MCMC for GLMMs

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Abstract

Generalized linear mixed models (GLMMs) are often used for analyzing correlated non-Gaussian data. The likelihood function in a GLMM is available only as a high dimensional integral, and thus closed-form inference and prediction are not possible for GLMMs. Since the likelihood is not available in a closed-form, the associated posterior densities in Bayesian GLMMs are also intractable. Generally, Markov chain Monte Carlo (MCMC) algorithms are used for conditional simulation in GLMMs and exploring these posterior densities. In this article, we present different state of the art MCMC algorithms for fitting GLMMs. These MCMC algorithms include efficient data augmentation strategies, as well as diffusions based and Hamiltonian dynamics based methods. The Langevin and Hamiltonian Monte Carlo methods presented here are applicable to any GLMMs, and are illustrated using three most popular GLMMs, namely, the logistic and probit GLMMs for binomial data and the Poisson-log GLMM for count data. We also present efficient data augmentation algorithms for probit and logistic GLMMs. Some of these algorithms are compared using a numerical example.

Key words: Bayesian GLMM; Data augmentation; EM; GLM; Hamiltonian Monte Carlo; MALA; Metropolis-Hastings; Mixed models; Monte Carlo maximum likelihood; spatial GLMM

1 Introduction

Generalized linear mixed models (GLMMs) are a natural extension of both the linear mixed models and the generalized linear models (GLMs). GLMMs allow for non-Gaussian responses and the random effects in the GLMMs can accommodate overdispersion often
present in non-Gaussian data, as well as dependence among correlated observations arising from longitudinal or repeated measures studies. GLMM is one of the most frequently used statistical models (Jiang and Nguyen, 2007).

Unlike the linear mixed models and the GLMs, the likelihood function for the GLMM is not available in a closed-form. Since the likelihood function for the GLMM is obtained by integrating a GLM likelihood with respect to the distribution of the random effects, it is available only as a high-dimensional integral. Both analytical and Monte Carlo approximations for the GLMM likelihood have been proposed in the literature. For example, Breslow and Clayton (1993) considered the Laplace’s method, and Wolfinger and O’connell (1993) used a Taylor expansion for the integral approximation. Implementations involving Markov chain Monte Carlo (MCMC) methods include Zeger and Karim (1991) who used Gibbs sampling and McCulloch (1997) who used Metropolis-Hastings (MH) algorithm for making inference in GLMMs. Use of sampling-based methods in GLMMs can be found in McCulloch (1994); Gamerman (1997); Booth and Hobert (1999) among others.

Over the last two decades, extensive efforts have gone into producing efficient, fast mixing MCMC algorithms, in general, and in the context of GLMMs, in particular. For example, effective data augmentation (DA) strategies have been proposed for specific GLMMs (see e.g. Wang and Roy, 2018b; Polson et al., 2013; Wang and Roy, 2018a; Rao and Roy, 2021). Also novel MH algorithms based on Langevin diffusions and Hamiltonian dynamics such as the Metropolis adjusted Langevin algorithms (MALA) (Roberts and Tweedie, 1996) and the Hamiltonian Monte Carlo (HMC) algorithms (Neal, 2011) have now emerged as the popular methods for MCMC sampling due to their ability to make distant moves with high acceptance probability and favorable scalability with respect to increasing state space dimensions. MALA and HMC have also been applied for inference for GLMMs (see e.g. Roy and Zhang, 2021; Bürkner, 2017). The goal of this article is to present these efficient MCMC algorithms for fitting GLMMs.

The rest of the article is organized as follows. In Section 2 we present the likelihood function for GLMMs and describe two sampling-based approaches, namely the Monte Carlo EM and the Monte Carlo maximum likelihood methods for approximating this likelihood function. In Section 3 we construct different MCMC algorithms for conditional simulation in GLMMs. Thus, these algorithms can be used for sampling-based inference in GLMMs. Several popular GLMMs are used to illustrate these algorithms. Next, Section 4 presents MCMC algorithms for Bayesian GLMMs under popular priors on the fixed
effects and the variance components parameters. Section 5 contains comparisons of some of these MCMC algorithms using a publicly available dataset. Some concluding remarks are provided in Section 6.

2 Likelihood function for GLMMs

Let \( Y = (Y_1, \ldots, Y_m)^\top \) denote the vector of response variables. Let \( x_i \) and \( z_i \) be the \( p \times 1 \) and \( q \times 1 \) vectors of fixed and random effects covariates associated with the \( i \)th response, respectively, \( i = 1, \ldots, m \). Let \( \beta \in \mathbb{R}^p \) be the regression coefficients vector and \( u \in \mathbb{R}^q \) be the random effects vector. A GLMM can be built with a link function \( g \) that connects \( \mu_i \), the (conditional) expectation of \( Y_i \), with the covariates \( x_i, z_i \) satisfying \( g(\mu_i) = x_i^\top \beta + z_i^\top u \), and assuming that conditional on the random effects \( u \), the responses \( Y_i \)’s are independent with

\[
Y_i \mid \beta, u \sim f(y_i | \beta, u) \equiv \exp \left\{ \frac{y_i \xi_i - b(\xi_i)}{a_i(\iota)} + c_i(y_i, \iota) \right\} \quad \text{for } i = 1, \ldots, m, \tag{1}
\]

where \( \iota \) is the dispersion parameter and \( a_i(\cdot), b(\cdot), c_i(\cdot, \cdot) \) are known functions. To simplify the presentation, here we assume that \( \iota \) is known. The quantity \( \xi_i \) is associated with the conditional mean \( \mu_i \) and hence with \( \beta, u \). The description of a GLMM is completed by specifying the distribution of \( u \) and the exponential family pdf (1) with the forms of the functions \( a_i(\cdot), b(\cdot), c_i(\cdot, \cdot) \). Assume there are \( r \) random effects \( u_1^\top, u_2^\top, \ldots, u_r^\top \), where \( u_j \) is a \( q_j \times 1 \) vector with \( q_j > 0 \), with \( q_1 + q_2 + \ldots + q_r = q \) and \( u = (u_1^\top, \ldots, u_r^\top)^\top \). A common assumption is that \( u_j \overset{\text{ind}}{\sim} N(0, \Lambda_j \otimes R_j) \) where the low-dimensional covariance matrix \( \Lambda_j \) is unknown and need to be estimated, and the structured matrix \( R_j \) is usually known. Here, \( \otimes \) indicates the Kronecker product. Let \( y = (y_1, y_2, \ldots, y_m) \) denote the vector of observed responses. For specific examples of (1) and the link function \( g(\cdot) \), we consider the three most popular GLMMs, namely the logistic GLMM, the probit GLMM and the Poisson GLMM with the log link.

Example 1 (Logistic GLMM). For the logistic GLMM, (1) is the binomial pmf given by

\[
\binom{\ell_i}{y_i} (\mu_i / \ell_i)^{y_i} (1 - \mu_i / \ell_i)^{\ell_i - y_i}, \quad y_i = 0, 1, \ldots, \ell_i, \tag{2}
\]

where \( \ell_i \) is a positive integer indicating the number of trials. The logistic GLMM uses the logit link \( g(\mu_i) = \log(\mu_i / [\ell_i - \mu_i]) = x_i^\top \beta + z_i^\top u \).
Example 2 (Probit GLMM). In this case, (1) is also the binomial pmf (2) whereas, the probit link \( g(\mu_i) = \Phi^{-1}(\mu_i/\ell_i) = x_i^T \beta + z_i^T u \) is used in the probit GLMM. Here, \( \Phi(\cdot) \) is the cdf of the standard normal distribution.

Example 3 (Poisson-log GLMM). For the Poisson-log link model, (1) is the Poisson pmf given by
\[
\exp(-\mu_i)\mu_i^{y_i}/y_i!, \quad y_i = 0, 1, \ldots
\]
with \( g(\mu_i) = \log(\mu_i) = x_i^T \beta + z_i^T u \).

Let \( \Lambda = (\Lambda_1, \ldots, \Lambda_r) \). Then the likelihood function for \((\beta, \Lambda)\) is given by
\[
L(\beta, \Lambda \mid y) = \int_{R^q} \left[ \prod_{i=1}^m f(y_i \mid \beta, u) \right] \phi_q(u; 0, G) du. \tag{4}
\]
Here, \( \phi_q(u; 0, D) \) denotes the probability density function of the \( q \)-dimensional normal distribution with mean vector 0, covariance matrix \( D \), evaluated at \( u \). Also, \( G = \oplus_{j=1}^r \Lambda_j \otimes R_j \), with \( \oplus \) indicating the direct sum. Outside the linear mixed model where (1) is the normal density, \( L(\beta, \Lambda \mid y) \) in (4) nearly always involves intractable integrals and is not available in closed-form.

