Scalable Inference for Gaussian Hierarchical Models

Master Thesis
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Submitted in partial fulfillment of the requirements
for the Master's Degree in Data Science
at the Barcelona Graduate School of Economics, 2018

1. Introduction

Hierarchy is an organization of items into different levels based on a certain logic, such that items in a set are linked directly either to other items above and below it to produce an overall structure for all the items in a given set. For better or for worse, hierarchy is frequently observed both in human society and its institutions as well as in nature (such as dominance hierarchies in animal packs). Accordingly, much of the data that is available for statistical analysis can be modeled in a multilevel manner. For example, data about the performance of individuals in a company can be modeled as a 2-level hierarchy begining with the entire company, followed by departments, sub-teams within each department, and finally individuals. The frequently superior performance of multilevel[1] modeling (Gelman, 2006) in different contexts affirms the validity of understanding the world around us in a hierarchical manner.

This paper will attempt to highlight the advantages of hierarchical models and study scalable methods for inference on Gaussian hierarchical models. The aims of this thesis are three-fold. Firstly, it will explore the formulation of posterior inference of Gaussian hierarchical models using Gaussian simulation as a linear algebra problem which can be solved with efficient sparse linear algebra methods. The second goal is to provide tools for inference for Gaussian hierarchical models in the form of an R package. Finally, this paper will analyze the performance of existing linear algebra packages ***spam*** and ***Matrix*** in obtaining the optimal fill-in of the cholesky factor.

For the purposes of this paper, all observations are taken to be 0. The main issue of concern here is computational efficiency. This assumption is a valid one since performance of the methods considered in this paper depend only on the structure of the covariance alone, which remains unaffected by the specific values of the observations for Gaussian hierarchical models.

1.1 Notation

To keep the equations short and readable, I have adopted the following notation for hierarchical variables. The root variable is denoted as β.

For variables at the first level,

$$\beta_{1:I} = \beta_1, \beta_2, ..., \beta_I$$

At the second level,

$$\beta_{1:I,1:J} = \beta_{11}, \beta_{12}, ..., \beta_{21}, \beta_{22}, ..., \beta_{IJ}$$

And so on for deeper levels.

[1] For the purposes of this paper, the reader should take the terms “multilevel” and “hierarchical” to mean the same thing.

2. Gaussian Hierarchical Models

2.1 Advantages of Hierarchical Modeling

Since the structure of many institutions or objects being studied is either explicitly or implicitly hierarchical, hierarchical models can more accurately capture the multilevel dynamics of the data on these objects. The use of hierarchical models allows us to fit a regression model at an individual level while also simultaneously explain the systematic variation at higher grouping levels (Gelman, 2006). This allows specific traits of different groups at different levels to be identified and makes it easier to characterize these groupings while also accounting for individual variation within groups, making inferences from multilevel models more reasonable. Models which utilize complete pooling give identical estimates to all sub-groups, which is not ideal especially when there is substantial variation between sub-groups, whereas for models where no pooling is done, the model is likely to overfit the data and be more susceptible to outliers.

On an anecdotal level, this is easy to understand: A person from Catalonia is likely to have certain traits which are unique to Catalans but also have in common traits with Spanish people in other regions which are characteristic of people living in Spain.

Furthermore, hierarchical models offer a framework to combine information across units (such as individuals or counties) and have been empirically shown to provide well-calibrated and more accurate predictions of observable outcomes (Draper, 1995) by using cross-validation (Gelman, 2006), especially when predicting group averages.

Finally, under certain conditions (such as conditional conjugacy of the prior and posterior distributions), hierarchical models allows us to utilize Bayesian statistical tools and techniques which allows us to learn from the data at different levels and conduct sampling-based inference. The multilevel structure of these models allow us to organize inference into a directed acyclic graph such that the observations at the bottom layer are the leaves, and the top layer being the hyperparameters, with intermediate parameters in the levels in between. Such a graph is easy to sample conditionally from, which can be done simply by calculating posterior distributions. This allows us to sample both exactly (using the precision matrix) and approximately (through Markov Chain Monte Carlo methods like Gibbs sampling). It is this quality precisely which will be exploited and studied in this paper.

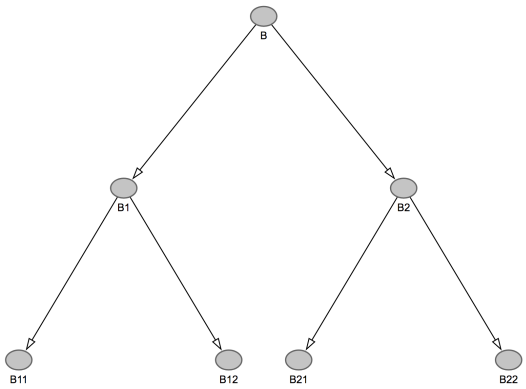


Figure 1. A simple hierarchical model generated using DAGitty. Sampling is easily done by sampling first from the leaves (B11, B12 ...) and then sampling conditional on the previously obtained samples.

2.2 Posterior inference on Gaussian hierarchical models

The rest of the paper will focus specifically on tree-structured hierarchical models where each parameter follows a Gaussian distribution. Tree-structured Gaussian hierarchical models depends only on the covariance of the parameters involved and not the mean, and thus allows exact sampling to be conducted and studied. It is also assumed that the variance of parameters within the same level are the same since the focus is on scalable inference, which is unaffected by specific values of the variances. Thus, all variance parameters are set to 1 and the mean for the root parameter β is set to 0 for the rest of this paper. For now, the focus of this paper is restricted to a 2-level multivariate Gaussian model with full-centered parameterizations (that is, the number of children nodes for each node in the first level is the same, resulting in a symmetric tree structure) (Zanella, Roberts, 2017). For i = 1, …, I and j = 1,…,J,

$$\beta \sim N(\mu, \tau) \quad -(2.1)$$

$$\beta_i \mid \beta \sim N(\beta, \tau_a) \quad -(2.2)$$
$$\beta_{ij} \mid \beta_i \sim N(\beta_i, \tau_b) \quad -(2.3)$$
$$y_{ij} \mid \beta_{ij} \sim N(\beta_{ij}, \sigma^2) \quad -(2.4)$$

where it is assumed that the variances for each level, $\tau, \tau_a, \tau_b, \sigma^2$, are the same for variables within the same level, and that there is only one observation y_{ij} for each parameter β_{ij}. Extension to a 3- or higher level model is simple and can be found in Appendix A1.

