Bayesian Joint Spike-and-Slab Graphical Lasso

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Abstract

In this article, we propose a new class of priors for Bayesian inference with multiple Gaussian graphical models. We introduce fully Bayesian treatments of two popular procedures, the group graphical lasso and the fused graphical lasso, and extend them to a continuous spike-and-slab framework to allow self-adaptive shrinkage and model selection simultaneously. We develop an EM algorithm that performs fast and dynamic explorations of posterior modes. Our approach selects sparse models efficiently with substantially smaller bias than would be induced by alternative regularization procedures. The performance of the proposed methods are demonstrated through simulation and two real data examples.

1 Introduction

Bayesian formulations of graphical models have been widely adopted as a way to characterize conditional independence structure among complex high-dimensional data. These models are popular in scientific domains including genomics [1, 25], public health [6, 17], and economics [7]. In practice, data often come from several distinct groups. For example, data may be collected under various conditions, at different locations and time periods, or correspond to distinct subpopulations. Assuming a single graphical model in such cases can lead to unreliable estimates of network structure, whereas the alternative, estimating different graphical models separately for each group, may not be feasible for high dimensional problems.

Several approaches have been proposed to learn graphical models jointly for multiple classes of data. Much of this work extends the penalized maximum likelihood approach to incorporate additional penalty terms that encourage the class-specific precision matrices to be similar [10, 3, 29, 20]. In the Bayesian literature, Peterson et al. [26] and Lin et al. [18] utilize Markov Random Field priors to model a super-graph linking different graphical models. Tan et al. [31] uses a logistic regression model to link the connectivity of nodes to covariates specific to each graph. These approaches only model the similarity of the underlying graphs, and thus are limited in their ability to borrow information when estimating the precision matrices. Borrowing strength is especially important when some classes have small sample sizes.

In this work, we introduce a new Bayesian formulation for estimating multiple related Gaussian graphical models by leveraging similarities in the underlying sparse precision matrices directly. We first present two shrinkage priors for multiple related precision matrices, as the Bayesian counterpart
of joint graphical lasso estimators [4]. We then propose a doubly spike-and-slab mixture extension to these priors, which allows us to achieve simultaneous shrinkage and model selection, as well as handle missing observations. In Section 5 and 6 we provide a fast Expectation-Maximization (EM) algorithm to quickly identify the posterior modes in a manner similar to [16] and [5]. We also propose a procedure to sequentially explore a series of posterior modes. We then demonstrate the substantial improvements in both model selection and parameter estimation over the original joint graphical lasso approach using both simulated data and two real datasets in Section 7. Finally, in Section 8 we discuss future directions for improvements.

2 Preliminaries

2.1 The joint graphical lasso

We first briefly introduce the notation used throughout this paper. We let $G$ denote the number of classes in the data, and let $\Omega_g$ and $\Sigma_g$ denote the precision and covariance matrix for the $g$-th class.

We let $\omega^{(g)}_{jk}$ denote the $(j,k)$-th element in $\Omega_g$ and $\omega_{jk} = \{\omega^{(g)}_{jk}\}_{g=1,...,G}$ denote the vector of all the $(j,k)$-th elements in $\{\Omega\}$. Suppose we are given $G$ datasets, $X^{(1)},...,X^{(G)}$, where $X^{(g)}$ is a $n_g \times p$ matrix of independent centered observations from the distribution $\text{Normal}(0,\Omega^{-1}_g)$. As maximum likelihood estimates of $\Omega_g$ can have high variance and are ill-defined when $p > n_g$, the joint penalized log likelihood for the $G$ dataset is usually considered instead:

$$
\ell(\{\Omega\}) = \frac{1}{2} \sum_{g=1}^{G} n_g \log \det \Omega_g - tr(S_g \Omega_g) - \text{pen}(\{\Omega\}),
$$

where $S_g = (X^{(g)})^T X^{(g)}$. The penalty function encourages $\{\Omega\}$ to have zeros on the off-diagonal and be similar across groups. In particular, we consider two useful penalty functions studied in Danaher et al. [4], the group graphical lasso (GGL), and the fused graphical lasso (FGL):

$$
\text{pen}(\{\Omega\}) = \frac{\lambda_0}{2} \sum_g \sum_j |\omega^{(g)}_{jj}| + \lambda_1 \sum_g \sum_{j<k} |\omega^{(g)}_{jk}| + \lambda_2 \sum_{j<k} \overline{\text{pen}}(\omega_{jk}),
$$

where $\overline{\text{pen}}(\omega_{jk}) = \|\omega_{jk}\|_2$ for GGL and $\sum_{g<g'} |\omega^{(g)}_{jk} - \omega^{(g')}_{jk}|$ for FGL. Both penalties encourage similarity across groups when $\lambda_2 > 0$, and reduce to separate graphical lasso problems when $\lambda_2 = 0$. The group graphical lasso encourages only similar patterns of zero elements across the $G$ precision matrices, while the fused graphical lasso encourages a stronger form of similarity: the values of off-diagonal elements are also encouraged to be similar across the $G$ precision matrices. In practice, $\lambda_0$ is typically set to 0 when the diagonal elements are not to be penalized.

2.2 Bayesian formulation of Gaussian graphical models

One of the most popular approaches for Bayesian inference with Gaussian graphical models is the $G$-Wishart prior [14,22]. The $G$-Wishart prior estimates the precision matrices with exact zeros in the off-diagonal elements and enjoys the conjugacy with the Gaussian likelihood. However, posterior inference under the $G$-Wishart prior can be computationally burdensome and has to rely on stochastic search algorithms over the large model space, consisting of all possible graphs. In recent years, several classes of shrinkage priors have been proposed for estimating large precision matrices, including the graphical lasso prior [13,25], the continuous spike-and-slab prior [14,17], and the graphical horseshoe prior [15]. This line of work draws direct connections between penalized likelihood schemes and, as their names suggest, the posterior modes in a Bayesian setting. Unlike the $G$-Wishart prior, these shrinkage priors do not take point mass at zero for the off-diagonal elements in the precision matrix, and thus usually lead to efficient block sampling algorithms with improved scalability. However, fully Bayesian procedures still need to rely on stochastic search to achieve model selection, making it less appealing for many problems.

To address this issue, deterministic algorithms have been proposed to perform fast posterior exploration and mode searching in Gaussian graphical models [16,5]. Motivated by the EMVS [27] and spike-and-slab lasso [23] procedures in the linear regression literature, the idea is to use a two-component mixture distribution, i.e., spike-and-slab priors, to parameterize off-diagonal elements in the precision matrix, which allows simultaneous model selection and parameter estimation. We will utilize a similar strategy for model estimation in this paper.
3 Bayesian joint graphical lasso priors

We first provide a Bayesian interpretation of the group and fused graphical lasso estimators. From a probabilistic perspective, it is well understood that estimators that optimize a penalized likelihood can often be seen as the posterior mode estimator under some suitable prior distributions. The Bayesian formulation of the joint graphical lasso problems discussed in the previous section can be defined as

\[ p(\{\Omega\}) \propto \exp(-\text{pen}(\{\Omega\})) \]

where \( \lambda \) is the non-zero elements in \( \{\Omega\} \) represent the graph structure. Second, the fixed penalty term, which minimizes the bias from over-penalizing the large elements, different hyper-priors on \( \lambda \) as the non-zero elements in \( \{\Omega\} \).

\[ p(\{\Omega\}) \propto \exp\left(-\frac{\lambda_1^2}{2} \sum_{g} \tau_{jkg} - \frac{\lambda_2^2}{2} \sum_{g<g'} \phi_{jkgg'} \right) \]

where \( C_{\tau,\rho} \) is a normalizing constant and \( M^+ \) denotes the space of symmetric positive matrices. The normalizing constant is analytically intractable due to this constraint, but it cancels out in the marginal distribution of \( p(\{\Omega\}) \). Such cancellation has been studied by several authors. Similarly, the FGL prior can be defined as

\[ p(\{\Omega\}) = C_{\tau,\rho}^{-1} \prod_{j<k} \text{Normal}(\omega_{jkg}; 0, (\Theta_{jk}^{(G)})^{-1}) \prod_{g} \prod_{j} \text{Exp}(\omega_{jj}; \lambda_0) 1_{\{\Omega\} \in \{M^+\}}, \]

where \( \Theta_{jk}^{(G)} = \text{diag}\left(\frac{1}{\rho_{jk}} + \frac{1}{\tau_{jkg}}\right) \)

\[ p(\tau, \rho) \propto C_{\tau,\rho} \prod_{j<k} \left( \exp\left(-\frac{\lambda_1^2}{2} \sum_{g} \tau_{jkg} - \frac{\lambda_2^2}{2} \sum_{g<g'} \phi_{jkgg'} \right) \right) \]

It is also worth noting that both of the above priors are proper, and we leave the proof of the following proposition in the supplement.

