A Scalable Blocked Gibbs Sampling Algorithm
For Gaussian And Poisson Regression Models

Nicholas A. Johnson,* Frank O. Kuehnel, Ali Nasiri Amini
Google Inc
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Abstract

Markov Chain Monte Carlo (MCMC) methods are a popular technique in Bayesian statistical modeling. They have long been used to obtain samples from posterior distributions, but recent research has focused on the scalability of these techniques for large problems. We do not develop new sampling methods but instead describe a blocked Gibbs sampler which is sufficiently scalable to accommodate many interesting problems. The sampler we describe applies to a restricted subset of the Generalized Linear Mixed-effects Models (GLMM’s); this subset includes Poisson and Gaussian regression models. The blocked Gibbs sampling steps jointly update a prior variance parameter along with all of the random effects underneath it. We also discuss extensions such as flexible prior distributions.

1 Introduction

There has been a great deal of work on implementing efficient, large-scale regularized regressions, but there has been much less progress in scaling up fully Bayesian regression models. Bayesian and Empirical Bayes models (such as GLMM’s) have found wide use when applied to smaller datasets. Two of the more popular software packages are STAN [12] and the lme4 R package [1]. STAN is highly-customizable and it uses MCMC to draw posterior samples of model parameters. The lme4 software is perhaps the most popular R package for mixed effects models, but its implementation is based on Laplace approximation which involves factorization of large matrices.

Recent work to scale up Bayesian model inference includes consensus Bayes [13], stochastic gradient Langevin dynamics (SGLD) [18], and the Weierstrass sampler [17]. The intent of our publication is to present blocked Gibbs sampling in terms of simple, scalable operations for solving large regression models. The narrow class of Bayesian regression models that we consider also have associated MCMC moves which depend on a (relatively) small set of sufficient statistics.

In this section we first discuss an example of the type of data that our algorithm can model. We then give some background on random effects models and follow by

*e-mail:naj@google.com
Table 1: An example dataset for which n.actions could be modeled as a Poisson count depending on two features, “url” and “ad.id”, and on an observed offset “n.views”.

| n.views | n.actions | url    | ad.id  |
|---------|-----------|--------|--------|
| 52      | 4         | abc.com| 83473  |
| 73      | 5         | xyz.edu| 40983  |
| 19      | 0         | abc.com| 4658   |
| 532     | 16        | efg.com| 40983  |
| 3       | 0         | z.com  | 4658   |

Typically a Gaussian prior is placed on \( b \):
\[
b \sim N(0, \Sigma)\]

where \( \Sigma \) is a diagonal matrix with \( \sigma_1 \) appearing on the first \( L_1 \) diagonal elements, \( \sigma_2 \) on the next \( L_2 \), and so on (and \( L_1 + \ldots + L_F = r \)). In the language of the “lme4” R package [1] a Poisson model of the data in Table 1 can be specified as:

\[
n.\text{actions} \sim 1 + (1 | \text{url}) + (1 | \text{ad.id}) + \text{offset}(\log(n.\text{views}))
\]
To be more precise, we define the index set $J_k$ to be the $k$'th block of indices: 
\[ \{T_{k-1} + 1, ..., T_k - 1 + L_k \} \] where $T_k := \sum_{j=1}^{k} L_j$ and $T_0 = 0$. The random effect variance matrix has $(j, j)$'th diagonal element $\Sigma(\sigma)_{jj} = \sigma^2_k$ when $j \in J_k$.

The mixed effects model is then fit by maximizing the marginal likelihood:

\[
\ell(\beta, \sigma) := \int P(\{b_i\}_{i=1}^{r} | \sigma) \left[ \prod_{j=1}^{n} P(Y_j | D_j, X_j, Z_j, \beta, b) \right] db_1...db_r 
\]

where $P(\{b_i\}_{i=1}^{r} | \sigma) = \prod_{f=1}^{F} \prod_{j=1}^{L_f} P(b_{T_f-1+j} | \sigma_f)$

(3)

where $X_j$ and $Z_j$ denote the $j$'th rows of the respective matrices, and $D_j$ and $Y_j$ refer to the $j$'th element of the respective vectors. Usually the integral in (3) cannot be computed in closed form, so it is approximated by MCMC or Laplace approximation [1]. Gaussian models are an exception but even in that case calculating the marginal likelihood can involve matrix factorizations which are prohibitive to compute. Software such as lme4 can handle more general prior covariance structure than that described above, but we focus on the case where $\Sigma$ is diagonal.

