

# Package ‘BiDAG’

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**Type** Package

**Title** Bayesian Inference for Directed Acyclic Graphs

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**Description** Implementation of a collection of MCMC methods for Bayesian structure learning of directed acyclic graphs (DAGs), both from continuous and discrete data. For efficient inference on larger DAGs, the space of DAGs is pruned according to the data. To filter the search space, the algorithm employs a hybrid approach, combining constraint-based learning with search and score. A reduced search space is initially defined on the basis of a skeleton obtained by means of the PC-algorithm, and then iteratively improved with search and score. Search and score is then performed following two approaches: Order MCMC, or Partition MCMC. The BGe score is implemented for continuous data and the BDe score is implemented for binary data or categorical data. The algorithms may provide the maximum a posteriori (MAP) graph or a sample (a collection of DAGs) from the posterior distribution given the data. All algorithms are also applicable for structure learning and sampling for dynamic Bayesian networks.

References:

J. Kuipers, P. Suter and G. Moffa (2018) <arXiv:1803.07859v2>, N. Friedman and D. Koller (2003) <doi:10.1023/A:1020249912095>, D. Geiger and D. Heckerman (2002) <doi:10.1214/aos/1035844981>, J. Kuipers and G. Moffa (2017) <doi:10.1080/01621459.2015.1133426>, M. Kalisch et al.(2012) <doi:10.18637/jss.v047.i11>.

**Acknowledgments** We would like to thank Giusi Moffa for discussion and comments on the package and its manual.

**License** GPL (>= 2)

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<i>Asia</i>	<i>Asia dataset</i>
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### Description

A synthetic dataset from Lauritzen and Spiegelhalter (1988) about lung diseases (tuberculosis, lung cancer or bronchitis) and visits to Asia.

### Usage

*Asia*

### Format

A data frame with 5000 rows and 8 binary variables:

- D (dyspnoea), binary 1/0 corresponding to "yes" and "no"
- T (tuberculosis), binary 1/0 corresponding to "yes" and "no"
- L (lung cancer), binary 1/0 corresponding to "yes" and "no"
- B (bronchitis), binary 1/0 corresponding to "yes" and "no"
- A (visit to Asia), binary 1/0 corresponding to "yes" and "no"
- S (smoking), binary 1/0 corresponding to "yes" and "no"
- X (chest X-ray), binary 1/0 corresponding to "yes" and "no"
- E (tuberculosis versus lung cancer/bronchitis), binary 1/0 corresponding to "yes" and "no"

### Source

<https://www.bnlearn.com/bnrepository/>

### References

Lauritzen S, Spiegelhalter D (1988). 'Local Computation with Probabilities on Graphical Structures and their Application to Expert Systems (with discussion)'. Journal of the Royal Statistical Society: Series B 50, 157-224.

---

Asiamat

*Asiamat*

---

### Description

An adjacency matrix representing the ground truth DAG used to generate a synthetic dataset from Lauritzen and Spiegelhalter (1988) about lung diseases (tuberculosis, lung cancer or bronchitis) and visits to Asia.

### Usage

Asiamat

### Format

A binary matrix with 8 rows and 8 columns representing an adjacency matrix of a DAG with 8 nodes:

- D (dyspnoea), binary 1/0 corresponding to "yes" and "no"
- T (tuberculosis), binary 1/0 corresponding to "yes" and "no"
- L (lung cancer), binary 1/0 corresponding to "yes" and "no"
- B (bronchitis), binary 1/0 corresponding to "yes" and "no"
- A (visit to Asia), binary 1/0 corresponding to "yes" and "no"
- S (smoking), binary 1/0 corresponding to "yes" and "no"
- X (chest X-ray), binary 1/0 corresponding to "yes" and "no"
- E (tuberculosis versus lung cancer/bronchitis), binary 1/0 corresponding to "yes" and "no"

### Source

<https://www.bnlearn.com/bnrepository/>

### References

Lauritzen S, Spiegelhalter D (1988). 'Local Computation with Probabilities on Graphical Structures and their Application to Expert Systems (with discussion)'. *Journal of the Royal Statistical Society: Series B* 50, 157-224.

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Boston	<i>Boston housing data</i>
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**Description**

A dataset containing information collected by the U.S Census Service concerning housing in the area of Boston, originally published by Harrison and Rubinfeld (1978).

**Usage**

Boston

**Format**

A data frame with 506 rows and 14 variables:

- CRIM - per capita crime rate by town
- ZN - proportion of residential land zoned for lots over 25,000 sq.ft.
- INDUS - proportion of non-retail business acres per town.
- CHAS - Charles River dummy variable (1 if tract bounds river; 0 otherwise)
- NOX - nitric oxides concentration (parts per 10 million)
- RM - average number of rooms per dwelling
- AGE - proportion of owner-occupied units built prior to 1940
- DIS - weighted distances to five Boston employment centres
- TAX - full-value property-tax rate per \$10,000
- RAD - index of accessibility to radial highways
- PTRATIO - pupil-teacher ratio by town
- B -  $1000(B_k - 0.63)^2$  where  $B_k$  is the proportion of blacks by town
- LSTAT - percentage lower status of the population
- MEDV - Median value of owner-occupied homes in \$1000's

**Source**

<http://lib.stat.cmu.edu/datasets/boston>

**References**

Harrison, D and Rubinfeld, DL (1978) 'Hedonic prices and the demand for clean air', Journal of Environmental Economics and Management 5, 81-102.

---

compact2full                      *Deriving an adjacency matrix of a full DBN*

---

### Description

This function transforms a compact 2-slice adjacency matrix of DBN into full T-slice adjacency matrix

### Usage

```
compact2full(DBNmat, n.dynamic, n.slices, n.static = 0)
```

### Arguments

DBNmat	a square matrix, representing initial and transitional structure of a DBN; the size of matrix is $2*n.dynamic+n.static$
n.dynamic	integer, number of dynamic variables in one time slice
n.slices	integer, number of slices in an unrolled DBN
n.static	integer, number of static variables

### Value

an adjacency matrix of an unrolled DBN

### Examples

```
compact2full(DBNmat, n.dynamic=12, n.slices=5, n.static=3)
```

---

compareDAGs                      *Comparing two graphs*

---

### Description

This function compares one (estimated) graph to another graph (true graph), returning a vector of 8 values:

- the number of true positive edges ('TP') is the number of edges in the skeleton of 'egraph' which are also present in the skeleton of 'truegraph'
- the number of false positive edges ('FP') is the number of edges in the skeleton of 'egraph' which are absent in the skeleton of 'truegraph'
- the number of false negative edges ('FN') is the number of edges in the skeleton of 'truegraph' which are absent in the skeleton of 'egraph'
- structural Hamming distance ('SHD') between 2 graphs is computed as TP+FP+the number of edges with an error in direction

- TPR equals  $TP/(TP+FN)$
- FPR equals  $FP/(TN+FP)$  (TN stands for true negative edges)
- FPRn equals  $FP/(TP+FN)$
- FDR equals  $FP/(TP+FP)$

### Usage

```
compareDAGs(egraph, truegraph, cpdag = FALSE, rnd = 2)
```

### Arguments

egraph	an object of class <code>graphNEL</code> (package 'graph'), representing the graph which should be compared to a ground truth graph or an adjacency matrix corresponding to the graph
truegraph	an object of class <code>graphNEL</code> (package 'graph'), representing the ground truth graph or an adjacency matrix corresponding to this graph
cpdag	logical, if TRUE (FALSE by default) both graphs are first converted to their respective equivalence class (CPDAG); this affects SHD calculation
rnd	integer, rounding integer indicating the number of decimal places (round) when computing TPR, FPR, FPRn and FDR

### Value

a named numeric vector 8 elements: SHD, number of true positive edges (TP), number of false positive edges (FP), number of false negative edges (FN), true positive rate (TPR), false positive rate (FPR), false positive rate normalized to the true number of edges (FPRn) and false discovery rate (FDR)

### Examples

```
Asiascore<-scoreparameters("bde", Asia)
## Not run:
eDAG<-orderMCMC(Asiascore)
compareDAGs(eDAG$DAG,Asiamat)

## End(Not run)
```

---

compareDBNs

*Comparing two DBNs*

---

### Description

This function compares one (estimated) DBN structure to another DBN (true DBN). Comparisons for initial and transitional structures are returned separately if `equalstruct` equals TRUE.

