



BDgraph: An R Package for Bayesian Structure Learning in Graphical Models

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Abstract

We introduce an R package **BDgraph** which performs Bayesian structure learning in high-dimensional graphical models with either continuous or discrete variables. The package efficiently implements recent improvements in the Bayesian literature, including Mohammadi and Wit (2015b) and Mohammadi, Abegaz Yazew, van den Heuvel, and Wit (2015). The core of the **BDgraph** package consists of two main MCMC sampling algorithms efficiently implemented in C++ to maximize computational speed. In this paper, we give a brief overview of the methodology and illustrate the package's functionality in both toy examples and applications.

Keywords: Bayesian structure learning, Gaussian graphical models, Gaussian copula, Covariance selection, Birth-death process, Markov chain Monte Carlo, G-Wishart, **BDgraph**, R.

1. Introduction

Graphical models (Lauritzen 1996) can be used to describe the conditional independence relationships among large numbers of variables. In graphical models, each random variable is associated with a node in a graph and links represent conditional dependency between variables, whereas the absence of a link implies that the variables are independent conditional on the rest of the variables (called the pairwise Markov property).

In recent years, significant progress has been made to design efficient algorithms to discover graph structures from high-dimensional multivariate data (Dobra, Lenkoski, and Rodriguez 2011; Jones, Carvalho, Dobra, Hans, Carter, and West 2005; Mohammadi and Wit 2015b; Mohammadi *et al.* 2015; Friedman, Hastie, and Tibshirani 2008; Meinshausen and Bühlmann 2006; Murray and Ghahramani 2004). In this regard, Bayesian approaches provide a principled alternative to various penalized approaches.

In this paper, we describe the **BDgraph** package (Mohammadi and Wit 2015a) in R (R Core

Team 2013) for Bayesian structure learning in undirected graphical models. The package can deal with Gaussian, non-Gaussian, discrete and mixed data sets. The package includes several functional modules, including data generation for simulation, a search algorithm, a graph estimation routine, a convergence check and a visualization tool; see Figure 1. The package efficiently implements recent improvements in the Bayesian literature, including Mohammadi and Wit (2015b); Mohammadi *et al.* (2015); Lenkoski (2013); Uhler, Lenkoski, and Richards (2014); Hoff (2007). For a Bayesian framework of Gaussian graphical models, we implement the method developed by Mohammadi and Wit (2015b) and for Gaussian copula graphical models we use the method described by Mohammadi *et al.* (2015). To make our Bayesian methods computationally feasible for high-dimensional data, we efficiently implement the **BDgraph** package in C++ linked to R. To make the package easy to use, we use the S3 class. The package is available under the general public license (GPL ≥ 3) from the Comprehensive R Archive Network (CRAN) at <http://cran.r-project.org/packages=BDgraph>.

In the Bayesian literature, the **BDgraph** is the only R package which is available online for Gaussian graphical models and Gaussian copula graphical models. On the other hand, in frequentist literature, existing packages are **huge** (Zhao, Liu, Roeder, Lafferty, and Wasserman 2014), **glasso** (Friedman, Hastie, and Tibshirani 2014), **bnlearn** (Scutari 2010), **pcalg** (Kalisch, Mächler, Colombo, Maathuis, and Bühlmann 2012) and **gRain** (Højsgaard 2012). We compare the performance to several packages.

The article is organized as follows. In Section 2 we illustrate the user interface of **BDgraph** package. In Section 3 we explain some methodological background of the package. In this regard, in Section 3.1, we briefly explain the Bayesian framework for Gaussian graphical models for continuous data. In Section 3.2 we briefly describe the Bayesian framework in the Gaussian copula graphical models for the data that not follow the Gaussianity assumption, such as non-Gaussian continuous, discrete or mixed data. In Section 4 we describe the main functions implemented in the **BDgraph** package. In Section 5 by a simple simulation example, we explain the user interface and the performance of the package and we compare it with **huge** package. In Section 6, by using the functions implemented in the **BDgraph** package, we study two real data sets.

2. User interface

In R environment, we can access and load the **BDgraph** package by suing the following commands

```
R> install.packages( "BDgraph" )
R> library( "BDgraph" )
```

Loading the package automatically loads **igraph** (Csardi and Nepusz 2006) and **Matrix** (Bates and Maechler 2014) packages, since **BDgraph** package depends on these two packages. These packages are available on the Comprehensive R Archive Network (CRAN) at <http://CRAN.R-project.org>. We use **igraph** package for graph visualization and **Matrix** package for memory-optimization using sparse matrix output. In our package, all the functions operate on or return **Matrix** objects.

To maximize computational speed, we efficiently implement the **BDgraph** package with C++ code linked to R. For C++ code, we used the highly optimized **LAPACK** (Anderson, Bai,

Bischof, Blackford, Demmel, Dongarra, Du Croz, Greenbaum, Hammarling, McKenney, and Sorensen 1999) and **BLAS** (Lawson, Hanson, Kincaid, and Krogh 1979) linear algebra libraries on systems that provide them. We significantly improve program speed by using these libraries.

We design the **BDgraph** package to provide a Bayesian framework for high-dimensional undirected graph estimation for different types of data sets such as continuous, discrete or mixed data. The package facilitates a flexible pipeline for analysis by three functional modules; see Figure 1. These modules are as follows:

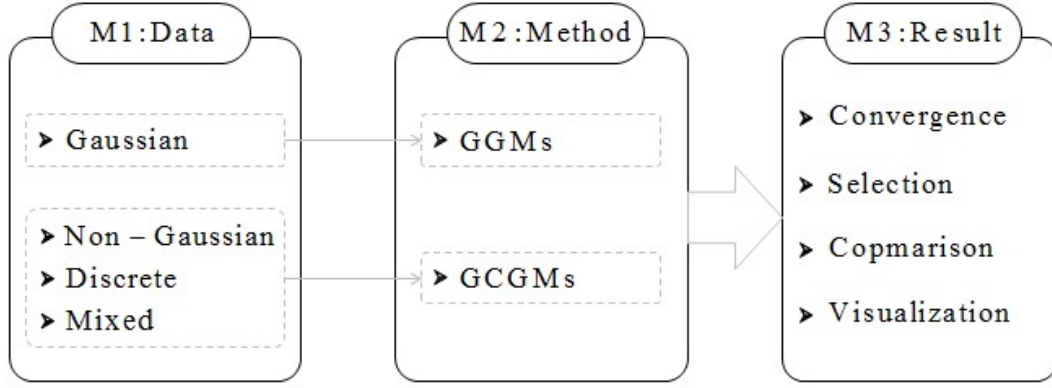


Figure 1: Configuration of the **BDgraph** package which includes three main parts: (M1) data generation, (M2) algorithm for sampling from joint posterior distribution and (M3) several functions to check convergence of BDMCMC algorithm, estimate the true graph, compare and model check and graph visualization.

Module 1. Data simulation: Function `bdgraph.sim` simulates multivariate Gaussian, discrete and mixed data with different undirected graph structures, including “random”, “cluster”, “hub”, “scale-free”, “circle” and “fixed” graphs. Users can set the sparsity of the graph structure. Users can generate mixed data, including “count”, “ordinal”, “binary”, “Gaussian” and “non-Gaussian” variables.

Module 2. Method: The function `bdgraph` provides two estimation methods with two different algorithms for sampling from the posterior distributions:

1. Graph estimation for normally distributed data which is based on the Gaussian graphical models (GGMs) by using the birth-death MCMC sampling algorithm, described in Mohammadi and Wit (2015b).
2. Graph estimation for non-Gaussian, discrete, and mixed data, which is based on Gaussian copula graphical models (GCGMs) by using the birth-death MCMC sampling algorithm, described in Mohammadi *et al.* (2015).

