Likelihood Inflating Sampling Algorithm

Reihaneh Entezari∗1, Radu V. Craiu†1, and Jeffrey S. Rosenthal‡1

1Department of Statistical Sciences, University of Toronto

April 2016

Abstract

Markov Chain Monte Carlo (MCMC) sampling from a posterior distribution corresponding to a massive data set can be computationally prohibitive since producing one sample requires a number of operations that is linear in the data size. In this paper, we introduce a new communication-free parallel method, the Likelihood Inflating Sampling Algorithm (LISA), that significantly reduces computational costs by randomly splitting the dataset into smaller subsets and running MCMC methods independently and in parallel on each subset using different processors. Each processor will draw sub-samples from sub-posterior distributions that are defined by “inflating” the likelihood function and the sub-samples are then combined using the importance re-sampling method to perform approximate full-data posterior samples. We test our method on several examples including the important case of Bayesian Additive Regression Trees (BART) using both simulated and real datasets. The method we propose shows significant efficiency gains over the existing Consensus Monte Carlo of Scott et al. (2013).

∗entezari@utstat.utoronto.ca
†craiu@ustat.toronto.edu web: http://www.utstat.toronto.edu/craiu/
‡jeff@utstat.toronto.edu web: http://probability.ca/jeff/
1 Introduction

Markov Chain Monte Carlo (MCMC) methods are fundamental tools for sampling highly complex distributions. They are of paramount importance in Bayesian inference as posterior distributions are generally difficult to characterize analytically (e.g., Brooks et al. 2011, Craiu and Rosenthal 2014). When the posterior distribution is based on a massive sample of size \( N \), posterior sampling can be computationally prohibitive since at least \( O(N) \) operations are needed to draw one MCMC sample. Additional issues include memory and storage bottlenecks where datasets are too large to be stored on one computer.

A common solution relies on parallelizing the computation task, i.e. dividing the load among a number of parallel workers, where a worker can be a processing unit, a computer, etc. Given the abundant availability of computer processors, such strategies can be extremely efficient as long as there is no need for frequent communication between workers. Some have discussed parallel MCMC methods (Wilkinson 2006, Rosenthal 2000, Laskey and Myers 2003) such that each worker runs on the full dataset. However, these methods do not resolve memory overload, and also face difficulties in assessing the number of burn-in iterations for each processor.

A truly parallel approach is to divide the dataset into smaller groups and run parallel MCMC methods on each subset using different workers. Such techniques benefit from not demanding space on each computer to store the full dataset. Generally, one needs to avoid frequent communication between workers, as it is time consuming. In a typical divide and conquer strategy the data is divided into non-overlapping parts, called shards, and each shard is analyzed by a different worker. For such strategies some essential MCMC-related questions are: 1) which sub-posterior distributions should one build for each shard, and
2) how to combine the MCMC sub-samples obtained from each sub-posterior so that we can recover the information that would have been obtained had we been able to sample from the full posterior distribution. Existing communication-free parallel methods proposed by Scott et al. (2013), Neiswanger et al. (2013) and Wang and Dunson (2013) present different approaches in combining sub-samples while they all share the fact that the product of the unnormalized sub-posteriors is equal to the unnormalized full posterior distribution. Specifically, Neiswanger et al. (2013) approximate each sub-posterior using kernel density estimators, while Wang and Dunson (2013) use the Weierstrass transformation. The independent product of sub-posteriors are then used to form global samples. The algorithm we propose here is an alternative to the popular Consensus Monte Carlo (CMC) method (Scott et al., 2013) that relies on a (weighted) averaging approach to combine sub-samples, a method that is known to be exact only for Gaussian posteriors. The approach we propose here is an alternative to CMC that shows superior performance in all the examples we examined, including the widely used regression model based on Bayesian Additive Regression Trees (BART) (Chipman et al., 1998, 2010; Kapelner and Bleich, 2013).

In this paper we consider the main theoretical challenge in Bayesian computation when sampling from a posterior distribution that is based on a massive data set. We introduce a new communication-free parallel method, the Likelihood Inflating Sampling Algorithm (LISA), that also relies on a partition of the dataset into subsets that are analyzed independently and in parallel by different workers to draw sub-samples from sub-posterior distributions that are defined differently than in the competing approaches described above. The sub-samples are then combined using different weighting schemes. Section 2 has a brief description of the CMC algorithm and in Section 3 we introduce LISA in detail with a theorem showing that its sub-posteriors are asymptotically equivalent to the full posterior distribution. Section 4 illustrates the potential difference brought by LISA over CMC in a simple Bernoulli example, and discusses the application of LISA
to linear regression models. The most important application of LISA is introduced in Section 5 where the BART model is discussed and we show the comparison between LISA and CMC when applied to this important model. Section 6 illustrates the performance of LISA on a Bayesian Logistic Regression model and ends with an open question. We end the paper with a discussion of ideas for future work. The Appendix contains the proof of the theorem mentioned in Section 3 and calculations related to the BART model.

2 Motivation

In what follows we assume that of interest is generating samples from a posterior distribution \( \pi(\theta) \) to compute say:

\[
I = \int h(\theta)\pi(\theta|\vec{y}_N)d\theta,
\]

where \( \vec{y}_N \) is an i.i.d. sample of size \( N \) which is large enough to prohibit a standard MCMC implementation in which draws from \( \pi \) can be obtained on a single computer, and \( \pi(\theta|\vec{y}_N) \) is the posterior distribution of \( \theta \), i.e. \( \pi(\theta|\vec{y}_N) \propto f(\vec{y}_N|\theta)p(\theta) \), where \( f(\vec{y}_N|\theta) \) is the likelihood function corresponding to the observed data \( \vec{y}_N \) and \( p(\theta) \) is the prior.