**Usage**

```
compareDBNs(eDBN, trueDBN, n.dynamic, n.static, struct = c("init", "trans"))
```

**Arguments**

eDBN	an object of class <code>graphNEL</code> (or an adjacency matrix corresponding to this DBN), representing the DBN which should be compared to a ground truth DBN
trueDBN	an object of class <code>graphNEL</code> (or an adjacency matrix corresponding to this DBN), representing the ground truth DBN
n.dynamic	number of dynamic variables in one time slice of a DBN
n.static	number of static variables in one time slice of a DBN; note that for function to work correctly all static variables have to be in the first n.static columns of the matrix
struct	option used to determine if the initial or the transitional structure should be compared; acceptable values are <code>init</code> or <code>trans</code>

**Value**

a vector of 5: SHD, number of true positive edges, number of false positive edges, number of false negative edges and true positive rate

**Examples**

```
testscore<-scoreparameters("bge", DBNdata, DBN=TRUE,
dbnpar=list(samestruct=TRUE, slices=5, b=3))
## Not run:
DBNfit<-iterativeMCMC(testscore, moveprobs=c(0.11,0.84,0.04,0.01))
compareDBNs(DBNfit$DAG,DBNmat, struct="trans", n.dynamic=12, n.static=3)

## End(Not run)
```

---

connectedSubGraph      *Deriving connected subgraph*

---

**Description**

This function derives an adjacency matrix of a subgraph whose nodes are connected to at least one other node in a graph

**Usage**

```
connectedSubGraph(adj)
```

**Arguments**

adj	square adjacency matrix with elements in $\{0, 1\}$ , representing a graph
-----	--



**Value**

adjacency matrix of a subgraph of graph represented by 'adj' whose nodes have at least one connection

**Examples**

```
dim(gsimmat) #full graph contains 100 nodes
gconn<-connectedSubGraph(gsimmat) #removing disconnected nodes
dim(gconn) #connected subgraph contains 93 nodes
```

---

DAGscore

*Calculating the BGe/BDe score of a single DAG*

---

**Description**

This function calculates the score of a DAG defined by its adjacency matrix. Acceptable data matrices are homogeneous with all variables of the same type: continuous, binary or categorical. The BGe score is evaluated in the case of continuous data and the BDe score is evaluated for binary and categorical variables.

**Usage**

```
DAGscore(scorepar, incidence)
```

**Arguments**

scorepar	an object of class scoreparameters, containing the data and scoring parameters; see constructor function <a href="#">scoreparameters</a>
incidence	a square matrix of dimensions equal to the number of nodes, representing the adjacency matrix of a DAG; the matrix entries are in $\{0, 1\}$ such that <code>incidence[i, j]</code> equals 1 if there is a directed edge from node i to node j in the DAG and <code>incidence[i, j]</code> equals 0 otherwise

**Value**

the log of the BGe or BDe score of the DAG

**Author(s)**

Polina Suter, Jack Kuipers, the code partly derived from the order MCMC implementation from Kuipers J, Moffa G (2017) <doi:10.1080/01621459.2015.1133426>

## References

Geiger D and Heckerman D (2002). Parameter priors for directed acyclic graphical models and the characterization of several probability distributions. *The Annals of Statistics* 30, 1412-1440.

Heckerman D and Geiger D (1995). Learning Bayesian networks: A unification for discrete and Gaussian domains. In *Eleventh Conference on Uncertainty in Artificial Intelligence*, pages 274-284.

Kuipers J, Moffa G and Heckerman D (2014). Addendum on the scoring of Gaussian directed acyclic graphical models. *The Annals of Statistics* 42, 1689-1691.

## Examples

```
myScore<-scoreparameters("bde", Asia)
DAGscore(myScore, Asiamat)
```

---

DBNdata

*Simulated data set from a 2-step dynamic Bayesian network A synthetic dataset containing 100 observations generated from a random dynamic Bayesian network with 12 continuous dynamic nodes and 3 static nodes. The DBN includes observations from 5 time slices.*

---

## Description

Simulated data set from a 2-step dynamic Bayesian network

A synthetic dataset containing 100 observations generated from a random dynamic Bayesian network with 12 continuous dynamic nodes and 3 static nodes. The DBN includes observations from 5 time slices.

## Usage

```
DBNdata
```

## Format

A data frame with 100 rows and 63 ( $3+12*5$ ) columns representing observations of 15 variables: 3 static variables (first 3 columns) which do not change over time and 12 dynamic variables observed in 5 consecutive time slices.

---

DBNmat	<i>An adjacency matrix of a dynamic Bayesian network</i>
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---

**Description**

An adjacency matrix representing the ground truth DBN used to generate a synthetic dataset [DBNdata](#). The matrix is a compact representation of a 2-step DBN, such that initial structure is stored in the first 15 columns of the matrix and transitional structure is stored in the last 12 columns of the matrix.

**Usage**

```
DBNmat
```

**Format**

A binary matrix with 27 rows and 27 columns representing an adjacency matrix of a DBN. Rows and columns of the matrix correspond to 15 variables of a DBN across 2 time slices.

---

DBNscore	<i>Calculating the BGe/BDe score of a single DBN</i>
----------	--

---

**Description**

This function calculates the score of a DBN defined by its compact adjacency matrix. Acceptable data matrices are homogeneous with all variables of the same type: continuous, binary or categorical. The BGe score is evaluated in the case of continuous data and the BDe score is evaluated for binary and categorical variables.

**Usage**

```
DBNscore(scorepar, incidence)
```

**Arguments**

scorepar	an object of class <code>scoreparameters</code> , containing the data and scoring parameters; see constructor function <a href="#">scoreparameters</a>
incidence	a square matrix, representing initial and transitional structure of a DBN; the size of matrix is $2 * n_{\text{small}} + b_{\text{gn}}$ , where $n_{\text{small}}$ is the number of variables per time slice excluding static nodes and $b_{\text{gn}}$ is the number of static variables the matrix entries are in $\{0, 1\}$ such that $\text{incidence}[i, j]$ equals 1 if there is a directed edge from node $i$ to node $j$ in the DAG and $\text{incidence}[i, j]$ equals 0 otherwise

**Value**

the log of the BGe or BDe score of the DBN

**Author(s)**

Polina Suter, Jack Kuipers

**Examples**

```
testscore<-scoreparameters("bge", DBNdata, DBN=TRUE, dbnpar=list(slices=5, b=3))
DBNscore(testscore, DBNmat)
```

---

DBNunrolled

*An unrolled adjacency matrix of a dynamic Bayesian network*

---

**Description**

An adjacency matrix representing the ground truth DBN used to generate a synthetic dataset [DBNdata](#). The matrix is an unrolled representation of a 2-step DBN, such that the static variables are represented in the first 3 columns/rows of the matrix.

**Usage**

```
DBNunrolled
```

**Format**

A binary matrix with 63 rows and 63 columns representing an adjacency matrix of a DBN. Rows and columns of the matrix correspond to 15 variables (s1, s2, s3, v1, v2, v3, v4, v5, v6, v7, v8, v9, v10, v11, v12) of a DBN across 5 time slices.

---

edgep

*Estimating posterior probabilities of single edges*

---

**Description**

This function estimates the posterior probabilities of edges by averaging over a sample of DAGs obtained via an MCMC scheme.

**Usage**

```
edgep(MCMCchain, pdag = FALSE, burnin = 0.2, endstep = 1)
```

**Arguments**

MCMCchain	an object of class <code>partitionMCMC</code> or <code>orderMCMC</code> , representing the output of structure sampling function <code>partitionMCMC</code> or <code>orderMCMC</code> (the latter when parameter <code>chainout=TRUE</code> );
pdag	logical, if <code>TRUE</code> ( <code>FALSE</code> by default) all DAGs in the <code>MCMCchain</code> are first converted to equivalence class (CPDAG) before the averaging
burnin	number between 0 and 1, indicates the percentage of the samples which will be discarded as ‘burn-in’ of the MCMC chain; the rest of the samples will be used to calculate the posterior probabilities; 0.2 by default
endstep	number between 0 and 1; 1 by default

**Value**

a square matrix with dimensions equal to the number of variables; each entry  $[i, j]$  is an estimate of the posterior probability of the edge from node  $i$  to node  $j$

**Author(s)**

Polina Suter

**Examples**

```
Bostonscore<-scoreparameters("bge", Boston)
## Not run:
samplefit<-orderMCMC(Bostonscore, iterations=25000,chainout=TRUE)
edgesposterior<-edgep(samplefit, pdag=TRUE, burnin=0.2)

## End(Not run)
```

---

full2compact

*Deriving a compact adjacency matrix of a DBN*

---

**Description**

This function transforms an unrolled adjacency matrix of DBN into a compact representation

**Usage**

```
full2compact(DBNmat, n.dynamic, n.static = 0)
```

**Arguments**

DBNmat	a square matrix, representing the structure of an unrolled DBN; the size of matrix is $n.slices * n.dynamic + n.static$ ; all static variables are assumed to be in the first $n.static$ rows and columns of the matrix
n.dynamic	integer, number of dynamic variables in each time slice
n.static	integer, number of static variables

**Examples**

```
full2compact(DBNunrolled,n.dynamic=12,n.static=3)
```

---

getSubGraph	<i>Deriving subgraph</i>
-------------	--------------------------

---

**Description**

This function derives an adjacency matrix of a subgraph based on the adjacency matrix of a full graph and a list of nodes

**Usage**

```
getSubGraph(adj, nodes)
```

**Arguments**

adj	square adjacency matrix with elements in $\{0, 1\}$ , representing a graph
nodes	vector of node names of the subgraph; should be a subset of column names of 'adj'

**Value**

adjacency matrix of a subgraph which includes all 'nodes'

**Examples**

```
getSubGraph(Asiamat,c("E","B","D","X"))
```

---

graph2m	<i>Deriving an adjacency matrix of a graph</i>
---------	--

---

**Description**

This function derives the adjacency matrix corresponding to a graph object

**Usage**

```
graph2m(g)
```

**Arguments**

g	graph, object of class <code>graphNEL</code> (package 'graph')
---	--

**Value**

a square matrix whose dimensions are the number of nodes in the graph  $g$ , where element  $[i, j]$  equals 1 if there is a directed edge from node  $i$  to node  $j$  in the graph  $g$ , and 0 otherwise

**Examples**

```
Asiagraph<-m2graph(Asiamat)
Asia.adj<-graph2m(Asiagraph)
```

---

gsim	<i>A simulated data set from a Gaussian continuous Bayesian network</i>
------	---

---

**Description**

A synthetic dataset containing 1000 observations generated from a random DAG with 100 continuous nodes. Functions 'randomDAG' and 'rmvDAG' from R-packages 'pcalg' were used to generate the data.

