Regression Based Bayesian Approach for Nonparanormal Graphical Models

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Abstract

A nonparanormal graphical model is a semiparametric generalization of a Gaussian graphical model for continuous variables in which it is assumed that the variables follow a Gaussian graphical model only after some unknown smooth monotone transformations. We consider a Bayesian approach in the nonparanormal graphical model in which we put priors on the unknown transformations through random series based on B-splines. We use a regression formulation to construct the likelihood through the Cholesky decomposition on the underlying precision matrix of the transformed variables and put shrinkage priors on the regression coefficients. We apply a plug-in variational Bayesian algorithm for learning the sparse precision matrix and compare the performance to a posterior Gibbs sampling scheme in a simulation study. We finally apply the proposed methods to a real data set.

Keywords: Bayesian inference, Cholesky decomposition, nonparanormal graphical models, continuous shrinkage prior.

1. Introduction

The Gaussian graphical model (GGM) is a mathematical model commonly used in machine learning to describe conditional independence relationships among normally distributed random variables. Zeros in the inverse covariance matrix, or the precision matrix, indicate that the corresponding variables in the data set are conditionally independent given the rest of the variables in the data set, and this relationship is represented by the absence of an edge in the graph. Similarly, nonzero entries in the precision matrix are represented by edges in the graph and correspond to conditionally dependent variables in the data set. An extension of the GGM is the nonparanormal graphical model (Liu et al., 2009) in which the random variables are replaced with transformed variables that are assumed to be normally

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distributed. Liu et al. (2009) use a truncated empirical distribution function to estimate the functions and then estimate the precision matrix of the transformed variables using the graphical lasso. The Bayesian nonparanormal graphical method (Mulgrave and Ghosal, 2018) uses a random series B-splines prior to estimate the functions and a Student-t spike-and-slab prior to estimate the resulting precision matrix. These extensions differ from the Gaussian copula graphical model (Pitt et al., 2006; Dobra and Lenkoski, 2011; Liu et al., 2012; Mohammadi and Wit, 2017) in that we concurrently estimate the transformation functions and the precision matrices.

Estimation of a sparse precision matrix is necessary to learn structure in GGMs and nonparanormal graphical models. For unstructured precision matrices, a commonly used algorithm in the frequentist literature is the graphical lasso (Friedman et al., 2008). A great number of algorithms have been proposed to solve this problem including (Meinshausen and Buhlmann, 2006; Yuan and Liu, 2007; Friedman et al., 2008; Banerjee et al., 2008; d’Aspremont et al., 2008; Rothman et al., 2008; Lu, 2009; Scheinberg et al., 2010; Witten et al., 2011; Mazumder and Hastie, 2012b).

Analogous methods in the Bayesian literature use priors to aid the edge selection procedure. For instance, off-diagonal entries of the precision matrix may be set to zero by allowing a point mass at zero in the prior (Banerjee and Ghosal, 2015), but the posterior is harder to compute or sample from. A normal spike-and-slab prior (Wang, 2015) replaces the point mass at zero by a highly concentrated normal distribution around zero and similarly, a Laplace spike-and-slab prior (Gan et al., 2018) has been used. From a computational point of view, continuous shrinkage priors such as the horseshoe prior (Carvalho et al., 2009), the Dirichlet-Laplace prior (Bhattacharya et al., 2015), and generalized double exponential prior (Armagan et al., 2013), bring in the effects of both a point mass and a thick tail by a single continuous distribution with an infinite spike at zero.

Ideally, we seek solutions that guarantee a sparse positive definite matrix using continuous shrinkage priors. Since continuous shrinkage priors do not assign exact zeros, a variable selection procedure needs to be used to determine which of the small and nonzero elements should be specified as exactly zero. Methods that use spike and slab priors naturally incorporate variable selection, whereas methods that use alternative priors need a thresholding procedure. However, post-hoc thresholding procedures do not guarantee a positive definite precision matrix. The methods in Wang (2015) and Wang (2012) guarantee a positive definite matrix by way of the sampling algorithm. Wang (2012) and Peterson et al. (2013) use the double exponential prior and improve on its use for sparsity by allowing each double exponential prior to have its own shrinkage parameter. More recent methods estimate the inverse covariance matrix by using the normal spike and slab prior (Wang, 2015; Peterson et al., 2016; Li and McCormick, 2017; Li et al., 2017) for variable selection in the graphical model context. Lastly, the recently developed method to construct Gaussian graphical models by estimating the partial correlation matrix (Williams et al., 2018) uses a horseshoe prior for regularization and for sparsity, uses projection predictive selection, a method that allows for variable exclusion based on predictive utility, with good results.
Utilizing a Cholesky decomposition is an alternative way to incorporate the positive definiteness constraint on precision matrices, but is very dependent on the ordering of the variables (Pourahmadi, 2011). We consider a prior based on Cholesky decomposition of the precision matrix that reduces this dependence. We derive a sparsity constraint that ensures a weak order invariance in that it maintains the same order of sparsity in the rows of the precision matrix by increasing the order of sparsity down the rows of the lower triangular matrix. We construct a pseudo-likelihood through regression of each variable on the preceding ones. The approach nicely scales with dimension because it splits the very high dimensional original problem to several lower dimensional ones and is parallelizable. The method in Wong et al. (2013) is also based on Cholesky decomposition, but it uses a noninformative Jeffreys’ prior and the ordering issue of the Cholesky decomposition is not addressed.

We consider two different priors, the horseshoe and the Bernoulli-Gaussian (Soussen et al., 2011). These priors have clear interpretations of the probability of nonzero elements (Soussen et al., 2011, van der Pas et al., 2014), which allows us to effectively calibrate sparsity. The strength of the Bernoulli-Gaussian prior is that it leads to a sparse positive definite precision matrix that does not require thresholding and the strength of the horseshoe prior is a better model of sparsity than the Bernoulli-Gaussian prior due to its heavier tails. We compare the performance of the methods using both a variational Bayesian algorithm and a full Markov Chain Monte Carlo (MCMC) sampling scheme. Mean field variational Bayes (Jordan et al., 1999, Wainwright and Jordan, 2007) is an alternative to MCMC that allows for faster fitting by deterministic optimization. A variational Bayesian method for Gaussian graphical models is developed in Chen et al. (2011). An expectation conditional maximization approach is used by Li and McCormick (2017) in Gaussian copula graphical models. Our method differs from previous approaches in that we apply it on the Cholesky decomposition of a sparse precision matrix and address nonparanormal graphical models.

The paper is organized as follows. In the next section, we describe the model and the sparsity constraint. In Section 3, we describe the variational Bayesian algorithm. In Sections 4 and 5, we discuss particular priors and their corresponding Markov Chain Monte Carlo algorithms. In Section 6, we describe a thresholding procedure and in Section 7, we detail the tuning procedure. In Section 8, we present a simulation study. In Section 9, we describe a real data application.

2. Model and Priors

2.1 Nonparanormal Transformation

We put prior distributions on the unknown transformation functions through a random series based on B-splines. We begin with a normal prior on the coefficients of the B-splines, $\theta \sim N_J(\zeta, \sigma^2 I)$, where $\sigma^2$ is some positive constant, $\zeta$ is some vector of constants,
and \( I \) is the identity matrix. To obtain a conjugate normal prior, we use the following two linear constraints on the coefficients through function values of the transformations: 
\[
0 = f_d(1/2) = \sum_{j=1}^{J} \theta_d B_j(1/2) \quad \text{and} \quad 1 = f_d(3/4) - f_d(1/4) = \sum_{j=1}^{J} \theta_d [B_j(3/4) - B_j(1/4)].
\]

The linear constraints can be written in matrix/vector form as \( A\theta = c \).

