Package: BDgraph (via r-universe)

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Title Bayesian Structure Learning in Graphical Models using Birth-Death MCMC

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Description

The R package **BDgraph** provides statistical tools for Bayesian structure learning in undirected graphical models for continuous, ordinal/count/dicrete, binary, and mixed data. The package is implemented the recent improvements in the Bayesian graphical models' literature, including Mohammadi and Wit (2015), Mohammadi et al. (2023), Mohammadi et al. (2017), and Dobra and Mohammadi (2018). To speed up the computations, the intensive tasks of the package are implemented in parallel using **OpenMP** in C++ and interfaced with R. Besides, the package contains several functions for simulation and visualization, as well as several multivariate datasets taken from the literature.

How to cite this package

To cite **BDgraph** in publications use:

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

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Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

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Lenkoski, A. (2013). A direct sampler for G-Wishart variates, *Stat*, 2(1):119-28, doi:10.1002/sta4.23

Pensar, J. et al (2017) Marginal pseudo-likelihood learning of discrete Markov network structures, *Bayesian Analysis*, 12(4):1195-215, doi:10.1214/16BA1032

See Also

bdgraph, bdgraph.mpl, bdgraph.dw, bdgraph.sim, compare, rgwish

Examples

```
## Not run:
library( BDgraph )
set.seed( 10 )
# Generating multivariate normal data from a 'scale-free' graph
data.sim <- bdgraph.sim( n = 100, p = 10, graph = "scale-free", vis = TRUE )
# Running algorithm based on GGMs
bdgraph.obj <- bdgraph( data = data.sim, iter = 5000 )</pre>
summary( bdgraph.obj )
# To compare the result with true graph
compare( bdgraph.obj, data.sim, main = c( "Target", "BDgraph" ), vis = TRUE )
# Confusion Matrix
conf.mat( actual = data.sim, pred = bdgraph.obj )
conf.mat.plot( actual = data.sim, pred = bdgraph.obj )
# Running algorithm based on GGMs and marginal pseudo-likelihood
bdgraph.mpl.obj <- bdgraph.mpl( data = data.sim, iter = 5000 )</pre>
summary( bdgraph.mpl.obj )
```

adj2link

End(Not run)

adj2link

Extract links from an adjacency matrix

Description

Extract links from an adjacency matrix or an object of calsses "sim" from function bdgraph.sim and "graph" from function graph.sim.

Usage

adj2link(adj)

Arguments

adj adjacency matrix corresponding to a graph structure in which $a_{ij} = 1$ if there is a link between notes *i* and *j*, otherwise $a_{ij} = 0$. It can be an object with S3 class "sim" from function bdgraph.sim. It can be an object with S3 class "graph" from function graph.sim.

Value

matrix corresponding to the extracted links from graph structure.

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References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

See Also

link2adj,graph.sim

Examples

```
# Generating a 'random' graph
adj <- graph.sim( p = 6, vis = TRUE )
adj2link( adj )
```

auc

Compute the area under the ROC curve

Description

This function computes the numeric value of area under the ROC curve (AUC) specifically for graph structure learning.

Usage

auc(pred, actual, cut = 200, calibrate = TRUE)

Arguments

pred	adjacency matrix corresponding to an estimated graph. It can be an object with S3 class "bdgraph" from function bdgraph. It can be an object of S3 class "ssgraph", from the function ssgraph::ssgraph() of R package ssgraph::ssgraph(). It can be a numeric or ordered vector of the same length than actual, containing the predicted value of each observation.
actual	adjacency matrix corresponding to the actual graph structure in which $a_{ij} = 1$ if there is a link between notes <i>i</i> and <i>j</i> , otherwise $a_{ij} = 0$. It can be an object with S3 class "sim" from function bdgraph.sim. It can be an object with S3 class "graph" from function graph.sim. It can be a factor, numeric or character vector of responses (true class), typically encoded with 0 (controls) and 1 (cases). Only two classes can be used in a ROC curve.
cut	number of cut points.
calibrate	If TRUE, compute the value of AUC by taking the level of the probabilities into account.

Value

The numeric AUC value

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bdgraph

References

Tom Fawcett (2006) "An introduction to ROC analysis". *Pattern Recognition Letters* **27**, 861–874, doi:10.1016/j.patrec.2005.10.010

Xavier Robin, Natacha Turck, Alexandre Hainard, *et al.* (2011) "pROC: an open-source package for R and S+ to analyze and compare ROC curves". *BMC Bioinformatics*, **7**, 77, doi:10.1186/1471-21051277.

See Also

plotroc, pROC::plot.roc(), pROC::auc(), pROC::print.roc(), bdgraph, bdgraph.mpl, compare

Examples

```
## Not run:
set.seed( 5 )
# Generating multivariate normal data from a 'scale-free' graph
data.sim = bdgraph.sim( n = 200, p = 15, graph = "scale-free", vis = TRUE )
# Running BDMCMC algorithm
sample.bdmcmc = bdgraph( data = data.sim, algorithm = "bdmcmc", iter = 10000 )
BDgraph::auc( pred = sample.bdmcmc, actual = data.sim, calibrate = TRUE )
## End(Not run)
```

bdgraph

Search algorithm in graphical models

Description

As the main function of the **BDgraph** package, this function consists of several MCMC sampling algorithms for Bayesian model determination in undirected graphical models. To speed up the computations, the birth-death MCMC sampling algorithms are implemented in parallel using **OpenMP** in C++.

Usage

```
bdgraph( data, n = NULL, method = "ggm", algorithm = "bdmcmc", iter = 5000,
            burnin = iter / 2, not.cont = NULL, g.prior = 0.2, df.prior = 3,
            g.start = "empty", jump = NULL, save = FALSE,
            cores = NULL, threshold = 1e-8, verbose = TRUE, nu = 1 )
```

Arguments

data	there are two options: (1) an $(n \times p)$ matrix or a data.frame corresponding to the data, (2) an $(p \times p)$ covariance matrix as $S = X'X$ which X is the data matrix $(n \text{ is the sample size and } p \text{ is the number of variables})$. It also could be an object of class "sim", from function bdgraph.sim. The input matrix is automatically identified by checking the symmetry.
n	number of observations. It is needed if the "data" is a covariance matrix.
method	character with two options "ggm" (default) and "gcgm". Option "ggm" is for Gaussian graphical models based on Gaussianity assumption. Option "gcgm" is for Gaussian copula graphical models for the data that not follow Gaussianity assumption (e.g. continuous non-Gaussian, count, or mixed dataset).
algorithm	character with two options "bdmcmc" (default) and "rjmcmc". Option "bdmcmc" is based on birth-death MCMC algorithm. Option "rjmcmc" is based on reverible jump MCMC algorithm. Option "bd-dmh" is based on birth-death MCMC algorithm using double Metropolis Hasting. Option "rj-dmh" is based on reverible jump MCMC algorithm using double Metropolis Hasting.
iter	number of iteration for the sampling algorithm.
burnin	number of burn-in iteration for the sampling algorithm.
not.cont	for the case method = "gcgm", a vector with binary values in which 1 indicates not continuous variables.
g.prior	for determining the prior distribution of each edge in the graph. There are two options: a single value between 0 and 1 (e.g. 0.5 as a noninformative prior) or an $(p \times p)$ matrix with elements between 0 and 1.
df.prior	degree of freedom for G-Wishart distribution, $W_G(b, D)$, which is a prior distribution of the precision matrix.
g.start	corresponds to a starting point of the graph. It could be an $(p \times p)$ matrix, "empty" (default), or "full". Option "empty" means the initial graph is an empty graph and "full" means a full graph. It also could be an object with S3 class "bdgraph" of R package BDgraph or the class "ssgraph" of R package ssgraph::ssgraph(); this option can be used to run the sampling algorithm from the last objects of previous run (see examples).
jump	it is only for the BDMCMC algorithm (algorithm = "bdmcmc"). It is for si- multaneously updating multiple links at the same time to update graph in the BDMCMC algorithm.
save	logical: if FALSE (default), the adjacency matrices are NOT saved. If TRUE, the adjacency matrices after burn-in are saved.
cores	number of cores to use for parallel execution. The case cores = "all" means all CPU cores to use for parallel execution.
threshold	threshold value for the convergence of sampling algorithm from G-Wishart for the precision matrix.
verbose	logical: if TRUE (default), report/print the MCMC running time.
nu	prior parameter for option method = "tgm".

bdgraph

Value

An object with S3 class "bdgraph" is returned:

p_links	upper triangular matrix which corresponds the estimated posterior probabilities of all possible links.	
K_hat	posterior estimation of the precision matrix.	
For the case "save = TRUE" is returned:		
sample_graphs	vector of strings which includes the adjacency matrices of visited graphs after burn-in.	
graph_weights	vector which includes the waiting times of visited graphs after burn-in.	
all_graphs	vector which includes the identity of the adjacency matrices for all iterations after burn-in. It is needed for monitoring the convergence of the BD-MCMC algorithm.	
all_weights	vector which includes the waiting times for all iterations after burn-in. It is needed for monitoring the convergence of the BD-MCMC algorithm.	

Author(s)

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References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

Mohammadi, A. and Wit, E. C. (2015). Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Bayesian Analysis*, 10(1):109-138, doi:10.1214/14BA889

Mohammadi, R., Massam, H. and Letac, G. (2023). Accelerating Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Journal of the American Statistical Association*, doi:10.1080/01621459.2021.1996377

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Mohammadi, R., Schoonhoven, M., Vogels, L., and Birbil, S.I. (2023) Large-scale Bayesian Structure Learning for Gaussian Graphical Models using Marginal Pseudo-likelihood, *arXiv preprint*, doi:10.48550/arXiv.2307.00127

Mohammadi, A. and Dobra A. (2017). The R Package **BDgraph** for Bayesian Structure Learning in Graphical Models, *ISBA Bulletin*, 24(4):11-16

See Also

bdgraph.mpl, bdgraph.dw, bdgraph.sim, summary.bdgraph, compare

Examples

```
## Not run:
set.seed( 10 )
# – – Example 1
# Generating multivariate normal data from a 'random' graph
data.sim <- bdgraph.sim( n = 100, p = 10, size = 15, vis = TRUE )</pre>
bdgraph.obj <- bdgraph( data = data.sim, iter = 1000, save = TRUE )</pre>
summary( bdgraph.obj )
# Confusion Matrix
conf.mat( actual = data.sim, pred = bdgraph.obj )
conf.mat.plot( actual = data.sim, pred = bdgraph.obj )
# To compare our result with true graph
compare( bdgraph.obj, data.sim, main = c( "Target", "BDgraph" ), vis = T )
# Running algorithm with starting points from previous run
bdgraph.obj2 <- bdgraph( data = data.sim, g.start = bdgraph.obj )</pre>
compare( list( bdgraph.obj, bdgraph.obj2 ), data.sim,
         main = c( "Target", "Frist run", "Second run" ) )
# - - Example 2
# Generating mixed data from a 'scale-free' graph
data.sim <- bdgraph.sim( n = 200, p = 7, type = "mixed", graph = "scale-free", vis = TRUE )</pre>
bdgraph.obj <- bdgraph( data = data.sim, method = "gcgm" )</pre>
summary( bdgraph.obj )
compare( bdgraph.obj, data.sim, vis = T )
conf.mat( actual = data.sim, pred = bdgraph.obj )
conf.mat.plot( actual = data.sim, pred = bdgraph.obj )
## End(Not run)
```

bdgraph.dw

Search algorithm for Gaussian copula graphical models for count data

Description

This function consists of several sampling algorithms for Bayesian structure learning in undirected graphical models for count data. It is based on Gaussian copula graphical models with discrete Weibull distributed marginals. To speed up the computations, the birth-death MCMC sampling algorithms are implemented in parallel using **OpenMP** in C++.