**Proposition 1.** The priors defined in (3) – (5) and (6) – (8) are proper and the posterior mode of \( \{\Omega\} \) is the solution of the group and fused graphical lasso problem with penalty terms defined in (2).

4 Bayesian joint spike-and-slab graphical lasso priors

The Bayesian formulation of the joint graphical lasso problems discussed in the previous section provide shrinkage effects at the level of both individual precision matrices and across different classes. However, two issues remain. First, shrinkage priors alone do not produce sparse models since the posterior draws are never exactly 0. Thus, additional thresholding is needed to obtain a sparse representation of the graph structure. Second, the fixed penalty term, \( \lambda_1 \) and \( \lambda_2 \) may be too restrictive, as the non-zero elements in \( \{\Omega\} \) are penalized equally to elements close to zero. To reduce the bias from over-penalizing the large elements, different hyper-priors on \( \lambda_1 \) have been proposed to adaptively estimate the penalty term in Bayesian graphical lasso.

Here we address both challenges simultaneously using the spike-and-slab approaches in Bayesian variable selection. In particular, we employ a set of latent indicators to construct a “selection” prior on both the group level and within-groups for the similarity penalties. We first let binary variables \( \delta = \{\delta_{jk}\}_{j<k} \) denote the existence of each edge in the graph, indexing the \( 2^{p(p-1)/2} \) possible models at the group level, so that \( \delta_{jk} = 1 \) indicates the \( (j,k) \)-th edge is selected for all precision matrices. We then let another set of binary variables \( \xi = \{\xi_{jk}\}_{j<k} \) denote the non-existence of ‘similarities’ among the elements in the same cell of different precision matrices, so that \( \xi_{jk} = 0 \) indicates the \( (j,k) \)-th element is expected to be similar. We use the term ‘similarity’ here as a broad term parameterized by \( \lambda_2 \), since the behavior of the similarity depends on the form of the penalization. Conditional
on the two binary indicators, we replace the fixed penalty parameters $\lambda_1$ and $\lambda_2$ by a mixture of edge-wise penalties that take values from $\{\lambda_1/v_0, \lambda_1/v_1\}$, and $\{\lambda_2/v_0, \lambda_2/v_1\}$ respectively, with fixed $v_1 > v_0 > 0$. That is, we introduce the following penalties conditional on $\delta$ and $\xi$, and we propose the doubly spike-and-slab extensions to GGL and FGL as

$$pen(\{\Omega\}|\delta, \xi) = \frac{\lambda_0}{2} \sum_g \sum_j |\omega_{jj}^{(g)}| + \lambda_1 \sum_j \sum_{g<j<k} \frac{|\omega_{jk}^{(g)}|}{v_{jk}} + \lambda_2 \sum_{j<k} \tilde{pen}(\omega_{jk}),$$

where $\tilde{pen}(\omega_{jk})$ is defined as before and $\xi_{jk} = \xi_{jk} \delta_{jk}$. The prior defined in (9) relate to the unconditional penalties by $pen(\{\Omega\}) = pen(\{\Omega\}|\delta, \xi) - \log(p(\delta, \xi))$, and we will refer to them as DSS-FGL and DSS-GGL.

In practice, we find it usually reasonable to enforce all elements from the spike distribution to also be similar, as the spike distribution is always chosen to have large penalization and leads to posterior modes at exactly 0. However, other types of edge-wise dependence between $\delta_{jk}$ and $\xi_{jk}$ are also possible with minor modifications. For example, we can also fix $\xi_{jk}$ to be 1, so that the two penalty terms will always be proportional. We refer to this setting as spike-and-slab group and fused lasso (SS-GGL and SS-FGL) and discuss their behavior in the supplements.

The original GGL and FGL suffer from the same bias induced by the excessive shrinkage of lasso estimates. With the introduction of $v_0$ and $v_1$, we can adaptively estimate which $\omega_{jk}$ to penalize in a data-driven way. As we discuss in more detail in Section 6, this adaptive shrinkage property can indeed significantly reduce bias imposed on the lasso penalty. That is, by choosing the hyperparameters so that $\lambda_1/v_0 \gg \lambda_1/v_1$, we impose only minimal shrinkage on values arising from the slab distribution.

For a fully Bayesian setup, we employ standard priors on the binary indicators to further share information on the sparsity level. The full generative model for $\{\Omega\}$ is:

$$p(\{\Omega\}|\delta, \xi, \theta) = C_{\delta}^{-1} C_{\xi}^{-1} \exp(-pen(\{\Omega\}|\delta, \xi)) \mathbf{1}_{\{\Omega\} \in \mathbb{M}_+^{G \times G}}$$

$$p(\delta, \xi|\pi_{\delta}, \pi_{\xi}) \propto C_{\delta, \xi} \prod_{j<k} \pi_{\delta}^{\delta_{jk}} (1 - \pi_{\delta})^{1-\delta_{jk}} \pi_{\xi}^{\xi_{jk}} (1 - \pi_{\xi})^{1-\xi_{jk}}$$

where $\theta$ denote $(\tau, \rho)$ for DSS-GGL, and $(\tau, \phi)$ for DSS-FGL. $C_{\delta, \xi}$ is another intractable normalization constant. We put standard Beta hyperpriors on the sparsity parameters so that $\pi_{\delta} \sim \text{Beta}(a_1, b_1)$ and $\pi_{\xi} \sim \text{Beta}(a_2, b_2)$. Throughout this paper, we let $a_1 = a_2 = 1$ and $b_1 = b_2 = \rho$. Additionally, the above prior can be easily reparameterized with scale mixture of normal prior distributions similar as before by modifying the precision matrix $\Theta$ into the following form, and they can be shown to be proper priors (the proofs can be found in the supplement):

$$\Theta^{(F)}_{jk} = \begin{cases} \theta_{gg} = \frac{v_{jk}^{\delta}}{\tau_{jk}^{\delta}} + \sum_{g'<g} \frac{v_{g'k}^{\delta}}{\sigma_{g'kg}^{\delta}} & g = 1, ..., G \\ \theta_{gg'} = \frac{v_{jk}}{\sigma_{g'kg}^{\delta}} & g' \neq g \end{cases}$$

$$\Theta^{(G)}_{jk} = \text{diag}(\{ \frac{v_{jk}^{\delta}}{\rho^{jk}} + \frac{v_{g'k}^{\xi}}{\tau_{jk}^{\xi}} \}_{g=1,...,G}).$$

**Proposition 2.** The priors defined in (10) - (12) are proper, and the posterior mode of $\{\Omega\}$ is the solution to the corresponding spike-and-slab version of joint graphical lasso penalties.

Finally, it is straightforward to see that the proposed DSS-GGL and DSS-FGL penalties reduce to their non spike-and-slab counterparts when $\delta$ and $\xi$ are fixed to be 1. Several other spike-and-slab formulations in the literature can be seen as the special case of this prior when $G = 1$ as well. For example, the spike-and-slab mixture of double exponential priors considered in [5] is a special case with $\lambda_2 = 0$. The spike-and-slab Gaussian mixtures in [16] can also be considered as a special case where we further fix $\tau_{jk} = \infty$. This approach is also related to the work on sparse group selection in linear regression, as has been discussed in [35] and [36]. As opposed to the point mass priors for the spike distribution commonly in the literature, our doubly spike-and-slab formulation of continuous mixtures allows the spike distribution to absorb small non-zero noises and facilitates fast dynamic explorations, as we will show in Section 6.
5 Model estimation

Given fixed $\lambda_1$, $\lambda_2$, and $v_0$, the representation of $p(\{\Omega\})$ with the scale mixture of normal distributions allows the posterior to be sampled using a block Gibbs algorithm, as described in the supplement. However, choosing the hyperparameters can usually be a nontrivial task. Instead, we focus on faster deterministic methods to detect posterior modes under different choices of hyperparameters [27]. We present an EM algorithm that maximizes the complete-data posterior distribution $p(\{\Omega\}, \delta, \xi, \pi_\delta, \pi_\xi | X)$ by treating the binary latent variables as “missing data.” Similar ideas have been explored in recent work for linear regression [27, 28] and single graphical model estimation [5, 16]. Our EM algorithm maximizes the objective function $E_{\delta,\xi | \{\Omega\}}(\pi_\delta^{(t)}, \pi_\xi^{(t)}, X) \log p(\{\Omega\}, \delta, \xi | X | \{\Omega\}^{(t)}, \pi_\delta^{(t)}, \pi_\xi^{(t)}, X)$ by iterating between the E-step and M-step until changes in $\{\Omega\}$ are within a small threshold.