**Usage**

```
gsim
```

**Format**

A data frame with 1000 rows representing observations of 100 continuous variables: V1, ..., V100

---

gsim100	<i>A simulated data set from a Gaussian continuous Bayesian network</i>
---------	---

---

**Description**

A synthetic dataset containing 100 observations generated from a random DAG with 100 continuous nodes. Functions 'randomDAG' and 'rmvDAG' from R-packages 'pcalg' were used to generate the data.

**Usage**

```
gsim100
```

**Format**

A data frame with 100 rows representing observations of 100 continuous variables: V1, ..., V100

---

`gsimmat`*An adjacency matrix of a simulated dataset*

---

**Description**

An adjacency matrix representing the ground truth DAG used to generate a synthetic dataset with observations of 100 continuous variables.

**Usage**`gsimmat`**Format**

A binary matrix with 100 rows and 100 columns representing an adjacency matrix of a DAG with 100 nodes: V1, ..., V100

---

`interactions`*interactions dataset*

---

**Description**

A data frame containing possible interactions between genes from kirp and kirc data sets

**Usage**`interactions`**Format**

A data frame with 179 rows and 3 columns;

- node1 character, name of a gene
- node2 character, name of a gene
- combined\_score interaction score, reflecting confidence in the fact that interaction between gene1 and gene2 is possible

each row represents a possible interaction between two genes

**Source**

<https://string-db.org/>



---

iterativeMCMC	<i>Structure learning with an iterative order MCMC algorithm on an expanded search space</i>
---------------	--

---

### Description

This function implements an iterative search for the maximum a posteriori (MAP) DAG, by means of order MCMC (arXiv:1803.07859v3). At each iteration, the current search space is expanded by allowing each node to have up to one additional parent not already included in the search space. By default the initial search space is obtained through the PC-algorithm (using the functions `skeleton` and `pc` from the 'pcalg' package [Kalisch et al, 2012]). At each iteration order MCMC is employed to search for the MAP DAG. The edges in the MAP DAG are added to the initial search space to provide the search space for the next iteration. The algorithm iterates until no further score improvements can be achieved by expanding the search space. The final search space may be used for the sampling versions of `orderMCMC` and `partitionMCMC`.

### Usage

```
iterativeMCMC(
  scorepar,
  MAP = TRUE,
  posterior = 0.5,
  softlimit = 9,
  hardlimit = 12,
  alpha = 0.05,
  gamma = 1,
  verbose = TRUE,
  chainout = FALSE,
  scoreout = FALSE,
  cpdag = FALSE,
  mergetype = "skeleton",
  iterations = NULL,
  moveprobs = NULL,
  stepsave = NULL,
  startorder = NULL,
  accum = FALSE,
  pluslit = NULL,
  startspace = NULL,
  blacklist = NULL,
  addspace = NULL,
  scoretable = NULL
)

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

```

    main = "iterative MCMC, DAG scores",
    xlab = "MCMC step",
    ylab = "DAG logscore",
    type = "l",
    col = "blue"
)

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

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

```

### Arguments

scorepar	an object of class <code>scoreparameters</code> , containing the data and scoring parameters; see constructor function <a href="#">scoreparameters</a>
MAP	logical, if TRUE (default) the search targets the MAP DAG (a DAG with maximum score), if FALSE at each MCMC step a DAG is sampled from the order proportionally to its score; when expanding a search space when MAP=TRUE all edges from the maximum scoring DAG are added to the new space, when MAP=FALSE only edges with posterior probability higher than defined by parameter posterior are added to the search space
posterior	logical, when MAP set to FALSE defines posterior probability threshold for adding the edges to the search space
softlimit	integer, limit on the size of parent sets beyond which adding undirected edges is restricted; below this limit edges are added to expand the parent sets based on the undirected skeleton of the MAP DAG (or from its CPDAG, depending on the parameter <code>mergecp</code> ), above the limit only the directed edges are added from the MAP DAG; the limit is 9 by default
hardlimit	integer, limit on the size of parent sets beyond which the search space is not further expanded to prevent long runtimes; the limit is 12 by default
alpha	numerical significance value in $\{0, 1\}$ for the conditional independence tests in the PC-stage (by default 0.4 for $n < 50$ , $20/n$ for $n > 50$ )
gamma	tuning parameter which transforms the score by raising it to this power, 1 by default
verbose	logical, if TRUE (default) prints messages on the progress of execution
chainout	logical, if TRUE the saved MCMC steps are returned, FALSE by default
scoreout	logical, if TRUE the search space from the last plus1 iterations and the corresponding score tables are returned, FALSE by default
cpdag	logical, if set to TRUE the equivalence class (CPDAG) found by the PC algorithm is used as a search space, when FALSE (default) the undirected skeleton used as a search space
mergetype	defines which edges are added to the search space at each expansion iteration; three options are available 'dag', 'cpdag', 'skeleton'; 'skeleton' by default

iterations	integer, the number of MCMC steps, the default value is $3.5n^2 \log n$
moveprobs	a numerical vector of 4 values in $\{0, 1\}$ corresponding to the probabilities of the following MCMC moves in the order space: <ul style="list-style-type: none"> <li>• exchanging 2 random nodes in the order</li> <li>• exchanging 2 adjacent nodes in the order</li> <li>• placing a single node elsewhere in the order</li> <li>• staying still</li> </ul>
stepsave	integer, thinning interval for the MCMC chain, indicating the number of steps between two output iterations, the default is $\text{iterations}/1000$
startorder	integer vector of length $n$ , which will be used as the starting order in the MCMC algorithm, the default order is random
accum	logical, when TRUE at each search step expansion new edges are added to the current search space; when FALSE (default) the new edges are added to the starting space
plus1it	(optional) integer, a number of iterations of search space expansion; by default the algorithm iterates until no score improvement can be achieved by further expanding the search space
startspace	(optional) a square matrix, of dimensions equal to the number of nodes, which defines the search space for the order MCMC in the form of an adjacency matrix; if NULL, the skeleton obtained from the PC-algorithm will be used; if $\text{startspace}[i, j]$ equals to 1 (0) it means that the edge from node $i$ to node $j$ is included (excluded) from the search space; to include an edge in both directions, both $\text{startspace}[i, j]$ and $\text{startspace}[j, i]$ should be 1
blacklist	(optional) a square matrix, of dimensions equal to the number of nodes, which defines edges to exclude from the search space; if $\text{blacklist}[i, j]$ equals to 1 it means that the edge from node $i$ to node $j$ is excluded from the search space <ul style="list-style-type: none"> <li>• "dag", then edges from maximum scoring DAG are added;</li> <li>• "cpdag", then the maximum scoring DAG is first converted to the CPDAG, from which all edges are added to the search space;</li> <li>• "skeleton", then the maximum scoring DAG is first converted to the skeleton, from which all edges are added to the search space</li> </ul>
addspace	(optional) a square matrix, of dimensions equal to the number of nodes, which defines the edges, which are added at to the search space only at the first iteration of iterative search and do not necessarily stay afterwards; defined in the form of an adjacency matrix; if $\text{addspace}[i, j]$ equals to 1 (0) it means that the edge from node $i$ to node $j$ is included (excluded) from the search space; to include an edge in both directions, both $\text{addspace}[i, j]$ and $\text{addspace}[j, i]$ should be 1
scoretable	(optional) object of class <code>scoretable</code> . When not NULL, parameters <code>startspace</code> and <code>addspace</code> are ignored.
x	object of class 'iterativeMCMC'
...	ignored
main	name of the graph; "iterative MCMC, DAG scores" by default

xlab	name of x-axis; "MCMC step"
ylab	name of y-axis; "DAG logscore"
type	type of line in the plot; "1" by default
col	colour of line in the plot; "blue" by default
object	object of class 'iterativeMCMC'

### Value

Object of class `iterativeMCMC`, which contains log-score trace as well as adjacency matrix of the maximum scoring DAG, its score and the order score. The output can optionally include DAGs sampled in MCMC iterations and the score tables. Optional output is regulated by the parameters `chainout` and `scoreout`. See [iterativeMCMC class](#) for a detailed class structure.

### Author(s)

Polina Suter, Jack Kuipers

### References

- Kuipers J, Super P and Moffa G (2020). Efficient Sampling and Structure Learning of Bayesian Networks. (arXiv:1803.07859v3)
- Friedman N and Koller D (2003). A Bayesian approach to structure discovery in bayesian networks. *Machine Learning* 50, 95-125.
- Kalisch M, Maechler M, Colombo D, Maathuis M and Buehlmann P (2012). Causal inference using graphical models with the R package `pcalg`. *Journal of Statistical Software* 47, 1-26.
- Geiger D and Heckerman D (2002). Parameter priors for directed acyclic graphical models and the characterization of several probability distributions. *The Annals of Statistics* 30, 1412-1440.
- Kuipers J, Moffa G and Heckerman D (2014). Addendum on the scoring of Gaussian directed acyclic graphical models. *The Annals of Statistics* 42, 1689-1691.
- Spirtes P, Glymour C and Scheines R (2000). *Causation, Prediction, and Search*, 2nd edition. The MIT Press.

### Examples