We impose the monotonicity constraint on the coefficients, which is equivalent with the series of inequalities \( \theta_2 - \theta_1 > 0, \ldots, \theta_J - \theta_{J-1} > 0 \). The monotonicity constraint can be expressed in matrix/vector form as \( F\theta > 0 \). We work with a dimension-reduced coefficient vector by removing two coefficients to ensure that we have a Lebesgue density on \( \mathbb{R}^{J-2} \) for the remaining components and we denote this reduction with a bar.

The final prior on the coefficients is given by a truncated normal prior distribution \( \theta | \{ A\theta = c \} \sim \text{TN}_{J-2}(\xi, \Gamma, \mathcal{T}) \), where \( \mathcal{T} = \{ \theta : F\theta + \bar{g} > 0 \} \), and the \( \text{N}_p(\mu, \Sigma) \)-distribution restricted on a set \( \mathcal{T} \) is denoted by \( \text{TN}_p(\mu, \Sigma, \mathcal{T}) \). In addition, \( \xi = \zeta + A'(AA')^{-1}(c - A\zeta) \), \( \Gamma = \sigma^2[I - A'(AA')^{-1}A] \), and \( \bar{g} \) is a constant vector. Any choice of \( \zeta \) is acceptable, but we use \( \zeta_j = \nu + \tau \Phi^{-1}(j-0.375, J-0.75+1) \), \( j = 1, \ldots, J \) where \( \nu \) is a constant, \( \tau \) is a positive constant, and \( \Phi^{-1} \) is the inverse of the cumulative distribution function of the standard normal distribution.

The idea is that by increasing the original components of the mean vector \( \zeta \), we can put a substantial probability of the truncation set \( \mathcal{T} \) in the final prior of the B-spline coefficients.

Finally, we put an improper uniform prior on the mean \( p(\mu) = \prod_{d=1}^{p} p_d(\mu_d) \propto 1 \). The resulting transformed variables are used to estimate the precision matrix and learn the structure of the underlying graph.

### 2.2 Cholesky Decomposition Reformulated as Regression Problems

We learn the structure of the precision matrix using a Cholesky decomposition. Denote the Cholesky decomposition of \( \Omega \) as \( \Omega = LL^T \), where \( L \) is a lower triangular matrix. Define the coefficients \( \beta_{kd} = -l_{kd}/l_{dd} \) and the precision as \( \phi_d = 1/\sigma_d^2 = \ell_{dd}^2 \). Then as described in (Wong et al., 2013), the lower triangular entries of \( \Omega \) are given by
\[
\omega_{kd} = \sum_{m=1}^{d} l_{km}l_{dm} = \sum_{m=1}^{d} \beta_{km}\beta_{dm}\phi_m, \quad \text{for } k \geq d.
\]

Accordingly, the multivariate Gaussian model \( Z \sim \text{Normal}(0, \Sigma) \) is equivalent to the set of independent regression problems,
\[
Z_d = \sum_{k>d} \beta_{kd} Z_k + \epsilon_d, \quad \epsilon_d \sim \text{Normal}(0, \sigma_d^2), \quad d = 1, \ldots, p,
\]
where \( \beta_{kd} \) are the regression coefficients for \( k = d+1, \ldots, p \) and \( d = 1, \ldots, p \) and \( Z_d \) and \( Z_k \) are, respectively, the \( d \)th column and \( k \)th columns selected from matrix \( Z \).

We use a standard conjugate noninformative prior on the variances. We consider two different continuous shrinkage priors on the regression coefficients, the horseshoe prior and
Bayesian Regression Approach

the Bernoulli-Gaussian prior. Using these priors, we enforce a sparsity constraint along
the rows of the lower triangular matrix. The sparsity constraint is one in which the global
sparsity parameter of the continuous shrinkage prior is scaled by $\sqrt{k}$, where $k > d$ and
d $= 1, \ldots, p$. Using this constraint, we expect that the precision matrix will be sparse
through weak order invariance. The sparsity constraint is derived in the next subsection.

2.3 Sparsity Constraint

In order to ensure that the probability that an entry is nonzero (i.e. sparsity) remains
roughly the same over different rows we cannot simply impose the same degree of sparsity
on the rows of the Cholesky factor $L$, but need to change it over rows appropriately. To
see how it depends on the row index, we observe that

$$P(\omega_{kd} \neq 0) = P(\sum_{m} l_{km} l_{dm} \neq 0)$$

$$= P(l_{km} l_{dm} \neq 0 \text{ for some } m)$$

$$= 1 - P(l_{km} l_{dm} = 0 \text{ for all } m) = 1 - P(\bigcap_{m=1}^{\min(k,d)} \{l_{km} l_{dm} = 0\})$$

$$= 1 - \prod_{m=1}^{\min(k,d)} P(l_{km} l_{dm} = 0) = 1 - \prod_{m=1}^{\min(k,d)} \{1 - P(l_{km} l_{dm} \neq 0)\}$$

$$= 1 - \prod_{m=1}^{\min(k,d)} \{1 - P(l_{km} \neq 0)P(l_{dm} \neq 0)\}$$

Let $\rho_k = P(\text{Nonzero entry in the } k^{th} \text{ row of } L)$. Then

$$P(\omega_{kd} \neq 0) = 1 - (1 - \rho_k \rho_d)^{\min(k,d)}.$$

If $k \asymp d$, the expression is roughly $1 - (1 - \rho_k^2)^k$, which remains stable in $k$ if $\rho_k = c_p / \sqrt{k}$, where $c_p$ depends on $p$ but not on $k$. Then we obtain the probability of non-zero to be

$$1 - \exp(-c_p^2).$$

Further, choosing $c_p$ to be small for $p \rightarrow \infty$ makes the probability small,
which is essential in higher dimension. We choose $\rho_k = P(\text{nonzero in } k^{th} \text{ row}) = c / (p \sqrt{k})$, and tune the value of $c \in \{0.1, 1, 10\}$ to cover a range of three orders of magnitude, i.e. $10^{-1}$, $10^{0}$, $10^{1}$.

3. Variational Bayes Estimation

Ideally, one would want to construct a complete variational Bayesian algorithm in which the
B-spline coefficients, mean, and inverse covariance matrix are estimated all in one setting.
However, for our problem, there is no closed form solution for the truncated multivariate
normal distribution, and closed form solutions are needed for the mean field variational
Bayesian algorithms. Instead, we use an exact Hamiltonian Monte Carlo within Gibbs
scheme to sample the B-spline coefficients and the mean. We obtain the Bayes estimate
of the B-spline coefficients, $\hat{\theta}_d = E(\theta_d)$, and the Bayes estimate of the mean, $\hat{\mu}_d = E(\mu_d)$,
where $E$ is the posterior mean operator. We then apply the variational Bayes method on
the synthetic data obtained by transforming the original observations using the estimated
transformations. Thus we estimate the transformed variables using

$$Z_{id} = \sum_{j=1}^{J} \hat{\theta}_{jd} B_j(X_{id}) - \hat{\mu}_d.$$  

Ideally, instead of plugging in, one can obtain samples from the posterior distributions of
the transformations and draw samples from the variational distributions of the precision
matrix for each generated samples and accumulate them. However, even in moderately
high dimension, such an approach is extremely computationally intensive. Since the poste-
rior distributions of the transformations are consistent (Mulgrave and Ghosal, 2018), they
concentrate near the Bayes estimate. As the main goal is structure learning, the inability of
the plug-in to assess the posterior variability of the transformations is not a highly deter-
ing issue. Thus, although the proposed algorithm is not fully Bayesian, it utilizes the strength
of the variational Bayesian approach to identify conditional independence relations in a
nonparanormal graphical model within a manageable time. We illustrate the variational
method on the Bernoulli-Gaussian prior, following the strategy described in Ormerod et al.
(2017). Let