There are two widely used Monte Carlo approaches for approximating the likelihood function (4) and making inference on \((\beta, \Lambda)\), namely the Monte Carlo EM algorithm (Booth and Hobert, 1999) and the Monte Carlo maximum likelihood based on importance sampling (Geyer and Thompson, 1992; Geyer, 1994). The EM is an iterative method and each iteration of this algorithm consists of an ‘E-step’ and an ‘M-step’. The \((j + 1)\)st E-step entails the calculation of
\[
E[\log f(y, u \mid \beta, \Lambda) \mid \beta^{(j)}, \Lambda^{(j)}], \tag{5}
\]
where
\[
f(y, u \mid \beta, \Lambda) = \left[ \prod_{i=1}^m f(y_i \mid \beta, u) \right] \phi_q(u; 0, G) \tag{6}
\]
is the joint density of \((y, u)\) and \((\beta^{(j)}, \Lambda^{(j)})\) is the value of \((\beta, \Lambda)\) from the \(j\)th iteration. The expectation in (5) is with respect to \( f(u \mid y, \beta^{(j)}, \Lambda^{(j)}) \), where \( f(u \mid y, \beta, \Lambda) \) is the conditional density of \( u \) given \( y \)
\[
f(u \mid \beta, \Lambda, y) = \frac{f(y, u \mid \beta, \Lambda)}{L(\beta, \Lambda \mid y)}, \tag{7}
\]
with \( f(y, u \mid \beta, \Lambda) \) and \( L(\beta, \Lambda \mid y) \) given in (6) and (4), respectively. Since closed-form expressions of (4) and hence (7) are not available, so are the means (5) with respect to the
conditional density (7). In the Monte Carlo EM algorithm (Wei and Tanner, 1990), (5) is approximated by a Monte Carlo estimate which is then maximized in the M-step. Indeed, if \( \{u^{(n,j)}, n = 1, \ldots, N\} \) are samples obtained by running a Markov chain with invariant density \( f(u^{(j)}, \Lambda^{(j)}, y) \), then a Monte Carlo estimate of (5) is \( \sum_{n=1}^{N} \log[f(y, u^{(n,j)}|\beta, \Lambda)]/N \) (McCulloch, 1994).

In the Monte Carlo maximum likelihood (Geyer and Thompson, 1992; Geyer, 1994), the likelihood function (4) is expressed as

\[
L(\beta, \Lambda|y) = \int_{\mathbb{R}^s} f(y, u|\beta, \Lambda)du = \int_{\mathbb{R}^s} \frac{f(y, u|\beta, \Lambda)}{f(y, u|\beta^{(0)}, \Lambda^{(0)})} f(y, u|\beta^{(0)}, \Lambda^{(0)})du \propto E\left[\frac{f(y, u|\beta, \Lambda)}{f(y, u|\beta^{(0)}, \Lambda^{(0)})}\right],
\]

where the expectation is with respect to the density (7) at some value \((\beta^{(0)}, \Lambda^{(0)})\). Since the expectation in (8) can be approximated by \((1/N) \sum_{n=1}^{N} f(y, u^{(n,0)}|\beta, \Lambda)/f(y, u^{(n,0)}|\beta^{(0)}, \Lambda^{(0)})\), maximum likelihood estimates of \((\beta, \Lambda)\) are calculated by maximizing this Monte Carlo approximation. Geyer (1994) recommends making a few pilot iterations to find an appropriate value for \((\beta^{(0)}, \Lambda^{(0)})\). The importance sampling technique has been successfully used for analyzing spatial generalized linear mixed models (SGLMMs) which are GLMMs with the random effects \(u\) being derived from a spatial process (see e.g. Christensen, 2004; Roy et al., 2016, 2018; Evangelou and Roy, 2019).

### 3 Conditional simulation for GLMMs

Both the Monte Carlo EM and the Monte Carlo maximum likelihood methods for making inference on \((\beta, \Lambda)\) requires effective methods for sampling from the density \( f(u|y, \beta, \Lambda) \) given in (7). To simplify notations, we use \( f(u|y) \) to denote this conditional density. In the context of some numerical examples involving SGLMMs, Roy and Zhang (2021) observe poor performance of random walk Metropolis compared to some other Metropolis-Hastings algorithms for sampling from (7). In this section, we present different variants of the MALA and HMC methods for exploring (7). We also describe some data augmentation algorithms for the two particular GLMMs, namely the logistic and the probit GLMMs.
3.1 MALA for GLMMs

MCMC methods are based on discrete time Markov chains. For example, as mentioned in Section 2, both Monte Carlo EM and Monte Carlo maximum likelihood methods require Markov chains \( \{u^{(n)}\}_{n \geq 1} \) with appropriate stationary densities. However, often, there are great benefits to first considering an appropriate continuous time stochastic process that possesses desirable properties. In particular, one can specify these continuous time processes by some differential equations as illustrated in this Section as well as in Section 3.2. For example, MALA is a discrete time Markov chain based on the Langevin diffusion \( u_t \) defined as

\[
du_t = \frac{1}{2} \nabla \log f(u_t|y) dt + ds_t,
\]

where \( s_t \) is the \( q \)–dimensional standard Brownian motion. It is known that \( f(u|y) \) is stationary for \( u_t \) given in (9). On the other hand, discretizations of (9), say, by using the Euler-Maruyama method may fail to maintain the stationarity with respect to \( f(u|y) \). MALA is an MH chain \( \{u^{(n)}\}_{n \geq 1} \) where, in each iteration, the proposal \( u' \) is drawn following a simple discretization of (9) given by

\[
u' = u^{(n-1)} + \epsilon \nabla \log f(u^{(n-1)}|y)/2 + \sqrt{\epsilon} v^{(n)} \]

for a chosen step-size \( \epsilon \) with \( v^{(n)} \overset{iid}{\sim} N(0, I_q) \). The proposal \( u' \) is accepted with probability

\[
\alpha(u^{(n-1)}, u') = 1 \land \frac{f(u'|y)k(u', u^{(n-1)})}{f(u^{(n-1)}|y)k(u^{(n-1)}, u')}.
\]

where the proposal density \( k(u, u') \) is the \( N(u + \epsilon \nabla \log f(u|y)/2, \epsilon I_q) \) density evaluated at \( u' \). Since the mean of the proposal density of the MALA is governed by the gradient of log of the target distribution, it is likely to make moves in the directions in which \( f \) is increasing. That way, the chain is encouraged to move towards the nearest mode of \( f(u|y) \) and stay near the high mass regions of the target density.

**Algorithm 1** The \( n \)th iteration for the MALA

1: Given \( u^{(n-1)} \) draw \( u' \sim N(u^{(n-1)} + \epsilon \nabla \log f(u^{(n-1)}|y)/2, \epsilon I_q) \).
2: Draw \( \delta \sim \text{Uniform} (0, 1) \). If \( \delta < \alpha(u^{(n-1)}, u') \) then set \( u^{(n)} \leftarrow u' \), else set \( u^{(n)} \leftarrow u^{(n-1)} \). Here, \( \alpha(\cdot, \cdot) \) is as defined in (11).

The MALA chain \( \{u^{(n)}\}_{n \geq 1} \) can be used to approximate (5) or (8). In particular, if \( f(u|\beta^{(j)}, \Lambda^{(j)}, y) \) is used for the stationary density \( f(u|y) \) in (10) then the corresponding
MALA chain can be used for the $j$th E-step in the EM algorithm and when $f(u|y)$ in (10) is replaced with $f(u|\beta(0), \Lambda(0), y)$, it results in a MALA chain that can be used for estimating (13). In practice, the step-size $\epsilon$ is chosen as $O(q^{-1/3})$ obtaining an acceptance rate of between 40% and 70% (Roberts and Rosenthal, 1998). For implementing MALA we need the derivatives of $\log f(u|y)$. Here, we derive $\nabla \log f(u|y)$ for the three popular GLMMs mentioned in Section 4. Let $X$ and $Z$ be the $m \times p$ and $m \times q$ known design matrices with $i$th row being $x_i^T$ and $z_i^T$, $i = 1, \ldots, m$ respectively. Let $\gamma_i = x_i^T \beta + z_i^T u$, $i = 1, \ldots, m$ and $\gamma = X \beta + Zu$.