For posterior inference, it is useful to first look at the joint posterior distribution of the parameters conditional on the observations (and also conditional on the variance parameters which have been set to 1). This is easy to calculate since the joint distribution is Gaussian. Let $\boldsymbol{\beta}$ represent $(\beta, \beta_1, ..., \beta_I, \beta_{11}, ..., \beta_{IJ})$, let $\boldsymbol{y}$ represent $(y_{11}, ..., y_{IJ})$. The posterior density $P(\boldsymbol{\beta} \mid \boldsymbol{y})$ is given by:

$$\begin{aligned} P(\boldsymbol{\beta} \mid \boldsymbol{y}) &= \frac{P(\boldsymbol{y} \mid \boldsymbol{\beta}) P(\boldsymbol{\beta})}{P(\boldsymbol{y})} \\ &\propto P(\boldsymbol{y} \mid \boldsymbol{\beta}) P(\boldsymbol{\beta}) \quad -(2.5) \end{aligned}$$

Note that since the model in question is a tree graph such that each node is connected to, and thus by d-separation, dependent only on its parent node and child nodes, for any given i, j:

$$P(y_{ij} \mid \boldsymbol{\beta}) = p(y_{ij} \mid \beta_{ij}) \quad -(2.6)$$

This factorization can be repeated for $P(\boldsymbol{\beta})$ until the factorization in (2.7) is obtained. Since the variables are Gaussian, this equation can be expressed explicitly using the formula for Gaussian densities:

$$
\begin{aligned}
P(\boldsymbol{\beta} \mid \boldsymbol{y}) &\propto P(\boldsymbol{y} \mid \boldsymbol{\beta}) P(\boldsymbol{\beta}) \\
&= P(\beta) \prod_i P(\beta_i \mid \beta) \prod_{i,j} P(\beta_{ij} \mid \beta_i) \prod_{i,j} P(y_{ij} \mid \beta_{ij}) \\
&\propto \exp\{-\frac{1}{2\sigma^2} \sum_{i,j} (y_{ij} - \beta_{ij})^2 - \frac{1}{2\tau_b} \sum_{i,j} (\beta_{ij} - \beta_i)^2 - \frac{1}{2\tau_a} \sum_i (\beta_i - \beta)^2 - \frac{1}{2\tau} (\beta - \mu)^2\} \quad -(2.7) \\
&\propto \exp\{-\frac{1}{2} \boldsymbol{\beta^T} Q \boldsymbol{\beta}\} \quad -(2.8)
\end{aligned}
$$

Equation (2.7) is useful because the entries of the precision matrix of the posterior distribution can be easily calculated from it (Appendix A2).

Traditional inference using linear algebra methods become infeasible when the number of parameters involved grow to extremely large numbers. To obtain a sample $\boldsymbol{V}$ from a m-dimensional multivariate Gaussian such that $\boldsymbol{V} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, one first samples from a multivariate standard normal $\boldsymbol{z} \sim N(0, I_m)$, multiply it by the cholesky factor $\tilde{\boldsymbol{L}}$ of the covariance matrix , and add the mean of the parameters $\boldsymbol{\mu}$.

$$\boldsymbol{V} = \boldsymbol{\mu} + \tilde{L}\boldsymbol{z} \quad -(2.9)$$

where $\tilde{L}\tilde{L^T} = \Sigma$. In sampling these parameters, one would need to compute the cholesky factor of the covariance matrix, which require $O(n^3)$ flops where n is the total number of parameters for a dense matrix. Alternatively, if the covariance matrix is not known but the precision matrix is known, one can generate samples by using the cholesky factor $\boldsymbol{L}$ of the precision matrix $\boldsymbol{Q}$.

$$\boldsymbol{V} = \boldsymbol{\mu} + L^{-T}\boldsymbol{z} = \boldsymbol{\mu} + \boldsymbol{v} \quad -(2.10)$$

where $LL^T = \boldsymbol{Q}$. This still requires $O(n^3)$ flops to decompose a dense matrix (the cholesky decomposition is the limiting factor as it is quick to solve $L^T\boldsymbol{v} = \boldsymbol{z}$ since L is lower triangular).

However, more efficient methods are available when the model in question is a tree-structured hierarchical model. For such models, the precision matrix of the parameters is sparse due to the conditional independence structure of the parameters which arises from the tree-structure of the model. This sparsity can be exploited to speed up the matrix factorization step to require only $O(n)$ flops (Rue, Held, 2002). The issue of posterior inference on Gaussian hierarchical models thus becomes a linear algebra problem which can be solved with sparse linear algebra techniques.