$$Z_d|\beta, \sigma, \gamma \sim N(Z_{k>d} \Gamma_{k>d} \beta_{k>d}, \sigma^2_d \mathbf{I}), \quad \beta_{kd} \sim N(0, \zeta^2),$$

$$\gamma_{kd} \sim \text{Ber}(\rho_{kd}^*), \quad \sigma^2_d \sim \text{IG}(0.01, 0.01)$$  \hfill (1)

for $d = 1, \ldots, p$, where $\beta_{k>d} = (\beta_{d+1}, \ldots, \beta_p)$, and $Z_{k>d}$ and $\Gamma_{k>d}$ are the matrices pert-
taining to $Z$ and $\Gamma$ where the columns are greater than the $d$th column. The Bernoulli
distribution is denoted as Ber and the Inverse Gamma distribution is denoted as IG. The param-
ters $\zeta^2$ and $\rho_k$ are fixed hyperparameters and $\rho_k \in [0, 1]$. This variant of the spike-
and-slab prior indirectly models sparsity on the regression coefficients by putting a binary
indicator on the regression coefficients in the likelihood, instead of directly modeling spar-
sity on the regression coefficients. As such, if $\gamma_k = 0$ for the Bernoulli-Gaussian prior, then
$\beta_k|\gamma_k \sim N(0, \zeta^2)$, unlike in usual spike-and-slab priors. Note that the sparsity is controlled
by $\rho_{kd}^* = \rho c /(p \sqrt{K})$. The parameters $\rho$ and $c$ is tuned in an algorithm that is detailed in
Subsection 3.1.

The joint posterior distribution that we aim to estimate is

$$p(\beta, \Gamma, \sigma^2|Z) \propto \prod_{i=1}^{n} \prod_{d=1}^{p-1} p(Z_{id}|Z_{i,k>d}, \beta_{k>d}, \Gamma_{k>d}, \sigma^2_d) \times p(\beta_{k>d}) p(\Gamma_{k>d}) p(\sigma^2_d) p(\sigma^2_p) p(\sigma^2_p).$$
Bayesian Regression Approach

By plugging in the estimated transformed variables, we use a variational Bayesian algorithm to estimate the sparse precision matrix. Mean-field variational Bayesian (VB) inference involves minimizing the Kullback-Leibler divergence between the true posterior distribution and a factorized approximation of the posterior. Let \( \kappa \) represent the set of a parameters in the model and \( Z \) represent the matrix of estimated transformed variables. Then \( p(\kappa|Z) \) is approximated by \( q(\kappa) = \prod_{k=1}^{K} q_k(\kappa_k) \), where \( (\kappa_1, \ldots, \kappa_k) \) is a partition of \( \kappa \). The optimal \( q_k \) densities satisfy

\[
q_k(\kappa_k) \propto \exp[\mathbb{E}_{\{q_k(\kappa_k)\}}\{\log p(Z, \kappa)\}],
\]

where \( \mathbb{E}_{\{q_k(\kappa_k)\}} \) is the expectation with respect to all densities except \( q_k(\kappa_k) \) (Bishop, 2006). The variational lower bound (VLB) for the marginal likelihood for \( Z \) is then given by

\[
\text{VLB}(q) = \mathbb{E}_q[\log \{p(Z, \kappa)/q(\kappa)\}].
\]

Using the coordinate ascent method, optimizing each \( q_k \) while holding the others fixed will result in the algorithm converging to a local maximum of the lower bound.

Following (Ormerod et al., 2017), the choice of factorization that we use for the VB approximation is

\[
q(\beta, \gamma, \sigma^2) = q(\sigma^2_p)\prod_{d=1}^{p-1} q(\sigma_d^2)\prod_{k=d+1}^{p} q(\gamma_{kd}).
\]

Then the optimal \( q_k \) densities are, for each \( d = 1, \ldots, p-1 \), and \( k > d \), are given by

\[
q^*(\beta_d) \sim N(\mu_d, \Sigma_d), \; q^*(\sigma^2_d) \sim \text{IG}(A + \frac{n}{2}, s_d), \; q^*(\gamma_{kd}) \sim \text{Ber}(w_{kd}).
\]

We can derive the variational updates as in Ormerod et al. (2017). Introduce the notations \( \expit(x) = \exp(x)/(1 + \exp(x)) \), and \( \text{logit}(x) = \log(x/(1-x)) \), and let the symbol \( \circ \) denote the Hadamard product between two matrices. Then we have

\[
\Sigma_d = [\tau_d(Z'_{k>d}Z_{k>d}) \circ \Omega_d + \varsigma^{-2}I]^{-1},
\]

\[
\mu_d = \tau_d(\tau_dW_dZ'_{k>d}Z_{k>d}W_d + D_d)^{-1}W_dZ'_{k>d}Z_d
\]

\[
s_d = B + \frac{1}{2}\|Z_d\|^2 - 2Z_d'Z_{k>d}W_d\mu_d + \text{tr}\{(Z'_{k>d}Z_{k>d} \circ \Omega_d)(\mu_d\mu_d' + \Sigma_d)\},
\]

\[
\eta_{kd} = \text{logit}(\rho_{kd}^*) - \frac{\tau_d}{2}(\mu_k^2 + \Sigma_{k,k})\|Z_k\|^2 + \tau_d|\mu_kZ_k'Z_d - Z_kW_l(\mu_l\mu_k + \Sigma_{l,k})|,
\]

\[
s_p = B + \frac{1}{2}\|Z_p\|^2, \; w_{kd} = \expit(\eta_{kd}), \; \tau_d = \frac{2A + n}{2s_d}, \; \rho_{kd}^* = \frac{s_d}{p\sqrt{k}},
\]

for \( l = k+1, \ldots, p, \; k = d+1, \ldots, p \), where \( W_d = \text{diag}(w_{k>d}) \), where \( w_{k>d} = (w_{d+1}, \ldots, w_p) \), \( \Omega_d = w_dw_d' + W_d(I - W_d) \) and \( D_d = \tau_d(Z'_{k>d}Z_{k>d}) \circ W_d \circ (I - W_d) + \varsigma^{-2}I \).
Using these optimal \( q_k \) densities, the VLB simplifies to

\[
\text{VLB}(Z; \rho) = -\frac{pm}{2} \log(2\pi) + pA \log B - p \log \Gamma(A) - (A + \frac{n}{2}) \log s_p + p \log \Gamma(A + \frac{n}{2}) \\
+ \sum_{d=1}^{p-1} \left\{ \frac{#(k > d)}{2} - \frac{#(k > d)}{2} \log(\zeta^2) - (A + \frac{n}{2}) \log(s_d) + \frac{1}{2} \log |\Sigma_d| \right. \\
- \frac{1}{2 \zeta^2} \text{tr}(\mu_d \mu_d' + \Sigma_d) + \sum_{k=(d+1)}^{p} \left[ w_k \log \left( \frac{\rho_k}{w_k} \right) + (1 - w_k) \log \left( \frac{1 - \rho_k}{1 - w_k} \right) \right].
\]

(2)

3.1 Tuning Procedure

For every \((p - 1)\) regression problem, we choose the parameter \( \rho_{kd}^* = \rho_d c/(p \sqrt{k}) \) and the initial values for \( w_{k>d} \) based on the tuning algorithm described in Ormerod et al. (2017), with a few changes to incorporate the sparsity constraint: the fixed \( \rho_d \) that is used to maximize the lower bound is taken to be \( \rho_d = \expit(-0.5 \sqrt{n})/(p \sqrt{k}) \) and for fixed \( w_{k>d} \), the updated \( \rho_j = (\expit(\lambda_j c_j))/(p \sqrt{k}) \), where \( c_j \) is taken from an equally spaced grid of 50 points between 0.1 and 10 and \( \lambda_j \) is an equally spaced grid of 50 points between \(-15\) and \(5\). Note that the variational lower bound for the tuning procedure is only based on the \((p - 1)\) regressions and not the regression that involves \( Z_p \) and \( \sigma_p^2 \).