Usage

```
bdgraph.dw( data, x = NULL, formula = y ~ .,
    n = NULL, algorithm = "bdmcmc", iter = 5000,
    burnin = iter / 2, g.prior = 0.2, df.prior = 3,
    ZI = FALSE, iter_bdw = 5000,
    g.start = "empty", jump = NULL, save = FALSE,
    q = NULL, beta = NULL, pii = NULL,
    cores = NULL, threshold = 1e-8, verbose = TRUE )
```

Arguments

data	$(n \times p)$ matrix or a data.frame corresponding to the data on the p nodes of the graph. It can also be an object of class "sim", from the function bdgraph.sim.
х	$(n \times k)$ matrix or a data.frame corresponding to the predictors.
formula	object of class formula as a symbolic description of the model for linking each node to the predictors. For the case of data.frame, it is taken as the model frame (see model.frame).
n	number of observations. It is needed if the "data" is a covariance matrix.
algorithm	character with two options "bdmcmc" (default) and "rjmcmc". Option "bdmcmc" is based on a birth-death MCMC algorithm. Option "rjmcmc" is based on a reversible jump MCMC algorithm.
iter	number of iterations for the sampling algorithm for graph learning.
burnin	number of burn-in iterations for the sampling algorithm for graph learning.
g.prior	for determining the prior distribution of each edge in the graph. There are two options: a single value between 0 and 1 (e.g. 0.5 as a noninformative prior) or a $(p \times p)$ matrix with elements between 0 and 1.
df.prior	degree of freedom for G-Wishart distribution, $W_G(b, D)$, which is a prior distribution for the precision matrix.
ZI	logical. If FALSE (default), the conditional distribution of each response variable is assumed to be Discrete Weibull given the predictors x. If TRUE, a zero- inflated model will be applied to each response. ZI can be passed also as a vector, in order to specify which of the (p variables) should be fitted with zero- inflation (TRUE) or not (FALSE).

iter_bdw	number of iterations for the sampling algorithm to estimate the regression parameters for the Discrete Weibull distribution. It is passed to the bdw.reg function.
g.start	corresponds to a starting point of the graph. It could be an $(p \times p)$ matrix, "empty" (default), or "full". Option "empty" means that the initial graph is an empty graph and "full" means a full graph. It also could be an object with S3 class "bdgraph" of R package BDgraph or the class "ssgraph" of R package ssgraph::ssgraph(); this option can be used to run the sampling algorithm from the last objects of the previous run (see examples).
jump	it is only for the BDMCMC algorithm (algorithm = "bdmcmc"). It is for simul- taneously updating multiple links at the same time while updating the graph in the BDMCMC algorithm.
save	logical: if FALSE (default), the adjacency matrices are NOT saved. If TRUE, the adjacency matrices after burn-in are saved.
q, beta	parameters of the discrete Weibull distribution used for the marginals. They should be given either as a $(n \times p)$ matrix (if covariates are present) or as a vector (if covariates are not present). If NULL (default), these parameters are estimated by the bdw.reg function.
pii	vector or matrix of zero-inflation parameters of the zero-inflated discrete Weibull distributions used for the marginals. If NULL (default), this parameter is estimated by the bdw.reg function when ZI = TRUE.
cores	number of cores to use for parallel execution. The case cores = "all" means all CPU cores to use for parallel execution.
threshold	threshold value for the convergence of the sampling algorithm from G-Wishart for the precision matrix.
verbose	logical: if TRUE (default), report/print the MCMC running time.

Value

An object with S3 class "bdgraph" is returned, containing:

p_links	upper triangular matrix corresponding to the estimated posterior probabilities of all possible links.	
K_hat sample_marginal	posterior estimation of the precision matrix.	
	posterior samples of the regression coefficients of the marginal distributions.	
For the case "save = TRUE", the code returns:		
sample_graphs	vector of strings which includes the adjacency matrices of the graphs visited after burn-in.	
graph_weights	vector which includes the waiting times of the graphs visited after burn-in.	
all_graphs	vector which includes the identity of the adjacency matrices for all iterations after burn-in. It is needed for monitoring the convergence of the BDMCMC algorithm.	
all_weights	vector which includes the waiting times for all iterations after burn-in. It is needed for monitoring the convergence of the BDMCMC algorithm.	

bdgraph.dw

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References

Vinciotti, V., Behrouzi, P., and Mohammadi, R. (2022) Bayesian structural learning of microbiota systems from count metagenomic data, *arXiv preprint*, doi:10.48550/arXiv.2203.10118

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Mohammadi, R., Massam, H. and Letac, G. (2023). Accelerating Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Journal of the American Statistical Association*, doi:10.1080/01621459.2021.1996377

See Also

bdgraph, bdgraph.mpl, bdw.reg, bdgraph.sim, summary.bdgraph, compare

Examples

```
## Not run:
# - - Example 1
# Generating multivariate Discrete Weibull data based on 'random' graph
data.sim <- bdgraph.sim( n = 100, p = 10, type = "dw", vis = TRUE )
bdgraph.obj <- bdgraph.dw( data = data.sim, iter = 5000 )
summary( bdgraph.obj )
# To compare the result with true graph
compare( bdgraph.obj, data.sim, main = c( "Target", "BDgraph" ), vis = TRUE )
# - - Example 2
# Generating multivariate Discrete Weibull data based on a 'scale-free' graph
```

```
data.sim <- bdgraph.sim( n = 100, p = 10, type = "dw", graph = "scale-free", vis = TRUE )
```

```
bdgraph.obj <- bdgraph.dw( data = data.sim, iter = 10000 )
summary( bdgraph.obj )
compare( bdgraph.obj, data.sim, main = c( "Target", "BDgraph" ), vis = TRUE )
## End(Not run)</pre>
```

bdgraph.mpl

Search algorithm in graphical models using marginal pseudolikehlihood

Description

This function consists of several sampling algorithms for Bayesian model determination in undirected graphical models based on mariginal pseudo-likelihood. To speed up the computations, the birth-death MCMC sampling algorithms are implemented in parallel using **OpenMP** in C++.

Usage

Arguments

data	there are two options: (1) an $(n \times p)$ matrix or a data.frame corresponding to the data, (2) an $(p \times p)$ covariance matrix as $S = X'X$ which X is the data matrix (n is the sample size and p is the number of variables). It also could be an object of class "sim", from function bdgraph.sim. The input matrix is automatically identified by checking the symmetry.
n	number of observations. It is needed if the "data" is a covariance matrix.
method	character with two options "ggm" (default), "dgm" and "dgm-binary". Option "ggm" is for Gaussian graphical models based on Gaussianity assumption. Op- tion "dgm" is for discrete graphical models for the count data. Option "dgm-binary" is for discrete graphical models for the data that are binary.
transfer	for only 'count' data which method = "dgm" or method = "dgm-binary".
algorithm	character with two options "bdmcmc" (default) and "rjmcmc". Option "bdmcmc" is based on birth-death MCMC algorithm. Option "rjmcmc" is based on reveri- ble jump MCMC algorithm. Option "hc" is based on hill-climbing algorithm; this algorithm is only for count data which method = "dgm" or method = "dgm-binary".
iter	number of iteration for the sampling algorithm.
burnin	number of burn-in iteration for the sampling algorithm.

g.prior	for determining the prior distribution of each edge in the graph. There are two options: a single value between 0 and 1 (e.g. 0.5 as a noninformative prior) or an $(p \times p)$ matrix with elements between 0 and 1.
g.start	corresponds to a starting point of the graph. It could be an $(p \times p)$ matrix, "empty" (default), or "full". Option "empty" means the initial graph is an empty graph and "full" means a full graph. It also could be an object with S3 class "bdgraph" of R package BDgraph or the class "ssgraph" of R package ssgraph::ssgraph(); this option can be used to run the sampling algorithm from the last objects of previous run (see examples).
jump	it is only for the BDMCMC algorithm (algorithm = "bdmcmc"). It is for si- multaneously updating multiple links at the same time to update graph in the BDMCMC algorithm.
alpha	value of the hyper parameter of Dirichlet, which is a prior distribution.
save	logical: if FALSE (default), the adjacency matrices are NOT saved. If TRUE, the adjacency matrices after burn-in are saved.
cores	number of cores to use for parallel execution. The case cores = "all" means all CPU cores to use for parallel execution.
operator	character with two options "or" (default) and "and". It is for hill-climbing algorithm.
verbose	logical: if TRUE (default), report/print the MCMC running time.

Value

An object with S3 class "bdgraph" is returned:

p_links	upper triangular matrix which corresponds the estimated posterior probabilities of all possible links.	
For the case "save = TRUE" is returned:		
sample_graphs	vector of strings which includes the adjacency matrices of visited graphs after burn-in.	
graph_weights	vector which includes the waiting times of visited graphs after burn-in.	
all_graphs	vector which includes the identity of the adjacency matrices for all iterations after burn-in. It is needed for monitoring the convergence of the BD-MCMC algorithm.	
all_weights	vector which includes the waiting times for all iterations after burn-in. It is needed for monitoring the convergence of the BD-MCMC algorithm.	

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>, Adrian Dobra, and Johan Pensar

References

Mohammadi, R., Schoonhoven, M., Vogels, L., and Birbil, S.I. (2023) Large-scale Bayesian Structure Learning for Gaussian Graphical Models using Marginal Pseudo-likelihood, *arXiv preprint*, doi:10.48550/arXiv.2307.00127

Dobra, A. and Mohammadi, R. (2018). Loglinear Model Selection and Human Mobility, *Annals of Applied Statistics*, 12(2):815-845, doi:10.1214/18AOAS1164

Mohammadi, A. and Wit, E. C. (2015). Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Bayesian Analysis*, 10(1):109-138, doi:10.1214/14BA889

Vogels, L., Mohammadi, R., Schoonhoven, M., and Birbil, S.I. (2023) Bayesian Structure Learning in Undirected Gaussian Graphical Models: Literature Review with Empirical Comparison, *arXiv* preprint, doi:10.48550/arXiv.2307.02603

Mohammadi, A. and Dobra, A. (2017). The R Package **BDgraph** for Bayesian Structure Learning in Graphical Models, *ISBA Bulletin*, 24(4):11-16

Pensar, J. et al (2017) Marginal pseudo-likelihood learning of discrete Markov network structures, *Bayesian Analysis*, 12(4):1195-215, doi:10.1214/16BA1032

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

See Also

bdgraph, bdgraph.dw, bdgraph.sim, summary.bdgraph, compare

Examples

```
# Generating multivariate normal data from a 'random' graph
data.sim <- bdgraph.sim( n = 70, p = 5, size = 7, vis = TRUE )
bdgraph.obj <- bdgraph.mpl( data = data.sim, iter = 500 )
summary( bdgraph.obj )
# To compare the result with true graph
compare( bdgraph.obj, data.sim, main = c( "Target", "BDgraph" ) )
```

bdgraph.npn Nonparametric transfer

Description

Transfers non-Gaussian data to Gaussian.