Major issues with MCMC posterior sampling given large datasets include: 1) the data may be too large to be stored on a single computer or 2) if \( \pi \) is sampled via a Metropolis-Hastings type of algorithm, each iteration requires \( N \) likelihood calculations which may be too computationally expensive to be practical.

The CMC method [Scott et al., 2013] proposes to reduce these costs by randomly partitioning the sample into \( K \) batches (i.e. \( \vec{y}_N = \bigcup_{j=1}^{K} \vec{y}^{(j)} \)) and independently distributing each batch to a worker to perform MCMC sampling on the corresponding sub-posterior. More precisely, the \( j \)-th worker (\( j = 1, ..., K \)) will generate samples from the \( j \)-th sub-posterior distribution defined as:

\[
\pi_{j,Cons}(\theta|\vec{y}^{(j)}) \propto f(\vec{y}^{(j)}|\theta)p(\theta)^{1/K}.
\]
Note that the prior for each batch is considered to be \( p_j(\theta) = [p(\theta)]^{1/K} \) such that 
\[
    p(\theta) = \prod_{j=1}^{K} p_j(\theta)
\]
and thus the overall full-data unnormalized posterior distribution which we denote as \( \pi_{Full}(\theta|\vec{y}_N) \) is equal to the product of unnormalized sub-posterior distributions, i.e.
\[
    \pi_{Full}(\theta|\vec{y}_N) \propto \prod_{j=1}^{K} \pi_{j,Cons}(\theta|\vec{y}^{(j)}).
\]

Weighted averages of the sub-samples from all batches can be used as full-data posterior draws. That is, assuming \( \theta_1^{(k)}, ..., \theta_S^{(k)} \) are \( S \) sub-samples from the \( k \)th worker then the \( s \)-th approximate full posterior draw will be:
\[
    \theta_s = \left( \sum_k w_k \right)^{-1} \sum_k w_k \theta_s^{(k)}
\]
where the weights \( w_k = \Sigma_k^{-1} \) are optimal for Gaussian models with \( \Sigma_k = var(\theta|\vec{y}^{(k)}) \).

The fading effect of the modified prior \( p(\theta)^{1/K} \), especially when \( K \) is large, can lead to diminished efficiency in some models. In the next section we introduce an alternative method to define the sub-posteriors in each batch.

### 3 Likelihood Inflating Sampling Algorithm (LISA)

LISA is an alternative to CMC that still benefits from the random partition of the dataset followed by independently applying MCMC methods to each batch on a different worker. Assuming that the data have been divided into \( K \) batches (of approximately equal size), we define new sub-posterior distributions for each machine by adjusting the likelihood function without making changes to the prior. Thus the \( j \)-th sub-posterior distribution will be:
\[
    \pi_{j,LISA}(\theta|\vec{y}^{(j)}) \propto (f(\vec{y}^{(j)}|\theta))^K p(\theta).
\]
Since the data are assumed to be i.i.d., inflating the likelihood function is intuitive because the sub-posterior from each batch of data is a closer representation of the whole data posterior. We thus expect that the samples obtained by each worker will be closer to full posterior samples and thus improve the statistical efficiency of the Bayesian inference.

To ensure approximate full posterior draws, we propose to apply the importance re-sampling method. Given samples from $\pi_{j,LISA}(\theta | \tilde{y}^{(j)})$, we can simply re-sample $\theta^{(j)}_t$ from batch $j$, using weights:

$$w^{(j)}_t \propto \frac{\pi_{Full}(\theta^{(j)}_t | \tilde{y}_N)}{\pi_{j,LISA}(\theta^{(j)}_t | \tilde{y}^{(j)})}.$$

One may be concerned about the need to compute $\pi_{Full}(\theta^{(j)}_t | \tilde{y}_N)$, but in the next sections we will show that this step is unnecessary in many instances, including the important case of BART. Furthermore, we will prove in a theorem below that under mild conditions, LISA’s sub-posterior distributions are asymptotically closer to the full posterior than, for instance, those produced by CMC.

Using a Taylor expansion for $\log(\pi(\theta | y_n))$ around its posterior mode $\hat{\theta}_n$, we obtain

$$\log(\pi(\theta | y_n)) \approx \log(\pi(\hat{\theta}_n | y_n)) - \frac{1}{2}(\theta - \hat{\theta}_n)^T \hat{I}_n(\theta - \hat{\theta}_n)$$

where $\hat{I}_n = -\frac{\partial \log(\pi(\theta | y_n))}{\partial \theta \partial \theta} |_{\theta = \hat{\theta}_n}$ is the observed Fisher Information matrix. Exponentiating both sides yields

$$\pi(\theta | y_n) \approx \pi(\hat{\theta}_n | y_n)exp\left(\frac{1}{2}(\theta - \hat{\theta}_n)^T \hat{I}_n(\theta - \hat{\theta}_n)\right)$$

which shows asymptotic normality, i.e. $\pi(\theta | y_n) \overset{D}{\rightarrow} N(\hat{\theta}_n, \hat{I}_n^{-1})$ as $n \rightarrow \infty$. These simple considerations lead to the following theorem.

