Bayesian Multinomial Logistic Regression for Numerous Categories

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Abstract

While multinomial logistic regression is a useful tool for classification among multiple categories, the posterior sampling of Bayesian implementations is computationally burdensome when the number of categories is large. In this paper, we show that the appropriate data augmentation technique provides faster posterior sampling than alternatives in the literature. This speed up comes from two sources: simpler posterior conditional distributions on the coefficients and the ability to parallelize parameter draws. In simulation studies, we demonstrate that the effective sampling rate of our posterior sampling approach is double that of competing methods when working with a large number of categories, even without parallelized computations. Furthermore, this computation time only increases linearly as the number of categories increases. Our corresponding R package is available on Github.

1 Introduction

Standard logistic regression is one of the most popular approaches to binary classification: the problem of assigning a probability, of being in one of two categories, to an observation. Compared to popular black-box machine learning approaches used for classification, logistic regression has the added bonus of interpretability: we can clearly state, or even plot, the model’s functional relationship between any input variable and the probability of interest. This is possible as the core of the model is additive, namely a linear model of the log odds.

Multinomial logistic regression is the natural extension when considering more than two categories. To do this, we estimate the log odds between multiple possible outcomes using a linear function of covariates. Bayesian approaches to coefficient estimation in multinomial logistic regression may be more computationally difficult than other common methods, as the resulting posterior distribution of the coefficients is not in a convenient analytical form. Thus, in order to estimate these coefficients’ posterior distributions, it is often necessary to pursue Markov chain Monte Carlo (MCMC) strategies that can be computationally intensive. However, by adding latent variables through data augmentation techniques, akin to the Bayesian probit regression of [Albert and Chib (1993)], a modeler can actually improve the ability of MCMC to efficiently estimate posterior distributions, even though the parameter space has increased. This paper proposes two sampling methods that improve either the computational speed or the effective sample size compared to other methods, and both result in superior effective sampling rates.

2 Multinomial Logistic Regression and its Challenges

We first define the multinomial logistic regression model. For \( i \in \{1, \ldots, N\} \), let \( y_i \in \mathbb{N}_0^C \) to be a length-\( C \) vector of non-negative integers \( y_{ij}, j = 1, \ldots, C \), which represent the counts of categories observed from \( n_i \)

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independent observations pertaining to subject \(i\), with each observation classified in one of \(C\) total categories. Let \(\pi_{ij}\) be the probability that one of the \(n_i\) observations from subject \(i\) falls into category \(j\in\{1,\ldots,C\}\). Thus, for each \(i\), \(y_i\) will be distributed with a multinomial distribution:

\[
y_i|\cdot \sim MN(n_i, \pi_{i1}, \ldots, \pi_{iC}).
\] (1)

In most cases, there is only one observation per subject, such that \(n_i = 1\) for all \(i\).

Now suppose we were to fit a logistic regression model to each of the categorical probabilities. For each \(j\in\{1,\ldots,C\}\), let \(\beta_j\in\mathbb{R}^P\) be a vector of coefficients, and we model the probability that an observation from \(y_i\) falls into one of the \(C\) different categories with:

\[
\pi_{ij} = \pi_j(x_i) = \frac{\exp x_i^T \beta_j}{\sum_{k=1}^{C}\exp x_i^T \beta_k}
\] (2)

where each vector \(x_i\in\mathbb{R}^P\) contains the observed values of the \(P\) explanatory variables associated with observation \(y_i\). From here, the Bayesian approach also includes a prior on the \(\beta_j\), which we’ll leave as general/unspecified and denote as \(p(\beta_j)\) for now.

However, while the \(\pi_{ij}\) are identifiable as presently defined, the \(\beta_j\) are not. If identification and interpretability of the \(\beta_j\) are desirable properties, the common practice is to assume that \(\beta_j = 0\) for a chosen category \(j\). In this paper, when this assumption is made, we assume it is for the last category: without loss of generality, let \(\beta_C = 0\). The implication here though is that these coefficients \(\beta_j\) now represent the effects of \(x_i\) on the log odds between categories \(j\) and \(C\). Of course, there are some cases/applications where this is not a desirable property.