When modeling Poisson data, the algorithm will only apply to the restricted case that: (a) $p = 1$, $X = [1]_{n \times 1}$, (b) $Z$ is a 0-1 matrix (i.e. $Z_{jk} \in \{0, 1\}$), and (c) the partial row sums within a family’s block of columns are equal to one: $\sum_{t \in J_k} Z_{it} = 1$. It is easy to instead accommodate $\sum_{t \in J_k} Z_{it} \in \{0, 1\}$, but we omit the details. When modeling Gaussian data we relax this to allow any real valued entries but maintain a restriction on the sparsity pattern: $\sum_{t \in J_k} 1\{Z_{it} \neq 0\} = 1$ for $k = 1, 2, ..., F$.

Condition (c) states that we have conditional independence between the random effects parameters $b$ within a single feature family “k”. We also depend on this sparsity pattern to store $Z$ efficiently. We discuss this in more detail in section 2. Next we choose a Gamma prior distribution instead of the standard log-normal one for GLMMs: $\exp(b_j) \sim \text{Gamma}(\sigma^{-2}_k, \sigma^{-2}_k)$, where $E[\exp(b_j)] = 1$ and $\text{Var}(\exp(b_j)) = \sigma^2_k$ for $j \in J_k$. The mean-one restriction is for identifiability; without it the Gamma prior distributions could be scaled by any amount and an adjustment to the fixed effect would yield exactly the same data distribution. We will see that the conjugacy of the Gamma and Poisson distributions simplifies some sampling steps in our algorithm.

With these restrictions and conjugate priors in place, we develop a blocked Gibbs sampling iteration in which we update a single family at a time. We jointly update a prior parameter and all of the random effects beneath it.

We end this section with a review of background material and related work. Gibbs sampling is widely used, so we just cover some early papers, relevant textbooks, and related applications to Bayesian regression models.

Gelfand and Smith [4] introduced the statistics community to Gibbs sampling as a computational technique for inference in Bayesian models. This paper did not propose Gibbs sampling (they attributed it to [6]), but they showed the power of the technique through several examples. The paper has since been cited over six thousand times.
Conditions for ergodicity of Gibbs samplers and Metropolis-Hastings algorithms are given in [14] and simpler, less-general conditions for convergence of the Gibbs sampler are given in [11]. Gibbs sampling and many other MCMC algorithms are described in the text book by Jun Liu [8]. This includes blocked Gibbs samplers (also referred to as “grouped”) and other variations. The textbook “Bayesian Data Analysis” (BDA) [5] contains examples of Bayesian regression models and Gibbs samplers tailored to them. BDA also includes examples of blocked Gibbs samplers (e.g. chapter 15 section 5 in the third edition).

Blocked Gibbs sampling was evaluated in the context of Gaussian Mixed Effects models by Chib and Carlin [3]. They considered the Gaussian longitudinal model:

$$y_k = X_k \beta + W_k b_k + \epsilon_k \in \mathbb{R}^{n_k} \quad (5)$$

where $b_k \in \mathbb{R}^q$ and has Gaussian prior $b_k \sim N_q(0, \Sigma)$. They developed seven different Gibbs samplers with varying levels of blocking. These included samplers which integrated out $\{b_k\}$ and $\beta$ and drew $\Sigma$ conditional on only the observed data $\{y_k\}$. They also showed how to apply their algorithms to binary probit regression using the latent variable representation $z_k = \text{sign}(y_k)$ where $z_k$ is observed but $y_k$ is not. They found that blocking substantially reduced autocorrelation in their examples that the additional computational cost of the blocked updates was a good tradeoff.

In our experience the blocked updates are especially important when there is a long tail of levels which have little associated data. Consider advertisers as an example: there may be a small subset of advertisers responsible for a huge number of “views” and “actions”, and these are most informative when learning the prior variance parameters $\sigma$. Often though, there is also a much larger population of advertisers with very sparse data, and their presence slows down the mixing of a non-blocked Gibbs sampler.

The work of Volfosky and Hoff [16] is similar in that they build models with many random effect families: their focus is on Gaussian ANOVA models with multiple factors and interaction terms. They implement Gibbs samplers of balanced designs and suggest data augmentation as a technique to handle imbalanced designs (i.e. add missing data which would make the design balanced). They focused on relatively small datasets (i.e. $n < 10,000$, $F < 3$, and $L_k < 10$). The algorithm we describe below has been applied to much larger problems.

In the next section we give a detailed description of the algorithm and associated computations, and in section 3 we discuss some extensions to the algorithm.

## 2 Gibbs Sampling for Gamma-Poisson Regression Models

In this section we give a detailed description of the blocked Gibbs sampler for the Gamma-Poisson model. In an un-blocked Gibbs sampler with variables $(V_1, V_2, \ldots, V_n)$ we would iterate the updates:

$$v_k \sim p(V_k|V_1 = v_1, \ldots, V_{k-1} = v_{k-1}, V_{k+1} = v_{k+1}, \ldots, V_n = v_n) \quad (6)$$
In a “blocked” or “grouped” Gibbs sampler we can update several variables at a time:
\[
\{v_j : j \in I\} \sim p(\{V_j : j \in I\}|\{V_i : i \notin I\})
\]
(7)

We describe how the block \(I\) can be taken to be a large set of random effects as well as an associated prior variance parameter. This blocked update is just as scalable as unblocked updates (and much more scalable than a naive implementation of an unblocked Gibbs sampler).

