, L), collecting the regression coefficients and conditional variances of the SEM.

The DAG-Wishart distribution (Cao et. al, 2019) with shape hyperparameter  $a = (a_1, ..., a_q)$  and position hyperparameter U (a s.p.d. (q, q) matrix) provides a conjugate prior for parameters (D, L). In addition, to guarantee compatibility among Markov equivalent DAGs (same marginal likelihood), the default choice (here implemented)  $a_j = a + |pa(j)| - q + 1$  (a > q - 1), with |pa(j)| the number of parents of node j in the DAG, was introduced by Peluso and Consonni (2020).

#### Value

A list of two elements: a qxqxn array collecting n sampled matrices L and a qxqxn array collecting n sampled matrices D

#### Author(s)

Federico Castelletti and Alessandro Mascaro

## References

F. Castelletti and A. Mascaro (2021). Structural learning and estimation of joint causal effects among network-dependent variables. *Statistical Methods and Applications*, Advance publication.

X. Cao, K. Khare and M. Ghosh (2019). Posterior graph selection and estimation consistency for high-dimensional Bayesian DAG models. *The Annals of Statistics* 47 319-348.

S. Peluso and G. Consonni (2020). Compatible priors for model selection of high-dimensional Gaussian DAGs. *Electronic Journal of Statistics* 14(2) 4110 - 4132.

#### Examples

```
# Randomly generate a DAG on q = 8 nodes with probability of edge inclusion w = 0.2
q = 8
w = 0.2
set.seed(123)
DAG = rDAG(q = q, w = w)
# Draw from a compatible DAG-Wishart distribution with parameters a = q and U = diag(1,q)
outDL = rDAGWishart(n = 5, DAG = DAG, a = q, U = diag(1, q))
outDL
```

rnodeDAGWishart

Draw one observation from a Normal-Inverse-Gamma distribution (internal function)

## Description

This function performs one draw from the Multivariate-Normal-Inverse-Gamma (prior/posterior) distribution of the parameters of a Normal linear regression model. Response variable is node and covariates are given by the parents of node in DAG. It is implemented node-by-node in rDAGWishart to obtain draws from a compatible (prior/posterior) DAG-Wishart distribution.

## Usage

rnodeDAGWishart(node, DAG, aj, U)

## Arguments

node	numerical label of the node in DAG
DAG	(q,q) adjacency matrix of the DAG
aj	common shape hyperparameter of the compatible DAG-Wishart, $a > q - 1$
U	position hyperparameter of the compatible DAG-Wishart, a $(q,q)$ s.p.d. matrix

## Value

A list with two elements; a vector with one draw for the (vector) regression coefficient and a scalar with one draw for the conditional variance

summary.bcdag bcdag object summaries

## Description

bcdag object summaries

## Usage

## S3 method for class 'bcdag'
summary(object, ...)

#### Arguments

object	a bcdag object for which a summary is desired
	additional arguments affecting the summary produced

## Value

A printed message listing the inputs given to learn\_DAG, a graphical representation of the Median Probability DAG, a heatmap representing posterior probability of edge inclusion and an histogram of the number of edges in the visited DAGs.

## Examples

```
n <- 1000
q <- 4
DAG <- matrix(c(0,1,1,0,0,0,0,0,0,0,0,0,0,1,1,0), nrow = q)
L <- DAG
L[L != 0] <- runif(q, 0.2, 1)
diag(L) <- c(1,1,1,1)
D <- diag(1, q)
Sigma <- t(solve(L))%*%D%*%solve(L)
a <- 6
g <- 1/1000
U <- g*diag(1,q)
w = 0.2
set.seed(1)
X <- mvtnorm::rmvnorm(n, sigma = Sigma)
out <- learn_DAG(1000, 0, X, a, U, w, fast = TRUE, collapse = TRUE, save.memory = FALSE)</pre>
```

```
summary(out)
```

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