Usage

```
bdgraph.npn( data, npn = "shrinkage", npn.thresh = NULL )
```

bdgraph.npn

Arguments

data	$(n \times p)$ matrix or a data.frame corresponding to the data (<i>n</i> is the sample size and <i>p</i> is the number of variables).
npn	character with three options "shrinkage" (default), "truncation", and "skeptic". Option "shrinkage" is for the shrunken transformation, option "truncation" is for the truncated transformation and option "skeptic" is for the non-paranormal skeptic transformation. For more details see references.
npn.thresh	truncation threshold; it is only for the truncated transformation (npn= "truncation"). The default value is $1/(4n^{1/4}\sqrt{\pi \log(n)})$.

Value

 $(n \times p)$ matrix of transferred data, if npn = "shrinkage" or "truncation", and a non-paranormal correlation $(p \times p)$ matrix, if npn = "skeptic".

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>

References

Liu, H., et al (2012). High Dimensional Semiparametric Gaussian Copula Graphical Models, *Annals of Statistics*, 40(4):2293-2326

Zhao, T. and Liu, H. (2012). The **huge** Package for High-dimensional Undirected Graph Estimation in R, *Journal of Machine Learning Research*, 13:1059-1062

See Also

bdgraph.sim,bdgraph,bdgraph.mpl

Examples

```
## Not run:
# Generating multivariate normal data from a 'random' graph
data.sim <- bdgraph.sim( n = 6, p = 4, size = 4 )
data <- ( data.sim $ data - 3 ) ^ 4
data
# Transfer the data by truncation
bdgraph.npn( data, npn = "truncation" )
# Transfer the data by shrunken
bdgraph.npn( data, npn = "shrunken" )
# Transfer the data by skeptic
bdgraph.npn( data, npn = "skeptic" )
## End(Not run)
```

bdgraph.sim

Description

Simulating multivariate distributions with different types of underlying graph structures, including "random", "cluster", "smallworld", "scale-free", "lattice", "hub", "star", "circle", "AR(1)", and "AR(2)". Based on the underlying graph structure, the function generates different types of *multivariate* data, including "*Gaussian*", "*non-Gaussian*", "*categorical*", "*pois*" (Poisson), "*nbinom*" (negative binomial), "*dweibull*" (discrete Weibull), "*binary*", "t" (t-distribution), "*alternative-t*", or "*mixed*" data. This function can be used also for simulating only graphs by setting the option n=0 (default).

Usage

```
bdgraph.sim( p = 10, graph = "random", n = 0, type = "Gaussian", prob = 0.2,
    size = NULL, mean = 0, class = NULL, cut = 4, b = 3,
    D = diag( p ), K = NULL, sigma = NULL,
    q = exp(-1), beta = 1, vis = FALSE, rewire = 0.05,
    range.mu = c( 3, 5 ), range.dispersion = c( 0.01, 0.1 ), nu = 1 )
```

Arguments

р	number of variables (nodes).
graph	graph structure with options "random", "cluster", "smallworld", "scale-free", "lattice", "hub", "star", "circle", "AR(1)", and "AR(2)". It could also be an adjacency matrix corresponding to a graph structure (an upper triangular matrix in which $g_{ij} = 1$ if there is a link between nodes i and j , otherwise $g_{ij} = 0$).
n	number of samples required. Note that for the case $n = 0$, only the graph is generated.
type	type of data with options "Gaussian" (default), "non-Gaussian", "categorical", "pois", "nbinom", "dweibull", "binary", "mixed", "t", and "alternative-t". For the option "Gaussian", data are generated from a multivariate normal distri- bution. For the option "non-Gaussian", data are transfered from a multivariate normal distribution to a continuous multivariate non-Gaussian distribution via Exponential marginals. For the option "categorical", data are transfered from a multivariate normal distribution to multivariate 'categorical' data. For the op- tion "pois", data are transfered from a multivariate normal distribution to a mul- tivariate Poisson distribution. For the option "nbinom", data are transfered from a multivariate normal distribution to a multivariate Negative Binomial distribu- tion. For the option "dweibull", data are transfered from a multivariate normal distribution to a multivariate discrete Weibull distribution with parameters q and beta. For the option "binary", data are generated directly from the joint dis- tribution, in this case p must be less than 17. For the option "mixed", data are transfered from a multivariate normal distribution to a mixture of 'categorical', 'non-Gaussian', 'binary' and 'Gaussian', respectively.

prob	if graph = "random", it is the probability that a pair of nodes has a link.	
size	number of links in the true graph (graph size).	
mean	vector specifying the mean of the variables.	
class	if graph = "cluster", it is the number of classes.	
cut	if type = "categorical", it is the number of categories for simulating 'categor- ical' data.	
b	degree of freedom for G-Wishart distribution, $W_G(b, D)$.	
D	positive definite $(p \times p)$ "scale" matrix for G-Wishart distribution, $W_G(b, D)$. The default is an identity matrix.	
К	if graph = "fixed", it is a positive-definite symmetric matrix, corresponding to the true precision matrix.	
sigma	if graph = "fixed", it is a positive-definite symmetric matrix corresponding to the true covariance matrix.	
q, beta	if type = "dweibull", they are the parameters of the discrete Weibull distribu- tion with density	
	$p(x,q,\beta) = q^{x^{\beta}} - q^{(x+1)^{\beta}}, \forall x = \{0,1,2,\ldots\}.$	
	They can be given either as a vector of length p or as an $(n \times p)$ matrix, e.g. if covariates are available and a regression model is used.	
vis	visualize the true graph structure.	
rewire	rewiring probability for smallworld network. Must be between 0 and 1.	
range.mu, range.dispersion		
	if type = "nbinom", vector with two elements specifying the range of parameters for the Negative Binomial distribution.	
nu	if type = "t" or "alternative-t", it is the parameter of the t distribution with density.	

Value

An object with S3 class "sim" is returned:

data	generated data as an $(n \times p)$ matrix.
sigma	covariance matrix of the generated data.
К	precision matrix of the generated data.
G	adjacency matrix corresponding to the true graph structure.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>, Pariya Behrouzi, Veronica Vinciotti, Ernst Wit, and Alexander Christensen

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

See Also

graph.sim,bdgraph,bdgraph.mpl

Examples

```
## Not run:
# Generating multivariate normal data from a 'random' graph
data.sim <- bdgraph.sim( p = 10, n = 50, prob = 0.3, vis = TRUE )
print( data.sim )
# Generating multivariate normal data from a 'hub' graph
data.sim <- bdgraph.sim( p = 6, n = 3, graph = "hub", vis = FALSE )
round( data.sim $ data, 2 )
# Generating mixed data from a 'hub' graph
data.sim <- bdgraph.sim( p = 8, n = 10, graph = "hub", type = "mixed" )
round( data.sim $ data, 2 )
# Generating only a 'scale-free' graph (with no data)
graph.sim <- bdgraph.sim( p = 8, graph = "scale-free" )
plot( graph.sim )
graph.sim $ G
## End(Not run)
```

bdw.reg

Bayesian estimation of (zero-inflated) Discrete Weibull regression

Description

Bayesian estimation of the parameters for Discrete Weibull (DW) regression. The conditional distribution of the response given the predictors is assumed to be DW with parameters q and beta, dependent on the predictors, and, with an additional parameter pi under zero inflation.

Usage

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bdw.reg

Arguments

data	data.frame or matrix corresponding to the data, containing the variables in the model.	
formula	object of class formula as a symbolic description of the model to be fitted. For the case of data.frame, it is taken as the model frame (see model.frame).	
iter	number of iterations for the sampling algorithm.	
burnin	number of burn-in iterations for the sampling algorithm.	
dist.q	Prior density for the regression coefficients associated to the parameter q. The default is a Normal distribution (dnorm). Any density function which has two parameters and can support the log = TRUE flag can be used, e.g. dnorm, dlnorm, dunif etc.	
dist.beta	Prior density for the regression coefficients associated to the parameter beta. The default is a Normal distribution (dnorm). Any density function which has two parameters and can support the log = TRUE flag can be used, e.g. dnorm, dlnorm, dunif etc.	
par.q	vector of length two corresponding to the parameters of dist.q.	
par.beta	vector of length two corresponding to the parameters of dist.beta.	
par.pi	vector of length two corresponding to the parameters of the beta prior density on pi.	
initial.q, initial.beta, initial.pi		
	vector of initial values for the regression coefficients and for pi (if $ZI = TRUE$).	
ZI	logical: if FALSE (default), the conditional distribution of the response given the predictors is assumed to be DW with parameters q and beta. If TRUE, a zero-inflated DW distribution will be applied.	
scale.proposal	scale of the proposal function. Setting to lower values results in an increase in the acceptance rate of the sampler.	
adapt	logical: if TRUE (default), the proposals will be adapted. If FALSE, no adapting will be applied.	
print	logical: if TRUE (default), tracing information is printed.	