4. MCMC Estimation through Horseshoe Prior

4.1 Horseshoe Prior

We use the horseshoe prior described in Neville et al. (2014), to shrink the \( \beta \) coefficients:

\[
Z_d|(Z_{k>d}, \beta_{k>d}, \sigma_d^2) \sim \mathcal{N}(Z_{k>d} \beta_{k>d}, \sigma_d^2 I), \\
\beta_{kd}|(\lambda_d^2, b_{kd}, \sigma_d^2) \sim \mathcal{N}(0, \frac{\sigma_d^2 b_{kd}^2 \lambda_d^2}{p^2 k}), \\
\lambda_d^2|a_d \sim IG\left(\frac{1}{2}, \frac{1}{a_d}\right), \\
a_d \sim IG\left(\frac{1}{2}, 1\right), \tag{3}
\]

\[
b_{kd}|h_{kd} \sim IG\left(\frac{1}{2}, \frac{1}{h_{kd}}\right), \\
h_{kd} \sim IG\left(\frac{1}{2}, 1\right), \\
\sigma_d^2 \sim IG(0.01, 0.01),
\]

for \( d = 1, \ldots, p \), where \( \beta_{k>d} = (\beta_{d+1}, \ldots, \beta_p) \) and \( Z_{k>d} \) is the matrix pertaining to \( Z \) with columns higher than the \( d \).
Algorithm 1 Variational Bayesian Algorithm

1: Gibbs Sampler
2: for $d = 1 : p$ do
   (a) Sample $\hat{\theta}_d | (\hat{\Theta}_{-d}, Y, \mu, \Omega) \sim \mathcal{TN} (\gamma, \Psi, \{F_d \hat{\theta}_d + \hat{g}_d > 0\})$, where $\gamma = -\{\xi \Gamma^{-1} - \lambda_d^{-1} \sum_{n=1}^{n} (B_q d - \delta_d) (\bar{B} + B^* W_d) \}' \{\lambda_d^{-1} \sum_{n=1}^{n} (\bar{B} + B^* W_d) (\bar{B} + B^* W_d) + \Gamma^{-1}\}^{-1}$ and $\Psi = \{\lambda_d^{-1} \sum_{n=1}^{n} (\bar{B} + B^* W_d) (\bar{B} + B^* W_d) + \Gamma^{-1}\}^{-1}$.
   (b) Compute $Y_{id} = \sum_{j=1}^{J} \theta_{jd} B_j (X_{id})$.
   (c) Sample $\mu | (Y, \Omega) \sim N_p (\bar{Y}, \frac{1}{\eta} \Omega^{-1})$.
3: end for
4: Repeat Step 2 until convergence.
5: Compute $\hat{\theta}_d = \sum_{m=1}^{M} \theta_{dm}$ and $\hat{\mu}_d = \sum_{m=1}^{M} \mu_{dm}$, where $M$ is the number of Markov Chain Monte Carlo samples.
6: Compute $Z_{id} = \sum_{j=1}^{J} \theta_{jd} B_j (X_{id}) - \hat{\mu}_d$.
7: Using $Z$, tune $\rho_{kd}$ and find the initial values for $w_{k>0}$ using the tuning procedure described in Subsection 3.1.
8: Coordinate Ascent Variational Inference
   (a) Initialize with $t = 1, Z_d, Z_{k>0}, s^2, A, B, \tau_0, \rho_0, w_{k>0}$ where $w_{k>0}^{(1)} \in [0, 1][k>0]$
   (b) for $d = 1 : (p-1)$ do
      - $W_d^{(1)} = \text{diag}(w_{k>0})$
      - $\Omega_d = w_{d} (W_d^{(1)}) + W_d^{(1)} (I - W_d^{(1)})$
      - $\Sigma_d^{(1)} = \tau_d (Z_{k>0} + \Omega_d) + \zeta^{-2} I_{-1}$
      - $\mu_d^{(t)} = \tau_d (Z_{k>0} + \Omega_d) W_d^{(t)} + \text{tr} \{Z_{k>0} + \Omega_d \} (\mu_d^{(t)} + \Sigma_d^{(t)})$
      - $\tau_d^{(t)} = \frac{2 + n_{d}}{2 s_d}$
      - $w_{d}^{*} = w_{d}^{(t)}$
      - for $k = (d+1) : p$ do
         - $\eta_{kd} = \text{logit}(\rho_{kd}) - \frac{\tau_d^{(t)} (\mu_{k}^{(t)})^2 + \Sigma_{k}^{(t)} \|Z_k\|^2 + \tau_d^{(t)} \mu_{k}^{(t)} Z_k \Omega_d^{(t)} (\mu_d^{(t)} + \Sigma_{k}^{(t)}) \|Z_k\|^2}$
         - $w_{k>0}^{*} = \expit(\eta_{kd})$
      - end for
      - $w_{d}^{(t+1)} = w_{d}^{*}$
   (c) end for
   (d) $s_p^{(t)} = B + \frac{1}{2} \|Z_p\|^2$
   (e) Repeat (b)–(d) until $|\text{VLB}(Z, \rho)^{(t)} - \text{VLB}(Z, \rho)^{(t-1)}| < \epsilon$.
9: Sample $\beta_d \sim \mathcal{N}(\mu_d, \Sigma_d)$, $\gamma_{kd} \sim \text{Ber}(w_{kd})$, $\sigma_d \sim \text{IG}(A + n_s, s_d)$, and $\sigma_p \sim \text{IG}(A + n_p, s_p)$
10: Compute $l_{kd} = -\gamma_{kd} \beta_{kd} / \sigma_d$ and $l_{dd} = 1 / \sigma_d$
11: Compute $\Omega = LL'$. 
The global scale parameter $\lambda$ is roughly equivalent to the probability of a nonzero element (van der Pas et al., 2014). We enforce the sparsity constraint using, $(\lambda d c) / (p \sqrt{k})$. Thus, since we are working with the squared parameter, the factor in the variance term for $\beta_{kd}$ is $(\lambda^2 c^2) / (p^2 k)$, where $c \in \{0, 1, 10\}$.

### 4.2 Horseshoe Posterior

The joint posterior distribution is,

$$p(\beta, \lambda^2, \sigma^2, a, b, h, \theta, \mu | Z) \propto \prod_{i=1}^{n} \prod_{d=1}^{p} p(\sum_{j=1}^{J} \theta_{dj} B_j(X_{id}) \sum_{j=1}^{J} \theta_{kd,j} B_j(X_{i,k>d}), \beta_{kd}, \sigma^2)$$

$$\times p(\beta_{kd}) p(\sigma^2_d) p(\mu_d) \times p(a_d) p(b_{kd}) p(h_{kd})$$

$$\times p(\lambda^2_d) p(\sum_{j=1}^{J} \theta_{pj} B_j(X_{ip}) | \sigma^2, p(\theta_p) p(\mu_p)).$$

(4)