```
## Not run:  
Bostonpar<-scoreparameters("bge",Boston)  
itfit<-iterativeMCMC(Bostonpar, chainout=TRUE, scoreout=TRUE)  
plot(itfit)  
  
## End(Not run)
```

---

iterativeMCMC class    *iterativeMCMC class structure*

---

## Description

The structure of an object of S3 class `iterativeMCMC`.

## Details

An object of class `iterativeMCMC` is a list containing at least the following components:

- `DAG`: adjacency matrix of a maximum scoring DAG found/sampled in MCMC.
- `CPDAG`: adjacency matrix representing equivalence class of a maximum scoring DAG found/sampled in MCMC.
- `score`: score of a maximum scoring DAG found/sampled in MCMC.
- `maxorder`: order of a maximum scoring DAG found/sampled in MCMC.
- `maxtrace`: a list of maximum score graphs uncovered at each expansion of the search space; their scores and orders
- `info`: a list containing information about parameters and results of MCMC
- `trace`: a vector containing log-scores of sampled DAGs
- `startspace`: adjacency matrix representing the initial core space where MCMC was ran
- `endspace`: adjacency matrix representing the final core space where MCMC was ran

Optional components:

- `traceadd`: list which consists of three elements:
  - \* `incidence`: list containing adjacency matrices of sampled DAGs
  - \* `order`: list of orders from which the DAGs were sampled
  - \* `orderscores`: order log-scores
- `scoretable`: object of class [score space class](#)

## Author(s)

Polina Suter

---

itercomp	<i>Performance assessment of iterative MCMC scheme against a known Bayesian network</i>
----------	---

---

## Description

This function compute 8 different metrics of structure fit of an object of class `iterativeMCMC` to the ground truth DAG (or CPDAG). Object of class `iterativeMCMC` stores MAP graph at from each search space expansion step. This function computes structure fit of each of the stored graphs to the ground truth one. Computed metrics include: TP, FP, TPR, FPR, FPRn, FDR, SHD. See metrics description in see also [compareDAGs](#).

## Usage

```
itercomp(MCMCmult, truedag, cpdag = TRUE, p = 0.5, trans = TRUE)

## S3 method for class 'itercomp'
plot(x, ..., vars = c("FP", "TP"), type = "b", col = "blue", showit = c())

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

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

## Arguments

MCMCmult	an object which of class <code>iterativeMCMC</code> , see also <a href="#">iterativeMCMC</a> )
truedag	ground truth DAG which generated the data used in the search procedure; represented by an object of class <a href="#">graphNEL</a> or an adjacency matrix
cpdag	logical, if TRUE (FALSE by default) all DAGs are first converted to their respective equivalence classes (CPDAG)
p	threshold such that only edges with a higher posterior probability will be retained in the directed graph summarising the sample of DAGs at each iteration from MCMCmult if parameter <code>sample</code> set to TRUE
trans	logical, for DBNs indicates if model comparions are performed for transition structure; when <code>trans</code> equals FALSE the comparison is performed for initial structures of estimated models and the ground truth DBN; for usual BNs the parameter is disregarded
x	object of class <code>'itercomp'</code>
...	ignored
vars	a tuple of variables which will be used for <code>'x'</code> and <code>'y'</code> axes; possible values: "SHD", "TP", "FP", "TPR", "FPR", "FPRn", "FDR", "score"
type	type of line in the plot;"b" by default

col	colour of line in the plot; "blue" by default
showit	(optional) vector of integers specifying indices of search expansion iterations to be labelled; by default no iterations are labelled
object	object of class 'itercomp'

**Value**

an object of class `itersim`, a matrix with the number of rows equal to the number of expansion iterations in `iterativeMCMC`, and 8 columns reporting for the maximally scoring DAG uncovered at each iteration: the number of true positive edges ('TP'), the number of false positive edges ('FP'), the true positive rate ('TPR'), the structural Hamming distance ('SHD'), false positive rate ('FPR'), false discovery rate ('FDR') and the score of the DAG ('score').

**Author(s)**

Polina Suter

**Examples**

```
gsim.score<-scoreparameters("bge", gsim)
## Not run:
MAPestimate<-iterativeMCMC(gsim.score)
itercomp(MAPestimate, gsimmat)

## End(Not run)
```

---

kirc

*kirc dataset*


---

**Description**

Mutation data from TCGA kidney renal clear cell cohort (KIRC). Mutations are picked according to q-value computed by MutSig2CV ( $q < 0.1$ ) or connected in networks discovered by Kuipers et al. 2018.

**Usage**

```
kirc
```

**Format**

An object of class `matrix` with 476 rows and 70 columns.

**Details**

Each variable represents a gene. If in sample  $i$  gene  $j$  contains a mutation, then  $j$ -th element in row  $i$  equals 1, and 0 otherwise. The rows are named according to sample names in TCGA. The columns are named according to gene symbols.

**References**

<https://portal.gdc.cancer.gov/>

<http://firebrowse.org/iCoMut/?cohort=kirc>

Lawrence, M. et al. Mutational heterogeneity in cancer and the search for new cancer-associated genes. Nature 499, 214-218 (2013)

---

kirp

*kirp dataset*

---

**Description**

Mutation data from TCGA kidney renal papillary cell cohort (KIRP). Mutations are picked according to q-value computed by MutSigCV ( $q < 0.1$ ) or connected in networks discovered by Kuipers et al. 2018.

**Usage**

kirp

**Format**

An object of class `matrix` with 282 rows and 70 columns.

**Details**

Each variable represents a gene. If in sample  $i$  gene  $j$  contains a mutation, then  $j$ -th element in row  $i$  equals 1, and 0 otherwise. The rows are named according to sample names in TCGA. The columns are named according to gene symbols.

**References**

<https://portal.gdc.cancer.gov/>

<http://firebrowse.org/iCoMut/?cohort=kirc>

Lawrence, M. et al. Mutational heterogeneity in cancer and the search for new cancer-associated genes. Nature 499, 214-218 (2013)



---

`m2graph`*Deriving a graph from an adjacency matrix*

---

**Description**

This function derives a graph object corresponding to an adjacency matrix

**Usage**

```
m2graph(adj, nodes = NULL)
```

**Arguments**

`adj` square adjacency matrix with elements in  $\{0, 1\}$ , representing a graph  
`nodes` (optional) labels of the nodes, `c(1:n)` are used by default

**Value**

object of class `graphNEL` (package 'graph'); if element `adj[i, j]` equals 1, then there is a directed edge from node `i` to node `j` in the graph, and no edge otherwise

**Examples**

```
m2graph(Asiamat)
```

---

`mapping`*mapping dataset*

---

**Description**

A data frame containing mapping between names of genes used in kirp/kirc data sets and names used in STRING interactions list (see [interactions](#)).

**Usage**

```
mapping
```

**Format**

A data frame with 46 rows and two columns:

- `queryItem` character, name used for structure learning
- `preferredName` character, name used in STRING interactions data set

**Source**

<https://string-db.org/>

---

 modelp

*Estimating a graph corresponding to a posterior probability threshold*


---

### Description

This function constructs a directed graph (not necessarily acyclic) including all edges with a posterior probability above a certain threshold. The posterior probability is evaluated as the Monte Carlo estimate from a sample of DAGs obtained via an MCMC scheme.

### Usage

```
modelp(MCMCchain, p, pdag = FALSE, burnin = 0.2)
```

### Arguments

MCMCchain	object of class <code>partitionMCMC</code> or <code>orderMCMC</code> , representing the output of structure sampling function <code>partitionMCMC</code> or <code>orderMCMC</code> (the latter when parameter <code>chainout=TRUE</code> );
p	threshold such that only edges with a higher posterior probability will be retained in the directed graph summarising the sample of DAGs
pdag	logical, if <code>TRUE</code> ( <code>FALSE</code> by default) all DAGs in the <code>MCMCchain</code> are first converted to equivalence class (CPDAG) before the averaging
burnin	number between 0 and 1, indicates the percentage of the samples which will be the discarded as 'burn-in' of the MCMC chain; the rest of the samples will be used to calculate the posterior probabilities; 0.2 by default

### Value

a square matrix with dimensions equal to the number of variables representing the adjacency matrix of the directed graph summarising the sample of DAGs

### Author(s)

Polina Suter

### Examples

```
Bostonscore<-scoreparameters("bge", Boston)
## Not run:
orderfit<-orderMCMC(Bostonscore, MAP=FALSE, iterations=25000, chainout=TRUE)
hdag<-modelp(orderfit, p=0.9)

## End(Not run)
```

## Description

This function implements the order MCMC algorithm for the structure learning of Bayesian networks. This function can be used for MAP discovery and for sampling from the posterior distribution of DAGs given the data. Due to the superexponential size of the search space as the number of nodes increases, the MCMC search is performed on a reduced search space. By default the search space is limited to the skeleton found through the PC algorithm by means of conditional independence tests (using the functions `skeleton` and `pc` from the ‘pcalg’ package [Kalisch et al, 2012]). It is also possible to define an arbitrary search space by inputting an adjacency matrix, for example estimated by partial correlations or other network algorithms. Also implemented is the possibility to expand the default or input search space, by allowing each node in the network to have one additional parent. This offers improvements in the learning and sampling of Bayesian networks.