**Theorem 1.** Assume $\pi_{Full} \overset{D}{\rightarrow} N(\hat{\theta}_N, \hat{I}_N^{-1})$ and that asymptotically, both LISA and CMC’s sub-posterior distributions have the same mean and the same variance across all batches.
Then

\[ \pi_{i,\text{LISA}} \xrightarrow{D} N(\hat{\theta}_N, \hat{I}_N^{-1}) \quad \& \quad \pi_{i,\text{Cons}} \xrightarrow{D} N(\bar{\theta}_N, K\hat{I}_N^{-1}) \quad \forall \; i \in \{1, ..., K\} \]

**Proof.** See Appendix.

Theorem 1 states that LISA’s sub-posterior distributions are similar to the full posterior distribution, while CMC’s are over-dispersed. Hence, we expect that the sub-samples are asymptotically better approximations of full posterior samples than the ones generated by CMC.

In the next section we will illustrate LISA in a simple example and compare its performance to the full-data posterior sampling as well as CMC.

# 4 Motivating Examples

In this section we examine some simple examples where theoretical derivations can be carried out in detail. We emphasize the difference between LISA and CMC.

## 4.1 Bernoulli Random Variables

Consider \( y_1, ..., y_N \) to be \( N \) i.i.d. Bernoulli random variables with parameter \( \theta \) that is known to be small. Hence, let \( p(\theta) = \text{Beta}(a, b) \) with \( a << b \) to be the prior such that the full-data posterior will be \( \pi_{\text{Full}}(\theta | \underline{y}_N) = \text{Beta}(S + a, N - S + b) \) where \( S = \sum_{i=1}^{N} y_i \) is the total number of ones. Suppose we divide the data into \( K \) batches with \( S_k \) number of ones in batch \( k \), such that \( S_k = S/K \), i.e. the number of 1’s are divided equally between batches. Then the \( k^{th} \) sub-posterior based on batch-data of size \( n = N/K \) for each method will be:
CMC:

\[
\pi_{k,\text{Cons}}(\theta|\vec{y}^{(k)}) \sim \text{Beta}\left( \frac{S}{K} + \frac{a - 1}{K} + 1, \frac{N - S}{K} + \frac{b - 1}{K} + 1 \right)
\]

LISA:

\[
\pi_{k,LISA}(\theta|\vec{y}^{(k)}) \sim \text{Beta}(S_k K + a, (n - S_k) K + b) = \text{Beta}(S + a, N - S + b)
\]

which implies

\[
\pi_{k,LISA}(\theta|\vec{y}^{(k)}) = \pi_{\text{Full}}(\theta|\vec{y}_N).
\]

As it is seen, LISA’s sub-posterior distribution is equal to the full posterior distribution when the number of 1’s are equally grouped across all batches. Thus, LISA’s sub-samples are retained as samples from the full posterior under the importance re-sampling approach. On the other hand, since it is possible for \(K\) to be large enough and much larger than \(S\), CMC sub-posterior distributions will have equivalent distribution to Beta(1, 1) which is U(0,1). The true full posterior \(\pi_{\text{Full}}(\theta|\vec{y}_N)\) will be difficult to recover based on a large set draws from uniform distributions.

In the next section, we will apply LISA to a Bayesian Linear Regression model and discover that with a minor modification we can generate exact posterior samples by employing a weighted average approach to sub-samples. We will describe this result in a theorem which we will find useful for the remaining part of this paper.

### 4.2 Bayesian Linear Regression

Consider a standard linear regression model:

\[
y = X\beta + \epsilon
\]
where $\beta$ is a $p \times 1$ vector and $y$ is a $N \times 1$ vector with $\epsilon \sim N(0, \sigma^2 I_N)$. In a Bayesian framework, define conjugate priors as:

\[
p(\beta | \sigma^2) \sim N(\mu_0, \sigma^2 \Omega_0^{-1}), \quad p(\sigma^2) \sim Inv - Gamma(a_0, b_0).
\]

Hence the full posterior distribution will have the following expression:

\[
p(\beta, \sigma^2 | y, X) \propto p(y | X, \beta, \sigma^2) \cdot p(\beta | \sigma^2) \cdot p(\sigma^2) \\
\propto (\sigma^2)^{-N/2} \exp\left( -\frac{1}{2\sigma^2} (y - X\beta)^T (y - X\beta) \right) \\
\times (\sigma^2)^{-p/2} \exp\left( -\frac{1}{2\sigma^2} (\beta - \mu_0)^T \Omega_0 (\beta - \mu_0) \right) \\
\times (\sigma^2)^{-a_0 - 1} \exp\left( -\frac{b_0}{\sigma^2} \right)
\]

with conditional distributions given as:

\[
p(\beta | \sigma^2, y, X) \sim N(\mu_N, \sigma^2 \Omega_N^{-1}) \\
p(\sigma^2 | \beta, y, X) \sim Inv - Gamma(a_N, b_N),
\]

where

\[
\begin{aligned}
\Omega_N &= X^T X + \Omega_0 \\
\mu_N &= \Omega_N^{-1} (X^T X \hat{\beta} + \Omega_0 \mu_0) = \Omega_N^{-1} (X^T y + \Omega_0 \mu_0)
\end{aligned}
\]

and

\[
\begin{aligned}
a_N &= a_0 + \frac{N + p}{2} \\
b_N &= b_0 + \frac{1}{2} \left( (y - X\beta)^T (y - X\beta) + (\beta - \mu_0)^T \Omega_0 (\beta - \mu_0) \right).
\end{aligned}
\]