Details

The regression model uses a logit link function on q and a log link function on beta, the two parameters of a DW distribution, with probability mass function given by

$$DW(y) = q^{y^{\beta}} - q^{(y+1)^{\beta}}, y = 0, 1, 2, \dots$$

For the case of zero inflation (ZI = TRUE), a zero-inflated DW is considered:

$$f(y) = (1 - pi)I(y = 0) + piDW(y)$$

where $0 \le pi \le 1$ and I(y = 0) is an indicator for the point mass at zero for the response y.

bdw.reg

Value

sample	MCMC samples
q.est	posterior estimates of q
beta.est	posterior estimates of beta
pi.est	posterior estimates of pi
accept.rate	acceptance rate of the MCMC algorithm

Author(s)

Veronica Vinciotti, Reza Mohammadi <a.mohammadi@uva.nl>, and Pariya Behrouzi

References

Vinciotti, V., Behrouzi, P., and Mohammadi, R. (2022) Bayesian structural learning of microbiota systems from count metagenomic data, *arXiv preprint*, doi:10.48550/arXiv.2203.10118

Peluso, A., Vinciotti, V., and Yu, K. (2018) Discrete Weibull generalized additive model: an application to count fertility, *Journal of the Royal Statistical Society: Series C*, 68(3):565-583, doi:10.1111/ rssc.12311

Haselimashhadi, H., Vinciotti, V. and Yu, K. (2018) A novel Bayesian regression model for counts with an application to health data, *Journal of Applied Statistics*, 45(6):1085-1105, doi:10.1080/02664763.2017.1342782

See Also

bdgraph.dw,bdgraph,ddweibull,bdgraph.sim

Examples

```
## Not run:
# - - Example 1
  = 0.6
q
beta = 1.1
n
    = 500
y = BDgraph::rdweibull( n = n, q = q, beta = beta )
output = bdw.reg( data = y, y \sim ., iter = 5000 )
output $ q.est
output $ beta.est
traceplot( output $ sample[ , 1 ], acf = T, pacf = T )
traceplot( output $ sample[ , 2 ], acf = T, pacf = T )
# - - Example 2
q = 0.6
beta = 1.1
```

bdw.reg

```
pii = 0.8
n = 500
y_dw = BDgraph::rdweibull( n = n, q = q, beta = beta )
z = rbinom( n = n, size = 1, prob = pii )
y = z * y_dw
output = bdw.reg( data = y, iter = 5000, ZI = TRUE )
output $ q.est
output $ beta.est
output $ pi.est
traceplot( output $ sample[ , 1 ], acf = T, pacf = T )
traceplot( output $ sample[ , 2 ], acf = T, pacf = T )
traceplot( output $ sample[ , 3 ], acf = T, pacf = T )
# - - Example 3
theta.q = c(0.1, -0.1, 0.34) # true parameter
theta.beta = c(0.1, -.15, 0.5) # true parameter
n = 500
x1 = runif(n = n, min = 0, max = 1.5)
x^2 = runif(n = n, min = 0, max = 1.5)
reg_q = theta.q[1] + x1 * theta.q[2] + x2 * theta.q[3]
q = 1 / (1 + exp( - reg_q))
reg_beta = theta.beta[ 1 ] + x1 * theta.beta[ 2 ] + x2 * theta.beta[ 3 ]
beta = exp( reg_beta )
y = BDgraph::rdweibull( n = n, q = q, beta = beta )
data = data.frame( x1, x2, y )
output = bdw.reg( data, y ~. , iter = 5000 )
# - - Example 4
theta.q = c( 1, -1, 0.8 ) # true parameter
theta.beta = c( 1, -1, 0.3 ) # true parameter
pii = 0.8
n = 500
x1 = runif(n = n, min = 0, max = 1.5)
x^2 = runif(n = n, min = 0, max = 1.5)
reg_q = theta.q[1] + x1 * theta.q[2] + x2 * theta.q[3]
q = 1 / (1 + exp(-reg_q))
```

bf

```
reg_beta = theta.beta[ 1 ] + x1 * theta.beta[ 2 ] + x2 * theta.beta[ 3 ]
beta = exp( reg_beta )

y_dw = BDgraph::rdweibull( n = n, q = q, beta = beta )
z = rbinom( n = n, size = 1, prob = pii )
y = z * y_dw
data = data.frame( x1, x2, y )
output = bdw.reg( data, y ~. , iter = 5000, ZI = TRUE )
## End(Not run)
```

bf

Bayes factor for two graphs

Description

Compute the Bayes factor for two graph structures.

Usage

bf(num, den, bdgraph.obj, log = TRUE)

Arguments

num, den	adjacency matrix corresponding to the true graph structure in which $a_{ij} = 1$ if there is a link between notes <i>i</i> and <i>j</i> , otherwise $a_{ij} = 0$. It can be an object with S3 class "graph" from function graph.sim. It can be an object with S3 class "sim" from function bdgraph.sim.
bdgraph.obj	object of S3 class "bdgraph", from function bdgraph. It also can be an object of S3 class "ssgraph", from the function ssgraph::ssgraph() of R package ssgraph::ssgraph().
log	character value. If TRUE the Bayes factor is given as log(BF).

Value

single numeric value, the Bayes factor of the two graph structures num and den.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

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compare

See Also

bdgraph, bdgraph.mpl, compare, bdgraph.sim

Examples

```
## Not run:
    # Generating multivariate normal data from a 'circle' graph
    data.sim <- bdgraph.sim( n = 50, p = 6, graph = "circle", vis = TRUE )
    # Running sampling algorithm
    bdgraph.obj <- bdgraph( data = data.sim )
    graph_1 <- graph.sim( p = 6, vis = TRUE )
    graph_2 <- graph.sim( p = 6, vis = TRUE )
    bf( num = graph_1, den = graph_2, bdgraph.obj = bdgraph.obj )
## End(Not run)
```

compare

Graph structure comparison

Description

This function provides several measures to assess the performance of the graphical structure learning.

Usage

```
compare( pred, actual, main = NULL, vis = FALSE )
```

Arguments

pred	adjacency matrix corresponding to an estimated graph. It can be an object with S3 class "bdgraph" from function bdgraph. It can be an object of S3 class "ssgraph", from the function ssgraph::ssgraph() of R package ssgraph::ssgraph(). It can be an object of S3 class "select", from the function huge.select of R package huge. It also can be a list of above objects for comparing two or more different approaches.
actual	adjacency matrix corresponding to the true graph structure in which $a_{ij} = 1$ if there is a link between notes <i>i</i> and <i>j</i> , otherwise $a_{ij} = 0$. It can be an object with S3 class "sim" from function bdgraph.sim. It can be an object with S3 class "graph" from function graph.sim.
main	character vector giving the names for the result table.
vis	logical: if TRUE, visualize the true graph and estimated graph structures.

Value

True positive	number of correctly estimated links.
True negative	number of true non-existing links which is correctly estimated.
False positive	number of links which they are not in the true graph, but are incorrectly esti- mated.
False negative	number of links which they are in the true graph, but are not estimated.
F1-score	weighted average of the "positive predictive" and "true positive rate". The F1-score value reaches its best value at 1 and worst score at 0.
Specificity	Specificity value reaches its best value at 1 and worst score at 0.
Sensitivity	Sensitivity value reaches its best value at 1 and worst score at 0.
MCC	Matthews Correlation Coefficients (MCC) value reaches its best value at 1 and worst score at 0.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>, Antonio Abbruzzo, and Ivan Vujacic

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

See Also

bdgraph, bdgraph.mpl, bdgraph.sim, plotroc

Examples

```
## Not run:
# Generating multivariate normal data from a 'random' graph
data.sim <- bdgraph.sim( n = 50, p = 6, size = 7, vis = TRUE )
# Running sampling algorithm based on GGMs
sample.ggm <- bdgraph( data = data.sim, method = "ggm", iter = 10000 )
# Comparing the results
compare( sample.ggm, data.sim, main = c( "True", "GGM" ), vis = TRUE )
# Running sampling algorithm based on GCGMs
sample.gcgm <- bdgraph( data = data.sim, method = "gcgm", iter = 10000 )
# Comparing GGM and GCGM methods
compare( list( sample.ggm, sample.gcgm ), data.sim,
main = c( "True", "GGM", "GCGM" ), vis = TRUE )
```

conf.mat

Confusion Matrix

Description

Create a Confusion Matrix.

Usage

Arguments

pred	adjacency matrix corresponding to an estimated graph. It can be an object with S3 class "bdgraph" from function bdgraph. It can be an object of S3 class "ssgraph", from the function ssgraph::ssgraph() of R package ssgraph::ssgraph().
actual	adjacency matrix corresponding to the actual graph structure in which $a_{ij} = 1$ if there is a link between notes <i>i</i> and <i>j</i> , otherwise $a_{ij} = 0$. It can be an object with S3 class "sim" from function bdgraph.sim. It can be an object with S3 class "graph" from function graph.sim. It can be a factor, numeric or character vector of responses (true class), typically encoded with 0 (controls) and 1 (cases). Only two classes can be used in a ROC curve.
cutoff	cutoff value for the case that pred is vector of probabilites. The default is 0.5.
proportion	logical: FALSE (default) for a confusion matrix with number of cases. TRUE, for a confusion matrix with the proportion of cases.
dnn	names to be given to the dimensions in the result (the dimnames names).
	further arguments to be passed to table.

Value

the results of table on pred and actual.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>

See Also

conf.mat.plot, compare, roc, bdgraph

Examples

```
## Not run:
set.seed( 100 )
# Generating multivariate normal data from a 'random' graph
data.sim <- bdgraph.sim( n = 50, p = 6, size = 7, vis = TRUE )
# Running sampling algorithm based on GGMs
sample.ggm <- bdgraph( data = data.sim, method = "ggm", iter = 10000 )
# Confusion Matrix for GGM method
conf.mat( pred = sample.ggm, actual = data.sim )
## End(Not run)
```

conf.mat.plot Plot Confusion Matrix

Description

Plot a Confusion Matrix.

Usage

Arguments

pred	adjacency matrix corresponding to an estimated graph. It can be an object with S3 class "bdgraph" from function bdgraph. It can be an object of S3 class "ssgraph", from the function ssgraph::ssgraph() of R package ssgraph::ssgraph().
actual	adjacency matrix corresponding to the actual graph structure in which $a_{ij} = 1$ if there is a link between notes <i>i</i> and <i>j</i> , otherwise $a_{ij} = 0$. It can be an object with S3 class "sim" from function bdgraph.sim. It can be an object with S3 class "graph" from function graph.sim. It can be a factor, numeric or character vector of responses (true class), typically encoded with 0 (controls) and 1 (cases). Only two classes can be used in a ROC curve.
cutoff	cutoff value for the case that pred is vector of probabilites. The default is 0.5.
conf.level	confidence level used for the confidence rings on the odds ratios. Must be a single nonnegative number less than 1; if set to 0 (the default), confidence rings are suppressed.
margin	numeric vector with the margins to equate. Must be one of 1 (the default), 2, or $c(1, 2)$, which corresponds to standardizing the row, column, or both margins in each 2 by 2 table. Only used if std equals "margins".
color	vector of length 2 specifying the colors to use for the smaller and larger diagonals of each 2 by 2 table.
	options to be passed to fourfoldplot.

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covariance

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>

See Also

conf.mat, compare, roc, bdgraph

Examples

```
## Not run:
set.seed( 100 )
```

Generating multivariate normal data from a 'random' graph data.sim <- bdgraph.sim(n = 50, p = 6, size = 7, vis = TRUE)

Running sampling algorithm based on GGMs
sample.ggm <- bdgraph(data = data.sim, method = "ggm", iter = 10000)</pre>

Confusion Matrix for GGM method conf.mat.plot(pred = sample.ggm, actual = data.sim)

End(Not run)

covariance

Estimated covariance matrix

Description

Provides the estimated covariance matrix.

Usage

```
covariance( bdgraph.obj, round = 2 )
```

Arguments

bdgraph.obj	object of S3 class "bdgraph", from function bdgraph. It also can be an object
	of S3 class "ssgraph", from the function ssgraph::ssgraph() of R package
	<pre>ssgraph::ssgraph().</pre>
round	value for rounding all probabilities to the specified number of decimal places.