Module 3. Result: This module includes four types of functions as follow

- **Convergence check:** The functions `plotcoda` and `traceplot` provide several visualization plots to monitor the convergence of the sampling algorithms.
- **Graph selection:** The functions `select`, `phat`, `prob`, provide selected graph, the posterior link inclusion probabilities and posterior probability of each graph, respectively.

- **Comparison and goodness-of-fit:** The functions `compare` and `plotroc` provide several comparison measures and ROC plot for model comparison.
- **Visualization:** The plotting functions `plot.bdgraph` and `plot.simulate` provide visualizations of the simulated data and estimated graphs.

3. Methodological background

In Section 3.1, we briefly explain the Gaussian graphical model for normal data. Then we explain the birth-death MCMC algorithm for sampling from the joint posterior distribution in the Gaussian graphical models; for more detail see Mohammadi and Wit (2015b). In Section 3.2, we briefly describe the Gaussian copula graphical model, which can deal with non-Gaussian, discrete or mixed data. Then we explain the Birth-death MCMC algorithm which is designed for the Gaussian copula graphical models; for more detail see Mohammadi *et al.* (2015).

3.1. Bayesian Gaussian graphical models

In graphical models, each variable is associated with a node and conditional dependence relationships among random variables are presented as a graph $G = (V, E)$ in which $V = \{1, 2, \dots, p\}$ specifies a set of nodes and a set of existing links $E \subset V \times V$ (Lauritzen 1996). Our focus here is on undirected graphs in where $(i, j) \in E$ is equivalent with $(j, i) \in E$. The absence of a link between two nodes specifies the pairwise conditional independence of these two variables given the remaining variables, while a link between two variables determines their conditional dependence.

In the Gaussian graphical models (GGMs), we assume the observed data follow a multivariate Gaussian distribution $\mathcal{N}_p(\mu, K^{-1})$, here we assume $\mu = 0$. Let $\mathbf{Z} = (Z^{(1)}, \dots, Z^{(n)})^T$ be the observed data of n independent samples, then the likelihood function is

$$Pr(\mathbf{Z}|K, G) \propto |K|^{n/2} \exp \left\{ -\frac{1}{2} \text{tr}(KU) \right\}, \quad (1)$$

where $U = \mathbf{Z}'\mathbf{Z}$.

In GGMs, the conditional independence is implied by the form of the precision matrix. Based on pairwise Markov property, variables i and j are conditionally independence given the remaining variables, if and only if $K_{ij} = 0$. This property implies that the links in graph $G = (V, E)$ correspond with the nonzero elements of precision matrix K , it means $E = \{(i, j) | K_{ij} \neq 0\}$. Given graph G , the precision matrix K is constrained to the cone \mathbb{P}_G of symmetric positive definite matrices with elements K_{ij} equal to zeros for all $(i, j) \notin E$.

We consider the G-Wishart distribution $W_G(b, D)$ as a prior distribution for the precision matrix K with density

$$Pr(K|G) = \frac{1}{I_G(b, D)} |K|^{(b-2)/2} \exp \left\{ -\frac{1}{2} \text{tr}(DK) \right\} 1(K \in \mathbb{P}_G), \quad (2)$$

where $b > 2$ is the degree of freedom, D is a symmetric positive definite matrix, $I_G(b, D)$ is the normalizing constant with respect to the graph G and $1(x)$ evaluates to 1 if x holds and

to 0 otherwise. The G-Wishart distribution is a well-known prior for the precision matrix, since it represents the conjugate prior for normally distributed data.

When G is complete the G-Wishart distribution reduces to the standard Wishart distribution, hence, its normalizing constant has an explicit form (Muirhead 1982). Also, for decomposable graphs, the normalizing constant has an explicit form (Roverato 2002). But, for non-decomposable graphs, the normalizing constant does not have an explicit form.

Since the G-Wishart prior is a conjugate prior to the likelihood (1), the posterior distribution of K is

$$Pr(K|\mathbf{Z}, G) = \frac{1}{I_G(b^*, D^*)} |K|^{(b^*-2)/2} \exp \left\{ -\frac{1}{2} \text{tr}(D^* K) \right\},$$

where $b^* = b + n$ and $D^* = D + S$, that is, $W_G(b^*, D^*)$.

Direct sampler from G-Wishart

Several sampling methods from G-Wishart distribution have been proposed; to review existing methods see Wang and Li (2012). More recently, Lenkoski (2013) have developed an exact sampling algorithm to sample from G-Wishart distribution, which borrows an idea from Hastie, Tibshirani, and Friedman (2009). The algorithm is as follows.

Algorithm 1 Given a graph $G = (V, E)$ with precision matrix K and $\Sigma = K^{-1}$

- 1: Set $\Omega = \Sigma$
 - 2: **repeat**
 - 3: **for** $i = 1, \dots, p$ **do**
 - 4: Let $N_i \subset V$ be the neighbors set of node i in G . Form Ω_{N_i} and $\Sigma_{N_i, i}$ and solve $\hat{\beta}_i^* = \Omega_{N_i}^{-1} \Sigma_{N_i, i}$
 - 5: Form $\hat{\beta}_i \in R^{p-1}$ by padding the elements of $\hat{\beta}_i^*$ to the appropriate locations and zeros in those locations not connected to i in G
 - 6: Update $\Omega_{i, -i}$ and $\Omega_{-i, i}$ with $\Omega_{-i, -i} \hat{\beta}_i$
 - 7: **end for**
 - 8: **until** convergence
 - 9: **return** $K = \Omega^{-1}$
-

In the **BDgraph** package, we use Algorithm 1 to sample from the posterior distribution of the precision matrix. Besides, we implement the algorithm for general purposes in our package as a function `rgwish`; see the R code below for an illustration.

```
R> graph <- toeplitz( c( 0, 1, rep( 0, 2 ) ) )
R> graph
```

```
      [,1] [,2] [,3] [,4]
[1,]    0    1    0    0
[2,]    1    0    1    0
[3,]    0    1    0    1
[4,]    0    0    1    0
```

```
R> sample <- rgwish( n = 1, G = graph, b = 3, D = diag(4) )
R> round( sample, 2 )
```

```
      [,1] [,2] [,3] [,4]
[1,]  2.10 0.88 0.00 0.00
[2,]  0.88 2.75 0.23 0.00
[3,]  0.00 0.23 4.14 0.81
[4,]  0.00 0.00 0.81 4.22
```

BDMCMC algorithm for GGMs

Consider the joint posterior distribution of K and the graph G given by

$$Pr(K, G | \mathbf{Z}) \propto Pr(\mathbf{Z} | K) Pr(K | G) Pr(G). \quad (3)$$

For the graph-prior, as a non-informative prior, we consider a uniform distribution over all graph space, $pr(G) \propto 1$. For the prior distribution of K condition on graph G we consider a G-Wishart $W_G(b, D)$.

Here, we consider a computationally efficient birth-death MCMC sampling algorithm proposed by [Mohammadi and Wit \(2015b\)](#) for the Gaussian graphical models. The algorithm is based on a continuous time birth-death Markov process in which the algorithm explores over the graph space by adding/removing a link in a birth/death event.

In the birth-death process, at a particular pair of graph $G = (V, E)$ with precision matrix K , each link dies independently of the rest as a Poisson process with death rate $\delta_e(K)$. Since the links are independent, the overall death rate is $\delta(K) = \sum_{e \in G} \delta_e(K)$. Birth rates $\beta_e(K)$ for $e \notin G$ are defined similarly. Thus the overall birth rate is $\beta(K) = \sum_{e \notin G} \beta_e(K)$.

Since the birth and death events are independent Poisson processes, the time between two successive events exponentially distributed with mean $1/(\beta(K) + \delta(K))$. The time between successive events can be considered as support for any particular instance of graph G . The probability of the birth and death events are

$$Pr(\text{birth of link } e) = \frac{\beta_e(K)}{\beta(K) + \delta(K)}, \quad \text{for each } e \notin G, \quad (4)$$

$$Pr(\text{death of link } e) = \frac{\delta_e(K)}{\beta(K) + \delta(K)}, \quad \text{for each } e \in G. \quad (5)$$

The birth and death rates of links occur in continuous time with the rates determined by the stationary distribution of the process. The algorithm is designed in such a way that the stationary distribution equals the target joint posterior distribution of the graph and the precision matrix (3).