2.3 Sparsity

The sparsity of the precision matrix for Gaussian hierarchical models follows directly from the conditional independence properties of the model. To illustrate this more clearly, it is useful to consider the graph for Gaussian hierarchical models. Since each of the parameters follows a Gaussian distribution, the graph for tree-structured Gaussian hierarchical models can be represented as a Gaussian Markov Random Field (or GMRF) (Rue, Held, 2002). Note that due to the tree structure of the model, the structure of the graph is the same whether it is represented as a GMRF or a DAG. The set of parameters, $\boldsymbol{x} = (x_1, ..., x_n)$,

is a GMRF with respect to G if $G = (V, E)$ where $V = \{1, ..., n\}$ is the set of (labeled) nodes which represent the parameters in the graph, and E is the set of edges which connect the nodes such that there is no edge between node i and node j if and only if:

$$x_i \perp x_j \mid \boldsymbol{x}_{-\{ij\}} \quad -(2.11)$$

where $\boldsymbol{x_{-\{ij\}}} = \boldsymbol{x_{-\{i,j\}}}$. Equation (2.11) is also known as the pairwise Markov property. Using this information, the following result can be obtained (refer to appendix A3). For $i \neq j$,

$$x_i \perp x_j \mid \boldsymbol{x}_{-\{ij\}} \iff Q_{ij} = 0 \quad -(2.12)$$

where $\boldsymbol{Q}$ is the precision matrix of the parameters. This says that two parameters x_i and x_j are independent conditional on the other parameters if and only if the term in the i^{th} column and j^{th} row of the precision matrix is 0. Thus, for a given precision matrix, the conditional independence properties of the graph can be deduced. More importantly, for a given graph G, this result makes it easy to determine where the zero and non-zero elements of the precision matrix are and to calculate and store only the non-zero values.

In this framework, the precision matrix of Gaussian hierarchical models tend to be very sparse. The hierarchical structure of the model means that each node in the model is dependent only on its parent or child node. Since any two nodes which do not have an edge between them has a conditional precision of 0, most of the entries in the precision matrix are 0. This permits the use of sparse linear algebra algorithms for more efficient cholesky factorization.

2.4 Sparse linear algebra methods

To sample from the model, the cholesky factor of the precision matrix needs to be computed, as seen in equation (2.10). As mentioned before, cholesky decomposition of a dense matrix requires $O(n^3)$ flops but with the sparse precision matrix of Gaussian hierarchical models, the following method can be used to reduce the complexity to at best $O(n)$ flops by making use of the sparsity of the graph to find zeros in the cholesky factor.

Let L be the cholesky triangle of $\boldsymbol{Q}$, and define for $1 \leq i \leq j \leq n$ the set $F(i, j) = \{i + 1, ..., j - 1, j + 1, ..., n\}$, or the ***future*** of i except j. Then we have a similar result (refer to Appendix A4):

$$x_i \perp x_j \mid \boldsymbol{x}_{F(i,j)} \iff L_{ji} = 0 \quad -(2.13)$$

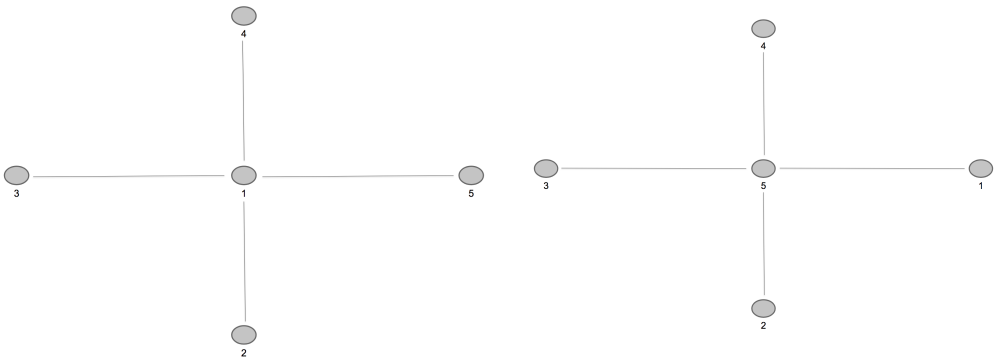
If $F(i, j)$ separates node $i < j$, then $x_i \perp x_j \mid \boldsymbol{x}_{F(i,j)}$ and $L_{ij} = 0$. However, if $F(i, j)$ does not separate the two nodes, then a calculation needs to be carried out to determine the value of L_{ij}, which may or may not be zero. In other words, if we can verify that L_{ij} is 0, then we do not have to compute it. Applying the global Markov property (Appendix A5), this verification can be done by ensuring that the future set $F(i, j)$ separates i and j in the graph G that defines the GMRF where $i < j$.

Therefore, to minimize computation, it is desirable to find a permutation such that $x_i \perp x_j \mid \boldsymbol{x}_{F(i,j)}$ for as many values of i and j as possible. It is the conditional independence structure of the graph which determines which nodes are connected to which, and therefore which nodes are separated by which, which

determines $F(i,j)$, thus affecting whether or not $L_{ij} = 0$. The more zeros we have in our cholesky factor $\boldsymbol{L}$, the less calculations needed to obtain the cholesky factor since only the non-zero elements are calculated.

Using again the global Markov property and equation (2.13) (maybe can be explained more in the appendix), L is more or equally dense than the lower triangular part of $\boldsymbol{Q}$, which has $n_Q = n-1$ entries (it is easy to see why the precision matrix has $n-1$ entries from equation (2.12)). In other words, the number of non-zero elements in the cholesky factor, n_L, is always greater than or equal to n_Q. The efficiency of the cholesky factorization can thus be measured by the fill-in ratio $\frac{n_L}{n_Q}$ since the closer the fill-in ratio to 1, the less non-zero elements need to be calculated. Optimal efficiency is thus achieved when the fill-in ratio is 1 and only $n-1$ entries need to be calculated, which is linear in the number of nodes.

Therefore, the ordering of individual nodes are important as they can be re-ordered so that overall, as many node pairs (i,j) as possible are separated by $F(i,j)$ for any i and j, leading to lower n_L and greater computational gains. In general, it is beneficial for nodes that are connected to many other nodes to have higher numbers, so that conditional independence between any 2 nodes given the set $F(i,j)$ is more likely. For instance, if all nodes depend on node 1, for any $1 < i < j \leq n$, the future set $F(i,j)$ will never separate i and j as every node is connected to node 1, leading to maximal fill-in. This is illustrated in Figure 2 below. This line of reasoning leads to the concept of nested dissection (Rue, Held, 2002).