In the E-step, we compute the conditional expectation terms in the objective function. It turns out that it suffices to find the conditional distribution of $(\delta_{jk}, \xi_{jk})$. The corresponding cell probabilities are proportional the the following mixture densities:

\[
p_{\delta_{jk}, \xi_{jk}}(j, k) \propto \begin{cases} 
\pi_{\delta}(1 - \pi_{\xi}) \frac{\lambda_1 \lambda_2}{v_0} \exp(-\lambda_1 \sum_{g} |\omega_{jk}^{(g)}|/v_1 - \lambda_2 \rho n(\omega_{jk})/v_0) & \delta_{jk} = 1, \xi_{jk} = 0 \\
\pi_{\delta} \pi_{\xi} \frac{\lambda_1 \lambda_2}{v_0^2} \exp(-\lambda_1 \sum_{g} |\omega_{jk}^{(g)}|/v_1 - \lambda_2 \rho n(\omega_{jk})/v_0) & \delta_{jk} = 1, \xi_{jk} = 1 \\
(1 - \pi_{\delta})(1 - \pi_{\xi}) \frac{\lambda_1 \lambda_2}{v_0} \exp(-\lambda_1 \sum_{g} |\omega_{jk}^{(g)}|/v_0 - \lambda_2 \rho n(\omega_{jk})/v_0) & \delta_{jk} = 0, \xi_{jk} = 0 
\end{cases}
\]

It is interesting to note that the three scenarios above represent three types of relationships among $\omega_{jk}$: weak shrinkage but strong similarity, weak shrinkage and weak similarity, and strong shrinkage across classes. $E_{\xi}(\delta_{jk})$ and $E_{\xi}(\xi_{jk})$ are then simply the marginal probabilities in this 2 by 2 table, i.e., $E_{\xi}(\delta_{jk}) = p_{\delta, 0}^{(1)}(j, k)$ and $E_{\xi}(\xi_{jk}) = E_{\xi}(\delta_{jk}, \xi_{jk}) = p_{1, 1}^{(t)}(j, k)$. The EM algorithm also handles missing cells in $X$ naturally. Assuming missing at random, the expectation can also be taken over the space of missing variables, by additionally computing $E_{\xi}(\text{tr}(S_g \Omega_g)) = \text{tr}(E_{\xi}(X^{(g)^T}X^{(g)})) \Omega_g)$, using the conditional Gaussian distribution of $\xi_{\alpha, \text{miss}}^{(g)} | \xi_{\alpha, \text{obs}}^{(g)}$. We relegate the derivations of the objective function to the supplement.

Given the expectations calculated in the E-step, one might proceed with conditional maximization steps using gradient ascent similar to the Gibbs sampler [16]. Alternatively, since the maximization step is equivalent to solving the following joint graphical lasso problem:

\[
\{\Omega\} = \text{argmax}_{\{\Omega\}} \frac{1}{2} \sum_{g} n_g \log |\Omega_g| - \frac{1}{2} \sum_{g} \text{tr}(S_g \Omega_g) - \frac{\lambda_0}{2} \sum_{j<k} |\omega_{jk}^{(g)}| - \lambda_1 \left(\frac{p_{\delta, 0}^{*}(0, j, k)}{v_0} + \frac{1 - p_{\delta, 0}^{*}(0, j, k)}{v_1}\right) \sum_{g} |\omega_{jk}^{(g)}| - \sum_{j<k} \lambda_2 \left(\frac{1 - p_{1, 1}^{*}(j, k)}{v_0} + \frac{p_{1, 1}^{*}(j, k)}{v_1}\right) \rho n(\omega_{jk}),
\]

meaning we can use the ADMM algorithm described in [4].

6 Dynamic posterior exploration

The algorithm proposed in the previous section requires a fixed set of hyperparameters, $(\lambda_0, \lambda_1, \lambda_2, v_0)$. The posterior is relatively insensitive to the choice of $\lambda_0$ as long as it is not too large [34]. Furthermore, unlike the original joint graphical lasso, where two tuning parameters need to be selected using cross-validation or model selection criterion, it turns out that we can leverage the self-adaptive property from the doubly spike-and-slab mixture setup to achieve automatic tuning using a path-following strategy [28]. Specifically, we consider a sequence of decreasing $v_0 = \{v_0^1, \ldots, v_0^L\}$ and some small $\lambda_1$ and $\lambda_2$. We initiate $\{\Omega\}_0$ so that $\Omega_{g0} = (S_g/n_g + cI)^{-1}$, and iterative estimate $\{\Omega\}_l$ with $v_0 = v_0^L$. After fitting the $t$-th model, we use the estimated graph structure to warm start the $(t + 1)$-th model by initiating $\Omega_{g0}$ to be $\Omega_{g0} \odot 1_{L \times 0}$, where $1_{L \times 0}$ denotes the group level graph structure at the $t$-th iteration. As $v_0$ decreases, the shrinkage imposed on the spike elements steadily increases and leads to sparser models. As noted in [28], the solution path from such dynamic reinitialization procedure usually ‘stabilizes’ as $v_0$ becomes closer to 0 in linear regression. We found similar behavior in our spike-and-slab joint graphical lasso models too, as illustrated in Figure [1].
Figure 1: The solution paths and estimated precision matrices of FGL (upper row) and DSS-FGL (lower row). The red nodes correspond to true edges and the gray nodes correspond to 0’s. The two vertical lines in the FGL solution path indicate the model that best matches the true sparsity (left) and the model with the lowest AIC (right). The block containing the edges is plotted for the estimated values (upper triangular) against the truth (lower triangular). The model that best matches the true graphs is plotted for FGL. The off-diagonal values are rescaled and negated to partial correlations, and 0’s are colored with light gray background for easier visual comparison. The bias of the estimated precision matrix as measured by the Frobenius norm, \( \| \hat{\Omega}_g - \Omega_g \|_F \), is also printed in the captions.

To demonstrate the dynamic posterior exploration in action, we simulated a small dataset from two classes, with \( n_g = 150 \) for \( g = 1, 2 \), and \( p = 100 \). The two underlying graphs differ by 5 edges: The first precision matrix contains a 10-node block with an AR(1) precision matrix where \((\Omega^{-1})_{jk} = \rho_1^{\mid j-k \mid} \), and \( \rho_1 = 0.7 \); the second precision matrix in the second class contains a common 5-node AR(1) block with \( \rho_2 = 0.9 \). The rest of the nodes are all independent. We fit the fused graphical lasso with a sequence of \( \lambda_1 \), and fixed \( \lambda_2 = 0.1 \), which leads to the best performance in this experiment; and DSS-FGL with \( \lambda_1 = 1 \), and \( \lambda_2 = 1 \). Figure[1] shows the FGL and DSS-FGL solution path. Unlike the continuous shrinkage of FGL, the zero and non-zero elements under DSS-FGL tend to be separated into two stable clusters as the effective shrinkage \( \lambda_1/\nu_0 \) increases beyond a critical point. Danaher et al. [4] noted that graph selection using AIC tends to favor large models. This example also confirms this observation as the likelihood evaluation for smaller models suffers from the overly aggressive shrinkage. In this example, AIC selects 27 edges in both classes, leading to 41 false positives. Assuming we know the true graphs, the best model in terms of edge selection along the FGL solution path contains one false negative edge as shown in Figure[1]. However, without accurate prior knowledge of graph sparsity, correctly identifying this model is typically difficult, if not impossible. On the other hand, the stable model from the DSS-FGL solution path yields 4 false positive edges in the second graph, but with clear visual separation from the regularization plot: only one false positive edge stabilizing to a larger value away from 0. Thus in practice, the solution path also provides a visual tool to threshold the small values close to 0. Additionally, the bias of the final precision matrices compared to the truth is also much smaller than the best FGL solution.

We also find that the converged region is insensitive to the choice of \( \lambda_1 \) and \( \lambda_2 \) in all our experiments, as the model allows a flexible combination of shrinkage through the adaptive estimation of \( p^* \). The supplement includes an empirical assessment of sensitivity in the simulation experiments.

7 Numerical results

Simulation experiments To assess the performance of the proposed models, we consider a three-class problem similar to the study carried out in [4]. We first generate three networks with \( p = 500 \) features with 10 equal sized unconnected subnetworks following power law degree distributions.
Exactly one and two subnetworks are removed from the second and third class. The details of the data generating process can be found in the supplement. The results comparing the proposed model and joint graphical lasso are shown in Figure 2. As discussed before, the DSS-FGL and DSS-GGL achieve model selection automatically. Thus we compare the selected models with the average curve of FGL and GGL under different tuning parameters. Figure 2(a) and (c) show that DSS-FGL and DSS-GGL usually achieves better structure learning performance for both identifying edges and differential edges. The differential edges are defined as the edges for the \((g, g')\) pair with \(|\omega_{jk}^g - \omega_{jk}^{g'}| > 0.01\). Figure 2(b) and (d) clearly demonstrate the bias-diminishing property of the proposed models. On average, both the sum of bias as measured by the Frobenius norm, \(\|\hat{\Omega}_g - \Omega_g\|_F\), and the Kullback-Leibler (KL) divergence achieved by the proposed model is much smaller.