Example 1 (Continued). For the binomial-logit link model, the log $f(u|y)$ (up to an additive constant) is

$$- \left[ u^T G^{-1} u + \log |G| \right]/2 + \sum_{i=1}^{m} \left[ y_i \gamma_i - \ell_i \log(1 + \exp(\gamma_i)) \right].$$  \hspace{1cm} (12)

Letting $\xi$ be the $m \times 1$ vector with $i$th element $\ell_i \exp(\gamma_i)/(1 + \exp(\gamma_i))$, $i = 1, \ldots, m$, we have

$$\nabla \log f(u|y) = -G^{-1} u + Z^T \xi.$$

Example 2 (Continued). For the binomial-probit model, the log $f(u|y)$ (up to an additive constant) is

$$- \left[ u^T G^{-1} u + \log |G| \right]/2 + \sum_{i=1}^{m} \left[ y_i \log(\Phi(\gamma_i)) + (\ell_i - y_i) \log(1 - \Phi(\gamma_i)) \right].$$  \hspace{1cm} (13)

Let $\tau_1$ and $\tau_2$ be the $m \times 1$ vectors with $i$th element $y_i \phi(\gamma_i)/\Phi(\gamma_i)$ and $[\ell_i - y_i] \phi(\gamma_i)/[1 - \Phi(\gamma_i)]$, respectively, $i = 1, \ldots, m$. Here, $\phi(\cdot) \equiv \phi_1(\cdot)$ is the standard normal pdf. For the probit GLMM we have

$$\nabla \log f(u|y) = -G^{-1} u + Z^T \tau_1 - Z^T \tau_2.$$

Example 3 (Continued). For the Poisson-log GLMM, we derive log $f(u|y)$ which (up to an additive constant) is

$$\log f(u|y) = - \left[ u^T G^{-1} u + \log |G| \right]/2 + \sum_{i=1}^{m} (y_i \gamma_i - \exp\{\gamma_i\}),$$  \hspace{1cm} (14)

implying

$$\nabla \log f(u|y) = -G^{-1} u + Z^T y - Z^T \exp(\gamma).$$
There are other variants of MALA, e.g., the pre-conditioned MALA (Stramer and Roberts, 2007), and the manifold MALA (Girolami and Calderhead, 2011) proposed in the literature. In the pre-conditioned MALA, the proposal density is $N(u + hM \nabla \log f(u|y)/2, hM)$ for some positive definite matrix $M$. For conditional simulation in SGLMMs, Roy and Zhang (2021) observe that the pre-conditioned MALA with an appropriately chosen $M$, and the manifold MALA can have superior performance over the standard MALA.

3.2 HMC for GLMMs

In the HMC algorithm (Duane et al., 1987; Neal, 2011), an auxiliary variable $\rho \sim f(\rho) \equiv N(0, M)$ is introduced for some $q \times q$ positive definite matrix $M$. The HMC chain $\{u^{(n)}, \rho^{(n)}\}_{n \geq 1}$ alternates between draws from $f(\rho^{(n)}|u^{(n-1)}) \equiv f(\rho^{(n)}) \equiv N(0, M)$ and $f(u^{(n)}|\rho^{(n)}, u^{(n-1)})$. We now describe how a draw from $f(u^{(n)}|\rho^{(n)}, u^{(n-1)})$ is made using ideas from classical mechanics. The negative of logarithm of the joint density of $u$ and $\rho$ given by

$$H(u, \rho) = -\log f(u|y) + \log((2\pi)^{q/2} M) + \rho^\top M^{-1} \rho/2$$

is a Hamiltonian function of the position ($u$) and the momentum ($\rho$). Intuitively, the Hamiltonian $H(u, \rho)$ measures the total energy of a physical system and it consists of the potential energy $-\log f(u|y)$ and the kinetic energy $\rho^\top M^{-1} \rho/2$. This is the reason $M$ is referred to as the mass matrix. The Hamiltonian equations are given by the following first order differential equations

$$\frac{du}{dt} = \frac{\partial H}{\partial \rho} = M^{-1} \rho \quad \text{and} \quad \frac{d\rho}{dt} = -\frac{\partial H}{\partial u} = \nabla \log f(u|y). \quad (15)$$

Solution of the Hamiltonian equations (15) results in the Hamiltonian flow from an initial $(u_0, \rho_0)$ to $(u_t, \rho_t)$. Here, $du/dt$ and $d\rho/dt$ denote the derivatives of $u$ and $\rho$ with respect to the (fictitious) continuous time $t$. To garner intuition behind (15) the following analogy in $\mathbb{R}^2$ is useful (Neal, 2011). Imagine a sledge sliding over a friction-less surface of varying height proportional to $1/f(u|y)$. The potential energy is based on the height of the surface at the current position, $u$, whereas the kinetic energy is determined by the sledge’s momentum, $\rho$, and its mass, $M$. In a flat surface, that is, when $\nabla \log f(u|y) = 0, \forall u$, the sledge moves at a constant velocity. On the other hand, when slope is positive ($\nabla \log f(u|y) < 0$), the kinetic energy decreases as the potential energy increases until it vanishes ($\rho = 0$). The sledge then slides back down the hill increasing its kinetic energy and decreasing the potential energy.
Over any interval, the Hamiltonian dynamics (15) defines the Hamiltonian flow \((u_0, \rho_0) \to (u_t, \rho_t)\) that satisfies three important properties, namely, (i) it is energy preserving, that is, \(H(u_t, \rho_t) = H(u_0, \rho_0)\), (ii) it is volume preserving, that is, \(du_t d\rho_t = du_0 d\rho_0\) and (iii) it is time reversible, which implies if, \((u_0, \rho_0) \sim \nu\) then \((u_t, \rho_t) \sim \nu\). Since (15) can not be solved analytically for practical examples, the Störmer-Verlet or the leapfrog method is a standard approach for approximating the solutions to (15) (Duane et al., 1987). In particular, this method uses a discrete step-size \(\epsilon\) to make a move, according to

\[
\begin{align*}
\rho_{t+\epsilon/2} &= \rho_t + (\epsilon/2) \nabla \log f(u_t|y) \\
u_{t+\epsilon} &= u_t + \epsilon M^{-1} \rho_{t+\epsilon/2} \\
\rho_{t+\epsilon} &= \rho_{t+\epsilon/2} + (\epsilon/2) \nabla \log f(u_{t+\epsilon}|y).
\end{align*}
\]

In HMC, in order to draw from \(f(u^{(n)}|\rho^{(n)}, u^{(n-1)})\), starting from \((u^{(n-1)}, \rho^{(n)})\), the above set of deterministic steps (16) (referred to as Leapfrog \((\cdot, \cdot, \epsilon, M)\)) is repeated \(L\) times to generate a proposal \((u', \rho')\) which is then accepted/rejected with an MH step. The Leapfrog method preserves the volume exactly and it is also reversible by simply negating \(\rho\) (see Neal, 2011, for details).

**Algorithm 2** The \(n\)th iteration for the HMC

1: Draw \(\rho^{(n)} \sim N(0, M)\).
2: Set \(u' \leftarrow u^{(n-1)}\), \(\rho' \leftarrow \rho^{(n)}\).
3: For \(i = 1, \ldots, L\) do \((u', \rho') \leftarrow \text{Leapfrog} (u', \rho', \epsilon, M)\).
4: \(\alpha \leftarrow \min \{1, \exp\{-H(u', \rho') + H(u^{(n-1)}, \rho^{(n)})\}\}\)
5: Draw \(\delta \sim \text{Uniform} (0, 1)\). If \(\delta < \alpha\) then set \(u^{(n)} \leftarrow u', \rho^{(n)} \leftarrow -\rho'\), else set \(u^{(n)} \leftarrow u^{(n-1)}\).

Note that, if we could simulate the Hamiltonian dynamics (15) exactly, by the energy preserving property (i), energy would be preserved exactly, and the MH acceptance probability would always be \(\min \{1, \exp(0)\} = 1\). Since we use the leapfrog integrator, that approximately simulates the dynamics, if the approximation is good, then \(H(u', \rho') - H(u^{(n-1)}, \rho^{(n)})\) would be small, and the acceptance rate will be high. Indeed, for HMC, \(\alpha\) still tends to be high even for proposals that are far from the current state, reducing the random walk behavior of some other MH algorithms. The marginal chain \(\{u^{(n)}\}_{n \geq 1}\) of the HMC chain \(\{u^{(n)}, \rho^{(n)}\}_{n \geq 1}\) can be used to approximate the expectations in (5) or (8).
The choices of $\epsilon, L$ and the mass matrix $M$ should be such that the resulting algorithm mixes well (that is, the sampled distribution is ‘close’ to the target distribution), leads to suitable acceptance rates and lower Monte Carlo errors. Often, in practice, the mass matrix $M$ is chosen to be the identity matrix and $\epsilon, L$ are adjusted to achieve around 70% acceptance rates. The No-U-Turn sampler (NUTS) (Hoffman and Gelman, 2014) is an extension of HMC that eliminates the need of manual tuning of $L$. Hoffman and Gelman (2014) also propose a method for dynamically adapting the $\epsilon$ parameter on the fly. NUTS is employed in the programming language Stan (Carpenter et al., 2017). Girolami and Calderhead (2011) propose the Riemannian manifold HMC algorithm that uses a position-dependent $M$ that changes in every iteration, eliminating the need for manually tuning the mass matrix. A comparison of performance of different HMC algorithms in the context of analyzing GLMMs can be found in Zhang (2022).

### 3.3 Data augmentation for GLMMs

Data augmentation (DA) is an MCMC algorithm that has been widely used for analyzing Bayesian probit and logistic GLMs (see e.g. Albert and Chib, 1993; Polson et al., 2013). Recently, DA algorithms have been developed and studied for Bayesian GLMMs (Wang and Roy, 2018b; Polson et al., 2013; Wang and Roy, 2018a; Rao and Roy, 2021). In this section, we propose DA algorithms for simulating from (7) corresponding to the probit and logistic mixed models. For constructing a valid and efficient DA algorithm (Tanner and Wong, 1987) for $f(u|\beta, \Lambda, y)$ in (7) we need to construct a joint density $f(u, d|\beta, \Lambda, y)$ with augmented variables $d$ satisfying the following two properties

(i) the $u$—marginal of the joint density $f(u, d|\beta, \Lambda, y)$ is the target density (7) and

(ii) sampling from the two corresponding conditional densities $f_{u|d}$ and $f_{d|u}$ is straightforward.