## Usage

```
orderMCMC(  
  scorepar,  
  MAP = TRUE,  
  plus1 = TRUE,  
  chainout = FALSE,  
  scoreout = FALSE,  
  moveprobs = NULL,  
  iterations = NULL,  
  stepsave = NULL,  
  alpha = 0.05,  
  cpdag = FALSE,  
  gamma = 1,  
  hardlimit = ifelse(plus1, 14, 20),  
  verbose = FALSE,  
  startspace = NULL,  
  blacklist = NULL,  
  startorder = NULL,  
  scoretable = NULL  
)  
  
## S3 method for class 'orderMCMC'  
plot(  
  x,  
  ...,  
  burnin = 0.2,  
  main = "DAG logscores",  
  xlab = "iteration",  
  ylab = "logscore",  
  type = "l",
```

```

    col = "#0c2c84"
)

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

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

```

## Arguments

scorepar	an object of class <code>scoreparameters</code> , containing the data and score parameters, see constructor function <code>scoreparameters</code>
MAP	logical, if TRUE (default) the search targets the MAP DAG (a DAG with maximum score), if FALSE at each MCMC step a DAG is sampled from the order proportionally to its score
plus1	logical, if TRUE (default) the search is performed on the extended search space
chainout	logical, if TRUE the saved MCMC steps are returned, TRUE by default
scoreout	logical, if TRUE the search space and score tables are returned, FALSE by default
moveprobs	a numerical vector of 4 values in $\{0, 1\}$ corresponding to the probabilities of the following MCMC moves in the order space <ul style="list-style-type: none"> <li>• exchanging 2 random nodes in the order</li> <li>• exchanging 2 adjacent nodes in the order</li> <li>• placing a single node elsewhere in the order</li> <li>• staying still</li> </ul>
iterations	integer, the number of MCMC steps, the default value is $6n^2 \log n$
stepsave	integer, thinning interval for the MCMC chain, indicating the number of steps between two output iterations, the default is $iterations/1000$
alpha	numerical significance value in $\{0, 1\}$ for the conditional independence tests at the PC algorithm stage (by default 0.4 for $n < 50$ , $20/n$ for $n > 50$ )
cpdag	logical, if TRUE the CPDAG returned by the PC algorithm will be used as the search space, if FALSE (default) the full undirected skeleton will be used as the search space
gamma	tuning parameter which transforms the score by raising it to this power, 1 by default
hardlimit	integer, limit on the size of parent sets in the search space; by default 14 when MAP=TRUE and 20 when MAP=FALSE
verbose	logical, if TRUE messages about the algorithm's progress will be printed, FALSE by default
startspace	(optional) a square matrix, of dimensions equal to the number of nodes, which defines the search space for the order MCMC in the form of an adjacency matrix. If NULL, the skeleton obtained from the PC-algorithm will be used. If <code>startspace[i, j]</code> equals to 1 (0) it means that the edge from node <i>i</i> to node <i>j</i> is included (excluded) from the search space. To include an edge in both directions, both <code>startspace[i, j]</code> and <code>startspace[j, i]</code> should be 1.

blacklist	(optional) a square matrix, of dimensions equal to the number of nodes, which defines edges to exclude from the search space. If <code>blacklist[i, j]</code> equals to 1 it means that the edge from node <i>i</i> to node <i>j</i> is excluded from the search space.
startorder	(optional) integer vector of length <i>n</i> , which will be used as the starting order in the MCMC algorithm, the default order is random
scoretable	(optional) object of class <code>scorespace</code> containing list of score tables calculated for example by the last iteration of the function <code>iterativeMCMC</code> . When not <code>NULL</code> , parameter <code>startspace</code> is ignored.
x	object of class 'orderMCMC'
...	ignored
burnin	number between 0 and 1, indicates the percentage of the samples which will be discarded as 'burn-in' of the MCMC chain; the rest of the samples will be used to calculate the posterior probabilities; 0.2 by default
main	name of the graph; "DAG logscores" by default
xlab	name of x-axis; "iteration"
ylab	name of y-axis; "logscore"
type	type of line in the plot; "l" by default
col	colour of line in the plot; "#0c2c84" by default
object	object of class 'orderMCMC'

### Value

Object of class `orderMCMC`, which contains log-score trace of sampled DAGs as well as adjacency matrix of the maximum scoring DAG, its score and the order score. The output can optionally include DAGs sampled in MCMC iterations and the score tables. Optional output is regulated by the parameters `chainout` and `scoreout`. See [orderMCMC class](#) for a detailed class structure.

### Author(s)

Polina Suter, Jack Kuipers, the code partly derived from the order MCMC implementation from Kuipers J, Moffa G (2017) <doi:10.1080/01621459.2015.1133426>

### References

- Friedman N and Koller D (2003). A Bayesian approach to structure discovery in bayesian networks. *Machine Learning* 50, 95-125.
- Kalisch M, Maechler M, Colombo D, Maathuis M and Buehlmann P (2012). Causal inference using graphical models with the R package `pcalg`. *Journal of Statistical Software* 47, 1-26.
- Geiger D and Heckerman D (2002). Parameter priors for directed acyclic graphical models and the characterization of several probability distributions. *The Annals of Statistics* 30, 1412-1440.
- Kuipers J, Moffa G and Heckerman D (2014). Addendum on the scoring of Gaussian acyclic graphical models. *The Annals of Statistics* 42, 1689-1691.
- Spirtes P, Glymour C and Scheines R (2000). *Causation, Prediction, and Search*, 2nd edition. The MIT Press.

**Examples**

```
## Not run:
#find a MAP DAG with search space defined by PC and plus1 neighbourhood
Bostonscore<-scoreparameters("bge",Boston)
#estimate MAP DAG
orderMAPfit<-orderMCMC(Bostonscore)
summary(orderMAPfit)
#sample DAGs from the posterior distribution
ordersamplefit<-orderMCMC(Bostonscore,MAP=FALSE,chainout=TRUE)
plot(ordersamplefit)

## End(Not run)
```

---

orderMCMC class	<i>orderMCMC class structure</i>
-----------------	----------------------------------

---

**Description**

The structure of an object of S3 class orderMCMC.

**Details**

An object of class orderMCMC is a list containing at least the following components:

- DAG: adjacency matrix of a maximum scoring DAG found/sampled in the MCMC scheme.
- CPDAG: adjacency matrix representing equivalence class of a maximum scoring DAG found/sampled in MCMC.
- score: score of a maximum scoring DAG found/sampled in MCMC.
- maxorder: order of a maximum scoring DAG found/sampled in MCMC.
- info: a list containing information about parameters and results of MCMC.
- trace: a vector containing log-scores of sampled DAGs.

Optional components:

- traceadd: list which consists of three or four elements (depending on MCMC scheme used for sampling):
  - \* incidence: list containing adjacency matrices of sampled DAGs
  - \* order: list of orders from which the DAGs were sampled
  - \* orderscores: order log-scores
- scoretable: object of class [score space class](#)

**Author(s)**

Polina Suter

---

partitionMCMC

*DAG structure sampling with partition MCMC*

---

## Description

This function implements the partition MCMC algorithm for the structure learning of Bayesian networks. This procedure provides an unbiased sample from the posterior distribution of DAGs given the data. The search space can be defined either by a preliminary run of the function `iterativeMCMC` or by a given adjacency matrix (which can be the full matrix with zero on the diagonal, to consider the entire space of DAGs, feasible only for a limited number of nodes).

## Usage

```
partitionMCMC(  
  scorepar,  
  moveprobs = NULL,  
  iterations = NULL,  
  stepsave = NULL,  
  gamma = 1,  
  verbose = FALSE,  
  scoreout = FALSE,  
  startspace = NULL,  
  blacklist = NULL,  
  scoretable = NULL,  
  startDAG = NULL  
)  
  
## S3 method for class 'partitionMCMC'  
plot(  
  x,  
  ...,  
  burnin = 0.2,  
  main = "DAG logscores",  
  xlab = "iteration",  
  ylab = "logscore",  
  type = "l",  
  col = "#0c2c84"  
)  
  
## S3 method for class 'partitionMCMC'  
print(x, ...)  
  
## S3 method for class 'partitionMCMC'  
summary(object, ...)
```