Figure 2: Performance of FGL, GGL, DSS-FGL, and DSS-GGL over 100 replications. The dots represent the metrics for the 100 selected models under DSS-FGL and DSS-GGL, and the lines represent the average performance of FGL and GGL over 100 replications under different tuning parameters.

**Symptom networks of verbal autopsy data** We applied the DSS-FGL and DSS-GGL to a gold-standard dataset of verbal autopsy (VA) surveys [23]. VA surveys are widely adopted in countries without full-coverage civil registration and vital statistics systems to estimate cause of death. They are conducted by interviewing caregiver of a recently deceased person about the decedent’s health history. The standard procedure of preparing the collected data is to dichotomize all continuous variables into binary indicators and many algorithms have been proposed to automatically assign causes of death using the binary input [3, 30, 21]. However, more information may be gained by modeling the continuous variables directly [17]. Here we focus on modeling the joint distribution of the continuous variables. The 27 continuous variables in this dataset contain representations of the duration of symptoms, such as response to the question ‘how many days did the fever last’, and age of the decedents. It is usually reasonable to assume the response to these questions are jointly distributed in similar ways conditional on each cause of death. We take the raw responses and transform raw duration \(x_{ij}\) by \(\log(x_{ij} + 1)\). We then let \(X_{ij}^{(g)}\) denote the \(j\)-th transformed variable for observation \(i\) due to the cause \(g\). The full dataset contains death assigned to 34 causes. We applied DSS-FGL with \(\lambda_1 = \lambda_2 = 1\) to the three largest determined causes of death in this data: Stroke (\(n = 630\)), Pneumonia (\(n = 540\)), and AIDS (\(n = 542\)) in Figure 3. The estimated graphs under other models are discussed in the supplement. Both DSS-FGL and DSS-GGL estimated similar graphs and discovered interesting differential symptom pairs, such as the strong conditional dependence between the duration of illness and paralysis in deaths due to stroke. Further incorporating the DSS-FGL and DSS-GGL formulation of multiple precision matrices into a classification framework would likely improve accuracy over existing methods (e.g. McCormick et al. [21], Byass et al. [3]) for automatic cause-of-death assignment.

**Prediction of missing mortality rates** Beyond structure learning, the bias reduction in estimating \(\{\Omega\}\) also makes the proposed method more appealing for prediction tasks involving sparse precision matrices. In this example, we illustrate the potential of using the proposed methods to impute missing mortality rates using a cross-validation study. We construct the data matrices \(X_{ij}^{(g)}\) as the log transformed central mortality rate of age group \(j\) in year \(i\) for subpopulation \(g\) (e.g., male and female). Standard approaches in demography, such as the Lee-Carter model [13], typically use dimension reduction techniques to estimate mean effects due to age and time, and consider the residuals as
independent measurement errors. However, residuals from such models are usually still highly correlated [8]. We consider estimating the residual structure with the $1 \times 1$ gender-specific mortality table up to age 100 in the US over the period of 1960 to 2010 using data obtained from the Human Mortality Database (HMD) [32]. For both the male and female mortality, we first randomly selected 25 years and remove 25 data points in each of those years. We then fit a Lee-Carter model to estimate the mean model and interpolate the missing rates. Next, we estimate the covariance matrices among the 101 age groups in both genders using FGL and DSS-FGL from the residuals. The estimated residuals for the missing values can then be obtained by the E-step in our EM algorithm, or as the expectation from the conditional Gaussian distributions with covariance matrices estimated by FGL. The average mean squared errors (MSEs) for the prediction of missing log rates are summarized in Table 1. Imputation based on DSS-FGL precision matrix reduces the MSE by 27.8% compared to simple interpolation of the mean model (i.e., assuming i.i.d errors), compared to the 6.5% reduction from the FGL precision matrix with the same complexity. The estimated graphs are in the supplement.

Table 1: Average and standard deviation of the mean squared errors from 50 cross-validation experiments. The FGL model is selected to have the same number of edges as the DSS-FGL.

|                  | i.i.d   | FGL    | DSS-FGL |
|------------------|---------|--------|---------|
| Average MSE      | 0.00372 | 0.00348| 0.00268 |
| Standard deviation of the MSEs | 0.00030 | 0.00031| 0.00028 |

8 Discussion

In this paper, we introduced a new class of priors for joint estimation of multiple graphical models. The proposed doubly spike-and-slab mixture priors, DSS-FGL and DSS-GGL, provide self-adaptive extensions to the joint graphical lasso penalties, and achieves simultaneous model selection and parameter estimation. Moreover, while taking advantage of the flexible class of penalty functions, the dynamic posterior exploration procedure allows the penalties to be adaptively estimated in a data-driven way, thus freeing practitioners from choosing multiple tuning parameters. This is especially useful in domains where sample sizes are too small to reliably perform cross-validation. Finally, while not discussed in the main paper, we note that the posterior uncertainty may be estimated using the Gibbs sampler described in the supplement.

The proposed framework can be extended in a few directions. First, we have assumed all classes to be exchangeable, as reflected in the penalty functions for the between-class similarity. When the classes exhibit hierarchical structures or different strengths of similarities, the indicator $\xi$ may be modeled as functions of the class membership as well. Markov Random Field priors discussed in Saegusa and Shojaie [29] and Peterson et al. [26] may also be used to model the between-class similarities. Second, we have considered the estimation of missing values in the data matrices. It is
also straightforward to extend to data with missing class labels. In this way, the proposed methods can be extended to classification or discriminant analysis based on sparse precision matrices [11]. Finally, the proposed model is estimated using an EM algorithm that is iteratively solving the joint graphical lasso problem. It may be interesting to construct coordinate ascent algorithms that optimize on the objective function directly, similar to that described in [28] for linear regression.

References

[1] Laurent Briollais, Adrian Dobra, Jinnan Liu, Matt Friedlander, Hilmi Ozcelik, Hélène Massam, et al. A Bayesian graphical model for genome-wide association studies (GWAS). The Annals of Applied Statistics, 10(2):786–811, 2016.

[2] Z Butt, S Haberman, and HL Shang. *ilc: Lee-Carter Mortality Models using Iterative Fitting Algorithms*, 2014. R package version 1.0.

[3] Peter Byass, Daniel Chandramohan, Samuel J Clark, Lucia D’Ambruoso, Edward Fottrell, Wendy J Graham, Abraham J Herbst, Abraham Hodgson, Sennen Hounton, Kathleen Kahn, et al. Strengthening standardised interpretation of verbal autopsy data: The new InterVA-4 tool. Global Health Action, 5, 2012.

[4] Patrick Danaher, Pei Wang, and Daniela M Witten. The joint graphical lasso for inverse covariance estimation across multiple classes. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 76(2):373–397, 2014.

[5] Sameer K Deshpande, Veronika Ročková, and Edward I George. Simultaneous variable and covariance selection with the multivariate spike-and-slab lasso. *arXiv preprint arXiv:1708.08911*, 2017.

[6] Adrian Dobra. Graphical modeling of spatial health data. *arXiv preprint arXiv:1411.6512*, 2014.

[7] Adrian Dobra, Theo S Eicher, and Alex Lenkoski. Modeling uncertainty in macroeconomic growth determinants using Gaussian graphical models. Statistical Methodology, 7(3):292–306, 2010.

[8] Bailey K Fosdick and Peter D Hoff. Separable factor analysis with applications to mortality data. The annals of applied statistics, 8(1):120, 2014.

[9] Edward I George and Robert E McCulloch. Variable selection via Gibbs sampling. Journal of the American Statistical Association, 88(423):881–889, 1993.

[10] Jian Guo, Elizaveta Levina, George Michailidis, and Ji Zhu. Joint estimation of multiple graphical models. Biometrika, 98(1):1–15, 2011.

[11] Botao Hao, Will Wei Sun, Yufeng Liu, and Guang Cheng. Simultaneous clustering and estimation of heterogeneous graphical models. *arXiv preprint arXiv:1611.09391*, 2016.

[12] Minjung Kyung, Jeff Gilly, Malay Ghoshz, and George Casellax. Penalized regression, standard errors, and Bayesian lassos. *Bayesian Analysis*, 5(2):369–412, 2010. ISSN 19360975. doi: 10.1214/10-BA607.

[13] Ronald D Lee and Lawrence R Carter. Modeling and forecasting us mortality. Journal of the American statistical association, 87(419):659–671, 1992.

[14] Alex Lenkoski and Adrian Dobra. Computational aspects related to inference in Gaussian graphical models with the G-Wishart prior. Journal of Computational and Graphical Statistics, 20(1):140–157, 2011.