Each iteration of the DA algorithm consists of two steps — a draw from $f_{d|u}$ followed by a draw from $f_{u|d}$. Thus, the DA Markov chain $\{u^{(n)}, d^{(n)}\}_{n \geq 1}$ is a two-variable Gibbs sampler. The DA algorithm, like its deterministic counterpart the EM algorithm, is widely used. In Sections 3.3.1 and 3.3.2 we provide appropriate DA algorithms for the probit and logistic mixed models, respectively.
### 3.3.1 Data augmentation for probit mixed models

In this Section, we consider probit GLMM for binary data, that is, \( \ell_i = 1 \) for \( i = 1, \ldots, m \) in Example 2. Thus, \( (Y_1, Y_2, \ldots, Y_m) \) are independent Bernoulli random variables with \( P(Y_i = 1) = \Phi(x_i^T \beta + z_i^T u) \). Following [Albert and Chib (1993)](#), let \( v_i \in \mathbb{R} \) be the continuous latent variable corresponding to binary observation \( Y_i \), such that \( Y_i = I(v_i > 0) \), where \( v_i | \beta, u \sim N(\gamma_i, 1) \) for \( i = 1, \ldots, m \). Then

\[
P(Y_i = 1) = P(v_i > 0) = \Phi(\gamma_i). \tag{17}
\]

Let \( v = (v_1, \ldots, v_m)^T \), then \( v | \beta, u \sim N(X\beta + Zu, I_m) \). Using the latent variables \( v \), we introduce the joint density

\[
f(u, v | \beta, \Lambda, y) = \frac{1}{L(\beta, \Lambda | y)} \left[ \prod_{i=1}^{m} \phi(v_i; \gamma_i, 1) \left[ 1_{(0, \infty)}(v_i) \right]^{y_i} \left[ 1_{(-\infty, 0]}(v_i) \right]^{1-y_i} \right] \times \phi_q(u; 0, G). \tag{18}
\]

From (17) it follows that

\[
\int_{\mathbb{R}^m} f(u, v | \beta, \Lambda, y) dv = f(u | \beta, \Lambda, y), \tag{19}
\]

where \( f(u | \beta, \Lambda, y) \), given in (17), is the target density. Thus, the condition (i) of DA construction mentioned before holds. From (18), it follows that

\[
v_i | u, \beta, \Lambda, y \sim TN(\gamma_i, 1, y_i), \ i = 1, \ldots, m, \tag{20}
\]

where \( TN(\mu, \sigma^2, e) \) denotes the distribution of the normal random variable with mean \( \mu \) and variance \( \sigma^2 \), that is truncated to have only positive values if \( e = 1 \), and, it has only negative values if \( e = 0 \).

From (18) it follows that the conditional density of \( u \) given \( \beta, \Lambda, v, y \) is

\[
f(u | \beta, \Lambda, v, y) \propto \left[ \prod_{i=1}^{m} \exp \left\{ -\frac{1}{2} \left[ (z_i^T u)^2 - 2(z_i^T u)(v_i - x_i^T \beta) \right] \right\} \right] \exp \left[ -\frac{1}{2} u^T G^{-1} u \right]
\]

\[
= \exp \left[ -\frac{1}{2} \left\{ u^T (Z^T Z + G^{-1}) u - 2u^T Z^T (v - X\beta) \right\} \right].
\]

Thus, the conditional distribution of \( u \) is

\[
u | v, \beta, \Lambda, y \sim N_q \left( (Z^T Z + G^{-1})^{-1} Z^T (v - X\beta), (Z^T Z + G^{-1})^{-1} \right). \tag{21}
\]
Thus, every iteration of the proposed DA algorithm for (18) consists of making the draws of $v$ and $u$ from (20) and (21), respectively.

**Algorithm 3** The $n$th iteration for the DA algorithm

1: Given $u^{(n-1)}$, draw $v^{(n)}_{i \text{ind}} \sim \text{TN}(x_i^T \beta + z_i^T u^{(n-1)}, 1, y_i)$ for $i = 1, \ldots, m$.
2: Draw $u^{(n)} \sim N_q\left(\left(Z^T Z + G^{-1}\right)^{-1}Z^T (v^{(n)} - X \beta), (Z^T Z + G^{-1})^{-1}\right)$.

The conditional distribution of $u$ in the above DA algorithm and several other conditional distributions appearing in this article are normal distributions of the form $N(S^{-1}t, S^{-1})$ for some positive definite matrix $S$ and a vector $t$. A naive method of drawing from $N(S^{-1}t, S^{-1})$ is inefficient when the dimension of $S$ is large as it involves calculating inverse of the matrix $S$. Rao and Roy (2021) advocate using the following method of drawing from $N(S^{-1}t, S^{-1})$ that does not require computing $S^{-1}$.

**Algorithm 4** An algorithm for drawing from $N(S^{-1}t, S^{-1})$

1: Let $S = LL^T$ be the Cholesky decomposition of $S$.
2: Solve $Lw = t$.
3: Draw $z \sim N(0, I_q)$ where $q$ is the dimension of $S$.
4: Solve $L^T x = w + z$. Then $x \sim N(S^{-1}t, S^{-1})$.

DA algorithms, although popular, they often suffer from slow convergence and high autocorrelations. Liu and Wu (1999) proposed the parameter expansion for data augmentation (PX-DA) algorithms for speeding up the convergence of DA algorithms. More recently, Hobert and Marchev (2008) compared the performance of PX-DA algorithms based on a Haar measure (called the Haar PX-DA algorithms), the PX-DA algorithms based on a probability measure and the DA algorithms. Hobert and Marchev (2008) showed that, under some mild conditions, the Haar PX-DA algorithms are better than the PX-DA and the DA algorithms in terms of different ordering. In PX-DA, an extra step is added (sandwiched) between the two steps of the original DA algorithm. In order to construct this extra step, we derive the marginal density of $v$ from the joint density (18) as

$$f(v|y) = \int_{\mathbb{R}^q} f(u,v|y)du \propto \prod_{i=1}^m \left[1_{(0,\infty)}(v_i)\right]^{y_i} \left[1_{(-\infty,0]}(v_i)\right]^{1-y_i} \exp\left\{-\frac{1}{2} \left[v^T Z_1 v - 2v^T Z_1 X \beta\right]\right\},$$

(22)
where
\[ Z_1 = \left[ I_m - Z \left( Z^\top Z + G^{-1} \right)^{-1} Z^\top \right]. \]

Let \( \mathcal{V} \) denote the subset of \( \mathbb{R}^m \) where \( v \) lives, that is, \( \mathcal{V} \) is the Cartesian product of \( m \) half (positive or negative) lines, where the \( i \)th component is \((0, \infty)\) (if \( y_i = 1 \)) or \((-\infty, 0]\) (if \( y_i = 0 \)). Let \( \psi \) be the unimodular multiplicative group on \( \mathbb{R}_+^m \) with Haar measure \( \nu(dh) = dh/h \), where \( dh \) is Lebesgue measure on \( \mathbb{R}_+^m \). For constructing an efficient extra step, as in Roy and Hobert (2007), we let the group \( \psi \) act on \( \mathcal{V} \) through a group action
\[ T(v) = hv = (hv_1, hv_2, \ldots, hv_m)^\top. \]

With the group action defined this way, it can be shown that the Lebesgue measure on \( \mathcal{V} \) is relatively left invariant with the multiplier \( \chi(h) = h^m \) (Roy, 2014; Hobert and Marchev, 2008). Following Hobert and Marchev (2008), consider a probability density function \( \omega(h) \) on \( \psi \) where
\[ \omega(h) \propto f(hv|y) \chi(h) \nu(dh) \propto h^{m-1} \exp \left\{ -\frac{1}{2} h^2 v^\top Z_1 v - 2hv^\top Z_1 X \beta \right\} dh. \quad (23) \]

Since \( Z_1 \) is a positive definite matrix, given \( v \), \( \omega(h) \) is a valid density. From Hobert and Marchev (2008), it follows that the transition \( v \rightarrow v' \equiv T(v) = hv \) where \( h \sim \omega(h) \), is reversible with respect to \( f(v|y) \) defined in (22). As mentioned in Roy (2014), intuitively, the extra step (23) reduces the correlation between \( u^{(n-1)} \) and \( u^{(n)} \) and thus improves the mixing of the DA algorithm. Below are the three steps involved in every iterations of the proposed Haar PX-DA algorithm.

**Algorithm 5** The \( n \)th iteration for the Haar PX-DA algorithm

1. Draw \( v_i^{(n)} \) \ind \TN(x_i^\top \beta + z_i^\top u^{(n-1)}_i, 1, y_i) \) for \( i = 1, \ldots, m \).
2. Draw \( h \) from (23).
3. Calculate \( v'_i = hv_i \) for \( i = 1, \ldots, m \), and draw \( u^{(n)} \) from (21) conditional on \( v' = (v'_1, \ldots, v'_m)^\top \), that is, draw
\[ u^{(n)} \sim N_q \left( \left( Z^\top Z + G^{-1} \right)^{-1} Z^\top (v' - X \beta) \right). \]

Since \( \omega(h) \) in (39) is log-concave, adaptive rejection sampling algorithm (Gilks and Wild, 1992) can be used to efficiently sample from \( \omega(h) \). The only difference between the Haar PX-DA algorithm (Algorithm 5) and the DA algorithm (Algorithm 3) is a single draw from
the univariate density \( \omega(h) \), which is easy to sample from. Thus, the computational burden, per iteration, for the Haar PX-DA algorithm is similar to that of the DA algorithm.