Using Gibbs sampling one can draw posterior draws of $\beta$ and $\sigma^2$ using the conditional distributions described in (1) and (2). However, since the main goal is prediction, we
focus the discussion on the posterior samples for $\beta$. Assume the data has been randomly divided into $K$ batches with $(X_k, y_k)$ representing the data in batch $k$ and $n$ denoting the number of observations in each batch ($n \approx N/K$). Thus, LISA’s conditional distribution of $\beta$ from batch $k$ will be:

$$p_L(\beta|\sigma^2, y_k, X_k) \sim N(\mu_{n,L}^{(k)}, \sigma^2 \Omega_{n,L}^{(k)})^{-1}$$

where

$$\begin{align*}
\Omega_{n,L}^{(k)} &= K X_k^T X_k + \Omega_0 = K(X_k^T X_k + \Omega_0/K) = K(X_k^T X_k + \Omega_0^*) \\
\mu_{n,L}^{(k)} &= \Omega_{n,L}^{(k)}^{-1} (K X_k^T y_k + \Omega_0 \mu_0) \\
&= \frac{1}{K} (X_k^T X_k + \Omega_0^*)^{-1} K (X_k^T y_k + \Omega_0 \mu_0/K) \\
&= (X_k^T X_k + \Omega_0^*)^{-1} (X_k^T y_k + \Omega_0^* \mu_0)
\end{align*}$$

(3)

Comparing (1) to (3), we can find similarities between LISA’s sub-posterior distributions and the original posterior distributions of each batch-data (which we call ”BatchSingleMachine”). Let $\mu_n^{(k)}$ and $\Omega_n^{(k)}$ denote the parameters for the conditional distribution of $\beta$ in BatchSingleMachine. Hence comparing to LISA, we have:

$$\begin{align*}
\Omega_{n,L}^{(k)} &= K \Omega_n^{(k)} \\
\mu_{n,L}^{(k)} &= \mu_n^{(k)}
\end{align*}$$

implying

$$p_L(\beta|\sigma^2, y_k, X_k) \sim N(\mu_n^{(k)}, \frac{\sigma^2}{K} \Omega_n^{(k)})^{-1}$$

(4)

As it is clear from (4), LISA has smaller residuals compared to BatchSingleMachine. We will show in the following theorem that with minor changes to the residuals in LISA,
we can achieve exact posterior samples by taking weighted averages of the sub-samples.

**Theorem 2.** Consider applying LISA to a Bayesian Linear Regression model. If the variance of the data in each batch is corrected by a factor of $K$ then a weighted average combination of LISA’s sub-samples will have as distribution the full posterior.

**Proof.** In the weighted average approach, we define the weights to be the inverse variance from each batch ($\Sigma_k^{-1}$). Since in this model, LISA’s sub-posterior distributions are normally distributed, taking weighted averages of sub-samples will also result in a normal distribution with mean and variance as calculated below (without any adjustments):

$$
\mu^* = \Sigma^*(\Sigma_1^{-1}\mu_1 + \ldots + \Sigma_K^{-1}\mu_K)
$$

$$
= \Sigma^*(\frac{1}{\sigma^2}\Omega_{n,L}^{(1)}\mu_{n,L}^{(1)} + \ldots + \frac{1}{\sigma^2}\Omega_{n,L}^{(K)}\mu_{n,L}^{(K)})
$$

$$
= \Sigma^*(\frac{K}{\sigma^2}\Omega_n^{(1)}\mu_n^{(1)} + \ldots + \frac{K}{\sigma^2}\Omega_n^{(K)}\mu_n^{(K)})
$$

$$
= \Sigma^*(\frac{K}{\sigma^2}(X_1^T y_1 + \Omega_0^*\mu_0) + \ldots + \frac{K}{\sigma^2}(X_K^T y_K + \Omega_0^*\mu_0))
$$

$$
= \Sigma^*(\frac{K}{\sigma^2}(X^T y + \Omega_0\mu_0))
$$

$$
= \frac{\sigma^2}{K}\Omega_N^{-1}\left(\frac{K}{\sigma^2}(X^T y + \Omega_0\mu_0)\right)
$$

implying that

$$
\mu^* = \Omega_N^{-1}((X^T y + \Omega_0\mu_0)) = \mu_N.
$$

(5)
Similarly,

\[ \Sigma^* = \left( \Sigma_1^{-1} + \ldots + \Sigma_K^{-1} \right)^{-1} \]

\[ = \left( \frac{1}{\sigma^2} \Omega_{n,L}^{(1)} + \ldots + \frac{1}{\sigma^2} \Omega_{n,L}^{(K)} \right)^{-1} \]

\[ = \left( \frac{K}{\sigma^2} \Omega_n^{(1)} + \ldots + \frac{K}{\sigma^2} \Omega_n^{(K)} \right)^{-1} \]

\[ = \left( \frac{K}{\sigma^2} (X_1^T X_1 + \Omega_0^*) + \ldots + \frac{K}{\sigma^2} (X_K^T X_K + \Omega_0^*) \right)^{-1} \]

\[ = \left( \frac{K}{\sigma^2} (X^T X + K\Omega_0^*) \right)^{-1} \]

yielding

\[ \Sigma^* = \left( \Sigma_1^{-1} + \ldots + \Sigma_K^{-1} \right)^{-1} = \frac{\sigma^2}{K} (X^T X + \Omega_0)^{-1} = \frac{\sigma^2}{K} \Omega_N^{-1}. \]  \( (6) \)

Thus, LISA’s combined posterior distribution is \( \beta | \sigma^2, X, y \sim N(\mu_N, \frac{\sigma^2}{K} \Omega_N^{-1}) \). Comparing this to the full posterior distribution, \( N(\mu_N, \sigma^2 \Omega_N^{-1}) \), we see that they are almost identical except that LISA has smaller variance by a factor of \( K \) (similar to its difference with BatchSingleMachine). Hence, adjusting \( \sigma^2 \rightarrow K \sigma^2 \), the variance will balance up to the variance of the full posterior distribution.