To estimate the posterior distribution of the \(\beta\) coefficients, Monte Carlo methods are typically employed. Generally speaking, and for several reasons, a “Gibbs” draw, i.e. sampling directly from a known conditional distribution, is typically preferable to a standard Metropolis-Hastings draw when sampling a parameter. These reasons include that 1) Metropolis-Hastings requires the tuning of proposal distribution parameters and 2) the acceptance rate in Metropolis-Hastings sampling is less than 1, which likely results in a lower effective sample size. However, as Holmes and Held (2006) point out, no conjugate priors exist for the linear model coefficients in Bayesian GLMs, and thus direct samples from the conditional posteriors are not possible with the model above with standard/typical priors on the \(\beta\)’s. There are data augmentation methods that allow Gibbs sampling though, which are discussed in the next section.

An additional issue with standard approaches is that the denominator in Equation [2] requires other categories’ parameter values/information, which means that the parameters must be sampled/updated in sequence, thus removing possibilities for enhanced computational speed through parallelization. We address this with our approach in Section [3].

2.1 Approaches in the Literature

Several papers have suggested data augmentation enhancements for logistic regression in the wake of/building upon the enhancements for probit regression from Albert and Chib (1993), Holmes and Held (2006) pursued multiple data augmentation strategies for the logistic regression model. The strategy most relevant to our paper represents the logistic regression model as a set of binary observations that are determined by the sign of an auxiliary variable. These auxiliary variables are distributed according to a linear model with logistic errors. They then introduced a set of auxiliary variables following a Kolmogorov-Smirnov distribution, which after squaring and scaling determine the variance of the logistic errors. Using a multivariate normal prior on the coefficients and conditioning on these auxiliary variables and the data, the coefficients will still have a multivariate normal distribution. Furthermore, this method allows for sampling from the full conditional distributions of all of the parameters, so a Gibbs sampling strategy can be adopted without any Metropolis steps. However, implementing this sampling strategy relies on sampling from a truncated logistic distribution.
Holmes and Held (2006) further extend these ideas to multinomial regression by fixing the coefficients for a category at 0, such that the posterior sampling reduces to the same Gibbs sampling procedure, but now looping over a sequence of $C - 1$ logistic regression models one at a time, holding the others fixed. We will call their sampling algorithm “HH”. In programming this sampling algorithm, we relied on the pseudo-code included in Holmes and Held (2006) with the corrections made by van der Lans (2011).

Frühwirth-Schnatter and Frühwirth (2010); Frühwirth-Schnatter and Frühwirth (2012) expanded upon these ideas, representing the multinomial logistic regression model as a difference random utility model. Auxiliary variables are introduced as linear functions of the predictors with an additive multivariate logistic distributed error term. One consequence of this representation is that the error terms across categories are not independent, and the correlation of the errors between categories must be dealt with, regardless of the sampling technique (Frühwirth-Schnatter and Frühwirth, 2012). Despite this challenge, they were able to implement efficient samplers that performed better in computation time and effective sample size compared to HH on some common binary and categorical data sets (Frühwirth-Schnatter and Frühwirth, 2010). We will call their sampling algorithm “FSF”.

While their paper does not address a multinomial/polychotomous version of their logistic regression approach, Polson et al. (2013)’s data-augmentation strategy has become a go-to approach for Bayesian logistic regression. Using the Polya-Gamma latent variables, they construct a posterior sampler that is both simple to write down and does not need Metropolis-Hastings. Though the paper does not extend to the multiclass case, early versions of their R package BayesLogit contained code and documentation for running the multinomial logistic (Windle, 2019), which we have built into our package.

2.2 MCMC Issue and a Data Augmentation Solution

Holmes and Held (2006) and Frühwirth-Schnatter and Frühwirth (2010) developed data augmentation methods that allowed for full Gibbs sampling as the MCMC method for posterior estimation, as opposed to using the usually-less-efficient Metropolis algorithms. We proceed with an approach that still relies on Metropolis sampling, but that achieves speed improvements by removing the denominator of Equation 2 from the posterior distribution of the coefficients $\beta_j$. We now describe both this problem and our solution.