[Mohammadi and Wit \(2015b, Section 3\)](#) prove by considering the birth and death rates as ratios of joint posterior distributions, as below, the birth-death MCMC sampling algorithm converges to the target joint posterior distribution of the graph and the precision matrix, if

$$\beta_e(K) = \frac{Pr(G^{+e}, K^{+e} | \mathbf{Z})}{Pr(G, K | \mathbf{Z})}, \quad \text{for each } e \notin G, \quad (6)$$

$$\delta_e(K) = \frac{Pr(G^{-e}, K^{-e} | \mathbf{Z})}{Pr(G, K | \mathbf{Z})}, \text{ for each } e \in G, \quad (7)$$

in which $G^{+e} = (V, E \cup \{e\})$ and $K^{+e} \in \mathbb{P}_{G^{+e}}$ and similarly $G^{-e} = (V, E \setminus \{e\})$ and $K^{-e} \in \mathbb{P}_{G^{-e}}$. Based on the above rates, we determine our BDMCMC algorithm as below.

Algorithm 2 Given a graph $G = (V, E)$ with a precision matrix K

for N iteration **do**

1. **Sample from the graph.** Based on birth and death process

1.1. Calculate the birth rates by (6) and $\beta(K) = \sum_{e \in \notin G} \beta_e(K)$

1.2. Calculate the death rates by (7) and $\delta(K) = \sum_{e \in G} \delta_e(K)$

1.3. Calculate the waiting time by $W(K) = 1/(\beta(K) + \delta(K))$

1.4. Simulate the type of jump (birth or death) by (4) and (5)

2. **Sample from the precision matrix.** By using Algorithm 1.

end for

We design our BDMCMC sampling algorithm in such a way that, we sample from (G, K) in each step of jumping to the new state, e.g., $\{t_1, t_2, \dots\}$ in Figure 2. For efficient inference, we compute the sample means based on the Rao-Blackwellized estimator (Cappé, Robert, and Rydén 2003, Section 2.5); see e.g., (12).

Note, our main aim is to estimate the posterior distribution of the graphs based on the data, $Pr(G | \text{data})$. By using the Rao-Blackwellized estimator the estimated posterior distribution of the graphs are proportion to the total waiting times of each graph; see Figure 2.

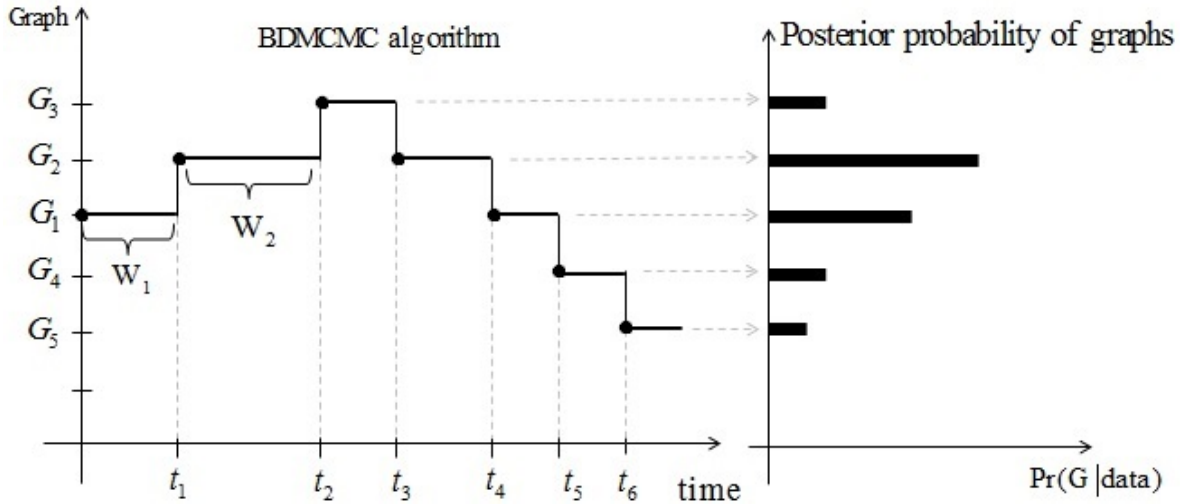


Figure 2: This image visualizes the Algorithm 2. Left side is a continuous time BDMCMC sampling algorithm where $\{W_1, W_2, \dots\}$ denote waiting times and $\{t_1, t_2, \dots\}$ denote jumping times. Right side denotes the estimated posterior probability of the graphs which are proportional to the total of their waiting times, according to the Rao-Blackwellized estimator.

3.2. Gaussian copula graphical models

In practice, we encounter both discrete and continuous variables; Gaussian copula graphical modelling has been proposed to describe dependencies between such heterogeneous variables. Let \mathbf{Y} (as an observed data) be a collection of continuous, binary, ordinal or count variables with the marginal distribution F_j of Y_j and F_j^{-1} its pseudo inverse. Towards constructing a joint distribution of \mathbf{Y} , we introduce a multivariate Gaussian latent variable as follows

$$\begin{aligned} Z_1, \dots, Z_n &\stackrel{iid}{\sim} \mathcal{N}(0, \Gamma(K)), \\ Y_{ij} &= F_j^{-1}(\Phi(Z_{ij})), \end{aligned} \quad (8)$$

where $\Gamma(K)$ is the correlation matrix for a given precision matrix K . The joint distribution of \mathbf{Y} is given by

$$Pr(Y_1 \leq Y_1, \dots, Y_p \leq Y_p) = C(F_1(Y_1), \dots, F_p(Y_p) \mid \Gamma(K)), \quad (9)$$

where $C(\cdot)$ is the Gaussian copula given by

$$C(u_1, \dots, u_p \mid \Gamma) = \Phi_p(\Phi^{-1}(u_1), \dots, \Phi^{-1}(u_p) \mid \Gamma),$$

with $u_v = F_v(Y_v)$ and $\Phi_p(\cdot)$ is the cumulative distribution of multivariate Gaussian and $\Phi(\cdot)$ is the cumulative distribution of univariate Gaussian distributions. It follows that $Y_v = F_v^{-1}(\Phi(Z_v))$ for $v = 1, \dots, p$. If all variables are continuous then the margins are unique; thus zeros in K imply conditional independence, as in Gaussian graphical models (Hoff 2007). For discrete variables, the margins are not unique but still well-defined (Nelsen 2007).

In semiparametric copula estimation, the marginals are treated as nuisance parameters and estimated by the rescaled empirical distribution. The joint distribution in (9) is then parametrized only by the correlation matrix of the Gaussian copula. We are interested to infer the underlying graph structure of the observed variables \mathbf{Y} implied by the continuous latent variables \mathbf{Z} . Since \mathbf{Z} are unobservable we follow the idea of Hoff (2007) to associate them to the observed data as follows.