Then the corresponding conditional posterior distributions are given by

$$\beta_{kd} \sim N(\sum_{j=1}^{J} \frac{\theta_{dj} B_j(X_{id}) \sum_{j=1}^{J} \theta_{kd,j} B_j(X_{i,k>d}) \beta_{kd}}{\sigma^2_d} + \frac{1}{2} \frac{1}{a_d} \beta_{kd} + \frac{1}{2} \frac{1}{b_{kd}}, \sigma^2_d)$$

$$\lambda^2_d \sim IG\left(\frac{\#(k > d)}{2} + 1, \frac{1}{2} \frac{1}{\lambda^2_d} \beta_{kd}^2 \sigma^2_d + \frac{1}{2} \beta_{kd} \right),$$

$$a_d \sim IG(1, \frac{1}{\lambda^2_d} + 1),$$

$$b_{kd} \sim IG\left(1, \frac{k \beta^2_{kd} \sigma^2_d}{2 \sigma^2_d \lambda^2_d c^2} + \frac{1}{h_{kd}}\right),$$

$$h_{kd} \sim IG(1, \frac{1}{b_{kd}} + 1),$$

$$\sigma^2_d \sim IG\left(\frac{n + \#(k > d)}{2} + 0.01, \frac{1}{2} \parallel Z_d - Z_{k>d} \beta_{kd} \parallel^2 + \frac{1}{2} \beta_{kd} \lambda^2_d \beta_{kd} + 0.01\right),$$

$$\sigma^2_p \sim IG\left(\frac{n}{2} + 0.01, \frac{1}{2} \parallel Z_p \parallel^2 + 0.01\right).$$

Since sampling the $\beta_{kd}$ can be expensive for large $p$, we use an exact sampling algorithm for Gaussian priors based on data augmentation (Bhattacharya et al., 2016).
Algorithm 2 Horseshoe Gibbs Algorithm

1: for $d = 1, \ldots, p$ do
   
   (a) $\tilde{\theta}_d | (\tilde{\Theta}_d, Y, \mu, \Omega) \sim \text{TN}(\gamma, \Psi, \{\tilde{E}_d \tilde{\theta}_d + g_d > 0\})$ where $\gamma = -\xi \bar{\Gamma}^{-1} - \lambda_d^{-1} \sum_{i=1}^{n} (B^* q_d - \delta_d, \delta_d)' (B + B^* W_d)' (B + B^* W_d) + \bar{\Gamma}^{-1}$, $\Psi = \{\lambda_d^{-1} \sum_{i=1}^{n} (B + B^* W_d)' (B + B^* W_d) + \bar{\Gamma}^{-1}\}^{-1}$.
   
   (b) Sample $Y_{id} = \sum_{j=1}^{I} \theta_{dj} B_{j}(X_{id})$.
   
   (c) Compute $Z_{id} = Y_{id} - \mu_d$.
   
   (d) for $d = 1, \ldots, n-1$ do
      
      (i) Sample $\beta_{k>d} | \sigma_{d}, b_{k>d}, \lambda_{d}^2 \sim N(A^{-1} Z_{k>d} Z_{d}, \sigma_{d}^2 A^{-1})$, where $A = (Z_{k>d} Z_{k>d} + \text{diag}(p^2 k/(\lambda_{d}^2 b_{k>d} c^2)))$.
      
      (ii) Sample $t \sim N(0, D)$ and $\delta \sim \text{Normal}(0, I_n)$, where $D = \sigma_{d}^2 \text{diag}(\lambda_{d}^2 b_{k>d} c^2) / (p^2 k)$.
      
      (iii) Set $v = t \Phi + \delta$, where $\Phi = Z_{k>d} / \sigma_d$.
      
      (iv) Solve $(D \Phi \Phi' + I_n)w = (\alpha - v)$, where $\alpha = Z_d / \sigma_d$.
      
      (v) Set $\beta = t + D \Phi' w$.
   
   (e) Sample $\lambda_{d}^2 \sim \text{IG}(\frac{#(k > d)}{2} + \frac{1}{2} \beta_{k>d} \text{diag}(\frac{p^2}{\sigma_{d}^2 b_{k>d} c^2}) \beta_{k>d} + \frac{1}{a_d})$.
   
   (f) Sample $a_d \sim \text{IG}(1, \lambda_d^2 + 1)$.
   
   (g) Sample $b_{kd} \sim \text{IG}(1, \frac{p^2 k^2 \beta_{kd}^2}{2 \sigma_d^2 \lambda_d^2 c^2} + \frac{1}{h_{kd}})$.
   
   (h) Sample $h_{kd} \sim \text{IG}(1, b_{kd}^{-1} + 1)$.
   
   (i) Sample $\sigma_{d}^2 \sim \text{IG}(\frac{n + \#(k > d)}{2} + 0.01, \frac{1}{2} \|Z_d - Z_{k>d} \beta_{k>d}\|^2 + \frac{1}{2} \beta_{k>d} \text{diag}(\frac{p^2}{\lambda_d^2 b_{k>d} c^2}) \beta_{k>d} + 0.01)$.
   
2: end for
3: Compute $\theta_{d} | (\tilde{\Theta}_d, Y, \mu, \Omega) \sim \text{IG}(\frac{n}{2} + 0.01, 0.01 \|Z_d\|^2 + 0.01)$.
4: Compute $l_{kd} = -\beta_{kd} / \sigma_d$ and $l_{dd} = 1 / \sigma_d$.
5: Compute $\Omega = \bar{\Gamma} L L'$.
6: These steps are repeated until convergence.
5. MCMC Estimation through Bernoulli-Gaussian Prior

5.1 Bernoulli-Gaussian Prior

We use the same Bernoulli-Gaussian prior described in (1).

5.2 Bernoulli-Gaussian Posterior

The joint posterior distribution is

\[
p(\beta, \Gamma | Z) \propto \prod_{i=1}^{n} \prod_{d=1}^{p-1} p\left(\sum_{j=1}^{J} \theta_{d,j} B_j(X_{id})\right) \prod_{j=1}^{J} \theta_{k>d,j} B_j(X_{i,k>d}), \beta_{k>d}, \Gamma_{k>d}, \sigma_d^2)
\]

\[
\times p(\beta_{k>d}) p(\Gamma_{k>d}) p(\sigma_d^2) p(\theta_d) p(\mu_d) p(\sum_{j=1}^{J} \theta_{pj} B_j(X_{ip})|\sigma_p^2) p(\sigma_p^2) p(\theta_p) p(\mu_p).
\]

Then the corresponding conditional posterior distributions are given by

\[
\beta_{k>d} | \cdot \sim N\left(\Gamma_{k>d} Z_k^\prime_d \Gamma_{k>d} + \frac{\sigma_d^2}{\zeta^2} I \right)^{-1} \Gamma_{k>d} Z_k^\prime_d Z_d,
\]

\[
(\Gamma_{k>d} Z_k^\prime_d Z_k^\prime_d \Gamma_{k>d} + \frac{\sigma_d^2}{\zeta^2} I)^{-1},
\]

\[
\gamma_k | \cdot \sim Ber\left[\expit\left\{\logit(\rho_{k>d}) - \frac{1}{2\sigma_d^2} \|Z_k\|^2 \beta_k^2 + \frac{1}{\sigma_d^2} \beta_k Z_k^\prime(Z_d - Z_{t>k} \Gamma_{t>k} \beta_{t>k})\right\}\right],
\]

\[
\sigma_d^2 \sim IG\left(\frac{n}{2} + 0.01, \frac{1}{2} \|Z_d - Z_{k>d} \Gamma_{k>d} \beta_{k>d}\|^2 + 0.01\right),
\]

\[
p(\sigma_p^2) \sim IG\left(\frac{n}{2} + 0.01, \frac{1}{2} \|Z_p\|^2 + 0.01\right),
\]

where \(k = d + 1, \ldots, p\), and \(d = 1, \ldots, p - 1\).

Again, to sample \(\beta_{k>d}\) we used an exact sampling algorithm for Gaussian priors that invokes data augmentation (Bhattacharya et al., 2016).