Value

matrix which corresponds the estimated covariance matrix.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

Mohammadi, A. and Wit, E. C. (2015). Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Bayesian Analysis*, 10(1):109-138, doi:10.1214/14BA889

Mohammadi, R., Massam, H. and Letac, G. (2023). Accelerating Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Journal of the American Statistical Association*, doi:10.1080/01621459.2021.1996377

See Also

bdgraph, precision, plinks

Examples

```
## Not run:
# Generating multivariate normal data from a 'circle' graph
data.sim <- bdgraph.sim( n = 70, p = 6, graph = "circle", vis = TRUE )
bdgraph.obj <- bdgraph( data = data.sim )
covariance( bdgraph.obj ) # Estimated covariance matrix
data.sim $ sigma # True covariance matrix
## End(Not run)
```

Discrete Weibull The Discrete Weibull Distribution (Type 1)

Description

Density, distribution function, quantile function and random generation for the discrete Weibull distribution (type I) with parameters q and β .

Usage

```
ddweibull( x, q = exp(-1), beta = 1, zero = TRUE )
pdweibull( x, q = exp(-1), beta = 1, zero = TRUE )
qdweibull( p, q = exp(-1), beta = 1, zero = TRUE )
rdweibull( n, q = exp(-1), beta = 1, zero = TRUE )
```

Discrete Weibull

Arguments

x	vector of quantiles.
р	vector of probabilities.
q, beta	shape and scale parameters, the latter defaulting to 1.
zero	logical; if TRUE (default), the support contains 0; FALSE otherwise.
n	number of observations. If $length(n) > 1$, the length is taken to be the number required.

Details

The discrete Weibull distribution has density given by

$$f(x) = q^{x^{\beta}} - q^{(x+1)^{\beta}}, x = 0, 1, 2, \dots$$

For the case zero = FALSE:

$$f(x) = q^{(x-1)^{\beta}} - q^{x^{\beta}}, x = 1, 2, \dots$$

Cumulative distribution function

$$F(x) = 1 - q^{(x+1)^{\beta}}$$

For the case zero = FALSE, x+1 should replaced by x.

Value

ddweibull gives the density, pdweibull gives the distribution function, qdweibull gives the quantile function, and rdweibull generates random values.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>, Pariya Behrouzi, Veronica Vinciotti

References

Nakagawa, T. and Osaki, S. (1975). The Discrete Weibull Distribution. *IEEE Transactions on Reliability*, R-24, 300-301, doi:10.1109/TR.1975.5214915

See Also

dweibull, bdw.reg, bdgraph.dw

Examples

n = 1000 q = 0.4 beta = 0.8 set.seed(7) rdw = rdweibull(n = n, q = q, beta = beta)

```
plot( prop.table( table( rdw ) ), type = "h", col = "gray50" )
x = 0:max( rdw )
lines( x, ddweibull( x = x, q = q, beta = beta ), type = "o", col = "blue", lwd = 2 )
hist( pdweibull( x = rdw, q = q, beta = beta ) )
plot( ecdf( rdw ) )
lines( x, pdweibull( x, q = q, beta = beta ), col = "blue", lwd = 2, type = "s" )
```

geneExpression Human gene expression dataset

Description

The dataset contains human gene expression of 100 transcripts (with unique Illumina TargetID) measured on 60 unrelated individuals.

Usage

```
data( geneExpression )
```

Format

The format is a matrix with 60 rows (number of individuals) and 100 column (number of transcripts).

References

Bhadra, A. and Mallick, B. K. (2013). Joint High Dimensional Bayesian Variable and Covariance Selection with an Application to eQTL Analysis, *Biometrics*, 69(2):447-457, doi:10.1111/ biom.12021

Mohammadi, A. and Wit, E. C. (2015). Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Bayesian Analysis*, 10(1):109-138, doi:10.1214/14BA889

Examples

```
data( geneExpression )
dim( geneExpression )
```

head(geneExpression)

gnorm

Description

Calculates log of the normalizing constant of G-Wishart distribution based on the Monte Carlo method, developed by Atay-Kayis and Massam (2005).

Usage

gnorm(adj, b = 3, D = diag(ncol(adj)), iter = 100)

Arguments

adj	adjacency matrix corresponding to the graph structure. It is an upper triangular matrix in which $a_{ij} = 1$ if there is a link between notes <i>i</i> and <i>j</i> , otherwise
	$a_{ij} = 0.$
b	degree of freedom for G-Wishart distribution, $W_G(b, D)$.
D	positive definite $(p \times p)$ "scale" matrix for G-Wishart distribution, $W_G(b, D)$. The default is an identity matrix.
iter	number of iteration for the Monte Carlo approximation.

Details

Log of the normalizing constant approximation using Monte Carlo method for a G-Wishart distribution, $K \sim W_G(b, D)$, with density:

$$Pr(K) = \frac{1}{I(b,D)} |K|^{(b-2)/2} \exp\left\{-\frac{1}{2} \operatorname{trace}(K \times D)\right\}.$$

Value

Log of the normalizing constant of G-Wishart distribution.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>

References

Atay-Kayis, A. and Massam, H. (2005). A monte carlo method for computing the marginal likelihood in nondecomposable Gaussian graphical models, *Biometrika*, 92(2):317-335, doi:10.1093/ biomet/92.2.317

Mohammadi, R., Massam, H. and Letac, G. (2023). Accelerating Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Journal of the American Statistical Association*, doi:10.1080/01621459.2021.1996377

Uhler, C., et al (2018) Exact formulas for the normalizing constants of Wishart distributions for graphical models, *The Annals of Statistics* 46(1):90-118, doi:10.1214/17AOS1543

See Also

rgwish, rwish

Examples

graph.sim Graph simulation

Description

Simulating undirected graph structures, including "random", "cluster", "scale-free", "lattice", "hub", "star", and "circle".

Usage

Arguments

р	number of variables (nodes).
graph	undirected graph with options "random", "cluster", "smallworld", "scale-free", "lattice", "hub", "star", and "circle". It also could be an adjacency matrix corresponding to a graph structure (an upper triangular matrix in which $g_{ij} = 1$ if there is a link between notes <i>i</i> and <i>j</i> , otherwise $g_{ij} = 0$).
prob	if graph = "random", it is the probability that a pair of nodes has a link.
size	number of links in the true graph (graph size).
class	if graph = "cluster", it is the number of classes.
vis	visualize the true graph structure.
rewire	rewiring probability for smallworld network. Must be between 0 and 1.

Value

The adjacency matrix corresponding to the simulated graph structure, as an object with S3 class "graph".

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link2adj

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl> and Alexander Christensen

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

See Also

bdgraph.sim,bdgraph,bdgraph.mpl

Examples

```
# Generating a 'hub' graph
adj <- graph.sim( p = 8, graph = "scale-free" )
plot( adj )
adj
```

link2adj

Extract links from an adjacency matrix

Description

Extract links from an adjacency matrix or an object of calsses "sim" from function bdgraph.sim and "graph" from function graph.sim.

Usage

```
link2adj( link, p = NULL )
```

Arguments

link	$(2\times p)$ matrix or a data.frame corresponding to the links from the graph structure.
р	number of nodes of the graph.

Value

An adjacency matrix corresponding to a graph structure in which $a_{ij} = 1$ if there is a link between notes i and j, otherwise $a_{ij} = 0$.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

See Also

adj2link,graph.sim

Examples

```
# Generating a 'random' graph
adj <- graph.sim( p = 6, vis = TRUE )
link <- adj2link( adj )
link2adj( link, p = 6 )
```

mse

Graph structure comparison

Description

Computes (weighted) mean squared error.

Usage

```
mse( pred, actual, weight = FALSE )
```

Arguments

pred	adjacency matrix corresponding to an estimated graph. It can be an object with S3 class "bdgraph" from function bdgraph. It can be an object of S3 class "ssgraph", from the function ssgraph::ssgraph() of R package ssgraph::ssgraph(). It can be an object of S3 class "select", from the function huge.select of R package huge. It also can be a list of above objects for comparing two or more different approaches.
actual	adjacency matrix corresponding to the true graph structure in which $a_{ij} = 1$ if there is a link between notes <i>i</i> and <i>j</i> , otherwise $a_{ij} = 0$. It can be an object with S3 class "sim" from function bdgraph.sim. It can be an object with S3 class "graph" from function graph.sim.
weight	for the case of weighted MSE.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>; Lucas Vogels <l.f.o.vogels@uva.nl>

pgraph

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

See Also

compare, auc, bdgraph, bdgraph.mpl, bdgraph.sim, plotroc

Examples

```
## Not run:
# Generating multivariate normal data from a 'random' graph
data.sim <- bdgraph.sim( n = 50, p = 6, size = 7, vis = TRUE )
# Running sampling algorithm based on GGMs
sample.ggm <- bdgraph( data = data.sim, method = "ggm", iter = 10000 )
# To compute the value of MSE
mse( pred = sample.ggm, actual = data.sim )
# To compute the value of weighted MSE
mse( pred = sample.ggm, actual = data.sim, weight = 0.5 )
```

End(Not run)

pgraph

Posterior probabilities of the graphs

Description

Provides the estimated posterior probabilities for the most likely graphs or a specific graph.

Usage

```
pgraph( bdgraph.obj, number.g = 4, adj = NULL )
```

Arguments

bdgraph.obj	object of S3 class "bdgraph", from function bdgraph.
number.g	number of graphs with the highest posterior probabilities to be shown. This option is ignored if 'adj' is specified.
adj	adjacency matrix corresponding to a graph structure. It is an upper triangular matrix in which $a_{ij} = 1$ if there is a link between notes <i>i</i> and <i>j</i> , otherwise $a_{ij} = 0$. It also can be an object of S3 class "sim", from function bdgraph.sim.

plinks

Value

-	adjacency matrices which corresponding to the graphs with the highest posterior probabilities.
prob_g	vector of the posterior probabilities of the graphs corresponding to 'selected_g'.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl> and Ernst Wit

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

Mohammadi, A. and Wit, E. C. (2015). Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Bayesian Analysis*, 10(1):109-138, doi:10.1214/14BA889

Mohammadi, R., Massam, H. and Letac, G. (2023). Accelerating Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Journal of the American Statistical Association*, doi:10.1080/01621459.2021.1996377

See Also

bdgraph, bdgraph.mpl

Examples

```
## Not run:
# Generating multivariate normal data from a 'random' graph
data.sim <- bdgraph.sim( n = 50, p = 6, size = 6, vis = TRUE )
bdgraph.obj <- bdgraph( data = data.sim, save = TRUE )
# Estimated posterior probability of the true graph
pgraph( bdgraph.obj, adj = data.sim )
# Estimated posterior probability of first and second graphs with highest probabilities
pgraph( bdgraph.obj, number.g = 2 )
## End(Not run)
```

plinks

Estimated posterior link probabilities

Description

Provides the estimated posterior link probabilities for all possible links in the graph.

plinks

Usage

plinks(bdgraph.obj, round = 2, burnin = NULL)

Arguments

bdgraph.obj	object of S3 class "bdgraph", from function bdgraph. It also can be an object of S3 class "ssgraph", from the function ssgraph::ssgraph() of R package ssgraph::ssgraph().
round	value for rounding all probabilities to the specified number of decimal places.
burnin	number of burn-in iteration to scape.