### 3.3.2 Data augmentation for logistic mixed models

Since the highly cited paper of [Albert and Chib (1993)](cite) for probit GLMs, there have been several attempts to construct such a DA sampler for the logistic model. Recently, [Polson et al. (2013)](cite) have proposed an efficient DA Gibbs sampler for Bayesian logistic models with Pólya-Gamma (PG) latent variables. A random variable \( \varphi \) has PG distribution with parameters \( a, b \), that is, \( \varphi \sim \text{PG}(a, b) \), if

\[
\varphi \overset{d}{=} \left( \frac{1}{2\pi^2} \right) \sum_{i=1}^{\infty} \frac{\varphi_i}{\left( i - 1/2 \right)^2 + b^2/(4\pi^2)}.
\]

where \( \varphi_i \overset{iid}{\sim} \text{Gamma}(a, 1), a > 0, b \in \mathbb{R} \). From [Wang and Roy (2018c)](cite), the pdf for PG \((a, b)\) is

\[
p(\varphi | a, b) = \cosh \left( \frac{b}{2} \right) \frac{a^{2a-1}}{\Gamma(a)} \sum_{j=0}^{\infty} (-1)^j \frac{\Gamma(j+a)(2j+a)}{\Gamma(j+1)} \exp \left( -\frac{(2j+a)^2}{8\varphi} - \frac{\varphi b^2}{2} \right).
\]

for \( \varphi > 0 \), where the hyperbolic cosine function \( \cosh(t) = (e^t + e^{-t})/2 \).

Polson et al.’s (2013) DA technique can be extended to construct a Gibbs sampler for logistic GLMMs (Example [1]). Indeed, from Polson et al. (2013) we have

\[
\frac{[\exp(\gamma_i)]^{y_i}}{[1 + \exp(\gamma_i)]^{\ell_i}} = 2^{-\ell_i} \exp(\kappa_i \gamma_i) \int_0^{\infty} \exp[-w_i \gamma_i^2/2] p(w_i) dw_i,
\]

where \( \kappa_i = y_i - 1/2, i = 1, \ldots, m \) and \( p(w_i) \) is the pdf of \( \text{PG}(\ell_i, 0) \). Using PG latent variables \( w = (w_1, w_2, \ldots, w_m) \), we construct the joint density

\[
f(u, w | \beta, \Lambda, y) \propto \left[ \prod_{i=1}^{m} \exp\{\kappa_i \gamma_i - w_i \gamma_i^2/2\} p(w_i) \right] \phi_q(u; 0, G).
\]

(25)

From (24) it follows that the \( u \)- marginal of (25) is the target density \( f(u | \beta, \Lambda, y) \). The conditional density for \( w_i \) is

\[
f(w_i | u, \beta, \Lambda, y) \propto \exp(-w_i \gamma_i^2/2) p(w_i).
\]

From [Rao and Roy (2021)](cite) we then have

\[
w_i | u, \beta, \Lambda, y \overset{iid}{\sim} \text{PG}(\ell_i, \gamma_i), i = 1, \ldots, m.
\]

(26)
Polson et al. (2013) describe an efficient method for sampling from the PG distribution. Also, from (25), as in Rao and Roy (2021), the conditional density of \( u \) given \( \beta, \Lambda, w, y \) is

\[
f(u \mid \beta, \Lambda, w, y) \propto \prod_{i=1}^{m} \exp \left\{ \kappa_i z_i^T u - \frac{w_i}{2} \left( (z_i^T u)^2 + 2(z_i^T u)(x_i^T \beta) \right) \right\} \exp \left[ -\frac{1}{2} u^T G^{-1} u \right]
\]

\[
= \exp \left[ -\frac{1}{2} u^T (Z^T W Z + G^{-1}) u + u^T (Z^T \kappa - Z^T W X \beta) \right],
\]

where \( W \) is the \( m \times m \) diagonal matrix with \( i^{th} \) diagonal element \( w_i \) and \( \kappa = (\kappa_1, \ldots, \kappa_m)^T \).

Thus, the conditional distribution of \( u \) is

\[
u \mid w, \beta, \Lambda, y \sim N_q \left( (Z^T W Z + G^{-1})^{-1} (Z^T \kappa - Z^T W X \beta), (Z^T W Z + G^{-1})^{-1} \right) .
\]

(27)

So, every iteration of the Pólya Gamma sampler for (25) consists of making the draws of \( w \) and \( u \) from (26) and (27), respectively.

**Algorithm 6** The \( n \)th iteration for the DA algorithm

1: Given \( u^{(n-1)} \), draw \( \omega_i^{(n)} \,^{\text{ind}} \sim \text{PG}(\ell_i, x_i^T \beta + z_i^T u^{(n-1)}) \), \( i = 1, \ldots, m \).
2: Draw \( u^{(n)} \sim N_q \left( (Z^T W Z + G^{-1})^{-1} (Z^T \kappa - Z^T W X \beta), (Z^T W Z + G^{-1})^{-1} \right) \) with \( w = w^{(n)} \).

### 4 MCMC for Bayesian GLMMs

Here, we consider MALA, HMC and DA algorithms for Bayesian GLMMs. In the Bayesian framework, one needs to specify the prior distributions of \( \beta \) and \( \Lambda \). We assume the Gaussian prior for \( \beta \) given by

\[
f(\beta) \propto \exp \left[ -\frac{1}{2} (\beta - \mu_0)^T Q (\beta - \mu_0) \right].
\]

(28)

where \( \mu_0 \in \mathbb{R}^p \) and \( Q \) is a \( p \times p \) positive definite matrix.

For simplifying the presentations, we assume that the structured matrices \( R_j \)'s to be identity matrices and the covariance matrices \( \Lambda_j \)'s correspond to scalar variances. Thus, \( \Lambda_j \otimes R_j = (1/\lambda_j)I_{q_j} \), where \( \lambda_j > 0 \), that is, the components in \( u_j \) are independent with a common variance \( 1/\lambda_j \). Let \( \lambda = (\lambda_1, \ldots, \lambda_r) \). We assume that the prior for \( \lambda_j \) is

\[
f(\lambda_j) \propto \lambda_j^{a_j - 1} e^{-b_j \lambda_j}, \ j = 1, \ldots, r,
\]

(29)
for $a_j > 0, b_j > 0$, that is, apriori $\lambda_j \sim \text{Gamma}(a_j, b_j)$, $j = 1, \ldots, r$. Finally, we assume that $\beta$ and $\lambda$ are apriori independent and all $\lambda_j$s are also apriori independent. Hence, the joint posterior density for $(u, \beta, \lambda)$ is

$$f(u, \beta, \lambda|y) \propto f(y, u|\beta, \lambda) \prod_{j=1}^{r} f(\lambda_j)$$

$$\propto \left[ \prod_{i=1}^{m} f(y_i|\beta, u) \right] f(\beta) \left[ \prod_{j=1}^{r} \lambda_j^{a_j-1+q_j/2} \exp\left[-(b_j + u_j^\top u_j/2)\lambda_j\right] \right], \quad (30)$$

where $f(y_i|\beta, u)$, $f(y, u|\beta, \lambda)$, $f(\beta)$ and $f(\lambda_j)$ are given in (1), (6), (28), and (29), respectively.

In (28) if $Q = 0$, then $\pi(\beta) \propto 1$, that is, in that case, (28) becomes the improper uniform prior on $\beta$. Similarly, the prior on $\lambda$ in (29) will be improper if $a_j$ and/or $b_j$ takes non-positive values. Several of the MCMC algorithms presented here are also applicable to the situations when $\pi(\beta) \propto 1$ and/or $\pi(\lambda)$ in (29) is improper. But, we do not pursue the use of improper priors here. Interested readers may look at Wang and Roy (2018) and Rao and Roy (2021). On the other hand, if improper priors are used, then the posterior density (30) is not guaranteed to be proper. Hence, in such cases, it is necessary to show that (30) is a proper pdf before carrying out further inference. Also, it is known that the usual (sample average) Monte Carlo estimators converge to zero with probability one if the MCMC chain corresponds to an improper target distribution (Athreya and Roy, 2014). We now present various MCMC algorithms for exploring the posterior density (30).