6. Thresholding

The thresholding procedure that we consider for the method using the horseshoe prior (3) is based on a 0-1 loss function described in (Wang, 2012) for classification under absolutely continuous priors. Although this procedure is heuristic, it seems to perform well in practice. Other thresholding rules may be used, such as those based on posterior credible intervals (Kondker et al., 2013), information criterion (Kuismin and Sillanp, 2016), clustering (Li and Pati, 2017), posterior model probabilities (Banerjee and Ghosal, 2015; Mohammadi and Wit, 2015), and projection predictive selection (Williams et al., 2018), but we chose to focus on the 0-1 loss procedure for this study.
Algorithm 3 Bernoulli-Gaussian Gibbs Algorithm

1: for \( d = 1, \ldots, p \) do
    (a) Sample \( \theta_d | (\bar{\theta}_d, Y, \mu, \Omega) \sim TN(\gamma, \Psi, \{F_d \theta_d + g_d > 0\}) \), where \( \gamma = -\{\xi \Gamma^{-1} - \lambda_d \sum_{i=1}^{n}(B^*q_d - \delta_{d,i})'(\bar{B} + B^*W_d)\}'\{\lambda_d^{-1} \sum_{i=1}^{n}(\bar{B} + B^*W_d)'(\bar{B} + B^*W_d) + \Gamma^{-1}\}^{-1}; \quad \Psi = \{\lambda_d^{-1} \sum_{i=1}^{n}(B + B^*W_d)'(B + B^*W_d) + \Gamma^{-1}\}^{-1}.

2: end for
3: Compute \( Y_{id} = \sum_{j=1}^{J} \theta_{dj} B_j (X_{id}) \).
4: Sample \( \mu | (Y, \Omega) \sim N(\bar{Y}, \frac{1}{n} \Omega^{-1}) \).
5: Compute \( Z_{id} = Y_{id} - \mu_d \).
6: for \( d = 1, \ldots, p-1 \) do
    (a) Sample \( \beta_{k>d} | \sigma_d, \Gamma_{k>d} \sim N(\Lambda^{-1}\Gamma_{k>d}Z_{k>d}^T Z_{d}, \sigma_d^2 A^{-1}) \), where \( \Lambda = (\Gamma_{k>d}Z_{k>d} \Gamma_{k>d} + \sigma_d^2 I) \).
        (i) Sample \( t \sim N(0, D) \) and \( \delta \sim N(0, I_n) \), where \( D = \zeta^2 I \);
        (ii) set \( v = \Phi t + \delta \), where \( \Phi = Z_{k>d} \Gamma_{k>d} / \sigma_d \);
        (iii) solve \( (\Phi D \Phi^T + I_n)q = (\alpha - v) \), where \( \alpha = Z_d / \sigma_d \);
        (iv) set \( \beta = t + D \Phi^T q \).
    (b) Sample \( \gamma_k | \beta_{k>d}, \sigma_d \sim Ber[expit\{\logit(\rho_{k,d}) - \frac{1}{2\sigma_d} \|Z_{k}\|^2 \beta_k^2 + \frac{1}{\sigma_d} \beta_k Z_{k}'(Z_{d} - Z_{l>k} \Gamma_{l>k} \beta_{l>k}) \}] \).
    (c) Sample \( \sigma_d^2 | \beta_{k>d}, \Gamma_{k>d} \sim IG(n \frac{1}{2} + 0.01, \frac{1}{2} \|Z_{d} - Z_{k>d} \Gamma_{k>d} \beta_{k>d} \|^2 + 0.01) \).

7: end for
8: Sample \( \sigma_p^2 | Z_p \sim IG(n \frac{1}{2} + 0.01, \frac{1}{2} \|Z_p\|^2 + 0.01) \).
9: Compute \( l_{kd} = -\gamma_{kd} \beta_{kd} / \sigma_d \) and \( l_{dd} = 1 / \sigma_d \).
10: Compute \( \Omega = LL' \).
11: These steps are repeated until convergence.
6.0.1 0-1 Loss Procedure

We find the posterior partial correlation using the precision matrices from the Gibbs sampler of the horseshoe prior (3) and the posterior partial correlation using the standard conjugate Wishart prior. The posterior samples of partial correlation using the precision matrices from the Gibbs sampler is defined as

$$\rho_{kd,m} = \frac{-\omega_{kd,m}}{\sqrt{\omega_{kd,m} \omega_{dd,m}}}$$

where $\omega_{kd,m}$ is the $m$th one of $M$ Markov chain Monte Carlo (MCMC) samples from the posterior distribution, $k, d = 1, \ldots, p$, $m = 1, \ldots, M$. The posterior partial correlation using the standard conjugate Wishart prior is found by starting with the latent observation, $Z_m$, which is obtained from the MCMC output. We put a standard Wishart prior on the precision matrix, $\Omega_m \sim W_p(3, I)$, where $I$ is the identity matrix. Note that this Wishart prior does not assume sparsity, but $Z_m$ is obtained from the MCMC output assuming sparsity of the precision matrix. Through conjugacy, the posterior distribution is $\Omega_m \sim W_p(n + 3, (I + S_m)^{-1})$, where $S_m = Z_m^\prime Z_m$. We then calculate the mean of the posterior distribution, $\Lambda_m = E(\Omega_m | Z_m) = (n + 3)(I + S_m)^{-1}$. Finally, we compute the posterior samples of partial correlation coefficients by conjugate Wishart prior as

$$\phi_{kd,m} = \frac{-\lambda_{kd,m}}{\sqrt{\lambda_{kd,m} \lambda_{dd,m}}}$$

where $\lambda_{kd,m}$ stands for the $(k, d)$th element of $\Lambda_m$.

We link these two posterior partial correlations for the 0-1 loss method. We claim the event $\{\omega_{kd,m} \neq 0\}$ if and only if

$$\frac{\rho_{kd,m}}{\phi_{kd,m}} > 0.5$$

for $k, d = 1, \ldots, p$ and $m = 1, \ldots, M$. The idea is that we are comparing the regularized precision matrix from the horseshoe prior to the non-regularized precision matrix from the Wishart prior. If the absolute value of the partial correlation coefficient from the regularized precision matrix is similar in size or larger than the absolute value of the partial correlation coefficient from the Wishart precision matrix, then there should be an edge in the edge matrix. If the absolute value of the partial correlation coefficient from the regularized precision matrix is much smaller than the absolute value of the coefficient from the Wishart matrix, then there should not be an edge in the edge matrix.

7. Choice of Prior Parameters

For the precision matrix being estimated with a horseshoe prior (3), we need to select the value of the parameter $c_p$, which controls the sparsity. We solve a convex constrained optimization problem in order to use the Bayesian Information Criterion (BIC), as described
in Dahl et al. (2005). First, we find the Bayes estimate of the inverse covariance matrix, \( \hat{\Omega} = \mathbb{E}(\Omega|\mathbf{Z}) \). We also find the average of the transformed variables, \( \bar{\mathbf{Z}} = \mathbf{M}^{-1} \sum_{m=1}^{M} \mathbf{Z}_m \), where \( \mathbf{Z}_m, m = 1, \ldots, M \), are obtained from the MCMC output. Then, using the sum of squares matrix \( \mathbf{S} = \bar{\mathbf{Z}}'\bar{\mathbf{Z}} \), we solve for \( \hat{\Omega}_{\text{MLE}} \), the maximum likelihood estimate of the inverse covariance matrix,

\[
\minimize_{\hat{\Omega}} -n \log \det \hat{\Omega} + \text{tr}(\hat{\Omega}\mathbf{S}), \quad \text{subject to } \mathcal{C}(\hat{\Omega}),
\]

where \( \mathcal{C} \) represents the constraint that all elements of \( \hat{\Omega} \) at the locations of the zeros of the estimated edge matrix from the MCMC sampler are zero. The estimated edge matrix from the MCMC sampler will be described in more detail in Section 8. For computational simplicity, in the code, we represent this problem as an unconstrained optimization problem as described in Dahl et al. (2005).