Value

An upper triangular matrix which corresponds the estimated posterior probabilities for all possible links.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl> and Ernst Wit

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

Mohammadi, A. and Wit, E. C. (2015). Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Bayesian Analysis*, 10(1):109-138, doi:10.1214/14BA889

Mohammadi, R., Massam, H. and Letac, G. (2023). Accelerating Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Journal of the American Statistical Association*, doi:10.1080/01621459.2021.1996377

Dobra, A. and Mohammadi, R. (2018). Loglinear Model Selection and Human Mobility, *Annals of Applied Statistics*, 12(2):815-845, doi:10.1214/18AOAS1164

Mohammadi, A. et al (2017). Bayesian modelling of Dupuytren disease by using Gaussian copula graphical models, *Journal of the Royal Statistical Society: Series C*, 66(3):629-645, doi:10.1111/rssc.12171

See Also

bdgraph, bdgraph.mpl

Examples

```
## Not run:
# Generating multivariate normal data from a 'circle' graph
data.sim <- bdgraph.sim( n = 70, p = 6, graph = "circle", vis = TRUE )
bdgraph.obj <- bdgraph( data = data.sim, iter = 10000 )
plinks( bdgraph.obj, round = 2 )
```

End(Not run)

plot.bdgraph

Plot function for S3 class "bdgraph"

Description

Visualizes structure of the selected graphs which could be a graph with links for which their estimated posterior probabilities are greater than 0.5 or graph with the highest posterior probability.

Usage

Arguments

х	object of S3 class "bdgraph", from function bdgraph.	
cut	threshold for including the links in the selected graph based on the estimated posterior probabilities of the links; See the examples.	
number.g	number of graphs with the highest probabilities. This option works for the case running function bdgraph() with option save = TRUE; See the examples.	
main	Graphical parameter (see plot).	
layout	vertex placement which is according to R package igraph; For different layouts, see layout of R package igraph.	
vertex.size	vertex size which is according to R package igraph.	
vertex.color	vertex color which is according to R package igraph.	
vertex.frame.color		
	vertex frame color which is according to R package igraph.	
vertex.label vertex label. The default vertex labels are the vertex ids.		
	vertex label distance which is according to R package igraph.	
vertex.label.color		
	vertex label color which is according to R package igraph.	
edge.color	edge color which is according to R package igraph.	
	additional plotting parameters. For the complete list, see igraph.plotting of R package igraph.	

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl> and Ernst Wit

plot.graph

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

See Also

bdgraph, bdgraph.mpl

Examples

```
## Not run:
set.seed( 100 )
# Generating multivariate normal data from a 'random' graph
data.sim <- bdgraph.sim( n = 100, p = 15, graph = "random", prob = 0.2, vis = TRUE )
bdgraph.obj <- bdgraph( data = data.sim )
plot( bdgraph.obj )
bdgraph.obj <- bdgraph( data = data.sim, save = TRUE )
plot( bdgraph.obj, cut = 0.5 )
plot( bdgraph.obj, number.g = 4 )
## End(Not run)
```

plot.graph

Plot function for S3 class "graph"

Description

Visualizes structure of the graph.

Usage

Arguments

х	object of S3 class "graph", from function graph.sim.
cut	for the case where input 'x' is the object of class "bdgraph" or "ssgraph". Thresh-
	old for including the links in the selected graph based on the estimated posterior
	probabilities of the links.

mode	type of graph which is according to R package igraph.	
diag	logical which is according to R package igraph.	
main	graphical parameter (see plot).	
layout	vertex placement which is according to R package igraph; For different layouts, see layout of R package igraph.	
vertex.size	vertex size which is according to R package igraph.	
vertex.color	vertex color which is according to R package igraph.	
vertex.frame.co	blor	
	vertex frame color which is according to R package igraph.	
vertex.label	vertex label. The default vertex labels are the vertex ids.	
vertex.label.dist		
	vertex label distance which is according to R package igraph.	
vertex.label.color		
	vertex label color which is according to R package igraph.	
edge.color	edge color which is according to R package igraph.	
	additional plotting parameters. For the complete list, see igraph.plotting of R package igraph.	

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

See Also

graph.sim, bdgraph.sim, plot.igraph

Examples

```
# Generating a 'scale-free' graph
adj <- graph.sim( p = 20, graph = "scale-free" )
plot( adj )
```

plot.sim

Description

Visualizes structure of the simulated graph for an object of S3 class "sim", from function bdgraph.sim.

Usage

```
## S3 method for class 'sim'
plot( x, ... )
```

Arguments

х	object of S3 class "sim", from function bdgraph.sim.
	additional plotting parameters. See plot.graph and for the complete list igraph.plotting of R package igraph.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl> and Ernst Wit

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

See Also

graph.sim, bdgraph.sim, plot.graph, plot.igraph

Examples

```
set.seed( 10 )
```

Generating synthetic multivariate normal data from a 'random' graph data.sim <- bdgraph.sim(n = 10, p = 15)

plot(data.sim)

plotcoda

Description

Visualizes the cumulative occupancy fractions of all possible links in the graph. It can be used for monitoring the convergence of the sampling algorithms, BDMCMC and RJMCMC.

Usage

Arguments

bdgraph.obj	object of S3 class "bdgraph", from function bdgraph. It also can be an object of S3 class "ssgraph", from the function ssgraph::ssgraph() of R package ssgraph::ssgraph().
thin	option for getting fast result for a cumulative plot according to part of the itera- tion.
control	logical: if TRUE (default) and the number of nodes is greater than 15, then 100 links randomly is selected for visualization.
main	graphical parameter (see plot).
verbose	logical: if TRUE (default), report/print the calculation progress.
	system reserved (no specific usage).

Details

Note that a spending time for this function depends on the number of nodes. For fast result, you can choose bigger value for the 'thin' option.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

See Also

bdgraph, bdgraph.mpl, traceplot

plotroc

Examples

```
## Not run:
# Generating multivariate normal data from a 'circle' graph
data.sim <- bdgraph.sim( n = 50, p = 6, graph = "circle", vis = TRUE )
bdgraph.obj <- bdgraph( data = data.sim, iter = 10000, burnin = 0 , save = TRUE )
plotcoda( bdgraph.obj )
## End(Not run)
```

plotroc

ROC plot

Description

Draws the receiver operating characteristic (ROC) curve according to the true graph structure for object of S3 class "bdgraph", from function bdgraph.

Usage

```
plotroc( pred, actual, cut = 200, smooth = FALSE, calibrate = TRUE,
    linetype = NULL, color = NULL, size = 1, main = "ROC Curve",
    xlab = "False Postive Rate", ylab = "True Postive Rate",
    legend = TRUE, legend.size = 17, legend.position = c( 0.7, 0.3 ),
    labels = NULL, auc = TRUE, theme = ggplot2::theme_minimal() )
```

Arguments

pred	upper triangular matrix corresponding to the estimated posterior probabilities for all possible links. It can be an object with S3 class "bdgraph" from func- tion bdgraph. It can be an object of S3 class "ssgraph", from the function ssgraph::ssgraph() of R package ssgraph::ssgraph(). It can be an object of S3 class "select", from the function huge.select of R package huge. Op- tions est2, est3 and est4 are for comparing two or more different approaches.
actual	adjacency matrix corresponding to the true graph structure in which $a_{ij} = 1$ if there is a link between notes <i>i</i> and <i>j</i> , otherwise $a_{ij} = 0$. It can be an object with S3 class "sim" from function bdgraph.sim. It can be an object with S3 class "graph" from function graph.sim.
cut	number of cut points.
smooth	logical: for smoothing the ROC curve.
calibrate	If TRUE, compute the value of AUC by taking the level of the probabilities into account.
linetype	specification for the default plotting line type.
color	specification for the default plotting color.

plotroc

size	specification for the default plotting line size.
main	overall title for the plot.
xlab	title for the x axis.
ylab	title for the y axis.
legend	logical: for adding legend to the ROC plot.
legend.size	title for the x axis.
legend.position	
	title for the y axis.
labels	for legends of the legend to the ROC plot.
auc	logical: to report AUC with legend.
theme	theme for the plot from the function ggplot2::ggplot() of R package ggplot2::ggplot().

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>; Lucas Vogels <1.f.o.vogels@uva.nl>

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

Mohammadi, A. and Wit, E. C. (2015). Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Bayesian Analysis*, 10(1):109-138, doi:10.1214/14BA889

Mohammadi, R., Massam, H. and Letac, G. (2023). Accelerating Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Journal of the American Statistical Association*, doi:10.1080/01621459.2021.1996377

See Also

roc, pROC::plot.roc(), pROC::auc(), bdgraph, bdgraph.mpl, compare

Examples

```
## Not run:
# To generate multivariate normal data from a 'random' graph
data.sim <- bdgraph.sim( n = 30, p = 6, size = 7, vis = TRUE )
# To Run sampling algorithm
bdgraph.obj <- bdgraph( data = data.sim, iter = 10000 )
# To compare the results
plotroc( bdgraph.ob2j, data.sim )
# To compare the results based on CGGMs approach
bdgraph.obj2 <- bdgraph( data = data.sim, method = "gcgm", iter = 10000 )
# To Compare the resultss
plotroc( list( bdgraph.obj, bdgraph.obj2 ), data.sim, legend = FALSE )
## End(Not run)
```

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posterior.predict Posterior Predictive Samples

Description

Provides samples from the posterior predictive distribution.

Usage

```
posterior.predict( object, iter = 1, ... )
```

Arguments

object	object of S3 class "bdgraph", from function bdgraph.
iter	number of predictions.
	additional parameters.

Value

a matrix containing the predicted datasets, corresponding to the samples from the joint posterior disribtuion.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl> and Ernst Wit

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

Mohammadi, A. and Wit, E. C. (2015). Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Bayesian Analysis*, 10(1):109-138, doi:10.1214/14BA889

Mohammadi, R., Massam, H. and Letac, G. (2023). Accelerating Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Journal of the American Statistical Association*, doi:10.1080/01621459.2021.1996377

Dobra, A. and Mohammadi, R. (2018). Loglinear Model Selection and Human Mobility, *Annals of Applied Statistics*, 12(2):815-845, doi:10.1214/18AOAS1164

Vogels, L., Mohammadi, R., Schoonhoven, M., and Birbil, S.I. (2023) Bayesian Structure Learning in Undirected Gaussian Graphical Models: Literature Review with Empirical Comparison, *arXiv* preprint, doi:10.48550/arXiv.2307.02603

Mohammadi, R., Schoonhoven, M., Vogels, L., and Birbil, S.I. (2023) Large-scale Bayesian Structure Learning for Gaussian Graphical Models using Marginal Pseudo-likelihood, *arXiv preprint*, doi:10.48550/arXiv.2307.00127

Mohammadi, A. et al (2017). Bayesian modelling of Dupuytren disease by using Gaussian copula graphical models, *Journal of the Royal Statistical Society: Series C*, 66(3):629-645, doi:10.1111/rssc.12171

See Also

bdgraph, bdgraph.mpl, bdgraph.dw

Examples

```
## Not run:
# Generating multivariate normal data from a 'random' graph
data.sim <- bdgraph.sim( n = 50, p = 6, size = 7, vis = TRUE )
bdgraph.obj <- bdgraph( data = data.sim )
posterior.predict( bdgraph.obj, iter = 20 )
## End(Not run)
```

precision

Estimated precision matrix

Description

Provides the estimated precision matrix.