(a) (b)

Figure 2. Two graphs which illustrate the importance of ordering of nodes to computational efficiency. In graph (a), every node is connected to node 1 and only node 1, making it in the future set of every node. Thus, fill-in is maximal and the cholesky factorization for its precision matrix is $O(n^3)$. However, in graph (b), every node is connected to node 6 and only node 6. It is thus in none of the future sets of any of the other nodes, making fill-in minimal and reducing complexity to $O(n)$

Permutation of the precision matrix can be done by finding a permutation matrix $\boldsymbol{P}$ such that $\boldsymbol{i}^p = \boldsymbol{P}\boldsymbol{i}$ where $\boldsymbol{i} = \{1,..,n\}^T$ is the original ordering of the nodes and $\boldsymbol{i}^p$ is the new ordering. $\boldsymbol{P}$ is then chosen such that the resulting permuted precision matrix $\boldsymbol{Q}^p = \boldsymbol{P}\boldsymbol{Q}\boldsymbol{P}^T$ leads to a reduction in fill-in for the cholesky factor. $\boldsymbol{P}$ can be chosen based on the principles of nested dissection. By selecting a small set of nodes whose removal divides the graph into two disconnected subgraphs of almost equal size and give them the highest numbers, re-ordering the nodes in each of the subgraphs, and repeating the same procedure to the rest of the nodes in each of the subgraphs. On average, algorithms based

on nested dissection ordering require $O(n^{3/2})$ flops and gives $O(nlogn)$ fill-ins (George, Liu, 1981). However, for graphs with cleaner structures such as Gaussian hierarchical models, optimal fill-in and faster performance is possible.

2.5 Gibbs Sampler

Efficient performance of above method is reliant on finding the right permutation matrix which can be hard to do without the right algorithm. The alternative to exact inference with sparse linear algebra methods is approximate inference belonging to the class of Monte Carlo Markov Chain methods such as the Gibbs sampler. The Gibbs sampler relies on calculating full conditionals of each parameter and sampling based on those conditionals (Appendix A6). In particular, the graph structure of the hierarchical model makes sampling from conditionals easily by sampling firstly from the leaves of the graph and then sampling upwards based on samples at lower levels. For a long enough time period, samples drawn from the Gibbs sampler with subsampling (since subsequent samples are highly correlated) resemble independent draws from the target distribution. The complexity is linear in the number of parameters and thus competitive with the sparse linear algebra methods. In particular, the Gibbs sampler used here is based off GS(0,0) in Zanella, Roberts (2017). The algorithm for the Gibbs sampler for a centered 2-level Gaussian hierarchical model is as follows:

Initialize $\beta^{*(0)} = \beta^{(0)}, \beta_1^{(0)}, ..., \beta_I^{(0)}, \beta_{11}^{(0)}, ..., \beta_{IJ}^{(0)}$ randomly;
for *t = 1 to T* do
  for *i = 1 to I* do
    for *j = 1 to J* do
      Sample $\beta_{ij}^{(t)} \mid \beta^{(t-1)},\ \beta_{1:I}^{(t-1)}$;
    end
    Sample $\beta_i^{(t)} \mid \beta^{(t-1)},\ \beta_{i,1:J}^{(t)}$
  end
  Sample $\beta^{(t)} \mid \beta_{1:I}^{(t)},\ \beta_{1:I,1:J}^{(t)}$
end

Algorithm 1: Gibbs Sampler

3. Experiments

3.1 ghInf

The R package ***ghInf*** was created to aid with the simulations conducted in this paper. ***ghInf*** provides multiple tools for inference with Gaussian hierarchical models. This includes functions which calculate the precision matrix for both centered and uncentered parametrizations of 2- and 3-level Gaussian hierarchical models and a Gibbs sampler for centered 2- and 3-level models. The code can be found here on Github.

3.2 Matrix and spam packages

The ***Matrix*** and ***spam*** packages are linear algebra packages for R. ***Matrix*** is a larger package with methods for a wide variety of functions which make use of linear algebra libraries such as BLAS (Basic Linear Algebra Subroutines), Lapack (dense matrix), CHOLMOD and Csparse (sparse matrix) routines (Maechler, Bates, 2006). On the other hand, ***spam*** is a more focused sparse matrix R package which an emphasis on Monte Carlo Markov Chain methods for Gaussian Markov Random Fields (Furrer, Sain, 2010). The main function of interest in both packages is the cholesky decomposition function, ***chol***, which is important in sampling-based inference of Gaussian hierarchical models. The ***chol*** function in ***Matrix*** uses CHOLMOD (Davis, 2009), a sparse supernodal Cholesky factorization routine, whereas ***spam*** uses the block sparse Cholesky algorithm (a supernodal left-looking - constructing the lower triangular factor R^T column-wise - Cholesky factorization) of Ng and Peyton (1993). For the purposes of this paper, the differences in the methods is not important since both routines return the same cholesky factor. This is because the precision matrix is positive definite and the cholesky factor of a positive definite matrix is unique.

Cholesky decomposition functions, especially for sparse matrices, often use permutation algorithms to permute the rows and columns of a matrix to reduce the fill-in and thus make computation more efficient. The ***spam*** package uses the multiple minimum degree algorithm (MMD) (George, Liu, 1989) by default to permute the matrix whereas the ***Matrix*** package uses the approximate minimum degree algorithm (AMD) (Amestoy, Davis, Duff, 1996). Both algorithms seek to directly reduce the fill-in of the cholesky factor as opposed to bandwith reduction methods. The difference between AMD and MMD are highly technical and irrelevant to the results of this paper.

Both ***Matrix*** and ***spam*** packages have cholesky decomposition functions which allow for pivot = FALSE. This means that the function attempts to compute the cholesky factor without using the AMD or MMD permutation algorithm. This allows performance comparisons to be made between the fill-in obtained using each package's respective permutation algorithm versus without to illustrate the importance of row and column permutation in factorizing sparse matrices.