Lastly, we calculate BIC = \(-2\ell(\hat{\Omega}_{\text{MLE}}) + k \log n \), where \( k = \#\mathcal{C}(\hat{\Omega}) \), the sum of the number of diagonal elements and the number of edges in the estimated edge matrix, and \(-\ell(\hat{\Omega}_{\text{MLE}}) = -n \log \det \hat{\Omega}_{\text{MLE}} + \text{tr}(\hat{\Omega}_{\text{MLE}}\mathbf{S}) \). We select the \( c_p \) that results in the smallest BIC.

8. Simulation Results

We conduct a simulation study to assess the performance of the proposed methods using the horseshoe MCMC, Bernoulli-Gaussian MCMC, and variational Bayesian algorithm. We compare the structure learning results of our methods to the nonparanormal graphical model (Liu et al., 2009) and to a Bayesian Gaussian copula graphical model (Mohammadi et al., 2017), indicated as the Bayesian copula, in which the rank likelihood is used to transform the random variables with a uniform prior on the graph, a G-Wishart prior on the inverse correlation matrix, and estimation is used with the birth-death MCMC (Mohammadi and Wit, 2015). We assess the effect of the transformation functions of our methods on parameter estimation.

The random variables, \( \mathbf{Y}_1, \ldots, \mathbf{Y}_p \), are simulated from a multivariate normal distribution such that \( \mathbf{Y}_{i1}, \ldots, \mathbf{Y}_{ip} \overset{\text{i.i.d.}}{\sim} \mathcal{N}(\mathbf{\mu}, \Omega^{-1}) \) for \( i = 1, \ldots, n \). The means \( \mathbf{\mu} \) are selected from an equally spaced grid between 0 and 2 with length \( p \). We consider nine different combinations of \( n, p, \) and sparsity for \( \Omega \):

- \( p = 25, n = 25 \), sparsity = 10\% non-zero entries in the off-diagonals;
- \( p = 50, n = 100 \), sparsity = 5\% non-zero entries in the off-diagonals;
- \( p = 100, n = 300 \), sparsity = 2\% non-zero entries in the off-diagonals;
- \( p = 25, n = 25 \), AR(2) model;
- \( p = 50, n = 100 \), AR(2) model;
$\bullet$ $p = 100$, $n = 300$, AR(2) model;

$\bullet$ $p = 25$, $n = 25$, circle model;

$\bullet$ $p = 50$, $n = 100$, circle model;

$\bullet$ $p = 100$, $n = 300$, circle model,

where the circle model and the AR(2) model are described by the relations

- Circle model: $\omega_{ii} = 2$, $\omega_{i,i-1} = \omega_{i-1,i} = 1$, and $\omega_{1,p} = \omega_{p,1} = 0.9$;

- AR(2) model: $\omega_{i,i} = 1$, $\omega_{i,i-1} = \omega_{i-1,i} = 0.5$ and $\omega_{i,i-2} = \omega_{i-2,i} = 0.25$.

The percent sparsity levels for $\Omega$ are computed using lower triangular matrices that have diagonal entries normally distributed with $\mu_{\text{diag}} = 1$ and $\sigma_{\text{diag}} = 0.1$, and non-zero off-diagonal entries normally distributed with $\mu_{\backslash \text{diag}} = 0$ and $\sigma_{\backslash \text{diag}} = 1$.

The observed variables $X = (X_1, \ldots, X_p)$ are constructed from the simulated variables $Y_1, \ldots, Y_p$. The functions used to construct the observed variables are three cumulative distribution functions (c.d.f.s): asymmetric Laplace, extreme value, and stable. Any values of the parameters for the c.d.f.s could be chosen, but instead of selecting 25, 50, and 100 sets of parameters, we automatically choose the values of the parameters to be the maximum likelihood estimates with the mle function in MATLAB. The values of the parameters for each of the c.d.f.s are the maximum likelihood estimates for the parameters of the corresponding distributions (asymmetric Laplace, extreme value, and stable), using the variables $Y_1, \ldots, Y_p$.

We follow the procedure in Mulgrave and Ghosal (2018) to estimate the transformation functions. The hyperparameters for the normal prior are chosen to be $\nu = 1, \tau = 1$, and $\sigma^2 = 1$. To choose the number of basis functions, we use the Akaike Information Criterion. Samples from the truncated multivariate normal posterior distributions for the B-spline coefficients are obtained using the exact Hamiltonian Monte Carlo (exact HMC) algorithm (Pakman and Paninski, 2014). The initial coefficient values, $\theta_{d,\text{initial}}$, for the exact HMC algorithm are calculated as described in (Mulgrave and Ghosal, 2018). After finding the initial coefficient values $\theta_d$, we construct initial values for $Y_{d,\text{initial}} = \sum_{j=1}^J \theta_{dj,\text{initial}} B_j(X_d)$ using the observed variables. These initial values $Y_{\text{initial}}$ are used to find initial values for $\Sigma, \mu$, and $\Omega$ for the algorithm, where $\Sigma_{\text{initial}} = \text{cov}(Y_{\text{initial}}), \mu_{\text{initial}} = Y_{\text{initial}}$, and $\Omega_{\text{initial}} = \Sigma_{\text{initial}}^{-1}$.

For the part of the simulation study in which we do not estimate the transformation functions, the initial values for the algorithm are constructed from the observed variables, $X$, where $\Sigma_{\text{initial}} = \text{cov}(X), \mu_{\text{initial}} = X$, and $\Omega_{\text{initial}} = \Sigma_{\text{initial}}^{-1}$. The mean $\mu$ and the precision matrix $\Omega$ are estimated by the algorithm as described in the previous sections.

The hyperparameter $\zeta^2$ for the Bernoulli-Gaussian prior and the variational Bayesian algorithm is fixed to be 10. The initial value $\tau^0$ for the variational Bayesian algorithm
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is chosen to be 1000. The threshold $\epsilon$ for stopping the variational Bayesian algorithm is set to $\epsilon = 10^{-6}$. For the MCMC algorithm using the Bernoulli-Gaussian prior, the tuning procedure described in Subsection 3.1 is used to find the hyperparameter for the Bernoulli distribution, $\rho^{*}_{kd} = (\rho_{d}/p\sqrt{k})$, and the initial indicator vector, $\gamma_{d}$. Since the vector $w_{k>d}$ from the tuning procedure consists of only 0 and 1 values, it is used as the initial indicator vector $\gamma_{d}$ for the MCMC algorithm. The data matrix that is used as input for the tuning procedure is $Z_{\text{initial}} = Y_{\text{initial}} - \mu_{\text{initial}}$.

For the MCMC algorithm for the horseshoe prior, all of the hyperparameters are initialized with ones. We consider three values of $c$ that are a range of three orders of magnitude: $c \in \{0.1, 1, 10\}$. The value of $c$ that yields the lowest BIC was selected for the final estimates of the precision matrix and edge matrix. The 0-1 loss procedure (5) was used to threshold the precision matrices and construct the edge matrices.

For the simulation study, we run 100 replications for each of the nine combinations and assess structure learning for each replication. We collect 10000 MCMC samples for inference after discarding a burn-in of 5000. We do not apply thinning. The Bayesian copula method is implemented using the R package BDGraph (Mohammadi and Wit, 2015, 2017; Dobra and Mohammadi, 2017; Mohammadi and Wit, 2018) using the option “gcgm”. Posterior graph selection is done using Bayesian model averaging, the default option in the BDGraph package, in which it selects the graph with links for which their estimated posterior probabilities are greater than 0.5. The nonparanormal graphical model is implemented using the R package huge (Zhao et al., 2015) using the option “truncation”. The graphical lasso method is selected for the graph estimation and the default screening method, lossless (Witten et al., 2011; Mazumder and Hastie, 2012a), is used. Three regularization selection methods are used to find the estimated precision matrix and select the graphical model: the Stability Approach for Regularization Selection (StARS) (Liu et al., 2010), the modified Rotation Information Criterion (RIC) (Lysen, 2009), and the Extended Bayesian Information Criterion (EBIC) (Foygel and Drton, 2010). The default parameters in the huge package are used for each selection method. As in Liu et al. (2009), the number of regularization parameters used is 50 and they are selected among an evenly spaced grid in the interval $[0.16, 1.2]$.