In the next section, we will examine LISA’s performance on a more complex model, the Bayesian Additive Regression Trees (BART), which will be our main focus in this paper. We will see similarities between applying LISA to BART and the Bayesian Linear Regression model. Hence the theorem stated in the previous section will play an important role in LISA’s implementation for BART.
5 Bayesian Additive Regression Trees (BART)

Consider the nonparametric regression model:

\[ y_i = f(x_i) + \epsilon_i \quad , \quad \epsilon_i \sim N(0, \sigma^2) \quad i.i.d. \]

where \( x_i = (x_{i1}, ..., x_{ip}) \) is a \( p \)-dimensional vector of inputs and \( f \) is approximated by a sum of \( m \) regression trees:

\[ f(x) \approx \sum_{j=1}^{m} g(x; T_j, M_j) \]

where \( T_j \) denotes a binary tree consisting of a set of interior node decision rules and a set of terminal nodes. \( M_j = \{\mu_{1j}, ..., \mu_{bj}\} \) is the set of parameter values associated with each \( b \) terminal nodes of \( T_j \). In addition, \( g(x; T_j, M_j) \) is the function that maps each \( x \) to a \( \mu_{ij} \in M_j \). Thus the regression model is approximated by a sum-of-trees model:

\[ y_i = \sum_{j=1}^{m} g(x_i; T_j, M_j) + \epsilon_i \quad , \quad \epsilon_i \sim N(0, \sigma^2) \quad i.i.d. \]

Let \( \tilde{\theta} := ((T_1, M_1), ..., (T_m, M_m), \sigma^2) \) denote the vector of model parameters. Below, we have briefly described the prior specifications stated in Chipman et al. (2010) and Chipman et al. (1998).

Prior Specifications:

- Prior Independence and Symmetry:

\[ p((T_1, M_1), ..., (T_m, M_m), \sigma) = \left[ \prod_j p(M_j|T_j)p(T_j) \right] p(\sigma) \]

where \( p(M_j|T_j) = \prod_i p(\mu_{ij}|T_j) \).

13
• Recommended number of trees: \( m=200 \) (Chipman et al. (2010)) and \( m=50 \) (Kapeler and Bleich (2013))

• Tree prior \( p(T_j) \), is characterised by three aspects:

  1. The probability that a node at depth \( d = 0, 1, \ldots \) is non-terminal, which is assumed to have the form \( \alpha(1 + d)^{-\beta} \), where \( \alpha \in (0, 1) \) and \( \beta \geq 0 \). (recommended values are \( \alpha = 0.95 \) and \( \beta = 2 \))

  2. The distribution on the splitting variable assignments at each interior node which is recommended to have a uniform distribution.

  3. The distribution on the splitting rule assignment in each interior node, conditional on the splitting variable which is also recommended to have a uniform distribution.

• The conditional prior for \( \mu_{ij} \) is considered as \( p(\mu_{ij}|T_j) \sim N(\mu, \sigma_\mu^2) \) such that:

\[
\begin{cases} 
  m\mu - k\sqrt{m}\sigma_\mu = y_{min} \\
  m\mu + k\sqrt{m}\sigma_\mu = y_{max}
\end{cases}
\]

with \( k = 2 \) recommended.

• The prior for \( \sigma^2 \) is considered as \( \sigma^2 \sim Inv-Gamma (\nu, \nu\lambda) \) where \( \nu = 3 \) is recommended and \( \lambda \) is chosen such that \( p(\sigma < \hat{\sigma}) = q \) with recommended \( q = 0.9 \) and sample variance \( \hat{\sigma} \).
Hence the posterior distribution will have the form:

\[
\pi(\bar{\theta}) = \pi(\bar{\theta}|Y, X) \propto \frac{1}{\text{Likelihood}} \times \frac{1}{\text{Prior of } \sigma^2}
\]

\[
\left[ (\sigma^2)^{-\frac{n}{2}} e^{-\frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - \sum_{j=1}^{m} g(x_i; M_j, T_j))^2} \right] \times \left[ \left( \sigma^2 \right)^{-\frac{\nu}{2} - 1} e^{-\frac{\nu\lambda}{2\sigma^2}} \prod_{j=1}^{m} \sigma_\mu^{-b_j} (2\pi)^{-\frac{b_j}{2}} e^{-\frac{1}{2\sigma_\mu^2} \sum_{k=1}^{b_j} (\mu_{kj} - \mu_{\bar{\mu}})^2} p(T_j) \right].
\]  

(7)

Gibbs Sampling is used to sample from this posterior distribution. The algorithm iterates between the following steps:

- \( \sigma^2 \mid (T_1, M_1), \ldots, (T_m, M_m), Y, X \propto \text{Inv - Gamma}(\rho, \gamma) \)
  where \( \rho = \frac{\nu + n}{2} \) and \( \gamma = \frac{1}{2} \left[ \sum_{i=1}^{n} (y_i - \sum_{j=1}^{m} g(x_i; M_j, T_j))^2 + \lambda \nu \right] \).