Usage

```
precision( bdgraph.obj, round = 2 )
```

Arguments

bdgraph.obj	object of S3 class "bdgraph", from function bdgraph. It also can be an object
	of S3 class "ssgraph", from the function ssgraph::ssgraph() of R package
	<pre>ssgraph::ssgraph().</pre>
round	value for rounding all probabilities to the specified number of decimal places.

Value

matrix which corresponds the estimated precision matrix.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

See Also

bdgraph, covariance, plinks

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predict.bdgraph

Examples

```
## Not run:
# Generating multivariate normal data from a 'circle' graph
data.sim <- bdgraph.sim( n = 70, p = 6, graph = "circle", vis = TRUE )
bdgraph.obj <- bdgraph( data = data.sim )
precision( bdgraph.obj ) # Estimated precision matrix
data.sim $ K # True precision matrix
## End(Not run)
```

predict.bdgraph Predict function for S3 class "bdgraph"

Description

Provides predict values of the results for function bdgraph.

Usage

S3 method for class 'bdgraph'
predict(object, iter = 1, ...)

Arguments

object	object of S3 class "bdgraph", from function bdgraph.
iter	number of predictions.
	additional parameters.

Value

a matrix containing the predicted datasets, corresponding to the samples from the joint posterior disribution.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl> and Ernst Wit

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03 Mohammadi, A. and Wit, E. C. (2015). Bayesian Structure Learning in Sparse Gaussian Graphical

Mohammadi, A. and Wit, E. C. (2015). Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Bayesian Analysis*, 10(1):109-138, doi:10.1214/14BA889

Mohammadi, R., Massam, H. and Letac, G. (2023). Accelerating Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Journal of the American Statistical Association*, doi:10.1080/01621459.2021.1996377

Dobra, A. and Mohammadi, R. (2018). Loglinear Model Selection and Human Mobility, *Annals of Applied Statistics*, 12(2):815-845, doi:10.1214/18AOAS1164

Vogels, L., Mohammadi, R., Schoonhoven, M., and Birbil, S.I. (2023) Bayesian Structure Learning in Undirected Gaussian Graphical Models: Literature Review with Empirical Comparison, *arXiv* preprint, doi:10.48550/arXiv.2307.02603

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Mohammadi, A. et al (2017). Bayesian modelling of Dupuytren disease by using Gaussian copula graphical models, *Journal of the Royal Statistical Society: Series C*, 66(3):629-645, doi:10.1111/rssc.12171

See Also

bdgraph, bdgraph.mpl, bdgraph.dw

Examples

```
## Not run:
# Generating multivariate normal data from a 'random' graph
data.sim <- bdgraph.sim( n = 50, p = 6, size = 7, vis = TRUE )
bdgraph.obj <- bdgraph( data = data.sim )
predict( bdgraph.obj, iter = 20 )
## End(Not run)
```

print.bdgraph

Print function for S3 class "bdgraph"

Description

Prints the information about the selected graph which could be a graph with links for which their estimated posterior probabilities are greater than 0.5 or graph with the highest posterior probability. It provides adjacency matrix, size and posterior probability of the selected graph.

Usage

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

print.sim

Arguments

Х	object of S3 class "bdgraph", from function bdgraph.
	system reserved (no specific usage).

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl> and Ernst Wit

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

See Also

bdgraph, bdgraph.mpl

Examples

```
## Not run:
# Generating multivariate normal data from a 'random' graph
data.sim <- bdgraph.sim( n = 50, p = 6, vis = TRUE )
bdgraph.obj <- bdgraph( data = data.sim )
print( bdgraph.obj )
## End(Not run)
```

print.sim

Print function for S3 class "sim"

Description

Prints the information about the type of data, the sample size, the graph type, the number of nodes, number of links and sparsity of the true graph.

Usage

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

Arguments

х	object of S3 class "sim", from function bdgraph.sim.
	system reserved (no specific usage).

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl> and Ernst Wit

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

See Also

graph.sim, bdgraph.sim

Examples

```
# Generating multivariate normal data from a 'random' graph data.sim <- bdgraph.sim( n = 20, p = 10, vis = TRUE )
```

print(data.sim)

reinis

Risk factors of coronary heart disease

Description

The dataset consist of 6 discrete variables as the potential risk factors of coronary heart disease. The data collected from 1841 men employed of a car factory in Czechoslovakia (Reinis et al. 1981).

Usage

data(reinis)

Format

The format is a matrix with 1841 rows (number of individuals) and 6 column (number of variables).

References

Edwards and Havranek (1985). A fast procedure for model search in multidimensional contingency tables, *Biometrika*, 72:339-351

Reinis et al (1981). Prognostic significance of the risk profile in the prevention of coronary heart disease, *Bratis. lek. Listy*, 76:137-150

Mohammadi, A. and Dobra, A. (2017). The R Package **BDgraph** for Bayesian Structure Learning in Graphical Models, *ISBA Bulletin*, 24(4):11-16

Examples

data(reinis)

summary(reinis)

rgwish

Description

Generates random matrices, distributed according to the G-Wishart distribution with parameters b and D, $W_G(b, D)$ with respect to the graph structure G. Note this function works for both non-decomposable and decomposable graphs.

Usage

```
rgwish( n = 1, adj = NULL, b = 3, D = NULL, threshold = 1e-8 )
```

Arguments

n	number of samples required.
adj	adjacency matrix corresponding to the graph structure which can be non-decomposable or decomposable. It should be an upper triangular matrix in which $a_{ij} = 1$ if there is a link between notes <i>i</i> and <i>j</i> , otherwise $a_{ij} = 0$. adj could be an ob- ject of class "graph", from function graph.sim. It also could be an object of class "sim", from function bdgraph.sim. It also could be an object of class "bdgraph", from functions bdgraph.mpl or bdgraph.
b	degree of freedom for G-Wishart distribution, $W_G(b, D)$.
D	positive definite $(p \times p)$ "scale" matrix for G-Wishart distribution, $W_G(b, D)$. The default is an identity matrix.
threshold	threshold value for the convergence of sampling algorithm from G-Wishart.

Details

Sampling from G-Wishart distribution, $K \sim W_G(b, D)$, with density:

$$Pr(K) \propto |K|^{(b-2)/2} \exp\left\{-\frac{1}{2}\operatorname{trace}(K \times D)\right\},$$

which b > 2 is the degree of freedom and D is a symmetric positive definite matrix.

Value

A numeric array, say A, of dimension $(p \times p \times n)$, where each A[, i] is a positive definite matrix, a realization of the G-Wishart distribution, $W_G(b, D)$. Note, for the case n = 1, the output is a matrix.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>

References

Lenkoski, A. (2013). A direct sampler for G-Wishart variates, Stat, 2:119-128, doi:10.1002/sta4.23

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

Mohammadi, A. and Wit, E. C. (2015). Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Bayesian Analysis*, 10(1):109-138, doi:10.1214/14BA889

See Also

gnorm, rwish

Examples

```
# Generating a 'circle' graph as a non-decomposable graph
adj <- graph.sim( p = 5, graph = "circle" )
adj  # adjacency of graph with 5 nodes
sample <- rgwish( n = 1, adj = adj, b = 3, D = diag( 5 ) )
round( sample, 2 )
sample <- rgwish( n = 5, adj = adj )
round( sample, 2 )
```

rmvnorm

Generate data from the multivariate Normal distribution

Description

Random generation function from the multivariate Normal distribution with mean equal to *mean* and covariance matrix *sigma*.

Usage

Arguments

n	Number of observations.
mean	Mean vector, default is $rep(0, length = ncol(sigma))$.
sigma	positive definite covariance matrix, default is $diag(length(mean)).$

Value

A numeric matrix with rows equal to n and columns equal to length(mean).

roc

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>

See Also

bdgraph.sim,rwish,rgwish

Examples

roc

Build a ROC curve

Description

This function builds a ROC curve specifically for graph structure learning and returns a "roc" object, a list of class "roc". This object can be printed, plotted, or passed to the functions pROC::roc(), pROC::ci(), pROC::smooth.roc() and pROC::coords(). Additionally, two roc objects can be compared with pROC::roc.test(). This function is based on the roc function of R package pROC.

Usage

roc(pred, actual, auc = TRUE, smooth = FALSE, plot = FALSE, quiet = TRUE, ...)

Arguments

pred	adjacency matrix (or a vector) corresponding to an estimated graph. It can be an object with S3 class "bdgraph" from function bdgraph. It can be an object of S3 class "ssgraph", from the function ssgraph::ssgraph() of R package ssgraph::ssgraph(). It can be a numeric or ordered vector of the same length than actual, containing the predicted value of each observation.
actual	adjacency matrix (or a vector) corresponding to the actual graph structure in which $a_{ij} = 1$ if there is a link between notes <i>i</i> and <i>j</i> , otherwise $a_{ij} = 0$. It can be an object with S3 class "sim" from function bdgraph.sim. It can be an object with S3 class "graph" from function graph.sim. It can be a factor, numeric or character vector of responses (true class), typically encoded with 0 (controls) and 1 (cases). Only two classes can be used in a ROC curve.
smooth	if TRUE, the ROC curve is passed to smooth to be smoothed.
auc	compute the area under the curve (AUC)? If TRUE (default), additional arguments can be passed to pROC::auc().

plot	plot the ROC curve? If TRUE, additional arguments can be passed to pROC::plot.roc().
quiet	if TRUE, turn off messages when direction and levels are auto-detected.
	further arguments to be passed to pROC::roc().

Value

If the data contained any NA value and na.rm=FALSE, NA is returned. Otherwise, if smooth=FALSE, a list of class "roc" with the following fields:

auc	if called with auc=TRUE, a numeric of class "auc" as defined in pROC::auc().
ci	if called with ci=TRUE, a numeric of class "ci" as defined in pROC::ci().
response	the response vector. Patients whose response is not %in% levels are discarded. If NA values were removed, a na.action attribute similar to na.omit stores the row numbers.
predictor	predictor vector converted to numeric as used to build the ROC curve. Patients whose response is not %in% levels are discarded. If NA values were removed, a na.action attribute similar to na.omit stores the row numbers.
original.predi	ctor, original.response
	response and predictor vectors as passed in argument.
levels	levels of the response as defined in argument.
controls	predictor values for the control observations.
cases	predictor values for the cases.
percent	if the sensitivities, specificities and AUC are reported in percent, as defined in argument.
direction	direction of the comparison, as defined in argument.
fun.sesp	function used to compute sensitivities and specificities. Will be re-used in boot- strap operations.
sensitivities	sensitivities defining the ROC curve.
specificities	specificities defining the ROC curve.
thresholds	thresholds at which the sensitivities and specificities were computed. See below for details.
call	how the function was called. See function match.call for more details.