[15] Yunfan Li, Bruce A Craig, and Anindya Bhadra. The graphical horseshoe estimator for inverse covariance matrices. *arXiv preprint arXiv:1707.06661*, 2017.

[16] Zehang R Li and Tyler H McCormick. An Expectation Conditional Maximization approach for Gaussian graphical models. Submitted, *arXiv:1709.06970*, 2017.
[17] Zehang Richard Li, Tyler H McCormick, and Samuel J Clark. Bayesian inference of latent Gaussian graphical models for mixed data. *arXiv preprint arXiv:1711.00877*, 2017.

[18] Zhixiang Lin, Tao Wang, Can Yang, and Hongyu Zhao. On joint estimation of Gaussian graphical models for spatial and temporal data. *Biometrics*, 73(3):769–779, 2017.

[19] Fei Liu, Soumik Chakraborty, Fan Li, Yan Liu, Aurelie C Lozano, et al. Bayesian regularization via graph laplacian. *Bayesian Analysis*, 9(2):449–474, 2014.

[20] Jing Ma and George Michailidis. Joint structural estimation of multiple graphical models. *Journal of Machine Learning Research*, 17(166):1–48, 2016.

[21] Tyler H. McCormick, Zehang Richard Li, Clara Calvert, Amelia C. Crampin, Kathleen Kahn, and Samuel J. Clark. Probabilistic cause-of-death assignment using verbal autopsies. *Journal of the American Statistical Association*, 111(515):1036–1049, 2016. doi: 10.1080/01621459.2016.1152191. URL http://dx.doi.org/10.1080/01621459.2016.1152191.

[22] Abdolreza Mohammadi, Ernst C Wit, et al. Bayesian structure learning in sparse Gaussian graphical models. *Bayesian Analysis*, 10(1):109–138, 2015.

[23] Christopher JL Murray, Alan D Lopez, Robert Black, Ramesh Ahuja, Said M Ali, Abdullah Baqui, Lalit Dandona, Emily Dantzer, Vinita Das, Usha Dhingra, et al. Population health metrics research consortium gold standard verbal autopsy validation study: design, implementation, and development of analysis datasets. *Population health metrics*, 9(1):27, 2011.

[24] Jie Peng, Pei Wang, Nengfeng Zhou, and Ji Zhu. Partial correlation estimation by joint sparse regression models. *Journal of the American Statistical Association*, 104(486):735–746, 2009.

[25] Christine Peterson, Marina Vannucci, Cemal Karakas, William Choi, Lihua Ma, and Mirjana Meletić-Savatić. Inferring metabolic networks using the Bayesian adaptive graphical lasso with informative priors. *Statistics and its Interface*, 6(4):547, 2013.

[26] Christine Peterson, Francesco Stingo, and Marina Vannucci. Bayesian Inference of Multiple Gaussian Graphical Models. *Journal of the American Statistical Association*, 110(June):00–00, 2014. ISSN 0162-1459. doi: 10.1080/01621459.2014.896806. URL http://www.tandfonline.com/doi/abs/10.1080/01621459.2014.896806.

[27] Veronika Ročková and Edward I George. EMVS: The EM approach to Bayesian variable selection. *Journal of the American Statistical Association*, 109(506):828–846, 2014.

[28] Veronika Ročková and Edward I. George. The Spike-and-Slab LASSO. *Journal of the American Statistical Association*, 0(ja):0–0, 2016. doi: 10.1080/01621459.2016.1260469. URL https://doi.org/10.1080/01621459.2016.1260469.

[29] Takumi Saegusa and Ali Shojaie. Joint estimation of precision matrices in heterogeneous populations. *Electronic journal of statistics*, 10(1):1341, 2016.

[30] Peter Serina, Ian Riley, Andrea Stewart, Abraham D Flaxman, Rafael Lozano, Meghan D Mooney, Richard Luning, Bernardo Hernandez, Robert Black, Ramesh Ahuja, et al. A shortened verbal autopsy instrument for use in routine mortality surveillance systems. *BMJ medicine*, 13(1):1, 2015.

[31] Linda SL Tan, Ajay Jasra, Maria De Iorio, Timothy MD Ebbels, et al. Bayesian inference for multiple Gaussian graphical models with application to metabolic association networks. *The Annals of Applied Statistics*, 11(4):2222–2251, 2017.

[32] University of California, Berkeley (USA), and Max Planck Institute for Demographic Research (Germany). Human Mortality Database. Available at [www.mortality.org](http://www.mortality.org) or [www.humanmortality.de](http://www.humanmortality.de) (data downloaded on 05/02/2018).

[33] Hao Wang. Bayesian graphical lasso models and efficient posterior computation. *Bayesian Analysis*, 7(4):867–886, 2012. ISSN 19360975. doi: 10.1214/12-BA729.

[34] Hao Wang. Scaling it up: Stochastic search structure learning in graphical models. *Bayesian Analysis*, 10(2):351–377, 2015. ISSN 19316690. doi: 10.1214/14-BA916.
[35] Xiaofan Xu, Malay Ghosh, et al. Bayesian variable selection and estimation for group lasso. *Bayesian Analysis*, 10(4):909–936, 2015.

[36] Lin Zhang, Veerabhadran Baladandayuthapani, Bani K Mallick, Ganiraju C Manyam, Patricia A Thompson, Melissa L Bondy, and Kim-Anh Do. Bayesian hierarchical structured variable selection methods with application to molecular inversion probe studies in breast cancer. *Journal of the Royal Statistical Society: Series C (Applied Statistics)*, 63(4):595–620, 2014.
A Proof of Proposition 1 and 2

Here we provide a proof of Proposition 2 in the main paper. The same arguments generalize to Proposition 1 directly by fixing all binary indicators to 1 and thus are not repeated.

Proof of DSS-GGL prior We first consider the GGL and DSS-GGL penalties. The joint distribution of all the parameters under the parameterization of the scale mixture of Normal distributions is

\[ p(\{\Omega\}, \tau, \rho, \delta, \xi, \pi_\delta, \pi_\xi) = \prod_{g} \prod_{j < k} \exp\left(-\frac{1}{2}(\omega_{jk}^{(g)})^2 (\frac{v_{jk}^{(g)}}{\tau_{jk}} + \frac{v_{jk}^{(g)}}{\rho_{jk}})\right) \prod_{g} \prod_{j} \exp\left(-\frac{\lambda_0}{2} \omega_{jj}^{(g)}\right) \]

\times \prod_{g} \prod_{j < k} \tau_{jk}^{(-\frac{1}{2})} \exp\left(-\frac{\lambda_1^2}{2} \tau_{jk}\right) \prod_{j < k} \rho_{jk}^{(-\frac{1}{2})} \exp\left(-\frac{\lambda_2^2}{2} \rho_{jk}\right) \]

\times \prod_{j < k} \pi_{\delta}^{\delta - 1} (1 - \pi_{\delta})^{1 - \delta} \prod_{j < k} \pi_{\xi}^{\xi - 1} (1 - \pi_{\xi})^{1 - \xi} \]

\times \prod_{j < k} \pi_{\delta}^{a_{\delta} - 1} (1 - \pi_{\delta})^{b_{\delta} - 1} \prod_{j < k} \pi_{\xi}^{a_{\xi} - 1} (1 - \pi_{\xi})^{b_{\xi} - 1} \]

The following two identities provide the key steps to connect the scale mixture of normal distributions to the Laplace representation in the penalty function:

\[ \int_0^\infty \frac{1}{\sqrt{2\pi s}} \exp\left(-\frac{z^2}{2s}\right) \frac{\lambda^2}{2} \exp\left(-\frac{\lambda^2 s}{2}\right) ds \]

\[ = \frac{\lambda}{2} \exp\left(-\lambda |z|\right) \] (14)

\[ \int_0^\infty \frac{1}{\sqrt{2\pi s}} \exp\left(-\frac{|z|^2}{2s}\right) \frac{\lambda^2}{2} \exp\left(-\frac{\lambda^2 s}{2}\right) \frac{1}{\Gamma\left(\frac{p+1}{2}\right)} ds \]

\[ = \frac{\lambda}{2} \exp\left(-\lambda |z|^2\right) \] (15)

where \( z \) is a vector of length \( p \) and \( |z|^2 = \sum_{i=1}^p z_i^2 \). By rearranging the terms and plugging in the two identities above, it can be seen that

\[ p(\{\Omega\}|\delta, \xi) \propto \exp\left(- \sum_{j < k} \frac{\lambda_1}{2} v_{jk}^{(g)} |\omega_{jk}^{(g)}| - \sum_{j < k} \frac{\lambda_2}{2} v_{jk}^{(g)} |\omega_{jk}^{(g)}|^2 - \sum_{g} \sum_{j} \frac{\lambda_0}{2} \omega_{jj}^{(g)}\right). \]