- \( (T_j, M_j) \mid T_{(j)}, M_{(j)}, \sigma, Y, X \) which is the same as drawing from the conditional \( (T_j, M_j) \mid R_j, \sigma \) where \( T_{(j)} \) denotes all trees except the \( j \)-th tree, and residual \( R_j \) is defined as:

\[
R_j = g(x_i; M_j, T_j) + \epsilon = y - \sum_{k \neq j} g(x; M_k, T_k).
\]

This is equivalent to the following two steps:

1. \( T_j \mid R_j, \sigma \)
2. \( M_j \mid T_j, R_j, \sigma \implies \)

\[
\mu_{ij} \mid T_j, R_j, \sigma \sim N \left( \frac{\sigma^2}{\sigma_\mu^2} \mu_{\bar{\mu}} + \frac{n_i \bar{R}_{j(i)}}{\sigma^2}, \frac{\sigma^2}{\sigma_\mu^2} + \frac{1}{n_i} \right)
\]

where \( \bar{R}_{j(i)} \) denotes the average residual (computed without tree \( j \)) at terminal node \( i \) with total number of observations \( n_i \).
The density in $1$ can be expressed as:

$$p(T_j \mid R_j, \sigma) \propto p(T_j) \int p(R_j \mid M_j, T_j, \sigma) \: p(M_j \mid T_j, \sigma) \: dM_j$$  \hspace{1cm} (8)

Metropolis-Hastings (MH) algorithm is then applied to draw $T_j$ from (8) with four different proposal moves on trees:

- **GROW**: growing a terminal node (with probability 0.25)
- **PRUNE**: pruning a pair of terminal nodes (with probability 0.25)
- **CHANGE**: changing a non-terminal rule (with probability 0.4) (Kapelner and Bleich (2013) change rules only for parent nodes with terminal children)
- **SWAP**: swapping a rule between parent and child (with probability 0.1) (This proposal move was removed by Kapelner and Bleich (2013))

Detailed derivations involving the Metropolis-Hastings acceptance ratios are described in the Appendix.

Two existing packages in R called "BayesTree" and "bartMachine" can be used to run BART on any dataset, but as the sample size increases, these packages tend to run slower. In these situations we expect methods such as LISA to become useful, and for a fair illustration of the advantages gained we have used our own R implementation of BART and applied the same structure to implement LISA and CMC algorithm for BART. The Metropolis-Hastings acceptance ratios for LISA and CMC are also explained in Appendix. The following sub-section discusses the results of LISA and CMC applied to a simulated dataset.
5.1 A Numerical Experiment

We have simulated a 20,000 dataset from Friedman’s test function \cite{Friedman1991}:

\[
f(x) = 10 \sin(\pi x_1 x_2) + 20(x_3 - 0.5)^2 + 10x_4 + 5x_5
\]

where \( x = (x_1 : x_{10}) \) are simulated independently from a \( Uniform(0,1) \) and \( y \sim N(f(x), \sigma^2) \) with \( \sigma^2 = 9 \). Applying BART to this simulated dataset will generate posterior draws of \((T, M, \sigma^2)\) which equivalently produces posterior draws for \( f(x) \) using the approximation \( \hat{f}(x) \approx \sum_{j=1}^{m} g(x; \hat{T}_j, \hat{M}_j) \) for each \( x \). So one can compute the prediction root mean squared error (RMSE) using average posterior draws of \( \hat{f}(x) \) for each \( x \) as \( \hat{y} \) to measure its performance, i.e. prediction RMSE = \( \sqrt{\frac{1}{N} \sum_{i=1}^{N} (y_i - \hat{y}(x_i))^2} \).

As stated by \cite{Scott2013}, the CMC algorithm fails to draw true posterior samples of BART due to its over-dispersed posterior distribution. Thus, for comparison reasons, we applied both LISA and CMC to BART using the simulated dataset with \( K = 30 \) batches. We observed that most of the importance re-sampling weights in LISA vanish to zero, which indicates that these weights are not a good choice in BART. Moreover, as stated in Theorem 1, since LISA’s sub-posterior distributions are asymptotically equivalent to the full posterior distribution, we also examined applying uniform weights as well as a weighted average combination of LISA’s sub-samples from all batches. We will see further that both weighting schemes produced higher prediction accuracy compared to CMC. However, they all perform poorly in generating true posterior samples as they produce larger trees with biased estimates for \( \sigma^2 \). Specifically, both CMC and LISA with uniform weights generate over-dispersed posterior distributions.
5.2 Modified LISA for BART

The under estimation of $\sigma^2$ when applying LISA to BART is similar to the problem encountered when using LISA for the linear regression model discussed in Section 4.2. This is a coincidence since BART is also a linear regression model, albeit one where the set of independent variables is determined through a highly sophisticated process. We will show below that when applying a similar variance adjustment to the one stated in Theorem 2, the Modified LISA (modLISA) for BART will no longer require importance sampling and will exhibit superior computational and statistical efficiency compared to either LISA or CMC.

Just like in the regression model we “correct” the sampling algorithm by adjusting the residual variance. We start with the conditional distribution of tree $j$ from expression (8) which takes the form

$$p(T_j \mid R_j, \sigma) \propto p(T_j) \int p(R_j \mid M_j, T_j, \sigma) p(M_j \mid T_j, \sigma) \, dM_j.$$  

Note that the only part of this distribution that is effected by LISA is from the conditional distribution of the residuals, $R_j \mid M_j, T_j, \sigma$. Thus, the Metropolis-Hastings acceptance ratios for tree proposals consists of three parts: the transition ratio, the likelihood ratio and the tree structure ratio. The likelihood ratio is constructed from the conditional distributions of residuals which is effected by LISA. Consider the likelihood ratio for GROW proposal in LISA (full details are presented in the Appendix)

$$\frac{P(R \mid T_*, \sigma^2)}{P(R \mid T, \sigma^2)} = \sqrt{\frac{\sigma^2(\sigma^2 + Kn_l \sigma^2_{\mu})}{(\sigma^2 + Kn_l \sigma^2_{\mu})(\sigma^2 + Kn_r \sigma^2_{\mu})}} \times \exp \left( \frac{K^2 \sigma^2_{\mu} \left[ \left( \sum_{i=1}^{n_l} R_{l,i} \right)^2 + \left( \sum_{i=1}^{n_r} R_{r,i} \right)^2 \right]}{2 \sigma^2 \left[ \sigma^2 + Kn_l \sigma^2_{\mu} \right]} - \left( \sum_{i=1}^{n_l} R_{l,i} \right)^2 \right) \right) \left( \frac{\sigma^2}{\sigma^2 + Kn_l \sigma^2_{\mu}} \right) \left( \frac{\sigma^2}{\sigma^2 + Kn_r \sigma^2_{\mu}} \right)$$  