Given the observed data \mathbf{Y} from a sample of n observations, we constrain the latent samples \mathbf{Z} to belong to the set

$$\mathcal{D}(\mathbf{Y}) = \{\mathbf{Z} \in \mathbb{R}^{n \times p} : L_j^r(\mathbf{Z}) < z_j^{(r)} < U_j^r(\mathbf{Z}), r = 1, \dots, n; j = 1, \dots, p\},$$

where

$$L_j^r(\mathbf{Z}) = \max \left\{ Z_j^{(k)} : Y_j^{(s)} < Y_j^{(r)} \right\} \text{ and } U_j^r(\mathbf{Z}) = \min \left\{ Z_j^{(s)} : Y_j^{(r)} < Y_j^{(s)} \right\}. \quad (10)$$

Following Hoff (2007) we infer on the latent space by substituting the observed data \mathbf{Y} with the event $\mathcal{D}(\mathbf{Y})$ and defined the likelihood as

$$Pr(\mathbf{Y} \mid K, G, F_1, \dots, F_p) = Pr(\mathbf{Z} \in \mathcal{D}(\mathbf{Y}) \mid K, G) Pr(\mathbf{Y} \mid \mathbf{Z} \in \mathcal{D}(\mathbf{Y}), K, G, F_1, \dots, F_p).$$

The only part of the observed data likelihood relevant for inference on K is $Pr(\mathbf{Z} \in \mathcal{D}(\mathbf{Y}) \mid K, G)$. Thus, the likelihood function is given by

$$Pr(\mathbf{Z} \in \mathcal{D}(\mathbf{Y}) \mid K, G) = Pr(\mathbf{Z} \in \mathcal{D}(\mathbf{Y}) \mid K, G) = \int_{\mathcal{D}(\mathbf{Y})} Pr(\mathbf{Z} \mid K, G) d\mathbf{Z} \quad (11)$$

where $Pr(\mathbf{Z} | K, G)$ is defined in (1).

BDMCMC algorithm for GCGMs

The joint posterior distribution of the graph G and precision matrix K for our Gaussian copula graphical model is as follow

$$Pr(K, G | Z \in \mathcal{D}(\mathbf{Y})) \propto Pr(K, G) Pr(Z \in \mathcal{D}(\mathbf{Y}) | K, G).$$

Sampling from this posterior distribution can be done by using the birth-death MCMC algorithm. Mohammadi *et al.* (2015) have developed and extended the birth-death MCMC algorithm for more general case of GCGMs. We summarize their algorithm as follows.

Algorithm 3 Given a graph $G = (V, E)$ with a precision matrix K

for N iteration **do**

1. **Sample the latent data.** For each $r \in V$ and $j \in \{1, \dots, n\}$, we update the latent values from its full conditional distribution as follows

$$Z_r^{(j)} | Z_{V \setminus \{r\}} = z_{V \setminus \{r\}}^{(j)}, K \sim N(-\sum_{r'} K_{rr'} z_{r'}^{(j)} / K_{rr}, 1/K_{rr}),$$

truncated to the interval $[L_r^j(\mathbf{Z}), U_r^j(\mathbf{Z})]$ in (10).

2. **Sample from the graph.** Same as Step 1 in the Algorithm 2.

3. **Sample from the precision matrix.** By using Algorithm 1.

end for

In each iteration of the Algorithm 3, first conditional on the observed data (\mathbf{Y}) we sample from the latent variables (\mathbf{Z}). The other steps are the same as the Algorithm 2.

Remark. For the cases that all variables are continuous, we do not need to sample from latent variables in each iteration of the Algorithm 2, since all margins in Gaussian copula are unique. Therefore, for these cases, first based on Gaussian copula approach, we transfer our non-Gaussian data to Gaussian then we run the Algorithm 2.

4. The BDgraph environment

The **BDgraph** package provides a set of comprehensive tools related to Bayesian graphical models; here, we describe the essential functions available in the package.

4.1. Description of the bdgraph function

The main function of the package is **bdgraph**, which includes two Bayesian frameworks (GGMs and GCGMs). This function is based on an underlying sampling engine (Algorithms 2 and 3) takes the model definition and returns a sequence of samples from the joint posterior distribution of the graph and precision matrix (3), given the supplied data. By using the following function

```
bdgraph( data, n = NULL, method = "ggm", iter = 5000, burnin = iter / 2,
         b = 3, D = NULL, Gstart = "empty" )
```

we can sample from our target joint posterior distribution. `bdgraph` returns an object of S3 class type “bdgraph”. The functions `plot`, `print` and `summary` are working with the object “bdgraph”. The input data can be a `matrix` or a `data.frame` ($n \times p$) or a covariance matrix; it can also be an object of class “simulate”, which is output of the function `bdgraph.sim`.

The argument `method` determines the type of BDMCMC algorithm (Algorithms 2 and 3). Option “ggm” implements the BDMCMC algorithm based on the Gaussian graphical models (Algorithm 2). It is designed for the data that follow Gaussianity assumption. Option “gsgm” implements the BDMCMC algorithm based on the Gaussian copula graphical models (Algorithm 3). It is designed for the data that do not follow the Gaussianity assumption such as non-Gaussian continuous, discrete or mixed data. This option can deal with missing data.

4.2. Description of the `bdgraph.sim` function

The function `bdgraph.sim` is designed to simulate different types of data sets with different graph structures. The function

```
bdgraph.sim( n = 2, p = 10, graph = "random", size = NULL, prob = 0.2,
             class = NULL, type = "Gaussian", cut = 4, b = 3, D = diag(p),
             K = NULL, sigma = NULL, mean = 0, vis = FALSE )
```

can simulate multivariate Gaussian, non-Gaussian, discrete and mixed data with different undirected graph structures, including “random”, “cluster”, “hub”, “scale-free”, “circle” and “fixed” graphs. Users can determine the sparsity level of the obtained graph by option `prob`. By this function, users can generate mixed data from “count”, “ordinal”, “binary”, “Gaussian” and “non-Gaussian” distributions. `bdgraph.sim` returns an object of the S3 class type “simulate”. The `plot`, `print` and `summary` functions are working with this object type.

4.3. Description of the `plotcoda` and `traceplot` functions

In general, convergence in MCMC approaches can be difficult to evaluate. From a theoretical point of view, the sampling distribution will converge to the target joint posterior distribution as the number of iteration increases to infinity. We normally have little theoretical insight about how quickly convergence “KICKS IN”; therefore we rely on post hoc testing of the sampled output. In general, the sample is divided into two parts: a “burn-in” part of sample and the remainder, in which the chain is considered to have converged sufficiently close to the target posterior distribution. Two questions then arise: How many samples are sufficient? How long should the burn-in period be?

The `plotcoda` and `traceplot` are two visualization functions in the **BDgraph** package for checking the convergence of the BDMCMC algorithm. The function

```
plotcoda( output, thin = NULL, main = NULL, links = TRUE, ... )
```

provides the trace of posterior inclusion probability of all possible links to check convergence of the BDMCMC algorithm. The function

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

provides the trace of graph size to check convergence of the BDMCMC algorithm. The input of these two functions is the `output` of `bdgraph` function, which is the sample drawn from the joint posterior distribution of graph and precision matrix.

4.4. Description of the `phat` and `select` functions

In the **BDgraph** package, the functions `phat` and `select` provide the potential tools to do statistical inference from the samples drawn from the joint posterior distribution. The function

```
phat( output, round = 3 )
```

provides the estimated posterior link inclusion probabilities for all possible links. These probabilities, for all possible link $e = (i, j)$ in graph G , can be calculated by using the Rao-Blackwellization (Cappé *et al.* 2003, Section 2.5) as

$$Pr(e \in G | data) = \frac{\sum_{t=1}^N 1(e \in G^{(t)}) W(K^{(t)})}{\sum_{t=1}^N W(K^{(t)})}, \quad (12)$$

where N is the number of iteration and $W(K^{(t)})$ are the weights of the graph $G^{(t)}$ with the precision matrix $K^{(t)}$.

The function

```
select( output, cut = NULL, vis = FALSE )
```

provides the inferred graph, which is the graph with the highest posterior probability as a default. By option `cut`, users can select the inferred graph based on the estimated posterior link inclusion probabilities.