3.3 Effectiveness of permutation algorithms

In this section, the efficacy of the permutation algorithms are tested by comparing the performance of each package with versus without the permutation algorithm. Performance is measured in terms of the ratio of the fill-in of the cholesky factor with respect to the optimal fill-in $n-1$, where n is the total number of parameters.

The default node ordering / labeling system that was used in generating the precision matrix is a lexicographic one which began from the parameters at the lowest level. That is, for a 2-level model with I parameters in level 1 and J children per level 1 node has a column/row labeling of $\beta_{11}, ..., \beta_{1J}, ..., \beta_{IJ}, \beta_1, ..., \beta_I, \beta$. To illustrate how the permutations look like, the precision matrix of a centered 3-level model is used instead. let $I = 2$, $J = 1$, and $K = 2$ and all variances set to 1. An example of the labeled matrix is illustrated below in Table 1.

Table 1: Default labels of precision matrix

	B111	B112	B211	B212	B11	B21	B1	B2	B
B111	2	0	0	0	-1	0	0	0	0
B112	0	2	0	0	-1	0	0	0	0
B211	0	0	2	0	0	-1	0	0	0
B212	0	0	0	2	0	-1	0	0	0
B11	-1	-1	0	0	3	0	-1	0	0
B21	0	0	-1	-1	0	3	0	-1	0
B1	0	0	0	0	-1	0	2	0	-1
B2	0	0	0	0	0	-1	0	2	-1
B	0	0	0	0	0	0	-1	-1	2

This choice of labeling was determined out of convenience in constructing the precision matrix from the posterior density of the joint distribution. However, when calculating the fill-in of the cholesky factor of the precision matrix with the option pivot = FALSE, both packages returned the optimal fill-in ratio of 1. This indicates that this choice of labelling was somehow coincidentally an optimal permutation of the precision matrix to obtain the optimal fill-in. To investigate this further, three other permutations were experimented with. The three permutations are reverse lexicographic order, random order, and depth-first order (that is, labeling is done for each path upwards from the leaf parameters towards the root parameter). Illustrations of each permutation are provided below:

Table 2: Depth-first permutation of precision matrix

	B111	B112	B11	B1	B211	B212	B21	B2	B
B111	2	0	-1	0	0	0	0	0	0
B112	0	2	-1	0	0	0	0	0	0
B11	-1	-1	3	-1	0	0	0	0	0
B1	0	0	-1	2	0	0	0	0	-1
B211	0	0	0	0	2	0	-1	0	0
B212	0	0	0	0	0	2	-1	0	0
B21	0	0	0	0	-1	-1	3	-1	0
B2	0	0	0	0	0	0	-1	2	-1
B	0	0	0	-1	0	0	0	-1	2

Table 3: Random permutation of precision matrix

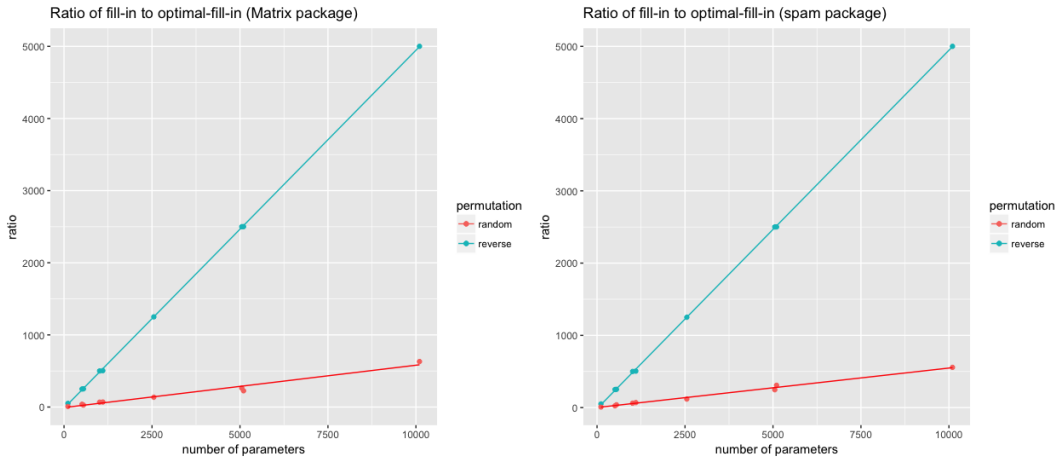
	B1	B111	B2	B212	B112	B21	B211	B11	B
B1	2	0	0	0	0	0	0	-1	-1
B111	0	2	0	0	0	0	0	-1	0
B2	0	0	2	0	0	-1	0	0	-1
B212	0	0	0	2	0	-1	0	0	0
B112	0	0	0	0	2	0	0	-1	0
B21	0	0	-1	-1	0	3	-1	0	0
B211	0	0	0	0	0	-1	2	0	0
B11	-1	-1	0	0	-1	0	0	3	0
B	-1	0	-1	0	0	0	0	0	2

Table 4: Reverse permutation of precision matrix

	B	B2	B1	B21	B11	B212	B211	B112	B111
B	2	-1	-1	0	0	0	0	0	0
B2	-1	2	0	-1	0	0	0	0	0
B1	-1	0	2	0	-1	0	0	0	0
B21	0	-1	0	3	0	-1	-1	0	0
B11	0	0	-1	0	3	0	0	-1	-1
B212	0	0	0	-1	0	2	0	0	0
B211	0	0	0	-1	0	0	2	0	0
B112	0	0	0	0	-1	0	0	2	0
B111	0	0	0	0	-1	0	0	0	2

For the depth-first permutation, the optimal fill-in was returned even with pivot = FALSE. However, non-optimal results were obtained for the reverse and random permutations. For these experiments, a centered 2-level model was used with i being the number of nodes in level 1 and j the number of children nodes per node in level 1. The fill-in ratio for reverse and random permutations are illustrated in figures 3(a) and 3(b) on the next page for combinations of values of i and j in the set $\{10, 50, 100\}$.