**Arguments**

scorepar	an object of class <code>scoreparameters</code> , containing the data and scoring parameters; see constructor function <code>scoreparameters</code> .
moveprobs	(optional) a numerical vector of 5 values in $\{0, 1\}$ corresponding to the following MCMC move probabilities in the space of partitions: <ul style="list-style-type: none"> <li>• swap any two elements from different partition elements</li> <li>• swap any two elements in adjacent partition elements</li> <li>• split a partition element or join one</li> <li>• move a single node into another partition element or into a new one</li> <li>• stay still</li> </ul>
iterations	integer, the number of MCMC steps, the default value is $20n^2 \log n$
stepsave	integer, thinning interval for the MCMC chain, indicating the number of steps between two output iterations, the default is $iterations/1000$
gamma	tuning parameter which transforms the score by raising it to this power, 1 by default
verbose	logical, if set to TRUE (default) messages about progress will be printed
scoreout	logical, if TRUE the search space and score tables are returned, FALSE by default
startspace	(optional) a square matrix, of dimensions equal to the number of nodes, which defines the search space for the order MCMC in the form of an adjacency matrix; if NULL, the skeleton obtained from the PC-algorithm will be used. If $startspace[i, j]$ equals to 1 (0) it means that the edge from node $i$ to node $j$ is included (excluded) from the search space. To include an edge in both directions, both $startspace[i, j]$ and $startspace[j, i]$ should be 1.
blacklist	(optional) a square matrix, of dimensions equal to the number of nodes, which defines edges to exclude from the search space; if $blacklist[i, j]=1$ it means that the edge from node $i$ to node $j$ is excluded from the search space
scoretable	(optional) object of class <code>scorespace</code> containing list of score tables calculated for example by the last iteration of the function <code>iterativeMCMC</code> . When not NULL, parameter <code>startspace</code> is ignored
startDAG	(optional) an adjacency matrix of dimensions equal to the number of nodes, representing a DAG in the search space defined by <code>startspace</code> . If <code>startspace</code> is defined but <code>startDAG</code> is not, an empty DAG will be used by default
x	object of class <code>'partitionMCMC'</code>
...	ignored
burnin	number between 0 and 1, indicates the percentage of the samples which will be discarded as 'burn-in' of the MCMC chain; the rest of the samples will be used to calculate the posterior probabilities; 0.2 by default
main	name of the graph; "DAG logscores" by default
xlab	name of x-axis; "iteration"
ylab	name of y-axis; "logscore"
type	type of line in the plot; "l" by default
col	colour of line in the plot; "#0c2c84" by default
object	object of class <code>'partitionMCMC'</code>



**Value**

Object of class `partitionMCMC`, which contains log-score trace as well as adjacency matrix of the maximum scoring DAG, its score and the order score. Additionally, returns all sampled DAGs (represented by their adjacency matrices), their scores, orders and partitions See [partitionMCMC class](#).

**Author(s)**

Polina Suter, Jack Kuipers, the code partly derived from the partition MCMC implementation from Kuipers J, Moffa G (2017) <doi:10.1080/01621459.2015.1133426>

**References**

Kuipers J and Moffa G (2017). Partition MCMC for inference on acyclic digraphs. *Journal of the American Statistical Association* 112, 282-299.

Geiger D and Heckerman D (2002). Parameter priors for directed acyclic graphical models and the characterization of several probability distributions. *The Annals of Statistics* 30, 1412-1440.

Heckerman D and Geiger D (1995). Learning Bayesian networks: A unification for discrete and Gaussian domains. In *Eleventh Conference on Uncertainty in Artificial Intelligence*, pages 274-284.

Kalisch M, Maechler M, Colombo D, Maathuis M and Buehlmann P (2012). Causal inference using graphical models with the R package `pcalg`. *Journal of Statistical Software* 47, 1-26.

Kuipers J, Moffa G and Heckerman D (2014). Addendum on the scoring of Gaussian directed acyclic graphical models. *The Annals of Statistics* 42, 1689-1691.

**Examples**

```
## Not run:
myScore<-scoreparameters("bge", Boston)
partfit<-partitionMCMC(myScore)
plot(partfit)

## End(Not run)
```

---

`partitionMCMC class`    *partitionMCMC class structure*

---

**Description**

The structure of an object of S3 class `partitionMCMC`.

**Details**

An object of class `partitionMCMC` is a list containing at least the following components:

- DAG: adjacency matrix of a maximum scoring DAG found/sampled in the MCMC scheme.

- CPDAG: adjacency matrix representing equivalence class of a maximum scoring DAG found/sampled in MCMC.
- score: score of a maximum scoring DAG found/sampled in MCMC.
- maxorder: order of a maximum scoring DAG found/sampled in MCMC.
- info: a list containing information about parameters and results of MCMC.
- trace: a vector containing log-scores of sampled DAGs.

Optional components:

- traceadd: list which consists of three or four elements (depending on MCMC scheme used for sampling):
  - \* incidence: list containing adjacency matrices of sampled DAGs
  - \* order: list of orders from which the DAGs were sampled
  - \* partition: list of partition from which the DAGs were sampled
  - \* partitionscores: partition log-scores
- scoretable: object of class `scorespace class`

### Author(s)

Polina Suter

---

plot2in1

*Highlighting similarities between two graphs*

---

### Description

This function plots nodes and edges from two graphs in one and indicates similarities between these graphs.

### Usage

```
plot2in1(graph1, graph2, bidir = FALSE, ...)
```

### Arguments

graph1	binary adjacency matrix of a graph
graph2	binary adjacency matrix of a graph, column names should coincide with column names of 'graph1'
bidir	logical, defines if arrows of bidirected edges are drawn; FALSE by default.
...	optional parameters passed to <b>Rgraphviz</b> plotting functions e.g. main, fontsize

### Value

plots the graph which includes nodes and edges two graphs; nodes which are connected to at least one other node in both graphs are plotted only once and coloured orange, edges which are shared by two graphs are coloured orange; all other nodes and edges are plotted once for each 'graph1' and 'graph2' and coloured blue and green accordingly.

**Author(s)**

Polina Suter

---

`plotDBN`*Plotting a DBN*

---

**Description**

This function can be used for plotting initial and transition structures of a dynamic Bayesian network.

**Usage**

```
plotDBN(DBN, struct = c("init", "trans"), n.dynamic, n.static)
```

**Arguments**

DBN	binary matrix (or a graph object) representing a 2-step DBN (compact or unrolled)
struct	option used to determine if the initial or the transition structure should be plotted; acceptable values are init or trans
n.dynamic	number of dynamic variables in one time slice of a DBN
n.static	number of static variables in one time slice of a DBN; note that for function to work correctly all static variables have to be in the first n.static columns of the matrix

**Value**

plots the DBN defined by the adjacency matrix 'DBN' and number of static and dynamic variables. When 'struct' equals "trans" the transition structure is plotted, otherwise initial structure is plotted

**Author(s)**

Polina Suter

**Examples**

```
plotDBN(DBNmat, "init", n.dynamic=12,n.static=3)  
plotDBN(DBNmat, "trans", n.dynamic=12,n.static=3)
```

---

`plotdiffs`*Plotting difference between two graphs*

---

### Description

This function plots edges from two graphs in one and indicates similarities and differences between these graphs. It is also possible to use this function for plotting mistakes in estimated graph when the ground truth graph is known.

### Usage

```
plotdiffs(  
  graph1,  
  graph2,  
  estimated = TRUE,  
  name1 = "graph1",  
  name2 = "graph2",  
  clusters = NULL,  
  ...  
)
```

### Arguments

<code>graph1</code>	object of class <code>graphNEL</code> or its adjacency matrix
<code>graph2</code>	object of class <code>graphNEL</code> or its adjacency matrix
<code>estimated</code>	logical, indicates if <code>graph1</code> is estimated graph and <code>graph2</code> is ground truth DAG, TRUE by default; this affects the legend and colouring of the edges
<code>name1</code>	character, custom name for 'graph1'
<code>name2</code>	character, custom name for 'graph2'
<code>clusters</code>	(optional) a list of nodes to be represented on the graph as clusters
<code>...</code>	optional parameters passed to <code>Rgraphviz</code> plotting functions e.g. <code>main</code> , <code>fontSize</code>

### Value

plots the graph which includes edges from `graph1` and `graph2`; edges which are different in `graph1` compared to `graph2` are coloured according to the type of a difference

### Author(s)

Polina Suter

**Examples**

```

Asiascore<-scoreparameters("bde",Asia)
Asiamap<-orderMCMC(Asiascore)
plotdiffs(Asiamap$DAG,Asiamat)
Asiacp<-pcalg::dag2cpdag(m2graph(Asiamat))
mapcp<-pcalg::dag2cpdag(m2graph(Asiamap$DAG))
plotdiffs(mapcp,Asiacp)

```

---

plotdiffs.DBN

*Plotting difference between two DBNs*


---

**Description**

This function plots an estimated DBN such that the edges which are different to the ground truth DBN are highlighted.

**Usage**

```

plotdiffs.DBN(
  eDBN,
  trueDBN,
  struct = c("init", "trans"),
  n.dynamic,
  n.static = 0
)

```

**Arguments**

eDBN	object of class graphNEL (or its adjacency matrix), representing estimated structure (not necessarily acyclic) to be compared to the ground truth graph
trueDBN	object of class graphNEL (or its adjacency matrix), representing the ground truth structure (not necessarily acyclic)
struct	option used to determine if the initial or the transition structure should be plotted; acceptable values are init or trans
n.dynamic	number of dynamic variables in one time slice of a DBN
n.static	number of static variables in one time slice of a DBN; note that for function to work correctly all static variables have to be in the first n.static columns of the matrix

**Value**

plots the graph highlights differences between 'eDBN' (estimated DBN) and 'trueDBN' (ground truth); edges which are different in 'eDBN' compared to 'trueDBN' are coloured according to the type of a difference: false-positive, false-negative and error in direction.