As mentioned earlier, we do not develop an algorithm for general \(X\) and \(Z\) model matrices. We will handle the case that \(X\) is the \(n \times 1\) matrix \([1]^n\) and so \(\beta \in \mathbb{R}\).

With the restriction on \(Z\) described above we can more compactly write the subsequent computations in terms of an \(n \times F\) matrix of indices \(I\). We define \(I_{jk} = t\) if \(Z_{j,(t+Tk-1)} = 1\). For example, if the first family of random effects is based on “url” and we enumerate the unique url’s as 1, 2, 3, ..., then \(I_{j1} = t\) if the \(j\)'th row of the input table contains the \(t\)'th url. To make some equations easier to read we will sometimes write \(I(j, k)\) in place of \(I_{jk}\).

The table below shows what the matrix \(I\) would look like for the dataset in the introduction (Table I). The columns with headings \(I_1\) and \(I_2\) show the first and second columns of the matrix \(I\).

| n.views | n.actions | url     | ad.id | \( I_1 \) | \( I_2 \) |
|---------|-----------|---------|-------|---------|---------|
| 52      | 4         | abc.com | 83473 | 1       | 1       |
| 73      | 5         | xyz.edu | 40983 | 2       | 2       |
| 19      | 0         | abc.com | 4658  | 1       | 3       |
| 532     | 16        | efg.com | 40983 | 4       | 2       |
| 3       | 0         | z.com   | 4658  | 5       | 3       |
| ...     | ...       | ...     | ...   | ...     |         |

Next we will define \(B_{kt} := \exp(b_{t+Tk-1})\). \(B\) is a ragged array rather than a matrix because the length \(\{B_{kt}\}_t \in \mathbb{R}^{L_k}\) can depend on the family index \(k\). As a shorthand we will simply write \(B_k := \{B_{kt}\}_t\) for the vector of random effects associated with the \(k\)'th family.

This representation is not just notationally convenient – it is also how we represent \(Z\) and \(b\) in our optimized implementation of the algorithm. Next we define three operations in terms of componentwise vector products/divisions, and these operations represent the bulk of the computation in large datasets. These operations are used to compute the sufficient statistics which appear in our Gibbs sampling steps.

\[
\text{Predict}(B, \beta) := \beta D \prod_{f=1}^F B_f[I] \in \mathbb{R}^n
\]
(8)

\[
\text{Predict}_k(B, \beta) := \text{Predict}(B, \beta)/B_k[I] \in \mathbb{R}^n
\]
(9)

\[
\text{SumBy}_k(V) := \{ \sum_{j : I_{(j,k)} = i} V_j \}_{i=1}^{L_k} \in \mathbb{R}^{L_k}, V \in \mathbb{R}^n
\]
(10)

where \(B_k[I] := \{B_{k,I_{(j,k)}}\}_{j=1}^{n} \in \mathbb{R}^n\). If we partitioned the columns of \(Z\) by family \(Z = [Z^{(1)} Z^{(2)} \ldots Z^{(F)}]\) then another way to define \(B_k[I]\) would simply be the matrix-
vector product $Z^{(k)} B_k$. In (10) we use a negative subscript 
$\neg k$ to remind the reader that the prediction is based on all but the $k’$th random effect family.

Our data distribution can be rewritten concisely in terms of $\text{Predict}()$:

$$\{Y|D, B, \beta, Z\} \sim \text{Poisson}(\text{Predict}(B, \beta)) \quad (11)$$

recalling that $I$ is just a different representation of the matrix $Z$.

To update $B_k$ we will perform two computations:

$$\text{events} := \text{SumBy}_k(Y) \in \mathbb{N}^{L_k} \quad (12)$$

$$\text{pevents} := \text{SumBy}_k(\text{Predict}_{\neg k}(B, \beta)) \in \mathbb{R}^{L_k} \quad (13)$$

“SumBy” can be computed in $O(n)$ time, and we will show that although the cost of “$\text{Predict}$” is $O(nF)$, this can be reduced through amortization.