The aforementioned papers consider logistic regression where the information in covariates $x_i$ enter into the model as parametric linear combinations, i.e. $x_i^T \beta_j$. However, these could be any category-specific function of the data, $f_j(x_i)$, such that

$$
\pi_{ij} = \pi_j(x_i) = \frac{f_j(x_i)}{\sum_{k=1}^C f_k(x_i)}.
$$

(3)

This is the case in Murray (2021), who fits these functions with Bayesian additive regression trees (Chipman et al., 2010). However, the denominator above presents a challenge with MCMC: the conditional posterior of $f_j$ depends on $f_k$ for all $k \neq j$. This yields two computational issues. First, you cannot parallelize the sampling of $f_j$ for all $j$. Second, and perhaps more importantly, the calculation of the sum in the denominator above grows in complexity as $C$ grows. However, Murray (2021) augments the data with the auxiliary variables $\phi_i$ where

$$(\phi_i | y_i, \cdot ) \sim \text{Gamma} \left( n_i, \sum_{j=1}^C f_j(x_i) \right)$$

(4)
akin to the ideas in [Nieto-Barajas et al. (2004) and Walker (2011)]. This yields the joint probability model

\[ p(y_i, \phi_i | \cdot) = p(\phi_i | y_i, \cdot) p(y_i | \cdot) \]

\[ = \sum_{j=1}^{c} f_j(x_i) \frac{n_i^{c-1} \exp \left\{ -\phi_i \sum_{j=1}^{c} f_j(x_i) \right\}}{(\phi_i)^{n_i}} \frac{1}{\Gamma(n_i)} \frac{n_i!}{y_{i1} y_{i2} \ldots y_{ic}!} \prod_{j=1}^{c} f_j(x_i)^{y_{ij}} \]  

\[ = \frac{n_i!}{y_{i1} y_{i2} \ldots y_{ic}!} \frac{\phi_i^{n_i-1}}{\Gamma(n_i)} \sum_{j=1}^{c} f_j(x_i)^{y_{ij}} \frac{1}{\phi_i} \prod_{j=1}^{c} f_j(x_i)^{y_{ij}} \frac{1}{\phi_i} \prod_{j=1}^{c} f_j(x_i)^{y_{ij}} \exp \left\{ -\phi_i f_j(x_i) \right\}. \]  

The product in Equation 8 means there are new avenues to computational efficiency (i.e. solves the two aforementioned computational issues) because the posterior parameters of \( f_j(x_i) \) need not depend on other \( f_k, k \neq j \). We illustrate this in the next section.

3 Our Approach

3.1 Our Model and Data Augmentation

We assume multinomial likelihood in Equation 1 with probabilities from Equation 2. We also assume a prior on the collection of coefficients, \( \beta_j \), such that the joint prior factors into a product of the marginal priors for each category. Independence across categories is sufficient for such factorization of priors. This should include most commonly-assumed priors. These assumptions yield the following posterior on the vector of coefficients \( \beta_j \).

\[ p(\beta_j | \cdot) \propto \prod_{i=1}^{N} \left( \frac{\exp \{ x_i^T \beta_j \}}{\sum_{k=1}^{C} \exp \{ x_i^T \beta_k \}} \right)^{y_{ij}} p(\beta_j) \]

Note that the denominator \( \sum_{k=1}^{C} \exp \{ x_i^T \beta_k \} \) implies that the posterior of \( \beta_j \) is conditional upon the coefficients \( \beta_k \) from all other categories \( k \neq j \). This is the same issue that the aforementioned general regression function case of Murray (2021), but now specifically with \( f_j(x_i) = \exp(x_i^T \beta_j) \), there are still the two issues for posterior sampling as the number of categories grows. First, this denominator grows in complexity as the number of categories grows. Second, the posterior samples must be drawn in sequence, whereas if that denominator was removed, then the coefficient vectors \( \beta_j \) could be drawn in parallel for all \( j \). Thus we likewise introduce auxiliary variables \( \phi_i \) as

\[ (\phi_i | y_i, \cdot) \sim \text{Gamma} \left( n_i, \sum_{k=1}^{C} \exp(x_k^T \beta_k) \right). \]

Now, conditioning the full joint likelihood on the data and the set of \( \phi_i \), we get a posterior distribution of \( \beta_j \) that is no longer proportional in \( \beta_j \) to any of the other categories coefficients, \( \beta_k \) (for \( k \neq j \)), as seen in Equation 13.