### 4.1 MALA and HMC for Bayesian GLMMs

The logarithm of the posterior density (30) (up to an additive constant) is

$$\log f(u, \beta, \lambda|y) = \sum_{i=1}^{m} \left[ (y_i-\xi_i - b(\xi_i))/a_i(u) \right] - (\beta - \mu_0)^\top Q(\beta - \mu_0)/2$$

$$+ \sum_{j=1}^{r} \left[ (a_j - 1 + q_j/2) \log \lambda_j - (b_j + u_j^\top u_j/2)\lambda_j \right]. \quad (31)$$

We can construct a MALA for (30) following Algorithm I given in Section 3.1 using the derivatives of $\log f(u, \beta, \log(\lambda)|y)$, but we propose a different algorithm. From (30), we know that conditional on $(u, \beta, y)$,

$$\lambda_j \overset{\text{ind}}{\sim} \text{Gamma}(a_j + q_j/2, b_j + u_j^\top u_j/2), \quad j = 1, \ldots, r. \quad (32)$$
Denoting \( \zeta = (u, \beta) \) and \( \zeta^{(n)} = (u^{(n)}, \beta^{(n)}) \), we suggest running a MALA within Gibbs chain \( \{\zeta^{(n)}, \lambda^{(n)}\}_{n \geq 1} \), where each iteration alternates between a MALA step for \( f(\zeta|\lambda, y) \) and a draw of \( \lambda \) from (32). Here, \( f(\zeta|\lambda, y) \) is the conditional density of \( \zeta \) given by

\[
f(\zeta|\lambda, y) = f(u, \beta|\lambda, y) \\
\propto \left[ \prod_{i=1}^{m} f(y_i|\beta, u) \right] \exp \left[ -\frac{1}{2} (\beta - \mu_0)^T Q (\beta - \mu_0) \right] \exp \left[ - \sum_{j=1}^{r} \lambda_j u_j^T u_j / 2 \right].
\]

**Algorithm 7** The \( n \)th iteration for the MALA

1. Given \( (\zeta^{(n-1)}, \lambda^{(n-1)}) \) draw \( \zeta' \sim N(\zeta^{(n-1)} + \epsilon \nabla \log f(\zeta^{(n-1)}|\lambda^{(n-1)}, y)/2, \epsilon I_{p+q}) \).
2. Draw \( \delta \sim \text{Uniform } (0, 1) \). If \( \delta < \alpha(\zeta^{(n-1)}, \zeta') \) then set \( \zeta^{(n)} \leftarrow \zeta' \), else set \( \zeta^{(n)} \leftarrow \zeta^{(n-1)} \). Here, \( \alpha(\cdot, \cdot) \) is obtained from (11) by replacing \( f(u|y) \) with \( f(\zeta|\lambda^{(n-1)}, y) \) and \( k(u, u') \) with \( k(\zeta, \zeta') \) which is \( N(\zeta + \epsilon \nabla \log f(\zeta|\lambda^{(n-1)}, y)/2, \epsilon I_{p+q}) \) density evaluated at \( \zeta' \).
3. Draw \( \lambda_j^{(n)} \sim \text{Gamma}(a_j + q_j/2, b_j + u_j^T u_j/2), j = 1, ..., r \) with \( u = u^{(n)} \).

For the three GLMM examples, \( \nabla_u \log f(\zeta|\lambda, y) \), the derivatives of \( \log f(\zeta|\lambda, y) \) with respect to \( u \) are given in Section 3.1 with \( G = D(\lambda)^{-1} \) where \( D(\lambda) = \bigoplus_{j=1}^{r} \lambda_j I_{q_j} \). Here, we derive \( \nabla_\beta \log f(\zeta|\lambda, y) \) for these three popular GLMMs.

**Example 1** (Continued). For the binomial-logit link model, from (12) and (31) it follows that

\[
\nabla_\beta \log f(\zeta|\lambda, y) = X^T y - X^T \xi - Q(\beta - \mu_0).
\]

**Example 2** (Continued). For the binomial-probit model, from (13) and (31) it follows that

\[
\nabla_\beta \log f(\zeta|\lambda, y) = X^T \tau_1 - X^T \tau_2 - Q(\beta - \mu_0).
\]

**Example 3** (Continued). For the Poisson-log GLMM, from (14) and (31) we have

\[
\nabla_\beta \log f(\zeta|\lambda, y) = X^T y - X^T \exp(\gamma) - Q(\beta - \mu_0).
\]

Also, in this case, we propose a HMC within Gibbs chain \( \{\zeta^{(n)}, \lambda^{(n)}\}_{n \geq 1} \), where each iteration alternates between a HMC step for \( f(\zeta|\lambda, y) \) as in Algorithm 2 for the Hamiltonian function \( H(\zeta, \rho) = - \log f(\zeta|\lambda, y) + [(p + q) \log(2\pi) + \log(|M|) + \rho^T M^{-1} \rho] / 2 \) with \( \rho \sim N(0, M) \) for a \( (p + q) \times (p + q) \) positive definite matrix \( M \) and a draw of \( \lambda \) from (32).
4.2 Data augmentation for Bayesian GLMMs

As mentioned in Section 3.3, for a successful DA for Bayesian GLMMs, we need to construct a joint density $f(u, \beta, \lambda, d|y)$ with augmented variables $d$ whose $(u, \beta, \lambda) -$ marginal is the density (30). In this Section, we show that the augmented variables derived in sections 3.3.1 and 3.3.2 can be used for constructing DA for the Bayesian probit and logistic mixed models, respectively.

4.2.1 Data augmentation for Bayesian probit mixed models

As in Section 3.3.1, we consider a vector of Bernoulli random variables $(Y_1, Y_2, \ldots, Y_m)$ and assume $P(Y_i = 1) = \Phi(\gamma_i)$, $i = 1, \ldots, m$. Using the latent variables $v$ introduced in Section 3.3.1, Wang and Roy (2018b) introduce the joint density

$$f(u, \beta, \lambda, v|y) \propto \prod_{i=1}^{m} \phi(v_i; x_i^T \beta + z_i^T u, 1) \left[1_{(0,\infty)}(v_i)\right]^{y_i} \left[1_{(-\infty,0]}(v_i)\right]^{1-y_i}$$

$$\times \phi_u(u; 0, D(\lambda)^{-1}) f(\beta) \prod_{j=1}^{r} f(\lambda_j).$$

(33)

From (19) it follows that

$$\int_{\mathbb{R}^m} f(u, \beta, \lambda, v|y) dv = f(u, \beta, \lambda|y).$$

Thus, $(u, \beta, \lambda) -$ marginal of (33) is the target density (30).

From (33), the conditional density of $\beta$ given $u, \lambda, v, y$ is

$$f(\beta | u, \lambda, v, y) \propto \prod_{i=1}^{m} \exp \left\{ -\frac{1}{2} \left[ (x_i^T \beta)^2 - 2(x_i^T \beta)(v_i - z_i^T u) \right] \right\}$$

$$\times \exp \left[ -\frac{1}{2}(\beta - \mu_0)^T Q(\beta - \mu_0) \right]$$

$$\times \exp \left[ -\frac{1}{2} \left\{ \beta^T (X^T X + Q) \beta - 2\beta^T (X^T v - X^T Zu + Q\mu_0) \right\} \right].$$

Thus, the conditional distribution of $\beta$ given $u, \lambda, v, y$ is

$$\beta | u, \lambda, v, y \sim N((X^T X + Q)^{-1}(X^T v + Q\mu_0 - X^T Zu), (X^T X + Q)^{-1}).$$

(34)

The conditional densities of $v, u$ and $\lambda$ are given in (20), (21) and (32), respectively. Using these conditional distributions, we develop the following full Gibbs sampler for Bayesian probit mixed models.
Algorithm 8 The \( n \)th iteration of the full Gibbs sampler

1: Draw \( \lambda_j^{(n)} \sim \text{Gamma}(a_j + q_j/2, b_j + u_j^\top u_j/2), j = 1, \ldots, r \) with \( u = u^{(n-1)} \).
2: Draw \( v_i \sim \text{TN}(\gamma_i, 1, y_i), i = 1, \ldots, m \), with \( u = u^{(n-1)} \) and \( \beta = \beta^{(n-1)} \).
3: Draw \( u^{(n)} \sim \text{N}(21) \) with \( \lambda = \lambda^{(n)} \) and \( v = v^{(n)} \).
4: Draw \( \beta^{(n)} \sim \text{N}(34) \) with \( v = v^{(n)} \) and \( u = u^{(n)} \).

It is known that blocking parameters can improve the performance of a Gibbs sampler in terms of reducing its operator norm (Liu et al., 1994). When one or more variables are correlated, sampling them jointly can generally improve efficiency of the MCMC algorithms. On the other hand, blocking may result in complex conditional distributions that are not easy to sample from. For the probit linear mixed models, Wang and Roy (2018b) show that an efficient two-block Gibbs sampler can be constructed by using the two blocks, \( \eta \equiv (\beta^\top, u^\top)^\top \) and \( v, \lambda \). Below we present Wang and Roy’s (2018b) block Gibbs sampler.