Our blocked Gibbs sampling update for the $k’$th family is then:

$$\sigma_k \sim P(\sigma_k|Y, D, B_{\neg k}, \sigma_{\neg k}, \beta) \quad \text{(integrating out } B_k) \quad (14)$$

$$B_k \sim P(B_k|Y, D, B_{\neg k}, \sigma, \beta) \quad \text{(conditioning on } \sigma_k) \quad (15)$$

This two stage process produces a sample from the joint posterior:

$$(B_k, \sigma_k) \sim P(B_k, \sigma_k|Y, D, B_{\neg k}, \sigma_{\neg k}, \beta)$$

Due to conditional independence this update is independent of $\sigma_{\neg k}$

$$(B_k, \sigma_k) \sim P(B_k, \sigma_k|Y, D, B_{\neg k}, \beta)$$

It is important to note that the conditional distributions will only depend on $2L_k$ sufficient statistics: events $\in \mathbb{N}^{L_k}$ and pevents $\in \mathbb{R}^{L_k}$. This is also true for the Gaussian regression described in section 3.3.

A second point worth noting is that we need not precisely sample the variance parameter in equation (14); to maintain the correct stationary distribution it is sufficient to use Metropolis-Hastings [15].

Earlier we mentioned that it was possible to speed up the computation of the $\text{Predict}$ functions defined above, and we describe this now. Suppose that $\Pi^{\text{old}} := \text{Predict}(B, \beta)$ was computed before sampling $(B_k, \sigma_k)$. Once we have drawn a new value $B_k^{\text{new}}$ we can update:

$$\Pi^{\text{new}} := \Pi^{\text{old}} \frac{B_k^{\text{new}}}{B_k^{\text{old}}} \in \mathbb{R}^n \quad \text{(componentwise multiplication/division)}$$

The un-amortized cost of the $\text{Predict}_{\neg k}(B, \beta)$ operations would be $O(nF^2)$ for a single scan over all $F$ families. In practice we compute $\text{Predict}(B, \beta)$ using equation (8) at the beginning of each scan to reduce the cost by a factor of $F$. Due to accumulation of numerical errors we cannot refresh once per scan for arbitrarily large

\footnote{This simplification does not occur for logistic models ($P(Y_k = 1) = (1 + \exp(-\theta))^{-1}$) or truncated Gaussian regressions which are used in a latent-variable representation of binary probit regressions [3].}
we have observed no practical consequences when applying this to models with $F$ in the hundreds.

If we let $\Pi \equiv \text{Predict}_{-k}(B, \beta)$ then data log likelihood for rows $j$ with index $I_{jk} = t$ is:

$$
\ell_t(B_{kt}) := \sum_{j: I(j, k) = t} (-B_{kt} \Pi_j + Y_j \log(B_{kt} \Pi_j) - \log(Y_j!))
$$

$$
= -\text{pevents}_t B_{kt} + \text{events}_t \log(B_{kt}) + c(t, Y, \Pi)
$$

where $c(t, Y, \Pi) := \sum_{j: I(j, k) = t} (Y_j \log \Pi_j - \log(Y_j!))$

The prior likelihood on $B_{kt}$ is

$$
P(B_{kt} = u \mid \sigma_k) = d\text{gamma}(u, \sigma_k^{-2}, \sigma_k^{-2})
$$

where $d\text{gamma}(x, \theta, \eta) := \frac{\Gamma(\theta, \eta)}{\Gamma(\theta)} x^{\theta-1} \exp(-\eta x)$

and $C_\Gamma(\theta, \eta) := \frac{\eta^\theta}{\Gamma(\theta)}$

Because the prior on $B_{kt}$ is a product of independent Gamma distributions, each element of $(B_{kt}, \{Y_j : I(j, k) = t\})_t$ is independent after conditioning on $(D, B_{-k}, \sigma_k, \beta)$. This conditional independence is used to simplify some high dimensional integrals into products of one-dimensional integrals in the formulas below.

Using this conditional independence we compute the marginal data likelihood after integrating out $B_{kt}$:

$$
P(Y \mid D, B_{-k}, \sigma_k) = \int \prod_t P(B_{kt} = u \mid \sigma_k) \exp(\ell_t(u)) du_1 ... du_{L_k}
$$

(16)

$$
= \prod_t \int P(B_{kt} = u \mid \sigma_k) \exp(\ell_t(u)) du
$$

(17)

$$
= \prod_t \exp(c(t, Y, \Pi)) \frac{C_\Gamma(\sigma_k^{-2}, \sigma_k^{-2})}{C_\Gamma(\sigma_k^{-2} + \text{events}_t, \sigma_k^{-2} + \text{pevents}_t)}
$$

(18)

In the equation above we did not condition on the other prior parameters, $\sigma_{-k}$, or integrate them out because $Y$ is independent of $\sigma_{-k}$ after conditioning on $B_{-k}$. For use in subsequent pseudocode we define the function $\text{PriorMarginal}()$ as

$$
\text{PriorMarginal}(\sigma_k, \text{events}, \text{pevents}) := \prod_t \frac{C_\Gamma(\sigma_k^{-2}, \sigma_k^{-2})}{C_\Gamma(\sigma_k^{-2} + \text{events}_t, \sigma_k^{-2} + \text{pevents}_t)}
$$