In general, the fill-in ratio is worse when the reverse order is used compared to when the nodes are randomly permuted. The fill-in ratio is also almost identical, with the only source of difference coming from the randomization of the permutations (which was averaged over multiple iterations), which is expected since the cholesky factor is unique.



(a) (b)

Figure 3. Fill-in ratio using both Matrix (a) and spam (b) packages

3.4 Future set $F(i, j)$ of Gaussian hierarchical models

For both the ***Matrix*** and ***spam*** packages, the optimal fill-in was obtained when pivot = TRUE for all 3 permutations constructed (depth-first, random, and reverse), confirming the efficacy of the row permutation algorithms used by both packages in finding the optimal configuration for matrix factorization. Both packages are thus robust to label permutations in the precision matrix. This result can possibly be explained by the cleanly divided multilevel structure of Gaussian hierarchical models which makes it easier to order nodes by nested dissection. Using the ***spam*** package's ***ordering*** function, the permuted precision matrix can be recovered and studied.

It turns out that the permuted precision matrix obtained using the ***ordering*** function is labelled in the same manner as the depth-first permutation (that the labels are not exactly the same is irrelevant since the positions in the matrix which are non-zero are the same)! Furthermore, this implies an interesting side result that there is more than one permutation which results in an optimal fill-in since the optimal fill-in was also obtained with the lexicographical ordering.

The results in section 3.3 can then be explained by considering the hierarchical structure together with the future set $F(i, j)$. Recall that if all the nodes depend on, or have an edge to, node 1, the fill-in will be maximal or close to maximal since the set $F(i, j)$ will never separate nodes i and j regardless of the values of i, j. Considered simply, this implies that nodes with fewer edges should be assigned lower numbers and nodes with more edges assigned higher numbers.

In a Gaussian hierarchical model, this means that the nodes at the bottom level, which are only connected to its parent, should be given lower numbers. This is exactly what was done for the lexicographical ordering as nodes are labelled 1 to n from the lowest level upwards. Likewise, this explains why the reversed lexicographical permutation had the worst fill-in ratio: the nodes which contained more edges in the higher levels are now given smaller numbers. Equation (2.13) tells us which entries of the cholesky factor are known to be 0 with certainty. With a reverseed lexicographical permutation, there is less information on and more uncertainty on which entries of the cholesky factor are zero and thus more computations need

to be carried out, leading to greater fill-in. This is because the conditional independence between two nodes i, j given the future set $F(i, j)$ cannot be established if they are both connected to a node k such that $1 \leq k < i < j \leq n$.

This also explains why the depth-first permutation is an optimal permutation since for any node i where $1 \leq i < n$, the future set $F(i, j)$ always contains the nodes which it is connected to. This is exactly due to the tree-like structure of the graph where each node is connected only to its parent and children (if available).

Thus, we can use the hierarchical structure to construct labelings for the precision matrices of Gaussian hierarchical model ***a priori*** so that little or no permutation is required before cholesky factorization. This will lead to computational gains since there is no longer any need to find a permutation matrix $\boldsymbol{P}$. Instead, one simply needs to construct a depth-first labeling as mentioned above.

4. Discussion

Hierarchical modeling is a practical approach with proven results in modeling real world data. This paper in particular studied Gaussian hierarchical models and methods which exploit the sparse conditional independence structure of such models to conduct scalable and efficient inference using sparse linear algebra methods. The efficiency of such methods is highly dependent on the row and column ordering of the precision matrix to be factorized. The key finding in this paper is that a depth-first permutation guarantees an optimal permutation of the precision matrix for Gaussian hierarchical models such that the fill-in ratio is optimal. This makes the use of permutation algorithms such as AMD or MMD unnecessary once it is known that the model used is a Gaussian hierarchical model, saving on computational efficiency. It was also found that the returned fill-in ratio is also optimal with a lexicographical ordering. Since the cholesky factor of a positive-definite matrix is unique, this implies that there is more than one optimal permutation of the precision matrix which returns minimal fill-in. A possible area of future research would be to determine if there are more permutations which also return an optimal fill-in ratio.

This paper illustrates how one can conduct scalable inference on Gaussian hierarchical models using a naive Gibbs sampler and sparse linear algebra methods. Other methods of scalable inference which can be explored include belief propagation (Papaspiliopoulos, Zanella, 2017), which allows exact draws from high-dimensional distributions at a cost which scales linearly in the number of parameters and data, at the expense of higher variable node dimensions.

Appendix

A1. Extension to 3-level model

For a 3-level model, we retain equations (2.1) to (2.3). However, we add an aditional level and a modified observation level.

$$\beta_{ijk} \mid \beta_{ij} \sim N(\beta_{ij}, \tau_c) \quad -(a.1)$$

$$y_{ijk} \mid \beta_{ijk} \sim N(\beta_{ijk}, \sigma^2)$$

A2. Calculating precision matrix entries

$$\begin{aligned}
P(\boldsymbol{\beta} \mid \boldsymbol{y}) &= \frac{P(\boldsymbol{y} \mid \boldsymbol{\beta})P(\boldsymbol{\beta})}{P(\boldsymbol{y})} \\
&\propto P(\boldsymbol{y} \mid \boldsymbol{\beta})P(\boldsymbol{\beta}) \\
&= P(\beta)\prod_i P(\beta_i \mid \beta)\prod_{i,j} P(\beta_{ij} \mid \beta_i)\prod_{i,j,k} P(\beta_{ijk} \mid \beta_{ij})\prod_{i,j,k} P(y_{ijk} \mid \beta_{ijk}) \\
&\propto \exp\{-\frac{1}{2\sigma^2}\sum_{i,j,k}(y_{ijk}-\beta_{ijk})^2 - \frac{1}{2\tau_c}\sum_{i,j,k}(\beta_{ijk}-\beta_{ij})^2 - \frac{1}{2\tau_b}\sum_{i,j}(\beta_{ij}-\beta_i)^2 - \frac{1}{2\tau_a}\sum_i(\beta_i-\beta)^2 - \\
&\frac{1}{2\tau}(\beta-\mu)^2\} \\
&\propto \exp\{-\frac{1}{2}\boldsymbol{\beta^T}Q\boldsymbol{\beta}\}
\end{aligned}$$