4.5. Description of the `compare` and `plotroc` functions

The function `compare` and `plotroc` are designed to check and compare the performance of the selected graph. This function is particularly useful for simulation studies. With the function

```
compare( G, est, est2 = NULL, colnames = NULL, vis = FALSE )
```

we can check the performance of our BDMCMC algorithm and compare it with other alternative approaches. This function provides several measures such as balanced F -score measure (Baldi, Brunak, Chauvin, Andersen, and Nielsen 2000) which is defined as follows

$$F_1\text{-score} = \frac{2TP}{2TP + FP + FN}, \quad (13)$$

where TP, FP and FN are the number of true positives, false positives and false negatives, respectively. The F_1 -score lies between 0 and 1, where 1 is for perfect identity and 0 for worst case.

The function

```
plotroc( G, prob, prob2 = NULL, cut = 20, smooth = FALSE )
```

provides a ROC plot for visualization comparison based on the estimated posterior link inclusion probabilities (12).

5. User interface by toy example

In this section, we illustrate the user interface of the **BDgraph** package with a simple simulation example. We perform all the computations on an Intel(R) Core(TM) i5 CPU 2.67GHz processor. By using the function `bdgraph.sim` we simulate 60 observations ($n = 60$) from a multivariate Gaussian distribution with 8 variables ($p = 8$) and “scale-free” graph structure, as below

```
R> data.sim <- bdgraph.sim( n = 60, p = 8, graph = "scale-free",
                           type = "Gaussian" )
R> round( head( data.sim $ data, 4), 2 )
```

	[,1]	[,2]	[,3]	[,4]	[,5]	[,6]	[,7]	[,8]
[1,]	-0.74	1.40	-0.85	0.56	-0.37	0.15	0.93	0.25
[2,]	0.67	-0.53	0.08	0.24	0.30	0.77	-0.44	-0.41
[3,]	-0.94	-1.74	1.25	-0.86	-0.25	-1.54	0.14	0.08
[4,]	0.34	-0.45	-0.53	-0.33	-0.28	-0.54	0.32	2.90

5.1. Running the BDMCMC algorithm

Since the generated data follow Gaussianity assumption, we run the BDMCMC algorithm which is based on the Gaussian graphical models. Therefore, we choose `method = "ggm"`, as follow

```
R> output.ggm <- bdgraph( data = data.sim, method = "ggm", iter = 50000 )
```

Running this function takes around 5 second which is computationally fast as main sampling part is in C++. Since the function `bdgraph` returns an object of class `S3`, users can see the summary result of BDMCMC algorithm as follows

```
R> summary( output.ggm )
```

```
$selected_graph
  1 2 3 4 5 6 7 8
1 . . . 1 . . . 1
2 . . 1 1 1 . . 1
3 . 1 . . . . .
4 1 1 . . . . 1 1
5 . 1 . . . 1 . .
6 . . . . 1 . 1 .
7 . . . 1 . 1 . .
8 1 1 . 1 . . . .
```

\$phat

	1	2	3	4	5	6	7	8
1	.	0.01	.	1.0	0.03	.	.	0.83
2	.	.	1	1.0	0.98	.	0.10	1.00
3	.	.	.	0.1	0.14	.	.	0.12
4	0.04	.	0.60	0.95
5	1	.	0.16
6	0.94	.
7
8

\$Khat

	[,1]	[,2]	[,3]	[,4]	[,5]	[,6]	[,7]	[,8]
[1,]	3.247	-0.002	0.000	-1.324	0.016	0.000	0.000	0.309
[2,]	-0.002	3.910	1.497	-2.749	-1.082	0.000	-0.046	0.746
[3,]	0.000	1.497	5.275	0.099	-0.061	0.000	0.000	0.044
[4,]	-1.324	-2.749	0.099	8.281	0.013	-0.001	-0.506	-0.730
[5,]	0.016	-1.082	-0.061	0.013	4.979	-1.432	0.000	0.065
[6,]	0.000	0.000	0.000	-0.001	-1.432	2.349	0.587	0.000
[7,]	0.000	-0.046	0.000	-0.506	0.000	0.587	3.091	0.000
[8,]	0.309	0.746	0.044	-0.730	0.065	0.000	0.000	0.667

The summary result are the adjacency matrix of the graph with the highest posterior probability (**selected_graph**), the estimated posterior probabilities of all possible links (**phat**) and the estimated precision matrix (**Khat**).

In addition, function **summary** reports a visualization summary of the results as we can see in Figure 3. In the top-left is the graph with the highest posterior probability. In the top-right is the estimated posterior probabilities of all the graphs which are visited by the BDMCMC algorithm. It indicates our algorithm visits more than 600 different graphs and the posterior probability of the selected graph is around 0.22. In the bottom-left is the estimated posterior probabilities of the size of graphs. It indicates our algorithm visited mainly graphs with size between 6 and 14 links. In the bottom-right is the trace of our algorithm based on the size of the graphs.

5.2. Convergence check

In our simulation example, we run the BDMCMC algorithm for 50,000 iteration, 25,000 of which as burn-in. To check whether the number of iteration is enough or not, we run

```
R> plotcoda( output.ggm )
```

The results in Figure 4 indicates that our BDMCMC algorithm, roughly speaking, converges after 20,000 iteration and that burn-in of 25,000 is sufficient.

5.3. Comparison and goodness-of-fit

The function **compare** provides several measures for checking the performance of our algorithms and compared with other alternative approaches, with respect to the true graph

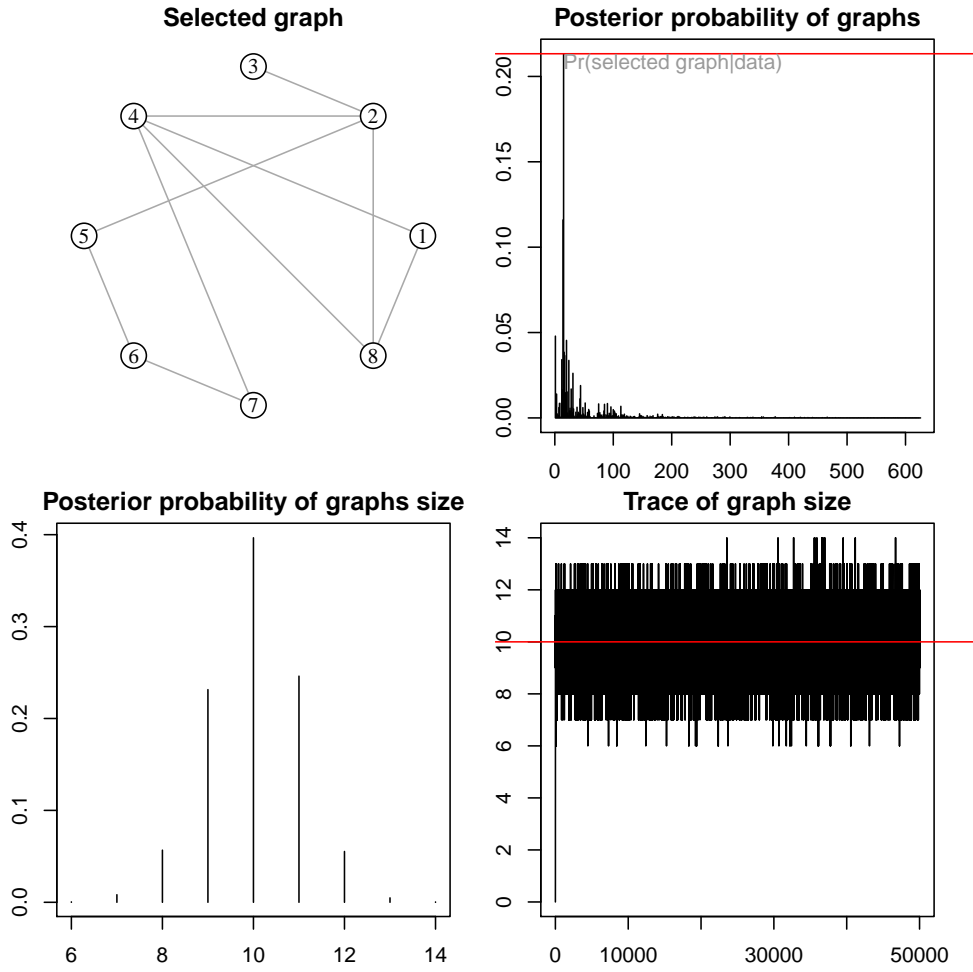


Figure 3: Visualization summary of the simulation data based on the output of `bdgraph` function. Figure in the top-left is the inferred graph with the highest posterior probability. Figure in the top-right is the estimated posterior probabilities of all visited graphs. Figure in the bottom-left is the estimated posterior probabilities of all visited graphs based on the size of the graph. Figure in the bottom-right is the trace of our algorithm based on the size of the graphs.

structure. To check the performance of our both algorithms (Algorithms 2 and 3), we also run the Algorithms 3 with the same condition as bellow

```
R> output.gcgm <- bdgraph( data = data.sim, method = "gcgm", iter = 50000 )
```

where `output.ggm` is 50,000 samples from the joint posterior distribution which are generated based on the Gaussian copula graphical models.