(19)

To sample $\sigma_k$ we take the product of the marginal data likelihood and the prior on $\sigma_k$

$$
P(Y, \sigma_k \mid D, B_{-k}) = P(Y \mid D, B_{-k}, \sigma_k) P(\sigma_k)
$$

which is proportional to the posterior $P(\sigma_k \mid Y, D, B_{-k})$ (as a function of $\sigma_k$). We assume a flat, improper prior $P(\sigma_k) \equiv 1$ because we have no preferred choice.
We do not bother to compute $\prod_t \exp(c(t, Y, \Pi))$ since we must renormalize or use Metropolis-Hastings anyway. The result is that we need only compute the aggregate statistics ‘events’ and ‘pevents’ to find $P(\sigma_k | Y, D, B_{-k})$.

Once $\sigma_k$ is drawn, the posterior distribution of $B_k$ is simply a product of Gamma distributions:

$$P(B_k | \sigma_k, Y, D, B_{-k}) = \prod_{t=1}^{L_k} \text{dgamma}(B_{kt}, (\text{events}_t + \sigma_k^{-2}), (\text{pevents}_t + \sigma_k^{-2}))$$

Finally, we discuss the update for the fixed effect parameter $\beta$. The fixed effect $\beta$ can be updated through a Monte Carlo EM algorithm, but for simplicity in the pseudocode we just put a $\text{Gamma}(1, 1)$ prior on $\beta$ and update it like the other random effects. We expect little difference in behavior when applied to large datasets.

The pseudocode in algorithm (1) summarizes the blocked Gibbs sampling algorithm described above. As mentioned earlier, step [10] in the algorithm could be a single Metropolis-Hastings update. The “griddy Gibbs sampler” updates described in [14] are another option. Finally, in subsequent pseudocode we write just “Sample $B_{new}^f \sim P(B_f | B_{-f}, Y, D, \beta, \sigma)$” in place of the for-loop on lines [11][13].

Algorithm 1 Gamma-Poisson Gibbs Sampling algorithm

1: initialize $B, \beta, \sigma$
2: for iter = 1, 2, ... do
3: $\Pi \leftarrow \text{Predict}(B, \beta)$
4: Sample $\beta_{new} \sim \text{dgamma}(\beta, 1 + \sum_j Y_j, 1 + \beta^{-1} \sum_j \Pi_j)$
5: $\Pi \leftarrow \Pi \beta_{new}/\beta$
6: $\beta \leftarrow \beta_{new}$ ▷ Update $\Pi$ for use in the next sampling step
7: for $f = 1, 2, ..., F$ do
8: events $\leftarrow \text{SumBy}_f(Y)$ ▷ For each feature family
9: pevents $\leftarrow \text{SumBy}_f(\Pi/B_f[I])$
10: Sample $\sigma_f$ from $\text{PriorMarginal}(\sigma_f, \text{events}, \text{pevents})$
11: for $t = 1, 2, ..., L_f$ do ▷ Sample $B_{new}^f \sim P(B_f | B_{-f}, Y, D, \beta, \sigma)$
12: $B_{new}^f \sim \text{dgamma}(\text{events}_t + \sigma_f^{-2}, \text{pevents}_t + \sigma_f^{-2})$
13: end for
14: $\Pi \leftarrow \Pi B_{new}^f[I]$ ▷ Update $\Pi$ for use in the next sampling step
15: $B_f \leftarrow B_{new}^f$
16: end for
17: end for

3 Extensions

In this section we discuss extensions which remain as scalable as the Gamma-Poisson regression described in the previous section.
3.1 Handling A More General Z Matrix

Suppose the matrix $Z$ from the introduction can be partitioned into two sets of columns $Z = [Z^{(1)} | Z^{(2)}]$ and that $Z^{(1)}$ is structured as we required for algorithm 1. If on the other hand $Z^{(2)}$ is not structured this way, then clearly we can use the algorithm 1 to update the random effects and priors associated with $Z^{(1)}$ and use more general updates for $Z^{(2)}$.

We take a moment to discuss one seemingly straightforward extension that turns out to not be as scalable in the Poisson model. Suppose the elements of $Z$ were not 0-1 but still had the sparsity pattern $\sum_{t \in J_k} \{Z_{it} \neq 0\} = 1$. We can represent the information in $Z$ compactly using two $n \times F$ matrices $I$ and $S$. While the index map $I$ stores the sparsity pattern, the additional matrix $S$ stores the non-zero values of $Z$ (i.e. $S_{jk}$ is equal to the $(j, T_{k-1} + I_{jk})$th element of $Z$ (recall the definition of $T_k$ in section 1 was $\sum_{j=1}^{k} L_k$).