The conditional distribution of \( \{\Omega\}|\delta, \xi \) takes the form of \( \exp(-\text{pen}(\{\Omega\}|\delta, \xi)) \) for DSS-GGL, and thus the mode of the posterior is equivalent to the DSS-GGL solution. It still remains to be seen that the intractable constant terms are all finite, so that each of the three conditional distributions are proper. This can be seen as follows:

\[ C_{\tau, \rho} | C_{\delta, \xi} = \int \prod_{j < k} \text{Normal}(\omega_{jk}; 0, \Theta) \prod_{g} \prod_{j} \text{Exp}(\omega_{jj}^{(g)}; \frac{\lambda_0}{2}) 1_{\{\Omega\} \in M} d\{\Omega\} \]

\[ < \int \prod_{j < k} \text{Normal}(\omega_{jk}; 0, \Theta) \prod_{g} \prod_{j} \text{Exp}(\omega_{jj}^{(g)}; \frac{\lambda_0}{2}) d\{\Omega\} = 1 \]

\[ C_{\tau, \rho}^{-1} \propto \int \prod_{j < k} \left( \exp\left(-\frac{\lambda_1^2}{2} \sum_{g} \tau_{jk} - \frac{\lambda_2^2}{2} \rho_{jk}\right) \tau_{jk}^{(-\frac{1}{2})} \prod_{g} (\tau_{jk} (\frac{1}{\tau_{jk}} + \frac{1}{\rho_{jk}}))^{-\frac{1}{2}} \right) d\{\tau_{jk}, \rho_{jk}\} \]

\[ < \int \prod_{j < k} \left( \exp\left(-\frac{\lambda_1^2}{2} \sum_{g} \tau_{jk} - \frac{\lambda_2^2}{2} \rho_{jk}\right) \rho_{jk}^{(-\frac{1}{2})} \right) d\rho_{jk} \]

\[ < \int \prod_{j < k} \left( \exp\left(-\frac{\lambda_2^2}{2} \rho_{jk}\right) \rho_{jk}^{(-\frac{1}{2})} \right) d\rho_{jk} = (2\pi/\lambda_2^2)^{\frac{p(p-1)}{4}} \]

The above inequalities complete the proof that the conditional prior distributions are all proper for DSS-GGL. For GGL prior, the proof is essentially the same by fixing \( \delta \) and \( \xi \) to be 1.
Proof of DSS-FGL prior  For DSS-FGL, the joint distribution of all the parameters using the scale Normal mixture representation is

\[
p(\{\Omega\}, \tau, \rho, \delta, \xi, \pi_\delta, \pi_\xi) = \prod_g \prod_{j<k} \exp\left(-\frac{1}{2}(\omega_{jk}^{(g)})^T \Theta_{jk} \omega_{jk}^{(g)} \right) \prod_g \prod_j \exp\left(-\frac{\lambda_0}{2} \omega_{jj}^{(g)} \right) \\
\times \prod_g \prod_{j<k} \tau_{jk}^{-\frac{1}{2}} \exp\left(-\frac{\lambda_1}{2} \rho_{jk} \right) \prod_j \exp\left(-\frac{\lambda_2}{2} \rho_{jk} \right) \\
\times \prod_j \pi_{\delta j} (1 - \pi_\delta)^{1 - \delta_j} \prod_j \pi_{\xi j} (1 - \pi_\xi)^{1 - \xi_j} \\
\times \prod_j \pi_{\delta j}^{-1} (1 - \pi_\delta)^{b_1 - 1} \prod_j \pi_{\xi j}^{-1} (1 - \pi_\xi)^{b_2 - 1}
\]

where the first term can be rewritten as the same form as \( \exp(-\text{pen}(\{\Omega\}|\delta, \xi)) \) for DSS-FGL:

\[
(\omega_{jk}^{(g)})^T \Theta_{jk} \omega_{jk}^{(g)} = \sum_g v_{\delta jk} (\omega_{jk}^{(g)})^2 + \sum_{g<g'} \sum_g v_{\xi jk} (\omega_{jk}^{(g)} - \omega_{jk}^{(g')})^2.
\]

Using the same identity as before, we can rewrite the conditional distribution below into the form of the DSS-FGL penalty:

\[
p(\{\Omega\}|\delta, \xi) \propto \exp\left(-\sum_{j<k} \frac{\lambda_1}{2} \omega_{jk}^{(g)} - \sum_{j<k} \sum_{g<g'} \frac{\lambda_2}{2} \omega_{jk}^{(g)} - \omega_{jk}^{(g')} - \sum_{g} \sum_{j} \frac{\lambda_0}{2} \omega_{jj}^{(g)} \right).
\]

The proof of the DSS-FGL conditional distributions being proper is similar to the previous case. We first note that

\[
\Theta_{jk} = \text{diag}(\{\frac{1}{\tau_{jk}}\}_g=1,...,\mathcal{G}) + L_{jk}
\]

where \( L_{jk} \) is a graph Laplacian matrix and is positive semi-definite. Then by Minkowski inequality, \( \det(\Theta_{jk}) \geq \det(\text{diag}(\{\frac{1}{\tau_{jk}}\}_g=1,...,\mathcal{G})). \) Then we have

\[
C_{\tau, \phi}^{-1} \propto \int \prod_{j<k} \left( \det(\Theta_{jk})^{-\frac{1}{2}} \exp\left(-\frac{\lambda_1}{2} \sum_g \tau_{jk} - \frac{\lambda_2}{2} \sum_{g<g'} \phi_{jk g g'} \right) \prod_g \tau_{jk}^{-\frac{1}{2}} \prod_{g<g'} \phi_{jk g g'} \right) d\{\tau, \phi\} \\
\leq \int \prod_{j<k} \left( \exp\left(-\frac{\lambda_1}{2} \sum_g \tau_{jk} - \frac{\lambda_2}{2} \sum_{g<g'} \phi_{jk g g'} \right) \prod_g \tau_{jk}^{-\frac{1}{2}} \prod_{g<g'} \phi_{jk g g'} \right) d\{\tau, \phi\} \\
\leq \int \prod_{j<k} \left( \exp\left(-\frac{\lambda_2}{2} \sum_{g<g'} \phi_{jk g g'} \right) \prod_{g<g'} \phi_{jk g g'} \right) d\phi,
\]

which is again finite since the integral consists of products of Gamma densities. The rest of the argument follows in the same way as the DSS-GGL case.
B Details of the EM algorithm implementation

Assuming no missing data, the full objective function in the t-th iteration of the EM algorithm described in \(5\) is the expectation of the complete data log likelihood, i.e.,

\[
Q(\Omega, \pi_\delta, \pi_\xi | \Omega^{(t)}, \pi_\delta^{(t)}, \pi_\xi^{(t)}) = \mathbb{E}_{\delta, \xi | \Omega^{(t)}, \pi_\delta^{(t)}, \pi_\xi^{(t)}, X} \{ \log p(\Omega, \pi_\delta, \pi_\xi | X) | \Omega^{(t)}, \pi_\delta^{(t)}, \pi_\xi^{(t)}, X \}
\]

\[
= \text{constant} + \sum_g \left[ \frac{n_g}{2} \log |\Omega_g| - \frac{1}{2} \text{tr}(S_g \Omega_g) - \frac{\lambda_0}{2} \sum_g \sum_{j<k} |\omega_{jk}^{(g)}| \right. \\
- \lambda_1 \sum_g \sum_{j<k} |\omega_{jk}^{(g)}| E_{|\cdot|}(\frac{1}{v_0(1-\delta_{jk}) + v_1\delta_{jk}}) + \sum_{j<k} \log(\frac{\pi_\delta}{1-\pi_\delta})E_{|\cdot|}(\delta_{jk}) \\
- \lambda_2 \sum_g \frac{\bar{p} \bar{m}(\omega_{jk})}{E_{|\cdot|}}(\frac{1}{v_0(1-\delta_{jk}\xi_{jk}) + v_1\delta_{jk}\xi_{jk}}) + \sum_{j<k} \log(\frac{\pi_\xi}{1-\pi_\xi})E_{|\cdot|}(\xi_{jk}) \\
+ (a_1 - 1) \log(\pi_\delta) + (b_1 + \frac{p(p-1)}{2} - 1) \log(1-\pi_\delta) \\
+ (a_2 - 1) \log(\pi_\xi) + (b_2 + \frac{p(p-1)}{2} - 1) \log(1-\pi_\xi),
\]

where \(E_{|\cdot|}\) denotes conditional expectation \(E_{\delta, \xi | \Omega^{(t)}, \pi_\delta^{(t)}, \pi_\xi^{(t)}, X}\), and \(\bar{p} \bar{m}(\omega_{jk}) = ||\omega_{jk}||_2\) for DSS-GGL and \(\bar{p} \bar{m}(\omega_{jk}) = \sum_{g<g'} |\omega_{jk}^{(g)} - \omega_{jk}^{(g')}|\) for DSS-FGL.