(9)
where \( n_l \) is the total number of observations from batch-data that end up in terminal node \( l \). The new grown tree, \( T_* \), splits terminal node \( l \) to two terminal nodes (children) \( l_L \) and \( l_R \), which will also divide \( n_l \) to \( n_{l_L} \) and \( n_{l_R} \) which are the corresponding number of observations in each new terminal node. By factoring out \( K \) in (9), we can re-write it as:

\[
\frac{P(R | T_* , \sigma^2)}{P(R | T, \sigma^2)} = \sqrt{\frac{\sigma^2 (\frac{\sigma^2}{K} + n_l \sigma^2)}{(\frac{\sigma^2}{K} + n_{l_L} \sigma^2) (\frac{\sigma^2}{K} + n_{l_R} \sigma^2)}} \times \exp \left( \frac{\sigma^2}{2 \sigma^2} \left[ \frac{(\sum_{i=1}^{n_{l_L}} R_{l_L,i})^2}{\frac{\sigma^2}{K} + n_{l_L} \sigma^2} + \frac{(\sum_{i=1}^{n_{l_R}} R_{l_R,i})^2}{\frac{\sigma^2}{K} + n_{l_R} \sigma^2} - \frac{(\sum_{i=1}^{n_l} R_{l,i})^2}{\frac{\sigma^2}{K} + n_l \sigma^2} \right] \right) \tag{10}
\]

Expression (10) in LISA is equivalent to BatchSingleMachine except for the smaller variance considered for the conditional distribution of residuals (\( \frac{\sigma^2}{K} \)), while in BatchSingleMachine each residual has conditional distribution given as \( R_j | M_j , T_j , \sigma \sim N(g(.; M_j, T_j), \sigma^2) \).

Hence, to preserve consistency and achieve similar variance for residuals as in BatchSingleMachine, we will also need to modify LISA for BART by changing \( \sigma^2 \rightarrow K \sigma^2 \) when updating trees and then taking a weighted average combination of sub-samples (similar to Bayesian linear regression – Theorem 2). Note that in modified LISA (modLISA), we don’t apply any changes in updating \( \sigma^2 \), i.e. we keep the same conditional distribution as in LISA:

\[
\sigma^2 \mid (T_1, M_1), \ldots, (T_m, M_m), y_k, X_k \propto Inv - Gamma(\rho, \gamma)
\]

where \( \rho = \frac{\nu + Kn}{2} \) and \( \gamma = \frac{1}{2} \left[ K \sum_{i=1}^{n} (y_{(k)} - \sum_{j=1}^{m} g(x_{(k)}; M_j, T_j))^2 + \lambda \nu \right] \). This is obviously different from the conditional distribution of \( \sigma^2 \) in BatchSingleMachine where there is no \( K \). All our numerical experiments show that, despite this difference, modLISA will still generate accurate predictions and the modification corrects the bias in the posterior draws of \( \sigma^2 \) and properly calibrates the size of the trees.
Table 1: Comparing training data prediction RMSE, average test data prediction RMSE from 5-fold cross-validation, average post burn-in $\hat{\sigma}^2$, and tree sizes in each method for $K = 30$ to SingleMachine BART.

<table>
<thead>
<tr>
<th>Method</th>
<th>Train Pred.RMSE</th>
<th>Avg Test Pred.RMSE</th>
<th>Avg $\hat{\sigma}^2$</th>
<th>Tree Nodes</th>
</tr>
</thead>
<tbody>
<tr>
<td>$CMC$</td>
<td>0.48</td>
<td>4.13</td>
<td>1.44</td>
<td>611</td>
</tr>
<tr>
<td>$LISA \text{ wgh avg}$</td>
<td>1.26</td>
<td>3.44</td>
<td>0.001</td>
<td>54</td>
</tr>
<tr>
<td>$LISA \text{ (Unif wgh)}$</td>
<td>3.15</td>
<td>3.26</td>
<td>0.001</td>
<td>54</td>
</tr>
<tr>
<td>$modLISA \text{ wgh avg}$</td>
<td>3.04</td>
<td>3.07</td>
<td>7.94</td>
<td>7</td>
</tr>
<tr>
<td>$SingleMachine$</td>
<td>2.99</td>
<td>3.06</td>
<td>9.09</td>
<td>9</td>
</tr>
</tbody>
</table>

5.3 Modified LISA Simulations

5.3.1 Comparison of modLISA with Competing Methods

Table 1 shows the results from a 5000-iteration run with 1000 posterior samples of BART drawn from CMC, LISA weighted average, LISA with uniform weights, and modLISA weighted average with $K = 30$. These results are compared to the SingleMachine which runs BART on the full dataset using only one machine. The table is reporting two prediction RMSE for each method, one is related to the training data prediction RMSE with all 20,000 data used as the training set, and the other is the average prediction RMSE for test data from a 5-fold cross-validation (80% training, 20% test). As it is seen from Table 1, training prediction RMSE for CMC and LISA weighted average are significantly smaller than their average test prediction RMSE, which shows overfitting issues. However, LISA in general is performing better than CMC as its average test prediction RMSEs are lower. On the other hand, CMC, LISA weighted average and LISA with uniform weights, all under-estimate $\sigma^2$ and generate larger trees compared to SingleMachine. In conclusion, modLISA weighted average has the best performance in prediction RMSE as well as tree sizes and $\sigma^2$ estimates which are significantly closer to SingleMachine.