In this more general model we would modify $\text{Predict}$ to instead be:

$$\text{ScaledPredict}(B, \beta) := \beta D \prod_{f=1}^{F} B_f[I]^{S_f} \in \mathbb{R}^n \quad (20)$$

where $S_f = \{S_{jf}\}_{j=1}^{n}$ is the $f$th column of $S$ and the exponentiation $B_f[I]^{S_f}$ is taken componentwise.

Under this generalization the vectors ‘events’ and ‘pevents’ are no longer the sufficient statistics for the conditional distribution of $(B_k, \sigma_k)$. We must instead aggregate by unique values of $(S_{jk}, I_{jk})$ rather than of $I_{jk}$.

Unless $S_f$ takes on few unique values, the vector of sufficient statistics can be as long as $2n$ elements. Another important difference is that the conditional distributions of the elements of $B_f$ will no longer have a Gamma distribution.

3.2 More Flexible Prior Distributions

In order to efficiently implement our blocked Gibbs sampler it is important that we can compute the marginal data likelihood $\int P(B_{kt} = u | \sigma_k) \exp(\ell_t(u)) du$ in closed form. This is possible because the Gamma distribution is a conjugate prior for the Poisson distribution.

We still have considerable flexibility because these integrals can be evaluated analytically for mixtures of discrete and Gamma distributions as well:

$$P(B_{kt} \in A) = \sum_{j=1}^{d} w_j^k 1\{\text{loc}_j^k \in A\} + \sum_{j=d+1}^{d+g} w_j^k \int_A d\text{gamma}(x, \frac{2}{\sigma_{kj}}, \frac{2}{\sigma_{kj}}) dx$$

where $\text{loc}_j^k \in \mathbb{R}_{\geq 0}, \sigma_{kj} \in \mathbb{R}_{>0}, \sum_j w_j^k = 1$

A common special case would be a sparse prior:

$$P(B_{kt} \in A) = w^k 1\{1.0 \in A\} + (1 - w^k) \int_A d\text{gamma}(x, \frac{2}{\sigma^2_k}, \frac{2}{\sigma^2_k}) dx$$
This is referred to as a “spike and slab” or “spike and bell” prior [7, 9].

Sampling from the two-dimensional conditional distribution of \((w^k, \lambda_k)\) may require more care to implement, but the likelihood is still a function of \(2L_k\) statistics.

3.3 Gaussian Regression Models

When defining the Gaussian model, we will refer to the matrix \(S\) defined in equation (20). In that section we pointed out that handling a more general \(Z\) matrix came at significant computational cost in the Poisson model; however, in the Gaussian model this is not the case. The updates are equally simple after lifting the 0-1 restriction on the entries of \(Z\). Again we consider the case with sparsity pattern \(\sum_{t \in J_k} \mathbb{1}\{Z_{it} \neq 0\} = 1\) for \(k = 1, 2, ..., F\).

The \texttt{Predict} functions are similar to those defined for the Poisson model:

\[
\text{GaussPredict}(B, \beta) := \beta + \sum_{f=1}^{F} B_f[I]S_f \in \mathbb{R}^n \tag{21}
\]

\[
\text{GaussPredict}_{-k}(B, \beta) := \beta + \sum_{f \neq k} B_f[I]S_f \in \mathbb{R}^n \tag{22}
\]

where \(B_f[I]S_f\) is a componentwise product. Our model of the data is now:

\[
Y \sim N(\text{GaussPredict}(B, \beta), D^{-1}) \tag{23}
\]

where \(D\) now serves as an residual inverse-variance rather than an offset in the regression. We do not develop the sampling steps needed to infer the residual variance in this report.

We next define the sufficient statistics for the Gibbs sampling steps:

\[
\text{invvar} := \text{SumBy}_k(S^2_kD) \in \mathbb{R}^{L_k} \tag{24}
\]

\[
\text{error} := \text{SumBy}_k((Y - \text{GaussPredict}_{-k}(B, \beta))S_kD) \in \mathbb{R}^{L_k} \tag{25}
\]

All operations are taken to be componentwise – including the squared term \(S^2_k\) in equation (24).

As in the Poisson model we will compute the data log likelihood associated with each level of the random effect:

\[
\ell_t(B_{kt}) := -(1/2) \sum_{j: I(j,k)=t} \left( (Y_j - \Pi_j - S_{jk}B_{kt})^2D_j + \log(2\pi/D_j) \right)
\]

\[
= -(1/2)\text{invvar}_tB^2_{kt} + \text{error}_tB_{kt} + c(t, Y, \Pi)
\]

where \(c(t, Y, \Pi) := -(1/2) \sum_{j: I(j,k)=t} \left( (Y_j - \Pi_j)^2D_j + \log(2\pi/D_j) \right)\)