Let \( E = (X, Z) \) with the \( i^{th} \) row being \( e_i^\top \) for \( i = 1, \ldots, n \). Thus, \( \gamma_i = x_i^\top \beta + z_i^\top u = e_i^\top \eta \). From (33), we have the conditional density of \( \eta \) given \( \lambda, v, y \) as

\[
\begin{align*}
    f(\eta|\lambda, v, y) &\propto \prod_{i=1}^{m} \exp \left[-\frac{1}{2} \left(v_i - x_i^\top \beta - z_i^\top u\right)^2\right] \prod_{j=1}^{r} \exp \left[-\frac{1}{2} \lambda_j u_j^\top u_j\right] \\
    &\times \exp \left[-\frac{1}{2} (\beta - \mu_0)^\top Q (\beta - \mu_0)\right] \\
    &\propto \exp \left[-\frac{1}{2} (v - E\eta)^\top (v - E\eta)\right] \cdot \exp \left[-\frac{1}{2} \eta^\top A(\lambda)\eta + \eta^\top \theta\right],
\end{align*}
\]

where

\[
\theta_{(p+q)\times 1} = \begin{pmatrix} Q\mu_0 \\ 0_{q\times 1} \end{pmatrix} \quad \text{and} \quad A(\lambda)_{(p+q)(p+q)} = \begin{pmatrix} Q & 0 \\ 0 & D(\lambda) \end{pmatrix}.
\]

Thus, from (35) we have

\[
\eta|\lambda, v, y \sim N_{p+q}( (E^\top E + A(\lambda))^{-1} (E^\top v + \theta), (E^\top E + A(\lambda))^{-1} ).
\]

From (33) note that conditional on \( (\eta, y) \), \( v \) and \( \lambda \) are independent. Thus, (37) together with (20) and (32) result in the following two-block Gibbs sampler for exploring the joint density (33).
Algorithm 9 The $n$th iteration for the two block Gibbs sampler

1: Draw $\lambda^{(n)} \sim \text{Gamma}(a_j + q_j/2, b_j + u^\top u_j/2)$, $j = 1, \ldots, r$ with $u = u^{(n-1)}$, and independently draw $v^{(n)}_i | \eta^{(n-1)}, y \sim \text{TN}(\varepsilon_i^\top \eta^{(n-1)}, 1, y_i)$ for $i = 1, \ldots, m$.

2: Draw $\eta^{(n)}$ from (37), that is,

$$
\eta^{(n)} \sim N\left(\left(E^\top E + A(\lambda^{(n)})\right)^{-1} \left(E^\top v^{(n)} + \theta\right), \left(E^\top E + A(\lambda^{(n)})\right)^{-1}\right).
$$

As in Section 3.3.1, we now construct a Haar PX-DA algorithm improving the block Gibbs sampler (Algorithm 9). In order to construct the extra step in the Haar PX-DA, we derive the marginal posterior density of $(\lambda, v)$ from the joint density (33) as

$$
f(\lambda, v | y) = \int_{\mathbb{R}^{p+q}} f(\eta, \lambda, v | y) d\eta
$$

$$
\propto \prod_{i=1}^m \left[1_{(0, \infty)}(v_i)\right]^{y_i} \left[1_{(-\infty, 0]}(v_i)\right]^{1-y_i} \prod_{j=1}^r \lambda_j^{q_j} 
\times \exp\left\{-\frac{1}{2} \left[v^\top E_1 v - 2v^\top E_2 - \theta^\top (E^\top E + A(\lambda))^{-1} \theta\right]\right\} \prod_{j=1}^r f(\lambda_j),
$$

where

$$
E_1 = \left[I_m - E \left(E^\top E + A(\lambda)\right)^{-1} E^\top \right] \quad \text{and} \quad E_2 = E \left(E^\top E + A(\lambda)\right)^{-1} \theta.
$$

For constructing an efficient sandwich step, Wang and Roy (2018b) let the group $\psi$ act on $\mathcal{V} \times \mathbb{R}_+^r$ through a group action $T^*(v, \lambda) = (hv, \lambda) = (hv_1, hv_2, \ldots, hv_m, \lambda)$. With the group action defined this way, it can be shown that the Lebesgue measure on $\mathcal{V} \times \mathbb{R}_+^r$ is relatively left invariant with multiplier $\chi(h) = h^m$ (Roy, 2014; Hobert and Marchev, 2008). Wang and Roy (2018b) then consider a probability density function $\omega^*(h)$ on $\psi$ where

$$
\omega^*(h) \, dh \propto f(\lambda, hv | y) \chi(h) \nu(dh)
\propto h^{m-1} \exp\left\{-\frac{1}{2} \left[h^2 v^\top E_1 v - 2hv^\top E_2\right]\right\} \, dh.
$$

Given $(\lambda, v), \omega^*(h)$ is a valid density since $E_1$ is a positive definite matrix. Below are the three steps involved in every iterations of Wang and Roy’s (2018b) Haar PX-DA algorithm.
Algorithm 10 The $n^{th}$ iteration for the Haar PX-DA algorithm

1: Draw $\lambda_i^{(n)} \overset{\text{ind}}{\sim} \text{Gamma}(a_j + q_j/2, b_j + u_j^T u_j/2)$, $j = 1, \ldots, r$ with $u = u^{(n-1)}$, and independently draw $v_i^{(n)}|\eta^{(n-1)}, y \overset{\text{ind}}{\sim} \text{TN}(e_i^T \eta^{(n-1)}, 1, y_i)$ for $i = 1, \ldots, m$.
2: Draw $h$ from (39).
3: Calculate $v'_i = hv_i$ for $i = 1, \ldots, m$, and draw $\eta^{(n)}$ from (37) conditional on $v' = (v'_1, \ldots, v'_m)^T$, that is, draw
   \[ \eta^{(n)} \sim N\left(\left(E^T E + A(\lambda^{(n)})\right)^{-1} \left(E^T v' + \theta\right), \left(E^T E + A(\lambda^{(n)})\right)^{-1}\right). \]

The adaptive rejection sampling algorithm (Gilks and Wild, 1992) can be used to sample from $\omega^*(h)$ as it log-concave. In general, the PX-DA algorithm is known to be theoretically more efficient than the DA (Hobert and Marchev, 2008; Roy, 2012b). In the context of some numerical examples of the probit GLMs, Roy and Hobert (2007) showed that huge gains in efficiency are possible by using the Haar PX-DA algorithm instead of the DA algorithm of Albert and Chib (1993) (see also Roy, 2012a, 2014, for comparisons of DA and PX-DA algorithms for the robit GLM). A numerical comparison of the three samplers presented in this section for the probit mixed models is given in Section 5.

4.2.2 Data augmentation for Bayesian logistic mixed models

Define the joint posterior density of $u, \beta, \lambda, w$ given $y$ as

\[ f(u, \beta, \lambda, w \mid y) \propto \prod_{i=1}^{m} \exp\{k_i(x_i^T \beta + z^T_i u) - w_i(x_i^T \beta + z^T_i u)^2/2\}p(w_i) \phi_q(u; 0, D(\lambda)^{-1})f(\beta)f(\lambda) \]

\[ = \prod_{i=1}^{m} \exp\{k_i(x_i^T \beta + z^T_i u) - w_i(x_i^T \beta + z^T_i u)^2/2\}p(w_i) \]

\[ \times \phi_q(u; 0, D(\lambda)^{-1}) \times \prod_{j=1}^{r} \lambda_j^{a_j-1} \exp(-b_j \lambda_j) \]

\[ \times \exp\left[-\frac{1}{2} (\beta - \mu_0)^T Q(\beta - \mu_0) \right], \]

(40)

where (40) follows from the priors on $\beta$ and $\lambda$ given in (28) and (29), respectively. From (24) it follows that the $(u, \beta, \lambda)$—marginal of (40) is the target density (30).
Based on (40), as in Rao and Roy (2021), the conditional density of $\beta$ given $u, \lambda, w, y$ is

$$f(\beta | u, \lambda, w, y) \propto \prod_{i=1}^{m} \exp \left[ \kappa_i x_i^T \beta - w_i (x_i^T \beta)^2 / 2 - w_i (x_i^T \beta) (z_i^T u) \right] \times \exp \left[ - \frac{1}{2} (\beta - \mu_0)^T Q (\beta - \mu_0) \right] \times \exp \left[ - \frac{1}{2} \beta^T (X^T WX + Q) \beta + \beta^T (X^T \kappa + Q \mu_0 - X^T W Zu) \right].$$

Thus, the conditional distribution of $\beta$ given $u, \lambda, w, y$ is

$$\beta | u, \lambda, w, y \sim N((X^T WX + Q)^{-1} (X^T \kappa + Q \mu_0 - X^T W Zu), (X^T WX + Q)^{-1}).$$

(41)

The conditional densities of $w, u$ and $\lambda$ are given in (26), (27) and (32), respectively. Rao and Roy (2021) use these conditional distributions to construct the following full Gibbs sampler for Bayesian logistic mixed models.

**Algorithm 11** The $n$th iteration of the full Gibbs sampler

1: Draw $\lambda_j^{(n)} \text{ind} \sim \text{Gamma}(a_j + q_j/2, b_j + u_j^T u_j/2)$, $j = 1, \ldots, r$ with $u = u^{(n-1)}$.
2: Draw $w_i^{(n)} \text{ind} \sim \text{PG}(\ell_i, \gamma_i)$, $i = 1, \ldots, m$ with $u = u^{(n-1)}$ and $\beta = \beta^{(n-1)}$.
3: Draw $u^{(n)} \sim (27)$ with $\lambda = \lambda^{(n)}$, $\beta = \beta^{(n-1)}$ and $w = w^{(n)}$.
4: Draw $\beta^{(n)} \sim (41)$ with $w = w^{(n)}$ and $u = u^{(n)}$.