Users can compare the performance of these two algorithms by using the code

```
R> plotroc( data.sim, output.ggm, output.gcgm )
```

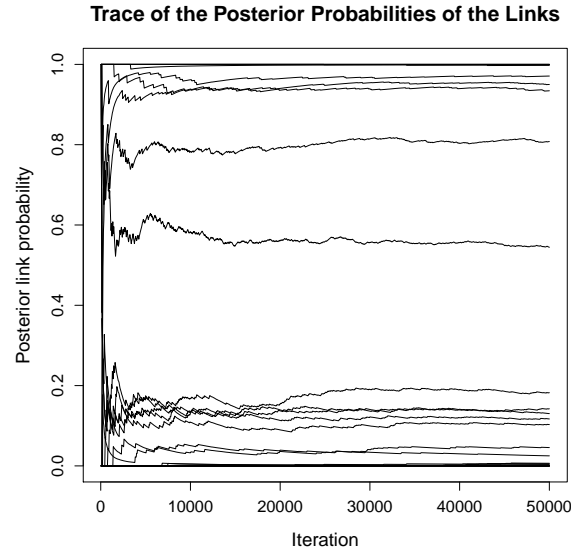


Figure 4: Plot for monitoring the convergence of BDMCMC algorithm. It shows the trace of the cumulative posterior probability of the all possible links of the graph.

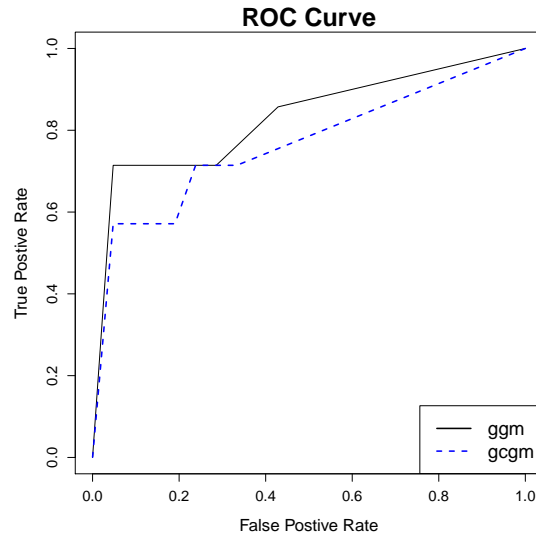


Figure 5: ROC plot to compare the performance of the GGM and GCGM approaches.

As expected, the result indicates that the “GGM” approach performs slightly better than the “GCGM”, since the data is generated from a Gaussian graphical model.

Here, we also compare our approach to the Meinshausen-Buhlmann approach `mb` (Meinshausen and Buhlmann 2006) by using the **huge** package (Zhao *et al.* 2014). We consider the following code

```
R> install.packages( "huge" )
R> library( "huge" )
```



```
R> huge <- huge( data.sim $ data, method = "mb" )
R> output.huge <- huge.select( mb )

R> compare( data.sim, output.ggm, output.gcgm, output.huge, vis = TRUE,
            colnames = c("True graph", "BDgraph(ggm)", "BDgraph(gcgm)",
                          "huge(mb)") )
```

	True graph	BDgraph(ggm)	BDgraph(gcgm)	huge(mb)
true positive	7	5	4	5
true negative	21	16	17	14
false positive	0	5	4	7
false negative	0	2	3	2
true positive rate	1	0.71	0.57	0.71
false positive rate	0	0.24	0.19	0.33
accuracy	1	0.75	0.75	0.68
balanced F-score	1	0.59	0.53	0.53
positive predictive	1	0.50	0.50	0.41

This result indicates that the **huge** package based on the **mb** discovers 5 true links, in addition, it finds 7 extra links which are not in the true graph. See Figure 6 for visualization. For more comparison see [Mohammadi and Wit \(2015b, Section 4\)](#).

6. Application to real data sets

In this section, we analyze two data sets from biology and sociology, by using the functions that are available in the **BDgraph** package. In Section 6.1, we analyze a Labor force survey data set, which are mixed data. In Section 6.2, we analyze Human gene expression data, which are high-dimensional data that do not follow the Gaussianity assumption. Both data sets are available in our package.

6.1. Application to labor force survey data

[Hoff \(2007\)](#) analyzes the multivariate dependencies among income, education and family background, by using data concerning 1002 males in the U.S labor force. The data is available in our package. Users can call the data via

```
R> data( "surveyData" )
R> dim( surveyData )
```

```
[1] 1002    7
```

```
R> head( surveyData, 5 )
```

	income	degree	children	pincome	pdegree	pchildren	age
[1,]	NA	1	3	3	1	5	59
[2,]	11	0	3	NA	0	7	59

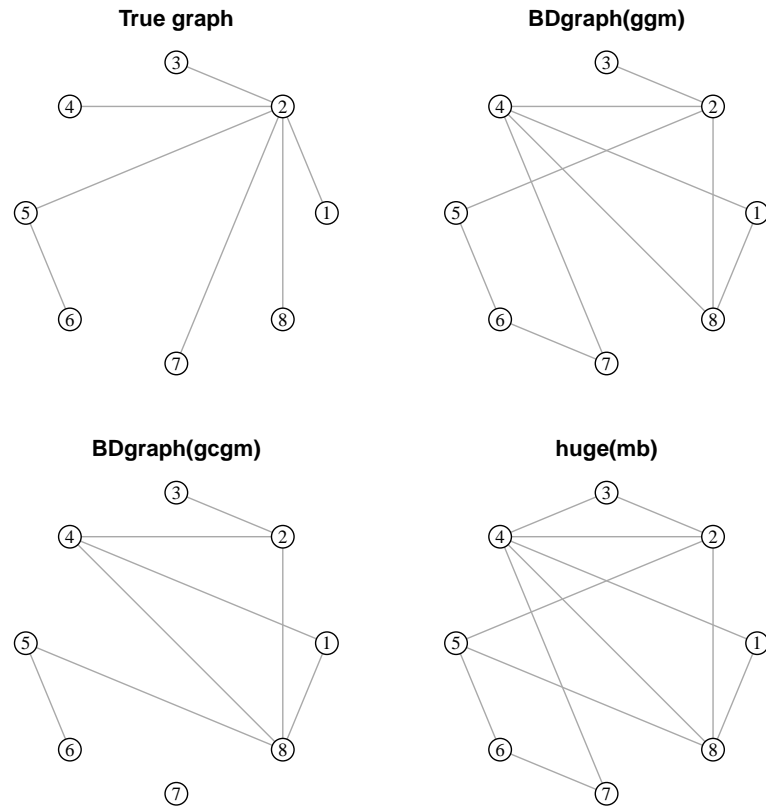


Figure 6: Comparing the performance of the **BDgraph** with **huge** packages. The graph in the top-left is the true graph. The graph in the top-right is the selected graph based on Gaussian graphical models. The graph in the bottom-left is the selected graph based on Gaussian copula graphical models. The graph in the bottom-right is the selected graph based on the **mb** approach in the **huge** package.