We place a \(N(0, \sigma^2_k)\) prior on \(B_{kt}\), and, as in equation (16), we will integrate over
the random effects:

\[ P(Y|D, B_{-k}, \sigma_k) = \int \prod_t P(B_{kt} = u_t|\sigma_k) \exp(\ell_t(u_t)) du_1...du_{L_k} \]

\[ = \prod_t \int P(B_{kt} = u|\sigma_k) \exp(\ell_t(u)) du \]

\[ = \prod_t \exp(c(t, Y, \Pi)) \left( \frac{\sigma^{-2}_k}{\text{invvar}_t + \sigma^{-2}_k} \right)^{1/2} \exp \left( \frac{1}{2} \frac{\text{error}_t^2}{\text{invvar}_t + \sigma^{-2}_k} \right) \]

We did not condition on \( \sigma_{-k} \) or integrate it out because \( Y \) is independent of \( \sigma_{-k} \) after conditioning on \( B_{-k} \). For the purpose of pseudocode we will define:

\[
\text{GaussPriorMarginal}(\sigma_k, \text{error}, \text{invvar}) := \prod_t \left( \frac{\sigma^{-2}_k}{\text{invvar}_t + \sigma^{-2}_k} \right)^{1/2} \exp \left( \frac{1}{2} \frac{\text{error}_t^2}{\text{invvar}_t + \sigma^{-2}_k} \right)
\]

This unnormalized likelihood is sufficient to update \( \sigma_k \) and can be computed from \( 2L_k \) sufficient statistics. Once \( \sigma_k \) is drawn, the random effects can be drawn from their Gaussian posterior distributions:

\[ P(B_k|Y, D, B_{-k}, \sigma_k) = \prod_{t=1}^{L_k} \text{dnorm} \left( B_{kt}, \frac{\text{error}_t}{\text{invvar}_t + \sigma^{-2}_k} \left( \text{invvar}_t + \sigma^{-2}_k \right)^{-1/2} \right) \]

where \( \text{dnorm}(x, \mu, s) \) is the normal density with mean \( \mu \) and variance \( s^2 \). Pseudocode for the Gaussian model is given in algorithm 2.

Finally we should note that the computational complexity of the updates (in terms of \( n \) and \( L_k \)) is unchanged if we generalize to say \( S_{jk}, B_{kt} \in \mathbb{R}^2 \) and let \( \sigma^2_k \) denote a \( 2 \times 2 \) covariance matrix. The update for \( \sigma_k \) would depend on a vector of \( 3L_k \) sufficient statistics rather than a vector of length \( 2L_k \), and the sampling step for each \( B_{kt} \) would be to draw from a bivariate rather than a univariate normal distribution.

### 3.4 Monte Carlo Expectation Maximization (MCEM) algorithm

We briefly describe the EM algorithm and discuss the similarities with the Gibbs sampling algorithm. Our approach is similar to that in [2] except that we integrate out some random effects - paralleling the prior updates we carried out in the full Bayesian approach described above.

The vanilla MCEM algorithm would generate samples \( B_1^T, ..., B^T \) by Gibbs sampling only the random effects while leaving the prior variance parameters \( \sigma \) fixed. The M-step then decomposes into independent one-dimensional optimizations which can be performed in parallel:

\[
\sigma_k := \arg\max_s \sum_{i=1}^{T} \sum_{t=1}^{L_k} \log (c\text{gamma}(B_{kt}^i, s^{-2}, s^{-2}))
\]
Algorithm 2 Gaussian Gibbs Sampling algorithm

1: initialize $B$, $\beta$, $\sigma$
2: for $\text{iter} = 1, 2, \ldots$ do
3: $\Pi \leftarrow \text{GaussPredict}(B, \beta)$
4: Sample $\beta^{\text{new}}$ $\triangleright$ Details omitted
5: $\Pi \leftarrow \Pi + \beta^{\text{new}} - \beta$ $\triangleright$ Update $\Pi$ for use in the next sampling step
6: for $f = 1, 2, \ldots, F$ do $\triangleright$ For each feature family
7: invvar $\leftarrow \text{SumBy}_f(S_f^2 D)$
8: error $\leftarrow \text{SumBy}_f((Y - \Pi + B_f[I]S_f)S_f D)$
9: Sample $\sigma_f$ from GaussPriorMarginal($\sigma_f$, error, invvar)
10: for $t = 1, 2, \ldots, L_f$ do $\triangleright$ Sample $B_{ft}^{\text{new}} \sim P(B_f | B_{-f}, Y, D, \beta, \sigma)$
11: Sample $B_{ft}^{\text{new}} \sim \text{dnorm} \left( B_{ft}, \frac{\text{error}}{\text{invvar} + \sigma_f^{-2}}, (\text{invvar} + \sigma_f^{-2})^{-1/2} \right)$
12: $\Pi \leftarrow \Pi + \left( B_{ft}^{\text{new}}[I] - B_f[I] \right) S_f$
13: $B_f \leftarrow B_f^{\text{new}}$
14: end for
15: end for
16: end for
17: end for

In practice this seems to converge much more slowly than the blocked Gibbs sampler we developed in section 2. The vanilla MCEM algorithm behaves like the unblocked Gibbs sampler which updates $\sigma_k$ conditional on $B_k$ rather than integrating over $B_k$.