\[ p(\beta_j | \cdot) \propto \prod_{i=1}^{N} p(y_i, \phi_i | \cdot) p(\beta_j) \]

\[ = \prod_{i=1}^{N} \frac{n_i!}{y_{i1} y_{i2} \ldots y_{ic}!} \frac{\phi_i^{n_i-1}}{\Gamma(n_i)} \prod_{j=1}^{c} f_j(x_i)^{y_{ij}} \frac{1}{\phi_i} \prod_{j=1}^{c} f_j(x_i)^{y_{ij}} \exp \left\{ y_{ij} x_i^T \beta_j - \phi_i \exp \{ x_i^T \beta_j \} \right\} \frac{1}{\phi_i} \prod_{j=1}^{c} f_j(x_i)^{y_{ij}} \exp \left\{ -\phi_i f_j(x_i) \right\} \]

\[ \propto \exp \left\{ \sum_{i=1}^{N} y_{ij} x_i^T \beta_j - \phi_i \exp \{ x_i^T \beta_j \} \right\} p(\beta_j) \]
Thus we can sample from this conditional distribution independently of the other categories. The ability to parallelize the sampling of the $\beta_j$ coefficients (as well as the latent variables $\phi_i$) is a key contribution of our paper.

However, this is without a free lunch. The posterior distribution in Equation [13] does not have an obvious conjugate prior to assume for $p(\beta_j)$, and thus we are unable to sample directly from conditional posterior distribution. Hence, the fastest Gibbs samplers are off the table, yet we find that simple Metropolis within Gibbs strategies are incredibly fast for our purposes.

3.2 Our Sampler

We have implemented these ideas and techniques into an R package, available at https://github.com/kylemcevoy/BayesMultiLogit. Our sampler has two main steps:

1. For each $i = 1, ..., N$, $\phi_i$ is sampled from the distribution in Equation [10] conditioning on the data and the current draws/values of $\beta_j$, $j = 1, ..., C$. These can be drawn in parallel across each $i$.

2. For each $j = 1, ..., C$, $\beta_j$ is sampled using a type of Metropolis algorithm conditioning on the data and the current draws/values of $\phi_i$, $i = 1, ..., N$. These can be drawn in parallel across each $j$.

To sample each $\beta_j$ we use a sequence of univariate random walk Metropolis samplers for each coefficient in the $\beta_j$ vector. This simple approach preserves flexibility and can generalize to many scenarios. In contrast, a multivariate normal proposal distribution would require a case-specific covariance matrix to sample efficiently. Thus, we set up simple, univariate normal proposal distributions for each individual coefficient.

Our univariate Metropolis samplers of the $\beta_j$ coefficients are set up to automatically tune the proposal distribution parameters during the burn in iterations, and this proceeds as follows. Let $\beta^{(t-1)}_{jp}$ be the coefficient in category $j = 1, ..., C$ for predictor $p = 1, ..., P$, drawn at MCMC iteration $t - 1$. The proposal distribution for generating $\beta^{(t)}_{jp}$ is $q(\beta^{(t-1)}_{jp}) = \beta^{(t-1)}_{jp} + W$ where $W \sim N(0, \sigma^2_{jp})$. While using univariate samplers mean there is no covariance matrix to tune, there is a variance term $\sigma^2_{jp}$ to tune for each coefficient’s proposal distribution, PC in total. While these can be pre-specified by the user, we have automated their tuning, akin to Fellingham and Fisher (2018). During the burn-in phase of MCMC, the value of $\sigma_{jp}$ is adjusted if the acceptance rate is outside of an acceptable range (currently 20%-40%). Specifically, for some predetermined number of MCMC iterations $\eta$, which is much less than the number of burn-in iterations, we check the number of values accepted during those $\eta$ iterations. If there were more than 0.4$\eta$ new values accepted in these $\eta$ iterations, we double the value of $\sigma_{jp}$. If there were fewer than 0.2$\eta$ new values accepted, we reduce $\sigma_{jp}$ by 10%, i.e. set its value to 0.9$\sigma_{jp}$.

In this way, as long as the initially provided values of both $\eta$ and $\sigma_{jp}$ are reasonable, $\sigma_{jp}$ will be automatically tuned to values that produce an acceptance/rejection rate in the desired range. For example, if performing 2000 burn-in iterations, then $\eta = 100$ provides $\eta/\eta = 20$ windows with which to tune $\sigma_{jp}$ for all $j, p$.