By expanding out the squared terms and rearranging them, we can deduce the terms of the posterior precision matrix Q. If we assume a flat prior,

$$\exp\{-\frac{1}{2}\boldsymbol{\beta}^T\boldsymbol{Q}\boldsymbol{\beta}\} \propto \exp\{-\frac{1}{2}(\sum_{i,j}(\frac{\beta_{ij}^2}{\sigma^2}+\frac{\beta_{ij}^2}{\tau_b}+\frac{\beta_i^2}{\tau_b}-\frac{2\beta_{ij}\beta_i}{\tau_b})+\sum_i(\frac{\beta_i^2}{\tau_a}+\frac{\beta^2}{\tau_a}-\frac{2\beta_i\beta}{\tau_a}))\} \quad -(a.2)$$

For example, the conditional precision of β_{ij} is $\frac{1}{\sigma^2}+\frac{1}{\tau_b}$, and the conditional precision between β_{ij} and β_i is $-\frac{1}{\tau_b}$. To better illustrate, for $I=3$ and $J=4$, the constructed precision matrix is shown below:

$$
\begin{array}{c}
 \\
\beta_{11} \\
\beta_{12} \\
\vdots \\
\beta_{1I} \\
\vdots \\
\beta_{IJ} \\
\beta_1 \\
\vdots \\
\beta_I \\
\beta
\end{array}
\begin{array}{c}
\begin{array}{ccccccccccc}
\beta_{11} & \beta_{12} & \cdots & \beta_{1I} & \cdots & \beta_{IJ} & \beta_1 & \cdots & \beta_I & \beta
\end{array} \\
\begin{pmatrix}
\frac{1}{\sigma^2}+\frac{1}{\tau_b} & 0 & \cdots & 0 & \cdots & 0 & -\frac{1}{\tau_b} & \cdots & 0 & 0 \\
0 & \frac{1}{\sigma^2}+\frac{1}{\tau_b} & \cdots & 0 & \cdots & 0 & -\frac{1}{\tau_b} & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & \frac{1}{\sigma^2}+\frac{1}{\tau_b} & \cdots & 0 & -\frac{1}{\tau_b} & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 0 & \cdots & \frac{1}{\sigma^2}+\frac{1}{\tau_b} & 0 & \cdots & -\frac{1}{\tau_b} & 0 \\
-\frac{1}{\tau_b} & -\frac{1}{\tau_b} & \cdots & -\frac{1}{\tau_b} & \cdots & 0 & \frac{1}{\tau_a}+\sum_j \frac{1}{\tau_b} & \cdots & 0 & -\frac{1}{\tau_a} \\
\vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 0 & \cdots & -\frac{1}{\tau_b} & 0 & \cdots & \frac{1}{\tau_a}+\sum_j \frac{1}{\tau_b} & -\frac{1}{\tau_a} \\
0 & 0 & \cdots & 0 & \cdots & 0 & -\frac{1}{\tau_a} & \cdots & -\frac{1}{\tau_a} & \sum_i \frac{1}{\tau_a}
\end{pmatrix}
\end{array}
$$

A3. Proof for equation (2.12):

Using the fact that $x \perp y \mid z \iff P(x,y,z) = f(x,z)g(y,z)$ for some functions f and g (Rue, Held, 2002), let $\mathbf{x} = (x_i, x_j, \mathbf{x}_{-\{ij\}})$, and setting the mean to be 0 without loss of generality, we have that for $i \neq j$:

$$
\begin{aligned}
P(x_i, x_j, \mathbf{x}_{-\{\mathbf{ij}\}}) &= f(x_i, \mathbf{x}_{-\{\mathbf{ij}\}}) g(x_j, \mathbf{x}_{-\{\mathbf{ij}\}}) \\
P(x_i, x_j, \mathbf{x}_{-\{\mathbf{ij}\}}) &\propto \exp\{-\frac{1}{2}\sum_{k,l} x_k Q_{kl} x_l\} \\
&\propto \exp\{-\frac{1}{2} x_i x_j (Q_{ij} + Q_{ji}) - \frac{1}{2} \sum_{\{k,l\} \neq \{i,j\}} x_k Q_{kl} x_l\} \quad -(a.3)
\end{aligned}
$$

Since in this case, it is already assumed that $x_i \perp x_j \mid \mathbf{x}_{-\{\mathbf{ij}\}}$, it follows that $Q_{ij} = Q_{ji} = 0$.