[3,]	8	1	1	NA	0	9	25
[4,]	25	3	2	NA	0	5	55
[5,]	100	3	2	4	3	2	56

Missing data are indicated by NA and in general the rate of missing data is around 0.09 with higher rates for variables **income** and **pincome**. In this data set, we have seven observed variables as follows

income: An ordinal variable indicating the respondent's income in 1000s of dollars.

degree: An ordinal variable with five categories indicating the respondent's highest educational degree.

children: A count variable indicating the number of children of the respondent.

pincome: An ordinal variable with five categories indicating financial status of respondent's parents.

pdegree: An ordinal variable with five categories indicating the highest educational degree of the respondent's parents.

pchildren: A count variable indicating the number of children of the respondent's parents.

age: A count variable indicating the respondent's age in years.

Since those variables are measured on various scales, the marginal distributions are heterogeneous, which makes the study of their joint distribution very challenging. However, we can apply our Bayesian framework based on the Gaussian copula graphical models to this data set. Thus, we run the function `bdgraph` with option `method = "gcgm"`. For the prior distributions of the graph and precision matrix, as default of the function `bdgraph`, we place a uniform distribution as a uninformative prior on the graph and a G-Wishart $W_G(3, I_7)$ on the precision matrix. We run our function for 50,000 iteration with 25,000 as burn-in.

```
R> output <- bdgraph( data = surveyData, method = "gcgm", iter = 50000 )
R> summary( output )
```

`$selected_graph`

	income	degree	children	pincome	pdegree	pchildren	age
income	.	1	1	.	.	.	1
degree	1	.	.	.	1	1	.
children	1	.	.	.	1	1	1
pincome	1	1	.
pdegree	.	1	1	1	.	1	1
pchildren	.	1	1	1	1	.	.
age	1	.	1	.	1	.	.

`$phat`

	income	degree	children	pincome	pdegree	pchildren	age
income	.	1	1.00	0.27	0.12	0.05	1.00
degree	.	.	0.53	0.03	1.00	0.84	0.11
children	.	.	.	0.14	0.88	1.00	1.00
pincome	1.00	0.53	0.07
pdegree	0.99	1.00
pchildren	0.03
age

`$Khat`

	[,1]	[,2]	[,3]	[,4]	[,5]	[,6]	[,7]
[1,]	3.546	-1.707	-0.949	-0.104	-0.041	0.019	-1.219
[2,]	-1.707	4.127	0.321	0.009	-1.853	0.413	-0.056
[3,]	-0.949	0.321	8.875	0.086	0.737	-1.074	-4.392
[4,]	-0.104	0.009	0.086	5.686	-2.050	0.355	0.036
[5,]	-0.041	-1.853	0.737	-2.050	6.510	1.029	1.028
[6,]	0.019	0.413	-1.074	0.355	1.029	7.826	0.022
[7,]	-1.219	-0.056	-4.392	0.036	1.028	0.022	9.250

The result of the function `summary` are the adjacency matrix of the graph with the highest

posterior probability (`selected_graph`), estimated posterior probabilities of all possible links (`phat`) and estimated precision matrix (`Khat`).

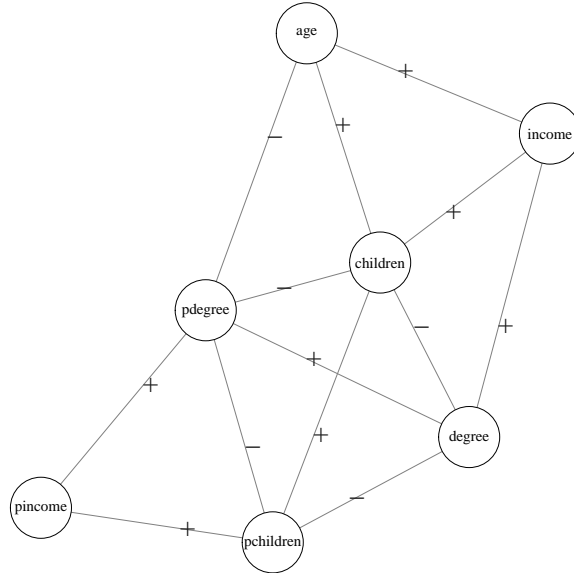


Figure 7: Graph with the highest posterior probability for the labor force survey data based on the output from **bdgraph**. Sign “+” represents a positively correlated relationship between associated variables and “-” represents a negatively correlated relationship.

Figure 7 shows the selected graph which is a graph with the highest posterior probability. Links in the graph are indicated by signs “+” and “-”, which represents a positively and negatively correlated relationship between associated variables, respectively.

The result indicate that education, fertility and age determinate income, since there are highly positively correlated relationships between income and those three variables, with posterior probability equal to one for all. It shows that respondent’s education and fertility are negatively correlated with posterior probability equal to 0.67. The respondent’s education is certainly related to his parent’s education, since there is positively correlated relationship with posterior probability equal to one. Moreover, the result indicate that relationships between income, education and fertility hold across generations.

For this data set, Hoff (2007) estimated the conditional independence between variables by inspecting whether the 95% credible intervals for the associated regression parameters do not contain zero. Our result is the same with Hoff’s result except for one link. Our result indicate there is a strong relationship between parent’s education (`pdegree`) and fertility (`child`), which is not selected by Hoff.

6.2. Application to human gene expression

Here, by using the functions that are available in the **BDgraph** package, we study the structure learning of the sparse graphs applied to the large-scale human gene expression data which was originally described by Stranger, Nica, Forrest, Dimas, Bird, Beazley, Ingle, Dunning, Flicek, Koller *et al.* (2007). They collected the data to measure gene expression in B-lymphocyte cells from Utah individuals of Northern and Western European ancestry. They consider 60

individuals whose genotypes are available online at <ftp://ftp.sanger.ac.uk/pub/genevar>. Here the focus is on the 3125 Single Nucleotide Polymorphisms (SNPs) that have been found in the 5' UTR (untranslated region) of mRNA (messenger RNA) with a minor allele frequency ≥ 0.1 . Since the UTR (untranslated region) of mRNA (messenger RNA) has been subject to investigation previously, it should have an important role in the regulation of the gene expression. The raw data were background corrected and then quantile normalized across replicates of a single individual and then median normalized across all individuals. Following [Bhadra and Mallick \(2013\)](#), among the 47,293 total available probes, we consider the 100 most variable probes that correspond to different Illumina TargetID transcripts. The data for these 100 probes are available in our package. To see the data, users can run the code

```
R> data( "geneExpression" )
R> dim( geneExpression )
```

```
[1] 60 100
```

The data consist of only 60 observations ($n = 60$) across 100 genes ($p = 100$). This data set is an interesting case study for graph structure learning, as it has been used in ([Bhadra and Mallick 2013](#); [Mohammadi and Wit 2015b](#); [Gu, Cao, Ning, and Liu 2015](#)).

In this data set, all the variables are continuous but they do not follow the Gaussianity assumption, as you can see in Figure 8. Thus, we apply the Gaussian copula graphical models. Therefore, we run function `bdgraph` with option `method = "ggm"`. For the prior distributions of the graph and precision matrix, as default of the function `bdgraph`, we place a uniform distribution as a uninformative prior on graph and the G-Wishart $W_G(3, I_{100})$ on the precision matrix.

We run our function for 100,000 iteration with 50,000 as burn-in as follows

```
R> output <- bdgraph( data = geneExpression, method = "ggm", iter = 100000 )
R> select( output )
```

This function takes around 13 hours. The function `select` gives as a default the graph with the highest posterior probability, which has 991 links. We use the following code to visualize the ones that we believe have posterior probabilities larger than 0.995.

```
R> select( output, cut = 0.995, vis = TRUE )
```

By using option `vis = TRUE`, this function plots the selected graph. Figure 9 shows the selected graph with 266 links, for which the posterior inclusion probabilities (12) are greater than 0.995.