Rao and Roy (2021) also construct an efficient two-block Gibbs sampler with the two blocks being $\eta$ and $(w, \lambda)$. From (40), the conditional density of $\eta$ given $\lambda, w, y$ is given by

$$f(\eta | \lambda, w, y) \propto \prod_{i=1}^{n} \exp \left[ \kappa_i e_i^T \eta - w_i (e_i^T \eta)^2 / 2 \right] \exp \left[ - u^T D(\lambda) u / 2 \right] \times \exp \left[ - (\beta - \mu_0)^T Q (\beta - \mu_0) / 2 \right].$$

Thus, the conditional distribution of $\eta$ given $\lambda, w, y$ is given by

$$\eta | \lambda, w, y \sim N((E^T WE + A(\lambda))^{-1} (E^T \kappa + \theta), (E^T WE + A(\lambda))^{-1}),$$

(42)

where $A(\lambda)$ and $\theta$ are defined in (36).

(42) together with (26) and (32) result in the following two-block Gibbs sampler.
Algorithm 12 The $n$th iteration of the block Gibbs sampler

1: Draw $\lambda^{(n)}_{j} \sim \text{Gamma}(a_j + q_j/2, b_j + u_j^\top u_j/2)$, $j = 1, \ldots, r$ with $u = u^{(n-1)}$, and independently draw $w^{(n)}_i \sim \text{PG}(\ell_i, e_i^\top \eta^{(n-1)})$, $i = 1, \ldots, m$.
2: Draw $\eta^{(n)} \sim (42)$ with $\lambda = \lambda^{(n)}$ and $w = w^{(n)}$.

A comparison of the full Gibbs sampler (Algorithm 11) and the block Gibbs sampler (Algorithm 11) in the context of some numerical examples as the dimensions of the design matrices vary can be found in Rao and Roy (2021).

5 Numerical example

In this section, we consider a publicly available simulated data set named “pbDat” from the R package pbnm to compare the full Gibbs sampler (Algorithm 8), the block Gibbs sampler (Algorithm 9) and the Haar PX-DA algorithm (Algorithm 10) for the probit mixed models. This data set has $m = 100$ binary observations. There are $p = 3$ covariates including an intercept term. There is $r = 1$ random effect with $q_1 = 12$ levels. We analyze the data set by fitting probit linear mixed models with a normal prior (28) on $\beta$ with $\mu_0 = 0$ and $Q = 0.001I_3$ and a Gamma prior (29) on $\lambda_1$ with $a_1 = 0.01$ and $b_1 = 0.01$. We ran the three samplers for $N = 100,000$ iterations starting at an initial value $(\beta^{(0)}, u^{(0)})$ with burn-in $B = 20,000$ iterations. Here $\beta^{(0)}$ is the estimate of $\beta$ obtained by fitting a probit linear model without any random effect. The initial value $u^{(0)}$ is a sample drawn from $N(0, (1/\lambda_1^{(0)})I_{12})$ where $1/\lambda_1^{(0)}$ is the estimate of random effect variance component obtained from the R package lme4. We use the R package ars to make draws from the density (39).

Next, we compare the performance of the full Gibbs (FG) sampler, the block Gibbs (BG) sampler and the Haar PX-DA algorithm in the context of this pbDat data. The samplers are compared using lag $k$ autocorrelation function (ACF) values $k = 1, \ldots, 5$, effective sample size (ESS) and multivariate ESS (mESS) (See Roy (2020) for a simple introduction to the different convergence diagnostic measures.). The ESS and mESS are calculated using the R package mcmcse. We also compute the mean squared jumps (MSJ) (defined as $\sum_{i=B+1}^{N} \|\beta^{(i+1)} - \beta^{(i)}\|^2 / (N - B)$ for the $\beta$ variable, and similarly for the other variables. Here, $\|\cdot\|$ denotes the Euclidian norm. Lower ACF values and higher ESS and MSJ...
numbers are preferred. Table 1 provides the values of ACF for the three samplers. Better performance of the Haar PX-DA and the block Gibbs samplers compared to the full Gibbs sampler is observed from their smaller ACF values. Table 2 provides the ESS values of the intercept parameter, first two regression coefficients and \( \lambda_1 \). It also gives the mESS values for \( \nu \) and \( (\beta, \lambda_1) \). Again, better efficiency of the Haar PX-DA and the block Gibbs samplers compared to the full Gibbs sampler is demonstrated from their larger ESS and mESS values. From Table 3, it can be seen that the Haar PX-DA sampler leads to higher MSJ values than the full Gibbs sampler. Also, the block Gibbs sampler results in higher MSJ values than the full Gibbs sampler with the exception of \( \lambda_1 \). Thus, Table 3 also corroborates better mixing of the Haar PX-DA and the block Gibbs samplers than the full Gibbs sampler.

Table 1: ACF for different samplers for the pbDat data

| Parameter | Sampler | lag 1 | lag 2 | lag 3 | lag 4 | lag 5 |
|-----------|---------|-------|-------|-------|-------|-------|
| \( \beta_0 \) | FG | 0.957 | 0.915 | 0.876 | 0.838 | 0.801 |
|           | BG | 0.085 | 0.062 | 0.042 | 0.023 | 0.026 |
|           | Haar | 0.089 | 0.061 | 0.038 | 0.030 | 0.020 |
| \( \beta_1 \) | FG | 0.724 | 0.539 | 0.410 | 0.317 | 0.249 |
|           | BG | 0.701 | 0.510 | 0.386 | 0.297 | 0.234 |
|           | Haar | 0.680 | 0.472 | 0.334 | 0.243 | 0.177 |
| \( \beta_2 \) | FG | 0.836 | 0.715 | 0.622 | 0.547 | 0.488 |
|           | BG | 0.812 | 0.681 | 0.584 | 0.509 | 0.449 |
|           | Haar | 0.720 | 0.528 | 0.395 | 0.297 | 0.223 |
| \( \lambda_1 \) | FG | 0.682 | 0.597 | 0.549 | 0.486 | 0.424 |
|           | BG | 0.635 | 0.521 | 0.442 | 0.375 | 0.320 |
|           | Haar | 0.636 | 0.442 | 0.344 | 0.266 | 0.207 |
Table 2: Multivariate ESS and ESS for different samplers for the pbDat data

| Sampler | mESS ($\beta \lambda$) | mESS ($u$) | ESS ($\beta_0$) | ESS ($\beta_1$) | ESS ($\beta_2$) | ESS ($\lambda_1$) |
|---------|--------------------------|-------------|-----------------|-----------------|-----------------|------------------|
| FG      | 4915                     | 14036       | 1565            | 8362            | 3481            | 4558             |
| BG      | 13142                    | 19156       | 47437           | 8867            | 4449            | 7093             |
| Haar    | 18865                    | 21940       | 47964           | 12891           | 10921           | 11177            |

Table 3: Mean squared jumps for different samplers for the pbDat data

|       | FG   | BG   | Haar |
|-------|------|------|------|
| $\beta$ | 0.018| 0.154| 0.155|
| $u$    | 0.224| 0.613| 0.622|
| $\lambda$ | 0.232| 0.198| 0.235|

6 Discussion

In this article, we have presented several MCMC algorithms for both frequentist as well as Bayesian GLMMs. While some of these algorithms discussed here are available in the literature, others are developed here. Since these algorithms result in Harris ergodic Markov chains, the (Monte Carlo) sample averages are consistent estimators of the means with respect to the corresponding target densities. On the other hand, in practice, it is important to ascertain the errors associated with these Monte Carlo estimates. An advantage of being able to calculate a valid standard error is that it can be used to decide ‘when to stop’ running the MCMC chain (Roy, 2020). A valid standard error for the Monte Carlo estimates can be formed if a central limit theorem is available for the time average estimator. Establishing geometric ergodicity (GE) of the underlying Markov chains is the most standard method for guaranteeing a central limit theorem for MCMC based estimators (Meyn and Tweedie, 1993). GE is also used for consistently estimating the asymptotic variance in the central limit theorem (Vats et al., 2019).

For several of the MCMC algorithms presented here, GE has been established in the literature. For example, Roy and Zhang (2021) demonstrates GE of Markov chains underlying different MALA for GLMMs. The GE of the Pólya Gamma block Gibbs sampler for Bayesian logistic mixed models under proper and improper priors have been established in Wang and Roy (2018a) and Rao and Roy (2021), respectively. Wang and Roy (2018b) derive conditions under which the block Gibbs sampler and the Haar PX-DA algorithm for
the probit mixed models are geometrically ergodic when improper priors are assumed on
the regression coefficients and the variance components.

It would be interesting to construct and study efficient DA samplers for other GLMMs,
for example the GLMMs with the robit link (Roy, 2012a). A potential future study can
be to extend Wang and Roy’s (2018b) GE results to the probit mixed models with proper
priors. Another potential project is to study convergence properties of the HMC chains in
the context of GLMMs.

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