A4. Proof for equation (2.13):

Let $\boldsymbol{x}$ be a GMRF with respect to the labelled graph G, with mean $\boldsymbol{\mu}$ and positive-definite precision matrix $\boldsymbol{Q}$. Let $\boldsymbol{L}$ be the Cholesky triangle of $\boldsymbol{Q}$. Then for $i \in V$,

$$
\begin{aligned}
E(x_i | \boldsymbol{x}_{(i+1):n}) &= \mu_i \frac{1}{L_i i} \sum_{j=i+1}^{n} L_{ji}(x_j \mu_j) \quad -(a.4) \\
Prec(x_i | \boldsymbol{x}_{(i+1):n}) &= L_{ii}^2 \quad -(a.5)
\end{aligned}
$$

Assume for simplicity that $\boldsymbol{\mu} = 0$ and fix $1 \leq i < j \leq n$, then:

$$P(\boldsymbol{x}_{i:n}) \propto \exp\left(-\frac{1}{2}\sum_{k=i}^{n} L_{kk}^2 \left(x_k + \frac{1}{L_{kk}}\sum_{j=k+1}^{n} L_{jk}x_j\right)^2\right)$$
$$= \exp\left(-\frac{1}{2}\boldsymbol{x}_{i:n}^T \boldsymbol{Q}^{(i:n)}\boldsymbol{x}_{i:n}\right) \quad -(a.6)$$

where $\boldsymbol{Q}^{i:n} = L_{ii}L_{ji}$. Using equation (2.12), it follows that:

$$x_i \perp x_j \mid \boldsymbol{x}_{F(i,j)} \iff L_{ii}L_{ji} = 0 \quad -(a.7)$$

which is equivalent to equation (2.13) since $L_{ii} > 0$ because the precision matrix is positive-definite.

A5. Markov properties of GMRF

This section is written with reference to Theorem 2.4 in Rue and Held (2002). From equation (2.12), a GMRF represented by the graph $G = (V, E)$ is defined by the non-zero pattern in the precision matrix $\boldsymbol{Q}$, since that tells you which nodes have edges to which other nodes. It turns out that for a GMRF, the pairwise Markov property defined in equation (2.11) is equivalent to the global Markov property:

$$\boldsymbol{x}_A \perp \boldsymbol{x}_B \mid \boldsymbol{x}_C \quad -(a.8)$$

for all disjoint sets A, B, and C where C separates A and B, and A and B are non-empty.

A6. Full conditionals for Gibbs sampler

Adopting the notation from Roberts & Zanella (2017),

$$\beta_{\cdot} = \frac{\sum_i \beta_i}{I}$$

$$\beta_{\cdot j} = \frac{\sum_i \beta_{ij}}{I},\ \beta_{\cdot\cdot k} = \frac{\sum_{i,j} \beta_{ijk}}{IJ}$$

and so on. Note that the following derivation for the full conditionals of the Gibbs sampler are for a centered parametrization with a flat prior.

Assuming that $\mu = 0$, the full conditional is proportional to the posterior density of the coefficients. Since we are only concerned with β, we can ignore all factors which do not contain β:

$$
\begin{aligned}
P(\beta \mid \beta_{1:I},\ \beta_{1:I,1:J},\ y^*) &= \frac{P(\beta^* \mid y^*)}{P(\beta_{1:I},\ \beta_{1:I,1:J} \mid y^*)} \\
&\propto \exp\{-\frac{1}{2\sigma^2}\ \sum_{i,j}(y_{ij}-\beta_{ij})^2 - \frac{1}{2\tau_b}\sum_{i,j}(\beta_{ij}-\beta_i)^2 - \frac{1}{2\tau_a}\sum_i(\beta_i-\beta)^2 - \frac{1}{2\tau}(\beta-\mu)^2\} \\
&\propto \exp\{-\frac{1}{2\tau_a}\sum_i(\beta^2-2\beta_i\beta) - \frac{1}{2\tau}\beta^2\}
\end{aligned}
$$

To generate samples from a Gaussian, all we need are the first and second moments. By expanding and manipulating the above, we can obtain a form to read off the mean and variance of the full conditional.

$$
\begin{aligned}
\exp\{-\frac{1}{2\tau_a}\sum_i(\beta^2-2\beta_i\beta) - \frac{1}{2\tau}\beta^2\} &= \exp\{-\frac{1}{2}\frac{\tau I\beta^2 - 2\tau\beta\sum_i\beta_i + \tau_a\beta^2}{\tau_a\tau}\} \\
&= \exp\{-\frac{1}{2}\frac{(\tau+\frac{\tau_a}{I})\beta^2 - 2\tau\beta\beta_\cdot}{\frac{\tau_a\tau}{I}}\} \\
&= \exp\{-\frac{1}{2}\frac{\beta^2 - 2\beta\beta_\cdot\frac{\tau}{\frac{\tau_a}{I}+\tau}}{\frac{\frac{\tau_a\tau}{I}}{\frac{\tau_a}{I}+\tau}}\} \\
&\propto \exp\{-\frac{1}{2}\frac{(\beta-\beta_\cdot\frac{\tau}{\frac{\tau_a}{I}+\tau})^2}{\frac{\frac{\tau_a\tau}{I}}{\frac{\tau_a}{I}+\tau}}\} \quad -(a.9)
\end{aligned}
$$

where $\beta_\cdot = \frac{\sum_i \beta_i}{I}$. From this, we can deduce the mean and variance of the posterior distribution of β.

$$
\beta \mid \beta_{1:I},\ \beta_{1:I,1:J}, \boldsymbol{y} \sim N(\frac{\beta_\cdot\tau}{\frac{\tau_a}{I}+\tau}, \frac{\frac{\tau_a\tau}{I}}{\frac{\tau_a}{I}+\tau}) \quad -(a.10)
$$

In the same way, the full conditionals for the other parameters can be derived.

$$
\beta_i \mid \beta,\ \beta_{1:I,1:J}, \boldsymbol{y} \sim N(\frac{(\frac{\tau_b}{J}\beta + \tau_a\beta_{i\cdot})}{\tau_a+\frac{\tau_b}{J}}, \frac{\frac{\tau_a\tau_b}{J}}{\frac{\tau_b}{J}+\tau_a}) \quad -(a.11)
$$

$$
\beta_{ij} \mid \beta,\ \beta_{1:I}, \boldsymbol{y} \sim N(\frac{\beta_i\sigma^2}{\tau_b+\sigma^2}, \frac{\tau_b\sigma^2}{\tau_b+\sigma^2}) \quad -(a.12)
$$

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