The function `phat` reports the estimated posterior probabilities of all possible links in the graph. For our data the output of this function is a 100×100 matrix. Figure 10 reports the visualization of that matrix.

Most of the links in our selected graph (graph with the highest posterior probability) conform the results in previous studies. For instance, [Bhadra and Mallick \(2013\)](#) found 54 significant interactions between genes, most of which are covered by our method. In addition, our approach indicates additional gene interactions with high posterior probabilities that are

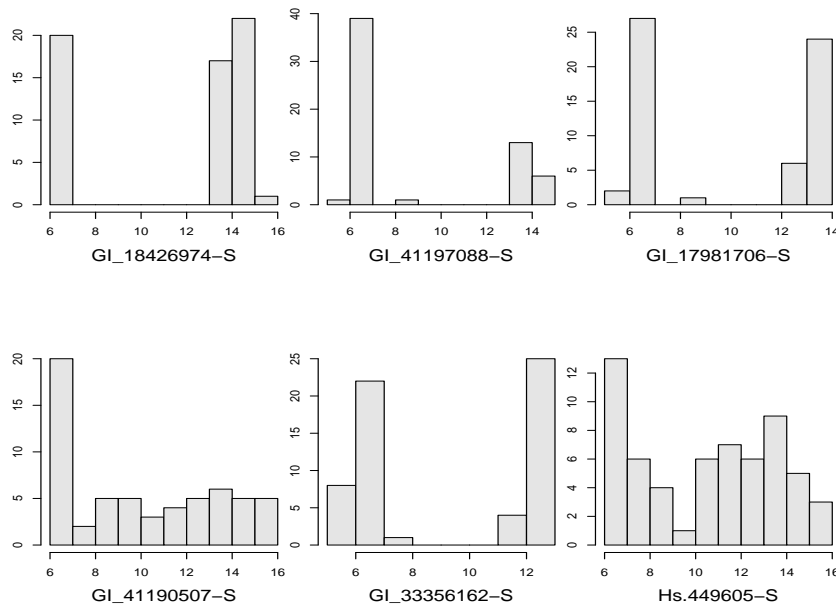


Figure 8: Univariate histograms of first 6 genes in human gene data set.

missed by previous work; thus our method may complement the analysis of human gene interaction networks.

7. Conclusion

The **BDgraph** package aims to help researchers in two ways. Firstly, the package provides a Bayesian framework which potentially can be extended, customized and adapted to address different requirements, in graphical models. Secondly, it is currently the only R package that provides a simple and complete range of tools for conducting Bayesian inference for graphical modelling based on conditional independence graph estimation.

We plan to maintain and develop the package in the future. Future versions of the package will contain more options for prior distributions of graph and precision matrix. On possible extension of our package, is to deal with outliers, by using robust Bayesian graphical modelling using Dirichlet **t**-Distributions (Finegold and Drton 2014; Mohammadi and Wit 2014). An implementation of this method would be desirable in real applications.

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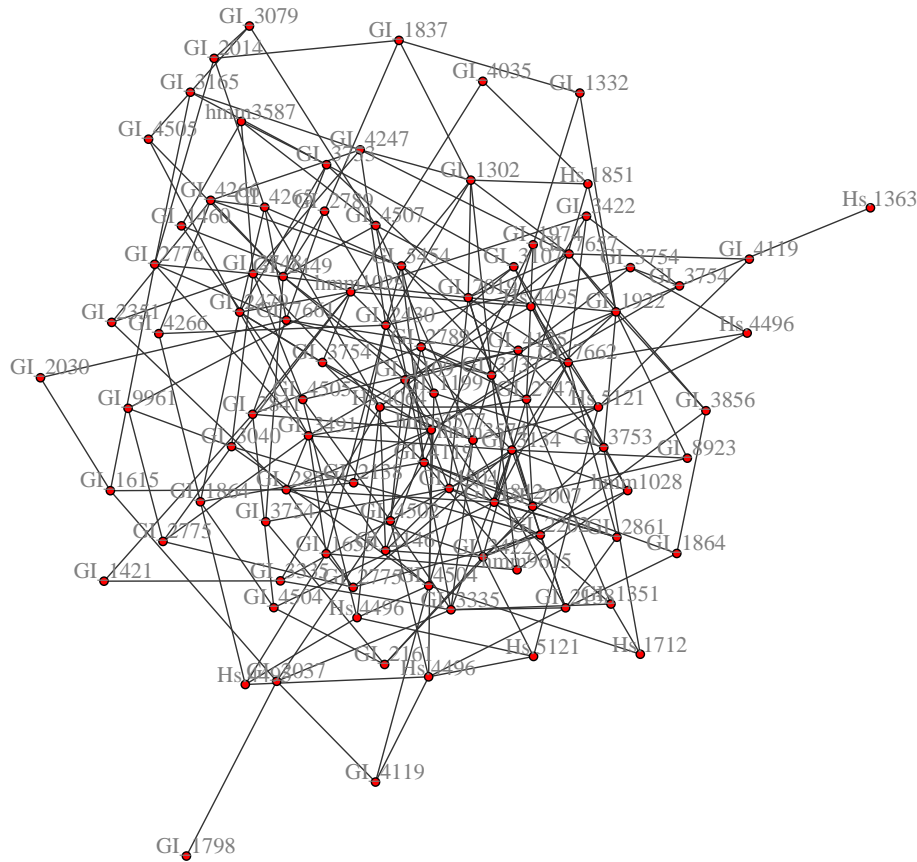


Figure 9: The inferred graph for the human gene expression data using Gaussian copula graphical models. This graph consists of links with posterior probabilities (12) larger than 0.995.

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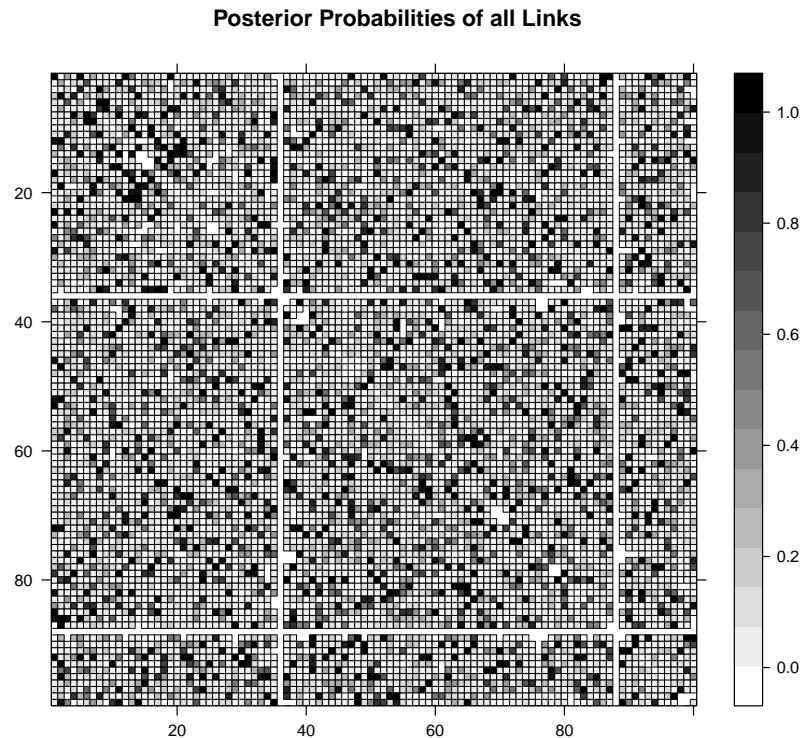


Figure 10: Image visualization of the estimated posterior probabilities for all possible links in the graph for the human gene expression data.

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