The code for the proposed Bayesian methods is written in MATLAB and sparse representations of the matrices are used when appropriate. For the variational Bayesian algorithm, when calculating $w^{*}_{kd} = \text{expit}(\eta_{kd})$, it is set to 0 if $\exp(\eta_{kd})$ is below $2^{-52}$, which is $\text{eps}$, the floating-point relative accuracy in MATLAB, while $w^{*}_{kd}$ is set to 1 if $\exp(\eta_{kd})$ is equal to infinity in MATLAB for numerical stability. Infinity results from operations that lead to results too large to represent as conventional floating-point values. Similar adjustments are also applied for the Bernoulli-Gaussian MCMC. The code is given in Appendix A.
8.1 Performance Assessment

We compute the Bayes estimate of the precision matrix $\hat{\Omega} = E(\Omega|Z)$ by averaging all MCMC samples after burn-in, or the variational Bayes estimate by averaging over 500 independent samples from the variational distribution. The median probability model (Berger and Barbieri, 2004) is used to obtain the Bayes estimate of the edge matrix. We find the estimated edge matrix by first using the 0-1 loss procedure to threshold the MCMC precision matrix samples, and then we take the mean of the thresholded precision matrices. If each off-diagonal element of the mean of the thresholded matrices is greater than 0.5, the element is registered as an edge in the estimated edge matrix, and if each off-diagonal element of the mean is not greater than 0.5, it is registered as no edge.

We compute specificity (SP), sensitivity (SE), and Matthews Correlation Coefficient (MCC) to assess the performance of the graphical structure learning. They are defined as follows:

$$\text{Specificity} = \frac{TN}{TN + FP}, \quad \text{Sensitivity} = \frac{TP}{TP + FN},$$

$$\text{MCC} = \frac{TP \times TN - FP \times FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}},$$

where TP is the number of true positives, TN is the number of true negatives, FP is the number of false positives, and FN is the number of false negatives. For all three metrics, the higher the values are, the better is the classification. If there are models that are estimated to have no edges, they result in NaNs as MCC values.

We also look at the effect of the transformation functions on parameter estimation for our methods. We consider the scaled $L_1$-loss function, the average absolute distance, as a measure of parameter estimation. Scaled $L_1$-loss is defined as

$$\text{Scaled } L_1\text{-loss} = \frac{1}{p^2} \sum_k \sum_d \left\| \hat{\Omega}_{kd} - \Omega_{true, kd} \right\|$$

where $\Omega_{true, kd}$ stands for the true covariance matrix. Note that for the Bayesian Copula method, we use the estimated inverse correlation matrix and the true correlation matrix in place of the precision matrix for loss calculation.

Overall, in terms of structure learning, the horseshoe prior, Bernoulli-Gaussian prior, and variational Bayesian methods outperform the nonparanormal and Gaussian copula graphical model. The Bayesian copula graphical model outperforms the horseshoe prior, Bernoulli-Gaussian prior, and variational Bayesian methods for only the AR(2) model for $p = 25$ and $p = 50$. Similarly, the horseshoe and Bernoulli-Gaussian models outperform the variational Bayesian methods for the AR(2) model for $p = 25$ and $p = 50$. Generally, the nonparanormal model selected by RIC outperforms the nonparanormal models selected by
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StARS and EBIC in terms of structure learning. No edges were selected by the nonparanormal model using EBIC for the sparsity models of dimension $p = 25$ and for the $p = 50$ AR(2) model. For the 10% and AR(2) models, the nonparanormal model selected by RIC performs similarly to the Bayesian methods for $p = 25$, but for $p = 50$ and $p = 100$, the Bayesian methods outperform the RIC-selected model in learning the structure. Compared to all other competing methods, the Bayesian nonparanormal methods is significantly better at learning the structure of the circle model and of models with $p = 100$ dimension. The horseshoe prior appears to be more sensitive to signals than the Bernoulli-Gaussian prior and variational Bayesian methods, but overall, the structure learning results are similar, as demonstrated by the MCC values.

In terms of parameter estimation, for the horseshoe prior, Bernoulli-Gaussian prior, and variational Bayesian methods, the transformation functions improves the scaled $L_1$-loss of the models, compared to the models without the transformation functions. In general, compared to the horseshoe and Bernoulli-Gaussian methods, the variational Bayesian method performs similar in terms of structure learning and the best in terms of parameter estimation. All three Bayesian nonparanormal methods proposed learn structure better than the available non-Bayesian methods, i.e. the nonparanormal graphical model selected using RIC and StARS. The results are presented in Figures 1–4. Note that Percent refers to the 10% model for dimension $p = 25$, 5% model for dimension $p = 50$ and 2% model for dimension $p = 100$.

9. Real Data Application

For the real data application, we consider the data set based on the GeneChip (Affymetrix) microarrays for the plant *Arabidopsis thaliana* originally referenced in (Wille et al., 2004). There are $n = 118$ microarrays and $p = 39$ genes from the isoprenoid pathway that are used. For pre-processing, the expression levels for each gene, $x_i$ for $i = 1, \ldots, 118$, are log-transformed. We study the associations among the genes using the Bayesian nonparanormal methods, the nonparanormal method of Liu et al. (2009), and the Bayesian copula graphical model of Mohammadi and Wit (2017). These data are treated as multivariate Gaussian originally in (Wille et al., 2004).

Using the same set-up as in the simulation study, we fit the Bayesian copula graphical model using the BDGraph package and we fit the nonparanormal graphical model using the huge package. The BDGraph package selected 211 edges using Bayesian model averaging. The huge package using the RIC selection resulted in 140 edges and using the StARS method resulted in 209 edges. The EBIC-selected model results in no edges.

In order to construct the graphical models using our methods, we converted the values to be between 0 and 1 using the equation $(x - \min(x_i)) / (\max(x_i) - \min(x_i))$. The variational Bayes method results in 98 edges, the horseshoe prior based method results in 257 edges, and the Bernoulli-Gaussian prior based method results in 102 edges. For $p = 39$, convergence of the variational Bayes method can be achieved in about 26 minutes,
the horseshoe prior based method in about 47 minutes for a given $c$, and the Bernoulli-Gaussian prior based method in about 52 minutes on a laptop computer. The graphs of our proposed methods are shown in Figure 1. The graphs of the existing methods are shown in Figure 2.

The variational Bayes and Bernoulli-Gaussian prior methods result in the sparsest graphs. The horseshoe prior method results in the densest graph. Out of the three proposed methods, the horseshoe prior method is the most sensitive method, so it appears for this data set, it is selecting more edges than the other models. The variational Bayes method is the fastest method out of the three proposed methods. The variational Bayes and Bernoulli-Gaussian prior methods proposed in this paper give sparser graphs than the Gaussian copula graphical model method, which uses a G-Wishart prior on the precision matrix. Sparse graphs can aid in simpler scientific interpretation.

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Figure 2: Specificity results.

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Appendix A.

GitHub Repository: https://github.com/jnj2102/BayesianRegressionApproach. The code used to run the methods described in this paper are available on GitHub.

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Figure 3: Matthews correlation coefficient results.

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Figure 4: Comparison of scaled $L_1$-loss with and without transformation.
Figure 5: Comparison of models from proposed methods.

(a) Variational Bayesian method.

(b) Horseshoe method.

(c) Bernoulli-Gaussian method.
Figure 6: Comparison of models from existing methods.

(a) Bayesian copula method.

(b) RIC method.

(c) StARS method.
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