Presently, our code allows for both normal and flat priors on the coefficients for the categories, $\beta_j$. In our code we assumed that these priors were an i.i.d. across the different categories. While the full i.i.d. assumption is not necessary for the sampling procedure we are using, the sampling procedure does rely on independence between the categories’ priors. We would not be able to sample the posterior of $\beta_j$ independently across categories, even with the data augmentation, if we chose a prior that had correlation across the categories. The program does allow the user to specify a mean vector and a covariance matrix if i.i.d. multivariate normal distributions are chosen as the prior distributions.

3.3 Our Alternative Sampler with Elliptical Slice Sampling

One issue with the standard Metropolis-Hastings sampler is that its random-walk behavior may not effectively explore spaces very well. Our simple sampler for the $\beta$ coefficients may be suboptimal given the development.

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1Our corresponding R package, and thereby the simulation results in Section [4] do not presently take advantage of the possibility to parallelize. It would make sense that doing so would improve our sampling efficiency even further, though we do not yet have any empirical evidence for or against.
of clever algorithms that move around the sampling space more elegantly, such as elliptical slice sampling from [Murray et al. (2010)](Murray et al., 2010). This method of slice sampling requires a multivariate normal prior on a vector of \( P \) parameters. For each sampling step, a random draw from the prior is combined with the current state of the sampler (both are \( P \)-length vectors) to create an ellipse of plausible values in \( \mathbb{R}^P \) space. Proposal values are taken from this ellipse and accepted/rejected based on the log likelihood. For further detail, please see [Murray et al. (2010)](Murray et al., 2010). This sampling method does not include our auto-tune during the burn-in iterations.

4 Simulation Study

4.1 Comparing Samplers

In order to compare the performance of these algorithms as the number of categories (\( C \)) increases in the classification problem, we conduct a simulation study using the following data-generating process. Given a fixed number of categories \( C \), \( N=1000 \) \( P \)-length vectors \( x_i \) were simulated, such that each subject \( i \) has \( P=15 \) predictors plus an intercept. These predictor variables were independently generated from univariate standard normal distributions. Likewise, \( C \) length-\((P + 1) \) vectors \( \beta_j \) of coefficients were generated in the same fashion. For simplicity of notation, let these coefficients be combined into a \((P + 1) \times C \) matrix \( B \).

To generate categorical probabilities, we set \( p_i = \text{softmax}(x_i B) \), then with \( n_i = 1 \), randomly draw the categorical variable \( y_i \) according to probabilities \( p_i \). To summarize,

\[
\begin{align*}
  x_{ip} &\sim N(0,1), \quad i = 1,...,N; \quad p = 1,...,P \\
  \beta_{jp} &\sim N(0,1), \quad j = 1,...,C; \quad p = 0,...,P \\
  p_i & = \text{softmax}(x_i B), \quad i = 1,...,N \\
  y_i &\sim \text{MN}(n_i = 1, p_i)
\end{align*}
\]

where \( N() \) is the normal/Gaussian distribution and \( \text{MN}() \) is the multinomial distribution.

Each posterior sampling algorithm was run for a total of 3000 MCMC iterations, discarding the first 2000 as burn in. We measured the elapsed time it took the code to complete execution with the `system.time()` function in R. The effective sample size of the algorithms was calculated using the R package \texttt{CODA} [Plummer et al., 2006] and used to compute the Effective Sampling Rate (ESR). The ESR is important as, of course, the main desire is for an MCMC algorithm that minimizes the computation time needed to obtain the desired effective sample size, not necessarily minimizing the time per iteration.

In the left panel of Figure 1, we show these values for both of our posterior sampling algorithms as well as for the multinomial version of the Polya-Gamma sampler which we construct by adapting the code [Windle (2019)](Windle, 2019) to include code from [Scott (2014)](Scott, 2014). We see that the run times for our data augmentation with Metropolis Hastings sampling of the coefficients (DA+MH) requires approximately the same run time as the PG method. However, data augmentation with elliptical slice sampling [Murray et al. (2010)](Murray et al., 2010) of the coefficients (DA+ESS) has much shorter run times. The Holmes-Held algorithm and a basic Metropolis-Hastings sampler were also ran for comparison, but the code run time for each was significantly higher (off this chart) and thus has been left off this figure.