If smooth=TRUE a list of class "smooth.roc" as returned by pROC::smooth(), with or without additional elements auc and ci (according to the call).

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>; Lucas Vogels <l.f.o.vogels@uva.nl>

References

Tom Fawcett (2006) "An introduction to ROC analysis". *Pattern Recognition Letters* **27**, 861–874, doi:10.1016/j.patrec.2005.10.010

Xavier Robin, Natacha Turck, Alexandre Hainard, *et al.* (2011) "pROC: an open-source package for R and S+ to analyze and compare ROC curves". *BMC Bioinformatics*, **7**, 77, doi:10.1186/1471-21051277.

rwish

See Also

plotroc, pROC::plot.roc(), pROC::auc(), pROC::print.roc(), bdgraph, bdgraph.mpl, compare

Examples

```
## Not run:
set.seed( 5 )
# Generating multivariate normal data from a 'scale-free' graph
data.sim = bdgraph.sim( n = 200, p = 15, graph = "scale-free", vis = TRUE )
# Running BDMCMC algorithm
sample.bdmcmc = bdgraph( data = data.sim, algorithm = "bdmcmc", iter = 10000 )
# ROC curve for BDMCMC algorithm
roc.bdmcmc = BDgraph::roc( pred = sample.bdmcmc, actual = data.sim, plot = TRUE )
# Running RJMCMC algorithm
sample.rjmcmc = bdgraph( data = data.sim, algorithm = "rjmcmc", iter = 10000 )
# ROC curve for RJMCMC algorithm
roc.rjmcmc = BDgraph::roc( pred = sample.rjmcmc, actual = data.sim, plot = TRUE )
# ROC curve for RJMCMC algorithm
roc.rjmcmc = BDgraph::roc( pred = sample.rjmcmc, actual = data.sim, plot = TRUE )
# ROC curve for both BDMCMC and RJMCMC algorithms
pROC::ggroc( list( BDMCMC = roc.bdmcmc, RJMCMC = roc.rjmcmc ) )
## End(Not run)
```

rwish

Sampling from Wishart distribution

Description

Generates random matrices, distributed according to the Wishart distribution with parameters b and D, W(b, D).

Usage

rwish(n = 1, p = 2, b = 3, D = diag(p))

Arguments

n	number of samples required.
р	number of variables (nodes).
b	degree of freedom for Wishart distribution, $W(b, D)$.
D	positive definite $(p \times p)$ "scale" matrix for Wishart distribution, $W(b, D)$. The default is an identity matrix.

Details

Sampling from Wishart distribution, $K \sim W(b, D)$, with density:

$$Pr(K) \propto |K|^{(b-2)/2} \exp\left\{-\frac{1}{2}\operatorname{trace}(K \times D)\right\},$$

which b > 2 is the degree of freedom and D is a symmetric positive definite matrix.

Value

A numeric array, say A, of dimension $(p \times p \times n)$, where each A[, i] is a positive definite matrix, a realization of the Wishart distribution W(b, D). Note, for the case n = 1, the output is a matrix.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>

References

Lenkoski, A. (2013). A direct sampler for G-Wishart variates, Stat, 2:119-128, doi:10.1002/sta4.23

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

See Also

gnorm, rgwish

Examples

sample <- rwish(n = 3, p = 5, b = 3, D = diag(5))</pre>

round(sample, 2)

select

Graph selection

Description

Provides the selected graph which, based on input, could be a graph with links for which their estimated posterior probabilities are greater than 0.5 (default) or a graph with the highest posterior probability; see examples.

Usage

```
select( bdgraph.obj, cut = NULL, vis = FALSE )
```

select

Arguments

bdgraph.obj	matrix in which each element response to the weight of the links. It can be an object of S3 class "bdgraph", from function bdgraph. It can be an object of S3 class "ssgraph", from the function ssgraph::ssgraph() of R package ssgraph::ssgraph().
cut	threshold for including the links in the selected graph based on the estimated posterior probabilities of the links; see the examples.
vis	visualize the selected graph structure.

Value

An adjacency matrix corresponding to the selected graph.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl> and Ernst Wit

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

Mohammadi, A. and Wit, E. C. (2015). Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Bayesian Analysis*, 10(1):109-138, doi:10.1214/14BA889

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Mohammadi, A. et al (2017). Bayesian modelling of Dupuytren disease by using Gaussian copula graphical models, *Journal of the Royal Statistical Society: Series C*, 66(3):629-645, doi:10.1111/rssc.12171

See Also

bdgraph, bdgraph.mpl

Examples

```
## Not run:
# Generating multivariate normal data from a 'random' graph
data.sim <- bdgraph.sim( n = 50, p = 6, size = 7, vis = TRUE )
bdgraph.obj <- bdgraph( data = data.sim )
select( bdgraph.obj )
bdgraph.obj <- bdgraph( data = data.sim, save = TRUE )</pre>
```

sparsity

```
select( bdgraph.obj )
select( bdgraph.obj, cut = 0.5, vis = TRUE )
## End(Not run)
```

sparsity

Compute the sparsity of a graph

Description

Compute the sparsity of a graph/network or an object of calss "graph" from function graph.sim or an object of calss "sim" from function bdgraph.sim.

Usage

sparsity(adj)

Arguments

adj

adjacency matrix corresponding to a graph structure in which $a_{ij} = 1$ if there is a link between notes *i* and *j*, otherwise $a_{ij} = 0$. It can be an object with S3 class "graph" from function graph.sim. It can be an object with S3 class "sim" from function bdgraph.sim.

Value

value corresponding to the graph sparsity which is the proportion of the non-links (non-zero elements) in adj.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl>

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

See Also

graph.sim, adj2link, link2adj

Examples

```
# Generating a 'random' graph
adj <- graph.sim( p = 10, graph = "random", prob = 0.4, vis = TRUE )
sparsity( adj )
```

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summary.bdgraph

Description

Provides a summary of the results for function bdgraph.

Usage

S3 method for class 'bdgraph'
summary(object, round = 2, vis = TRUE, ...)

Arguments

object	object of S3 class "bdgraph", from function bdgraph.
round	value for rounding all probabilities to the specified number of decimal places.
vis	visualize the results.
	additional plotting parameters for the case vis = TRUE. See plot.graph.

Value

selected_g	adjacency matrix corresponding to the selected graph which has the highest pos- terior probability.
p_links	upper triangular matrix corresponding to the posterior probabilities of all possible links.
K_hat	estimated precision matrix.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl> and Ernst Wit

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

See Also

bdgraph, bdgraph.mpl

Examples

```
## Not run:
# Generating multivariate normal data from a 'random' graph
data.sim <- bdgraph.sim( n = 50, p = 6, size = 7, vis = TRUE )
bdgraph.obj <- bdgraph( data = data.sim )
summary( bdgraph.obj )
bdgraph.obj <- bdgraph( data = data.sim, save = TRUE )
summary( bdgraph.obj )
summary( bdgraph.obj , vis = FALSE )
## End(Not run)
```

surveyData

Labor force survey data

Description

The survey dataset concerns 1002 males in the U.S labor force, described by Hoff (2007). The seven observed variables which have been measured on various scales are as follow: the income (income), degree (degree), the number of children (children), parents income (pincome), parents degree (pdegree), number of parents children (pchildren), and age (age).

Usage

data(surveyData)

Format

The format is a matrix with 1002 rows (number of individuals) and 7 column (number of variables).

References

Hoff, P. (2007). Extending the rank likelihood for semiparametric copula estimation, *The Annals of Applied Statistics*, 1(1), 265-283.

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

Examples

data(surveyData)

summary(surveyData)

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traceplot

Description

Trace plot for graph size for the objects of S3 class "bdgraph", from function bdgraph. It is a tool for monitoring the convergence of the sampling algorithms, BDMCMC and RJMCMC.

Usage

```
traceplot ( bdgraph.obj, acf = FALSE, pacf = FALSE, main = NULL, ... )
```

Arguments

bdgraph.obj	object of S3 class "bdgraph", from function bdgraph. It also can be an object of S3 class "ssgraph", from the function ssgraph::ssgraph() of R package ssgraph::ssgraph().
acf	visualize the autocorrelation functions for graph size.
pacf	visualize the partial autocorrelations for graph size.
main	graphical parameter (see plot).
	system reserved (no specific usage).

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl> and Ernst Wit

References

Mohammadi, R. and Wit, E. C. (2019). **BDgraph**: An R Package for Bayesian Structure Learning in Graphical Models, *Journal of Statistical Software*, 89(3):1-30, doi:10.18637/jss.v089.i03

Mohammadi, A. and Wit, E. C. (2015). Bayesian Structure Learning in Sparse Gaussian Graphical Models, *Bayesian Analysis*, 10(1):109-138, doi:10.1214/14BA889

Dobra, A. and Mohammadi, R. (2018). Loglinear Model Selection and Human Mobility, *Annals of Applied Statistics*, 12(2):815-845, doi:10.1214/18AOAS1164

Mohammadi, A. et al (2017). Bayesian modelling of Dupuytren disease by using Gaussian copula graphical models, *Journal of the Royal Statistical Society: Series C*, 66(3):629-645, doi:10.1111/rssc.12171

Mohammadi, A. and Dobra, A. (2017). The R Package **BDgraph** for Bayesian Structure Learning in Graphical Models, *ISBA Bulletin*, 24(4):11-16

See Also

plotcoda, bdgraph, bdgraph.mpl

Examples

```
## Not run:
# Generating multivariate normal data from a 'random' graph
data.sim <- bdgraph.sim( n = 50, p = 6, size = 7, vis = TRUE )
bdgraph.obj <- bdgraph( data = data.sim, iter = 10000, burnin = 0, save = TRUE )
traceplot( bdgraph.obj )
traceplot( bdgraph.obj, acf = TRUE, pacf = TRUE )
## End(Not run)
```

transfer transfer for count data

Description

Transfers count data, by counting the duplicated rows.

Usage

```
transfer( r_data )
```

Arguments

r_data	$(n \times p)$ matrix or a data. frame corresponding to the data (<i>n</i> is the sample size
	and p is the number of variables).

Value

 $(n \times p + 1)$ matrix of transferred data, in which the last column is the frequency of duplicated rows.

Author(s)

Reza Mohammadi <a.mohammadi@uva.nl> and Adrian Dobra

References

Mohammadi, A. and Dobra, A. (2017). The R Package **BDgraph** for Bayesian Structure Learning in Graphical Models, *ISBA Bulletin*, 24(4):11-16

Dobra, A. and Mohammadi, R. (2018). Loglinear Model Selection and Human Mobility, *Annals of Applied Statistics*, 12(2):815-845, doi:10.1214/18AOAS1164

See Also

bdgraph.mpl,bdgraph.sim

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transfer

Examples

```
# Generating multivariate binary data from a 'random' graph
data.sim <- bdgraph.sim( n = 12, p = 4, size = 4, type = "binary" )
r_data <- data.sim $ data
r_data
# Transfer the data
transfer( r_data )
```

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