**Author(s)**

Polina Suter

**Examples**

```

dbnscore<-scoreparameters("bge",DBNdata,
dbnpar = list(samestruct=TRUE, slices=5, b=3),
DBN=TRUE)
## Not run:
orderDBNfit<-iterativeMCMC(dbnscore,chainout = TRUE, mergetype = "skeleton",scoreout=TRUE,alpha=0.4)
plotdiffs.DBN(orderDBNfit$DAG,DBNmat,struct="trans",n.dynamic=12,n.static=3)
plotdiffs.DBN(orderDBNfit$DAG,DBNmat,struct="init",n.dynamic=12,n.static=3)

## End(Not run)

```

---

plotpcor

*Comparing posterior probabilities of single edges*


---

**Description**

This function can be used to compare posterior probabilities of edges in a graph

**Usage**

```
plotpcor(pmat, highlight = 0.3, printedges = FALSE, cut = 0.05, ...)
```

**Arguments**

pmat	a list of square matrices, representing posterior probabilities of single edges in a Bayesian network; see <a href="#">edgep</a> for obtaining such a matrix from a single MCMC run
highlight	numeric, defines maximum acceptable difference between posterior probabilities of an edge in two samples; points corresponding to higher differences are highlighted in red
printedges	when TRUE the function also returns squared correlation and RMSE of posterior probabilities higher than the value defined by the argument 'cut' as well as the list of all edges whose posterior probabilities in the first two matrices differ more than 'highlight'; FALSE by default
cut	numeric value corresponding to a minimum posterior probability which is included into calculation of squared correlation and MSE when 'printedges' equals TRUE
...	parameters passed further to the plot function (e.g. xlab, ylab, main) in case when the length of pmat equals 2

**Value**

plots concordance of posterior probabilities of single edges based on several matrices (minimum 2 matrices); highlights the edges whose posterior probabilities in a pair of matrices differ by more than 'highlight'; when 'printedges' set to TRUE, the function returns also squared correlation and RMSE of posterior probabilities higher than the value defined by the argument 'cut' as well as the list of all edges whose posterior probabilities in the first two matrices differ by more than 'highlight'.

**Author(s)**

Polina Suter

**Examples**

```
Asiascore<-scoreparameters("bde", Asia)
## Not run:
orderfit<-list()
orderfit[[1]]<-orderMCMC(Asiascore,MAP=FALSE)
orderfit[[2]]<-orderMCMC(Asiascore,MAP=FALSE)
pedges<-lapply(orderfit,edgep,pdag=TRUE)
plotpcor(pedges, xlab="run1", ylab="run2")

## End(Not run)
```

---

plotpedges

*Plotting posterior probabilities of single edges*

---

**Description**

This function plots posterior probabilities of all possible edges in the graph as a function of MCMC iterations. It can be used for convergence diagnostics of MCMC sampling algorithms order MCMC and partition MCMC.

**Usage**

```
plotpedges(
  MCMCtrace,
  cutoff = 0.2,
  pdag = FALSE,
  onlyedges = NULL,
  highlight = NULL,
  ...
)
```

**Arguments**

MCMCtrace	an object of class MCMCres
cutoff	number representing a threshold of posterior probability below which lines will not be plotted
pdag	logical, when true DAGs in a sample will be first covered to CPDAGs
onlyedges	(optional) binary matrix, only edges corresponding to entries which equal 1 will be plotted
highlight	(optional) binary matrix, edges corresponding to entries which equal 1 are highlighted with "red"
...	(optional) parameters passed to the plot function

**Value**

plots posterior probabilities of edges in the graph as a function of MCMC iterations

**Author(s)**

Polina Suter

**Examples**

```
score100<-scoreparameters("bde", Asia[1:100,])
orderfit100<-orderMCMC(score100,plus1=TRUE)
## Not run:
score5000<-scoreparameters("bde", Asia)
orderfit5000<-orderMCMC(score5000,plus1=TRUE)
plotpedges(orderfit100, pdag=TRUE)
plotpedges(orderfit5000, pdag=TRUE)

## End(Not run)
```

---

samplecomp

*Performance assessment of sampling algorithms against a known Bayesian network*

---

**Description**

This function compute 8 different metrics of structure fit of an object of classes `orderMCMC` and `partitionMCMC` to the ground truth DAG (or CPDAG). First posterior probabilities of single edges are calculated based on a sample stores in the object of class `orderMCMC` or `partitionMCMC`. This function computes structure fit of each of the consensus graphs to the ground truth one based on a defined range of posterior thresholds. Computed metrics include: TP, FP, TPR, FPR, FPRn, FDR, SHD. See metrics description in see also [compareDAGs](#).



**Usage**

```

samplecomp(
  MCMCchain,
  truedag,
  p = c(0.99, 0.95, 0.9, 0.8, 0.7, 0.6, 0.5, 0.4, 0.3, 0.2),
  pdag = TRUE,
  burnin = 0.2,
  trans = TRUE
)

## S3 method for class 'samplecomp'
plot(x, ..., vars = c("FP", "TP"), type = "b", col = "blue", showp = NULL)

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

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

```

**Arguments**

MCMCchain	an object of class <code>partitionMCMC</code> or <code>orderMCMC</code> , representing the output of structure sampling function <code>partitionMCMC</code> or <code>orderMCMC</code> (the latter when parameter <code>chainout=TRUE</code> );
truedag	ground truth DAG which generated the data used in the search procedure; represented by an object of class <code>graphNEL</code>
p	a vector of numeric values between 0 and 1, defining posterior probabilities according to which the edges of assessed structures are drawn, please note very low barriers can lead to very dense structures; by default $p = c(0.99, 0.95, 0.9, 0.8, 0.7, 0.6, 0.5, 0.4, 0.3, 0.2)$
pdag	logical, if TRUE (default) all DAGs in the MCMCchain are first converted to equivalence class (CPDAG) before the averaging
burnin	number between 0 and 1, indicates the percentage of the samples which will be the discarded as 'burn-in' of the MCMC chain; the rest of the samples will be used to calculate the posterior probabilities; 0.2 by default
trans	logical, for DBNs indicates if model comparisons are performed for transition structure; when trans equals FALSE the comparison is performed for initial structures of estimated models and the ground truth DBN; for usual BNs the parameter is disregarded
x	object of class 'samplecomp'
...	ignored
vars	a tuple of variables which will be used for 'x' and 'y' axes; possible values: "SHD", "TP", "FP", "TPR", "FPR", "FPRn", "FDR"
type	type of line in the plot; "b" by default
col	colour of line in the plot; "blue" by default

showp	logical, defines if points are labelled with the posterior threshold corresponding to the assessed model
object	object of class 'samplecomp'

**Value**

an object of class `samplesim`, a matrix with the number of rows equal to the number of elements in 'p', and 8 columns reporting for the consensus graphss (corresponding to each of the values in 'p') the number of true positive edges ('TP'), the number of false positive edges ('FP'), the number of false negative edges ('FN'), the true positive rate ('TPR'), the structural Hamming distance ('SHD'), false positive rate ('FPR'), false discovery rate ('FDR') and false positive rate normalized by TP+FN ('FPRn').

**Author(s)**

Polina Suter

**Examples**

```
gsim.score<-scoreparameters("bge", gsim)
## Not run:
mapest<-iterativeMCMC(gsim.score)
ordersample<-orderMCMC(gsim.score, MAP=FALSE, startspace=mapest$endspace)
samplecomp(ordersample, gsimmat)

## End(Not run)
```

---

scoreagainstDAG

*Calculating the score of a sample against a DAG*

---

**Description**

This function calculates the score of a given sample against a DAG represented by its incidence matrix.

**Usage**

```
scoreagainstDAG(scorepar, incidence, datatoscore = NULL, marginalise = FALSE)
```

**Arguments**

scorepar	an object of class <code>scoreparameters</code> ; see constructor function <a href="#">scoreparameters</a>
incidence	a square matrix of dimensions equal to the number of variables with entries in $\{0, 1\}$ , representing the adjacency matrix of the DAG against which the score is calculated

datatoscore	(optional) a matrix (vector) containing binary (for BDe score) or continuous (for the BGe score) observations (or just one observation) to be scored; the number of columns should be equal to the number of variables in the Bayesian network, the number of rows should be equal to the number of observations; by default all data from scorepar parameter is used
marginalise	(optional for continuous data), whether to use the posterior mean for scoring (default) or to marginalise over the posterior distribution (more computationally costly)

**Value**

the log of the BDe/BGe score of given observations against a DAG

**Author(s)**

Jack Kuipers

**References**

Heckerman D and Geiger D, (1995). Learning Bayesian networks: A unification for discrete and Gaussian domains. In Eleventh Conference on Uncertainty in Artificial Intelligence, pages 274-284, 1995.

**Examples**

```
Asiascore<-scoreparameters("bde", Asia[1:100,]) #we wish to score only first 100 observations
scoreagainstDAG(Asiascore, Asiamat)
```

---

scoreparameters      *Initializing score object*

---

**Description**

This function returns an object of class scoreparameters containing the data and parameters needed for calculation of the BDe/BGe score, or a user defined score.