The central panel of Figure 1 shows the median effective sample size from the 1000 post-burn-in iterations, where the median is taken across the effective samples sizes of all the simulated coefficients of a particular number of categories \( C \). We see two main things. First, PG easily has markedly the best effective sample size for a small number of categories. Second, at ten or more categories, DA+MH has the best sample size. Typically, DA+ESS has the worst effective sample size. The naive Metropolis-Hastings sampler (not shown) actually has a decreasing effective sample size as the number of categories increases.

Most importantly, the right panel of Figure 1 shows the effective sampling rate, which gives the efficiency of the posterior sampling algorithm. It shows that for 10 categories or more, the median ESR of either of
our data augmentation methods improves on that of the multinomial Polya-Gamma sampler. And for 15 or more categories, our samplers have about double the ESR of PG.

4.2 Accuracy of Estimates

Computational speed is not impactful if parameters are not estimated well. Using the same data generation methods as before but with 5 categories, 10 predictors and one intercept, we model these 44 parameters (one of the categories is set as the reference category with all coefficients set to zero). Figure 2 shows the estimated posterior densities of a particular coefficient using multiple sampling algorithms, including the popular STAN package (Stan Development Team, 2020, 2021). We chose the particular coefficient in Figure 2 as the density estimates were representative of the general trend amongst the estimated densities. The main finding is simply that all the samplers except for HH were centered at the likelihood-based value most of the time, while HH’s densities were usually shrunk toward zero though sometimes they had the same or a more extreme center.

As another indicator of the effectiveness of the posterior estimation, we present the coverage rates of the posterior intervals in Table 1 which are defined as the number of intervals that contain the true parameter value divided by the number of parameters estimated, 44. We see that our data augmentation methods as well as STAN yield the coverage rates that are closest to the ideal.

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3STAN is not included in the speed and sampling rate tests before as it is not built within our same package, and thus differences in performance may be due to programming efficiencies and not the MCMC posterior sampling algorithm itself.
Figure 2: The set of posterior densities for a chosen predictor’s coefficient. The solid black vertical line denotes that true parameter value from the data-generating process, while the dotted black vertical line shows the likelihood-based estimate of the parameter from the `multinom` function from the `nnet` package in R.
| Sampler    | Posterior Percentage |
|-----------|----------------------|
| DA+MH     | 0.990 0.955 0.932 0.773 0.523 |
| DA+ESS    | 1.000 0.955 0.909 0.705 0.500 |
| HH        | 0.500 0.364 0.341 0.295 0.250 |
| PG        | 0.909 0.886 0.841 0.773 0.500 |
| STAN      | 1.000 0.977 0.909 0.750 0.568 |

Table 1: Coverage rate of posterior credible intervals, as a proportion of the 44 parameters estimated.

5 Conclusion and Future Work

We have developed a multinomial logistic regression posterior sampling algorithm that yields a superior median effective sample size for large numbers of categories compared to the flagship Bayesian logistic regression algorithm (Polson et al., 2013). This is done without sacrificing computational speed, which results in an improved effective sampling rate. We also find that replacing the Metropolis sampler with elliptical slice sampling (Murray et al., 2010) decreases the median effective sample size while drastically improving computational speed, which results in a similar median effective sample rate as our original method.

Our R package on Github ([https://github.com/kylemcevoy/BayesMultiLogit](https://github.com/kylemcevoy/BayesMultiLogit)) also includes the other algorithms discussed in this paper, as some do not have readily-available implementations C++ that can be called in R. We use the Rcpp (Eddelbuettel and François, 2011) and RcppArmadillo packages (Eddelbuettel and Sanderson, 2014), giving us access to the Armadillo C++ library (Sanderson and Curtin, 2016) for linear algebra within an R framework. Our simulations could be expanded to include Frühwirth-Schnatter and Frühwirth (2010)’s algorithm as well as the multinomial version of Gramacy and Polson (2012)’s logistic regression, mentioned in their discussion and extensions section. There is also a different Polya-Gamma sampling function from Scott (2011) that would be worth exploring. In addition, our current code could be further improved by taking advantage of the opportunities for parallelization that are immediately present in our formulation, and such improvements would likely only further improve our computation time and effective sampling rate.

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