When missing data exists, we need to also calculate the expectation of \(S_g\) given the observed data. That is, We need to replace the \(\text{tr}(S_g \Omega_g)\) term in the above objective function by

\[
E_{|\cdot|}(S_g \Omega_g) = E_{|\cdot|}(\frac{1}{n_g} \sum_i n_g \sum_i x_i^{(g)}(x_i^{(g)})^T \Omega_g) = \frac{1}{n_g} \sum_i E_{|\cdot|}(x_i^{(g)}(x_i^{(g)})^T) \Omega_g,
\]

where \(x_i^{(g)}\) and \(x_{i,m}^{(g)}\) denote the observed and missing cells in \(x_i^{(g)}\) respectively. \(x_i^{(g)}\) follows a multivariate Gaussian distribution. Without loss of generality, if we let \(x_i^{(g)} = (x_{i,o}^{(g)}, x_{i,m}^{(g)})\), we know

\[
E_{x_{i,o}^{(g)}}(x_{i,o}^{(g)}) = \Sigma_{oo}^{-1} x_{i,o}^{(g)}
\]

\[
E_{x_{i,m}^{(g)}}(x_{i,m}^{(g)}(x_{i,m}^{(g)})^T) = E_{|\cdot|}(x_{i}^{(g)})E_{|\cdot|}(x_{i}^{(g)})^T + \begin{pmatrix} 0_{oo} & 0_{om} \\ 0_{mo} & 0_{mm} - \Sigma_{mm} \Sigma_{oo}^{-1} \Sigma_{om} \end{pmatrix}
\]

where \(\Sigma_{oo}, \Sigma_{om}, \Sigma_{mo} \) and \(\Sigma_{mm}\) are the corresponding submatrices of \(\Sigma_g\).

C Gibbs sampler of the proposed models

The EM algorithm introduced in the main paper maximizes the complete data likelihood by looking at the Laplace representation after integrating out all the latent parameters. In this section, we show that these latent parameters, \(\tau, \phi\) and \(\rho\), facilitates efficient block Gibbs sampling algorithms for fully Bayesian inference.

We start by describing the posterior sampling of \(\{\Omega\}\). The basic idea is to sample each column and row for all the precision matrices jointly. To simplify notation, we separate out the last column and row in \(\Omega_g\) and \(S_g\) and define

\[
\Omega_g = \begin{pmatrix} \Omega_1^{(g)} \\ \omega_2^{(g)} \end{pmatrix}, \quad S_g = \begin{pmatrix} S_1^{(g)} \\ s_2^{(g)} \end{pmatrix}
\]

We further let \(\omega_1 = (\omega_1^{(1)} \omega_1^{(2)} \omega_1^{(3)} \omega_1^{(4)})^T, \omega_2 = (\omega_2^{(1)} \omega_2^{(2)} \omega_2^{(3)} \omega_2^{(4)})^T\), and \(s_1 = (s_1^{(1)} s_1^{(2)} s_1^{(3)} s_1^{(4)})^T, s_2 = (s_2^{(1)} s_2^{(2)} s_2^{(3)} s_2^{(4)})^T\), each denoting a vector of length \((p-1)G\), and \(\omega_2 = [\omega_2^{(1)}, \omega_2^{(2)}, ..., \omega_2^{(G)}]\).
The conditional distribution of \((\omega_{12}, \omega_{22})\) given the rest of the elements in \(\{\Omega\}\) does not seem to take any standard form. However, if we perform a change of variables and let \(\theta_g = \omega_{22}^{(g)} - \omega_{21}^{(g)} \left( \Omega_{11}^{(g)} \right)^{-1} \omega_{12}^{(g)} \), the conditional distribution of \((\omega_{12}, \theta)\) becomes

\[
p(\omega_{12}, \theta) \propto \sum_g \theta_g^{n_g} \exp(-s_{22}^{(g)} + \frac{\lambda_0}{2} \theta_g - s_{12}^T \omega_{12} - \frac{1}{2} \omega_{12}^T A \omega_{12}) = \prod_g \text{Gamma}(\theta_g; \frac{n_g}{2} + 1, \frac{s_{22}^{(g)} + \lambda_0}{2}) \times \text{Normal}(\omega_{12}; -A^{-1}s_{12}, A^{-1}).
\]

The \(A\) matrix can be calculated by \(A = U + V\), where \(U\) is a matrix by rearranging the precision matrices so that its \(\left( (g - 1)(p - 1) + k, (g' - 1)(p - 1) + k \right)\)-th element is the \((g, g')\)-element in \(\tilde{\Theta}_{jk}\) defined in (12) and (13) of the main paper, and

\[
V = \left( \begin{array}{cc}
\left( \lambda_0 + s_{22}^{(1)} \left( \Omega_{11}^{(1)} \right)^{-1} \right) & \\
\vdots & \\
\left( \lambda_0 + s_{22}^{(G)} \left( \Omega_{11}^{(G)} \right)^{-1} \right)
\end{array} \right).
\]

For DSS-GGL, we notice that \(A\) is block diagonal, thus we can alternatively sample \(\omega_{12}^{(g)}\) independently by

\[
\omega_{12}^{(g)} \sim \text{Normal}(-A^{-1}_g s_{12}^{(g)}, A^{-1}_g)
\]

where \(A_g = \left( \lambda_0 + s_{22}^{(g)} \left( \Omega_{11}^{(g)} \right)^{-1} + \Theta_{11}^{(g)} \right)\).

Given \(\{\Omega\}\), the latent parameters in DSS-GGL have simple conditional distribution as follows:

\[
\tau_{jkg}^{-1} \sim \text{InvGaussian} \left( \frac{\lambda_1}{v_{jkg} \left| \omega_{jk}^{(g)} \right|}, \lambda_2^2 \right), \quad j, k = 1, ..., p, g = 1, ..., G
\]

\[
\rho_{jk}^{-1} \sim \text{InvGaussian} \left( \frac{\lambda_2}{v_{jk} \sum_g \left( \omega_{jk}^{(g)} \right)^2}, \lambda_2^2 \right), \quad j, k = 1, ..., p
\]

\[
\delta_{jk}, \xi_{jk} \sim \text{InvGaussian} \left( \frac{\rho_{jk}^{-1} \left( \delta_{jk}, \xi_{jk} \right)}{v_{jk} \sum_g \left( \omega_{jk}^{(g)} \right)^2}, \lambda_2^2 \right), \quad j, k = 1, ..., p
\]

\[
\pi_\delta \sim \text{Beta} \left( \sum_j \delta_{jk} + a_1; \sum_j (1 - \delta_{jk}) + b_1 \right)
\]

\[
\pi_\xi \sim \text{Beta} \left( \sum_j \xi_{jk} + a_2; \sum_j (1 - \xi_{jk}) + b_2 \right)
\]

where \(p^*(\delta, \xi)\) is defined in (5) in the main paper.

For DSS-FGL, the conditional distribution of \(\tau, \delta, \xi, \pi_\delta, \) and \(\pi_\xi\) are the same as DSS-GGL. The conditional distribution of \(\phi\) is

\[
\phi_{jkg}^{-1} \sim \text{InvGaussian} \left( \frac{\lambda_2}{v_{jkg} \left| \omega_{jk}^{(g)} - \omega_{jk}^{(g')} \right|}, \lambda_2^2 \right), \quad j, k = 1, ..., p, g, g' = 1, ..., G
\]

The Gibbs sampler is then complete by circling through and sampling each blocks of \(\{\Omega\}\) and the latent parameters with the above posterior conditional distributions.

**D Additional illustrating example**

In this section, we provide a more detailed description to the small 2-class simulated example described in Section [6] of the main paper. We let \(n_g = 150\) for \(g = 1, 2, p = 100\). The first 10 variables in the first class form a 10-node block with an AR(1) precision matrix, i.e., \(\left( \Omega^{-1} \right)_{jk} = 0.7|j-k|\). The rest of the 90 variables are independent noises from a standard Gaussian distribution. The second class shares the first 4 edges of the first class. The first 5 variables form another AR(1) block with different strength of correlations so that \(\left( \Omega^{-1} \right)_{jk} = 0.9|j-k|\). The rest of the 95 variables all follow independent standard Gaussian distribution.
The best performance of FGL in our experiments was achieved with $\lambda_2 = 0.1$. We then obtained the regularization path along different values of $\lambda_1$. We also fit DSS-FGL and SS-FGL with $\lambda_1 = 1, \lambda_2 = 1$. The latter assumes $\xi_{jk} = 1$ for all edges, i.e., the penalization of similarities is always proportional to the penalization of sparsity.