**Usage**

```
scoreparameters(
  scoretype = c("bge", "bde", "bdecat", "usr"),
  data,
  bgepar = list(am = 1, aw = NULL),
  bdepar = list(chi = 0.5, edgepf = 2),
  bdecatpar = list(chi = 0.5, edgepf = 2),
  dbnpar = list(samestruct = TRUE, slices = 2, b = 0),
  usrpar = list(pctesttype = c("bge", "bde", "bdecat")),
  DBN = FALSE,
```

```

    weightvector = NULL,
    bgnodes = NULL,
    edgepmat = NULL,
    nodeslabels = NULL
)

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

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

```

### Arguments

scoretype	the score to be used to assess the DAG structure: "bge" for Gaussian data, "bde" for binary data, "bdecat" for categorical data, "usr" for a user defined score; when "usr" score is chosen, one must define a function (which evaluates the log score of a node given its parents) in the following format: <code>usrDAG-corescore(j,parentnodes,n,param)</code> , where 'j' is node to be scores, 'parentnodes' are the parents of this node, 'n' number of nodes in the network and 'param' is an object of class 'scoreparameters'
data	the data matrix with n columns (the number of variables) and a number of rows equal to the number of observations
bgepar	a list which contains parameters for BGe score: <ul style="list-style-type: none"> <li>• am (optional) a positive numerical value, 1 by default</li> <li>• aw (optional) a positive numerical value should be more than n+1, n+am+1 by default</li> </ul>
bdepar	a list which contains parameters for BDe score for binary data: <ul style="list-style-type: none"> <li>• chi (optional) a positive number of prior pseudo counts used by the BDe score, 0.5 by default</li> <li>• edgepf (optional) a positive numerical value providing the edge penalization factor to be combined with the BDe score, 2 by default</li> </ul>
bdecatpar	a list which contains parameters for BDe score for categorical data: <ul style="list-style-type: none"> <li>• chi (optional) a positive number of prior pseudo counts used by the BDe score, 0.5 by default</li> <li>• edgepf (optional) a positive numerical value providing the edge penalization factor to be combined with the BDe score, 2 by default</li> </ul>
dbnpar	which type of score to use for the slices <ul style="list-style-type: none"> <li>• samestruct logical, when TRUE the structure of the first time slice is assumed to be the same as internal structure of all other time slices</li> <li>• slices integer representing the number of time slices in a DBN</li> <li>• b the number of static variables; all static variables have to be in the first b columns of the data; for DBNs static variables have the same meaning as bgnodes for usual Bayesian networks; for DBNs parameters parameter bgnodes is ignored</li> </ul>

usrpar	a list which contains parameters for the user defined score <ul style="list-style-type: none"> <li>• pctesttype (optional) conditional independence test ("bde","bge","bdecat")</li> </ul>
DBN	logical, when TRUE the score is initialized for a dynamic Bayesian network; FALSE by default
weightvector	(optional) a numerical vector of positive values representing the weight of each observation; should be NULL(default) for non-weighted data
bgnodes	(optional) a numerical vector which contains numbers of columns in the data defining background nodes, background nodes are nodes which have no parents but can be parents of other nodes in the network; in case of DBNs bgnodes represent static variables and defined via element b of the parameters dbnpar
edgepmat	(optional) a matrix of positive numerical values providing the per edge penalization factor to be added to the score, NULL by default
nodeslabels	(optional) a vector of characters which denote the names of nodes in the Bayesian network; by default column names of the data will be taken
x	object of class 'scoreparameters'
...	ignored
object	object of class 'scoreparameters'

**Value**

an object of class `scoreparameters`, which includes all necessary information for calculating the BDe/BGe score

**Author(s)**

Polina Suter, Jack kuipers

**References**

Geiger D and Heckerman D (2002). Parameter priors for directed acyclic graphical models and the characterization of several probability distributions. *The Annals of Statistics* 30, 1412-1440.

Kuipers J, Moffa G and Heckerman D (2014). Addendum on the scoring of Gaussian acyclic graphical models. *The Annals of Statistics* 42, 1689-1691.

Heckerman D and Geiger D (1995). Learning Bayesian networks: A unification for discrete and Gaussian domains. In *Eleventh Conference on Uncertainty in Artificial Intelligence*, pages 274-284.

Scutari M (2016). An Empirical-Bayes Score for Discrete Bayesian Networks. *Journal of Machine Learning Research* 52, 438-448

**Examples**

```
myDAG<-pcalg::randomDAG(20, prob=0.15, lB = 0.4, uB = 2)
myData<-pcalg::rmvDAG(200, myDAG)
myScore<-scoreparameters("bge", myData)
```

---

scorespace	<i>Prints 'scorespace' object</i>
------------	-----------------------------------

---

### Description

Prints 'scorespace' object  
 Summary of object of class 'scorespace'

### Usage

```
scorespace(
  scorepar,
  alpha = 0.05,
  hardlimit = 14,
  plus1 = TRUE,
  cpdag = TRUE,
  startspace = NULL,
  blacklist = NULL,
  verbose = FALSE
)

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

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

### Arguments

scorepar	an object of class <code>scoreparameters</code> , containing the data and score scoreparameters, see constructor function <code>scoreparameters</code>
alpha	numerical significance value in $\{0, 1\}$ for the conditional independence tests at the PC algorithm stage (by default 0.4 for $n < 50$ , $20/n$ for $n > 50$ )
hardlimit	integer, limit on the size of parent sets in the search space; by default 14 when MAP=TRUE and 20 when MAP=FALSE
plus1	logical, if TRUE (default) the search is performed on the extended search space
cpdag	logical, if TRUE the CPDAG returned by the PC algorithm will be used as the search space, if FALSE (default) the full undirected skeleton will be used as the search space
startspace	(optional) a square matrix, of dimensions equal to the number of nodes, which defines the search space for the order MCMC in the form of an adjacency matrix. If NULL, the skeleton obtained from the PC-algorithm will be used. If <code>startspace[i, j]</code> equals to 1 (0) it means that the edge from node <i>i</i> to node <i>j</i> is included (excluded) from the search space. To include an edge in both directions, both <code>startspace[i, j]</code> and <code>startspace[j, i]</code> should be 1.

blacklist	(optional) a square matrix, of dimensions equal to the number of nodes, which defines edges to exclude from the search space. If <code>blacklist[i, j]</code> equals to 1 it means that the edge from node <code>i</code> to node <code>j</code> is excluded from the search space.
verbose	logical, if TRUE messages about the algorithm's progress will be printed, FALSE by default
x	object of class 'scorespace'
...	ignored
object	object of class 'scorespace'

**Value**

Object of class `scorespace`, a list of three objects: 'adjacency' matrix representing the search space, 'blacklist' used to exclude edges from the search space and 'tables' containing score quantities for each node needed to run MCMC schemes

**Author(s)**

Polina Suter, Jack Kuipers

**References**

Friedman N and Koller D (2003). A Bayesian approach to structure discovery in bayesian networks. *Machine Learning* 50, 95-125.

**Examples**

```
#' #find a MAP DAG with search space defined by PC and plus1 neighbourhood
BostonScore<-scoreparameters("bge",Boston)
BostonSpace<-scorespace(BostonScore, 0.05, 14)
## Not run:
orderfit<-orderMCMC(BostonScore, scoretable=BostonSpace)
partitionfit<-orderMCMC(BostonScore, scoretable=BostonSpace)

## End(Not run)
```

---

scorespace class      *scorespace class structure*

---

**Description**

The structure of an object of S3 class `scorespace`.

**Details**

An object of class `scorespace` is a list containing at least the following components:

- `adjacency`: adjacency matrix representing the core search space
- `blacklist`: adjacency matrix representing the blacklist used for computing score tables
- `tables`: a list of matrices (for core search space) or a list of lists of matrices (for extended search space) containing quantities needed for scoring orders and sampling DAGs in MCMC schemes; this list corresponds to `adjacency` and `blacklist`

**Author(s)**

Polina Suter

---

string2mat

*Deriving interactions matrix*

---

**Description**

This transforms a list of possible interactions between proteins downloaded from STRING database into a matrix which can be used for blacklisting/penalization in BiDAG.

**Usage**

```
string2mat(curnames, int, mapping = NULL, type = c("int"), pf = 2)
```

**Arguments**

<code>curnames</code>	character vector with gene names which will be used in BiDAG learning function
<code>int</code>	data frame, representing a interactions between genes/proteins downloaded from STRING ( <a href="https://string-db.org/">https://string-db.org/</a> ); two columns are necessary 'node1' and 'node2'
<code>mapping</code>	(optional) data frame, representing a mapping between 'curnames' (gene names, usually the column names of 'data') and gene names used in interactions downloaded from STRING ( <a href="https://string-db.org/">https://string-db.org/</a> ); two columns are necessary 'queryItem' and 'preferredName'
<code>type</code>	character, defines how interactions will be reflected in the output matrix; <code>int</code> will result in a matrix whose entries equal 1 if interaction is present in the list of interactions <code>int</code> and 0 otherwise; <code>blacklist</code> results in a matrix whose entries equal 0 when interaction is present in the list of interactions and 1 otherwise; <code>pf</code> results in a matrix whose entries equal 1 if interaction is present in the list of interactions <code>int</code> and <code>pf</code> otherwise\$ "int" by default
<code>pf</code>	penalization factor for interactions, needed if <code>type=pf</code>

**Value**

square matrix whose entries correspond to the list of interactions and parameter `type`



**Examples**

```
curnames<-colnames(kirp)
intmat<-string2mat(curnames, mapping, interactions, type="pf")
```

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