At this point we depart from the description in [2] and change the update to mimic the blocked Gibbs sampler. We instead suggest updating just a single $\sigma_k$ at a time and remove $B_k$ from the complete data log likelihood (i.e. integrate over it). The update requires a sample of $B_{-k}$ from its marginal posterior, but sampling the complete random effect vector $B$ (including $B_k$) is an easy way to generate this. Algorithm 3 lists pseudocode which omits the maximum likelihood update for $\beta$.

Algorithm 4 reduces the number of sampling steps in algorithm 3 as a tradeoff between accuracy and efficiency. It may be surprising, but we have found in practice that algorithm 4 works well when both $n$ and $L_k$ are large; however, when the number of levels $L_k$ is small, we have seen that a single sample iteration is not sufficient. In those cases there is little additional cost in taking a fully Bayesian approach and sampling $\sigma_k$ from its posterior as well.

4 Discussion

First we should address what we mean by “scalable”. On a single workstation we have applied these algorithms on data sets with $n$ around 100 million, $F$ in the tens, and $L_k$ less than one million for each family.

The computational complexity of each update is $O(nF + L_k)$ i.e. linear in the number of input records and linear in the number of levels of the random effect. For
Algorithm 3 Gamma-Poisson MCEM algorithm

1: initialize $B$, $\beta$, $\sigma$
2: for iter = 1, 2, ... do
3:   for $k = 1, 2, ..., F$ do
4:     for $s = 1, 2, ..., T$ do
5:       $\Pi \leftarrow \text{Predict}(B, \beta)$
6:       for $f = 1, 2, ..., F$ do
7:         Sample $B_f^{\text{new}} \sim P(B_f|B_{-f}, Y, D, \beta, \sigma_f)$
8:         $\Pi \leftarrow \Pi \frac{B_f^{\text{new}}[i]}{B_f[i]}$
9:         $B_f \leftarrow B_f^{\text{new}}$
10:     end for
11:     $\text{pevents}(s) \leftarrow \text{SumBy}_k(\Pi / B_k[I])$
12:     end for
13:     $\text{events} \leftarrow \text{SumBy}_k(Y)$
14:     $\sigma_k \leftarrow \arg\max_v \sum_{s=1}^T \log \text{PriorMarginal}(v, \text{events}, \text{pevents}(s))$
15:     Sample $B_{-k}^{\text{new}} \sim P(B_{-k}|B_k, Y, D, \beta, \sigma_k)$
16:     $\Pi \leftarrow I \frac{B_{-k}^{\text{new}}[i]}{B_{-k}[i]}$
17:     $B_k \leftarrow B_{-k}^{\text{new}}$
18:     end for
19:     $\beta \leftarrow \beta \sum_j Y_j / \sum_j \Pi_j$
20: end for

Algorithm 4 Minimal Gamma-Poisson MCEM algorithm

1: initialize $B$, $\beta$, $\sigma$
2: for iter = 1, 2, ... do
3:   $\Pi \leftarrow \text{Predict}(B, \beta)$
4:   for $k = 1, 2, ..., F$ do
5:     $\text{pevents} \leftarrow \text{SumBy}_k(\Pi / B_k[I])$
6:     $\text{events} \leftarrow \text{SumBy}_k(Y)$
7:     $\sigma_k \leftarrow \arg\max_v \sum_{s=1}^T \log \text{PriorMarginal}(v, \text{events}, \text{pevents}(s))$
8:     Sample $B_k^{\text{new}} \sim P(B_k|B_{-k}, Y, D, \beta, \sigma_k)$
9:     $\Pi \leftarrow I \frac{B_k^{\text{new}}[i]}{B_k[i]}$
10:    $B_k \leftarrow B_k^{\text{new}}$
11: end for
12: $\beta \leftarrow \beta \sum_j Y_j / \sum_j \Pi_j$
an entire sequential scan it would be $O(nF^2 + r)$, recalling that $r = \sum_k L_k$ the total number of random effects and $F$ is the number of random effect families. Through the amortization described in section 2 we can effectively reduce the cost by a factor of $F$ to $O(nF^2 \min(F, M)^{-1} + r)$ where experimentally we have found that we can take $M > 100$.

The “Consensus Bayes” framework is another scalable approach to Bayesian hierarchical modeling \cite{10, 13}. We believe that it is possible to develop consensus versions of the models presented above, but we have not pursued this yet. However, the computations described above lend themselves to parallelized implementations even without the use of Consensus Bayes techniques.

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