Figure 4: The solution paths and estimated precision matrices of FGL (upper row), SS-FGL (middle row) and DSS-FGL (lower row). The red nodes correspond to true edges and the gray nodes correspond to 0’s. The two vertical lines in the FGL solution path indicate the model that best matches the true sparsity (left) and the model with the lowest AIC (right). The block containing the edges is plotted for the estimated values (upper triangular) against the truth (lower triangular). The model that best matches the true graphs is plotted for FGL. The off-diagonal values are rescaled and negated to partial correlations, and 0’s are colored with light gray background for easier visual comparison. The bias of the estimated precision matrix measured by the Frobenius norm, $\| \hat{\Omega}_g - \Omega_g \|_F$, is also printed in the captions.

Figure 4 shows both the two solution paths presented in the main paper, and the solution path from SS-FGL. It can be seen that although SS-FGL achieves similar bias as DSS-FGL, it also estimates several more false positive edges. This can be seen from the formulation of the doubly spike-and-slab selection: with only one spike-and-slab mixture of the penalties, the selected edges from the slab distributions receive also only weak penalization for between-class similarities. Thus it is more likely to pick up spurious edges due to noises that happen to exist in one class. This full illustration of the simple example shows the advantage of having the doubly spike-and-slab setup.

E Additional simulation evidence

Here we describe our procedure in simulating the dataset described in Section 7 of the main paper. We first generate three networks with $p$ features with 10 equal sized unconnected subnetwork. Each of the subnetwork follow a power law degree distribution, which is generally harder to estimate than simpler structures [24]. The first class contains all ten subnetworks, and the second and third classes each has one and two subnetworks removed. Given the network structure, we generate $\Omega_g$ from the
$G$-Wishart distribution $W_G(3, I_p)$, and rescale them so that $\Omega^{-1}$ have unit variances. Finally, we generate $n = 150$ independent and identically distributed samples from Normal$(0, \Omega_g)$ in each class. The resulted graph for $p = 500$ is shown in Figure 5. We fit GGL and FGL with various choice of fixed $\lambda_2$ and a sequence of $\lambda_1$. We fit DSS-GGL and DSS-FGL with $\lambda_1 = 1$, $\lambda_2 = 2/30$ in this case. We explore more choices of $\lambda_2$ in the moderate dimensional experiments below and found no substantial changes in the performance of the final models.

Additional results for $p = 100$ and $p = 200$ are shown in Figure 6 and 7. The dots correspond to DSS-GGL and DSS-FGL with $\lambda_1 = 1$, $\lambda_2 = 0.1$. We also examined different choices of $\lambda_2$ are found no substantial differences in performance. An exploratory sensitivity analysis is presented in the next subsection.

**Graph structure**

![Graph structure](image)

Figure 5: Graph structure of the simulated dataset. The edges between the red nodes are removed from the second class, and edges between both the red and blue nodes are removed from the third class.

![Performance graphs](image)

Figure 6: Performance of FGL, GGL, DSS-FGL, and DSS-GGL over 100 replications, $p = 100$. The dots represent the metrics for the 100 selected models under DSS-FGL and DSS-GGL, and the lines represent the average performance of FGL and GGL over 100 replications under different tuning parameters.
Figure 7: Performance of FGL, GGL, DSS-FGL, and DSS-GGL over 100 replications, \(p = 200\). The dots represent the metrics for the 100 selected models under DSS-FGL and DSS-GGL, and the lines represent the average performance of FGL and GGL over 100 replications under different tuning parameters.

E.1 Sensitivity to hyperparameters

Figure 8 and 9 shows the converged regions over 100 replications on space of the true positive against false positive discoveries for edges and differential edges respectively when \(p = 200\). It can be seen that the performance is relatively stable under different choices of \(\lambda_2\).

Figure 8: The density plot of true positive edges against false positive edges for DSS-FGL (top row), and DSS-GGL (bottom row) under different choices of \(\lambda_2\). \(\lambda_1\) is set to 1.
Figure 9: The density plot of true positive differential edges against false positive positive edges for DSS-FGL (top row), and DSS-GGL (bottom row) under different choices of $\lambda_2$. $\lambda_1$ is set to 1.
F Details on the verbal autopsy data analysis

F.1 List of symptoms

Table 2 shows the questions with continuous responses used in the analysis in the main paper.

Table 2: List of symptoms considered in this analysis.

| Abbreviation    | Questionnaire item                                                                 |
|-----------------|-----------------------------------------------------------------------------------|
| ill             | For how long was [name] ill before s/he died? [days]                              |
| fever           | How many days did the fever last? [days]                                          |
| rash            | How many days did [name] have the rash? [days]                                    |
| ulcer           | For how many days did the ulcer ooze pus? [days]                                 |
| yellow discoloration | For how long did [name] have the yellow discoloration? [days]                  |
| ankle swelling  | For how long did [name] have ankle swelling? [days]                              |
| puffiness face  | For how long did [name] have puffiness of the face? [days]                       |
| puffiness body  | For how long did [name] have puffiness all over his/her body? [days]             |
| cough           | For how long did [name] have a cough? [days]                                     |
| difficulty breathing | For how long did [name] have difficulty breathing? [days]      |
| fast breathing  | For how long did [name] have fast breathing? [days]                              |
| liquid stool    | For how long before death did [name] have loose or liquid stools? [days]         |
| vomit           | For how long before death did [name] vomit? [days]                                |
| difficulty swallowing | For how long before death did [name] have difficulty swallowing? [days]        |
| belly pain      | For how long before death did [name] have belly pain? [days]                     |
| protruding belly| For how long before death did [name] have a protruding belly? [days]             |
| mass belly      | For how long before death did [name] have a mass in the belly [days]             |
| headaches       | For how long before death did [name] have headaches? [days]                      |
| stiff neck      | For how long before death did [name] have stiff neck? [days]                     |
| unconsciousness | For how long did the period of loss of consciousness last? [days]                |
| confusion       | For how long did the period of confusion last? [days]                             |
| convulsion      | For how long before death did the convulsions last? [days]                       |
| paralysis       | For how long before death did [name] have paralysis? [days]                      |
| period overdue  | For how many weeks was her period overdue? [days]                                |
| tobacco         | How much pipe/chewing tobacco did [name] use daily?                               |
| cigarettes      | How many cigarettes did [name] smoke daily?                                      |
| age             | Age [years]                                                                     |

F.2 Comparing with JGL

The estimated symptom network from the DSS-FGL and DSS-GGL are summarized in Figure 10.

The estimated symptom network from the FGL and GGL are summarized in Figure 11. We fit both models under a 2-dimensional grids over $\lambda_1$ and $\lambda_2$. As expected, AIC selects very dense graphs (first two rows of Figure 11) and are difficult to interpret. We also compare the FGL and GGL graph with the closest number of edges as those from DSS-FGL and DSS-GGL in the third and forth row of Figure 11. The number of differential edges is typically smaller compared to DSS-FGL and DSS-GGL, which is likely due to over penalization of similarities, i.e., edges become too similar using FGL, and too sparse among half of the nodes using GGL.

G Details on prediction of missing mortality rates

The data we consider in this example consist of log mortality rates over $n = 51$ years for $p = 101$ age groups, and 2 classes representing female and male series respectively. The estimated graph structure from one of the cross-validation dataset using FGL and DSS-FGL are shown in Figure 12.

The Lee-Carter model are estimated using the R package ilc[2] for each gender separately.

The DSS-FGL is able to pick up more conditional dependence structures along the diagonal among several age groups, while the FGL estimates mostly within adults only. It is interesting that both
Figure 10: Estimated edges between the symptoms under the three causes using DSS-FGL (top row) and DSS-GGL (bottom row). The width of the edges are proportional to the size of $|\omega_{jk}|$. Common edges across all groups are colored in blue, and the differential edges are colored in red.

approaches identifies positive partial correlations between age $14 - 17$ and $30 - 40$ between male and female. This is likely due to the fact that male mortality around age 20 typically shows a hump of increase due to young adult accident mortality, which leads to the mean model more likely to underestimations for mortality during age $18 - 30$ and overestimations both before and after that period. This relationship of the age curve, however, is not seen in female mortality.
Figure 11: Estimated edges between the symptoms under the three causes using FGL using AIC (first row), GGL using AIC (second row), FGL with the same number of edges as selected by DSS-FGL (third row), and GGL with the same number of edges as selected by DSS-GGL (last row). The width of the edges are proportional to the size of $|\omega_{ij}|$. Common edges across all groups are colored in blue, and the differential edges are colored in red.
Figure 12: Estimated partial correlation matrix using one cross-validation dataset. The partial correlations among the 101 age groups are estimated using FGL with the same number of edges as selected by DSS-FGL (top row), and DSS-FGL (bottom row). DSS-FGL estimates 197 and 199 edges respectively for female and male. The closet configuration of FGL estimates 157 and 241 edges respectively. The precision matrices are rescaled and negated to partial correlations for easier interpretation.