The main reason that trees grow large or balance up in different methods, can be seen in Table 2 which shows the average acceptance rates of each tree proposal move. As
seen in Table 2, CMC and LISA have significant difference in average acceptance rates between growing a tree and pruning one, which indicates why they generate larger trees. In addition, this difference is smaller in LISA which is why LISA generates smaller trees compared to CMC (0.5/1.8 ≈ 0.28 in LISA versus 0.03/21 ≈ 0.0014 in Consensus), while still having larger trees compared to SingleMachine. On the other hand, modLISA has overall larger acceptance rates with the smallest difference between growing and pruning compared to LISA and Consensus (20/26 ≈ 0.77 in modLISA is closer to 1) and a closer difference to SingleMachine (9/10 = 0.9). Overall, modLISA induced a significant reduction in tree sizes by preserving a balance between growing and pruning trees which also improves exploring the posterior distribution.

### 5.3.2 Comparison with SingleMachine BART

To investigate the closeness of posterior samples in each method to the benchmark, the SingleMachine BART, we have plotted the empirical distribution functions of \( \hat{f}(x) \) generated from each algorithm for four different observations in the dataset as shown in Figure 1. We can see that LISA with uniform weights, LISA with weighted average and CMC perform poorly as none of their distributions match the SingleMachine. In addition, the distributions from LISA with uniform weights and CMC look over-dispersed as they cover larger range of \( x \) values within \( F_n(x) \in (0, 1) \). However, indistinguishable empirical distribution functions are seen between modLISA weighted average and SingleMachine, which
Figure 1: Comparing empirical distribution functions of \( \hat{f}(x) \) in modLISA weighted average, Consensus, LISA weighted average, LISA (Unif weights) with \( K = 30 \), to SingleMachine BART for four different observations.

specifies the best performance among other methods.

In order to compute quantitative comparisons between sampling procedures, we propose to use the Cramér-von Mises criterion test statistic to measure the distance between two empirical distribution functions. This distance is defined to be

\[
\omega^2 = \int_{-\infty}^{\infty} (F_n(x) - F(x))^2 dF(x)
\]

where in our case we assume \( F(x) = F_{\text{BART}}(x) \) to be the empirical distribution function generated from posterior samples in SingleMachine BART and \( F_{\text{LISA}}(x) \) similarly generated from LISA (or any other alternative method that is considered for
comparison). Note that in all the following comparisons, $F_{BART}(x)$ will be our benchmark when comparing performances.

![Graphs showing fitted polynomial trends](image)

**Figure 2:** Blue lines: Fitted polynomial trends of average squared difference between empirical distribution functions for the SingleMachine and the following: (a) CMC, (b) LISA with weighted average, (c) LISA with uniform weights and (d) modLISA with weighted average. The difference is plotted against the mean prediction $\hat{f}(x)$ produced by SingleMachine. Grey areas represent the 95% credible intervals constructed based on 100 replicates.

We have computed the average squared difference between $F_{BART}(\cdot)$ and $F_{LISA}(\cdot)$ (and all other alternative methods) for each observation in the dataset as an estimation to the distance between the two distributions, i.e. $\hat{\omega}_{LISA}^2 = \frac{1}{T} \sum_{j=1}^{T} (F_{LISA}(t_j) - F_{BART}(t_j))^2$
where \( T = 1000 \) inner-interval points are equally distributed on the overall interval.

Figure 2 is comparing the fitted polynomial trends of \( \hat{\omega}^2 \) (for each method) versus mean predicted \( \hat{f}(x) \) in SingleMachine with their corresponding 95\% credible regions. Clearly in each plot, there are small variation around the trend with no significant changes in values of \( \hat{\omega}^2 \) among different mean predicted \( \hat{f}(x) \), which specifies consistency within different observations.

To emphasize the difference in performance between modLISA and its competitors, Figure 3 shows in a single plot all the fitted polynomial trends without the credible regions. One can see that there is a large gap between \( \hat{\omega}^2 \) values in modLISA weighted average and other alternative methods. The weighted average of samples produced by modLISA yields the closest results to SingleMachine. This can also be justified by comparing average \( \hat{\omega}^2 \) over all observations for each trend, which is calculated to be 0.013 for modLISA weighted average that is significantly smaller than 0.058, 0.056, and 0.047 for CMC, LISA weighted average, and LISA with uniform weights, respectively. Hence we conclude that modLISA weighted average generates true posterior draws of BART and has the best performance among its alternative methods.

At last we will compare run time per iteration for each method to conclude the most efficient method.

### 5.4 Run Time Comparisons

The main goal of methods such as LISA and CMC was to reduce run times regarding big data applications. Here we have compared average run times per iteration (from one processor) for each method using our implementation of BART.

As it is seen in Table 3, modLISA, LISA and CMC are all faster compared to SingleMachine since they are influenced by the smaller subsets of data used. However, since LISA and CMC generate much larger trees, they become slower compared to modLISA.
Figure 3: Comparing fitted polynomial trends of average squared difference in empirical distribution functions of each method and SingleMachine, as functions of mean predicted $\hat{f}(x)$ in SingleMachine.

which is the fastest method. We have also reported the speed-up percentages with respect to SingleMachine, which is defined to be $(1 - t/17.28) \times 100\%$ where $t$ is the average time per iteration in each method. Clearly, CMC has the least speed-up (31%) while modLISA has the highest (90%), which counts as the most computational efficient method.

In the next section we will apply modLISA weighted average BART to a real big dataset.
<table>
<thead>
<tr>
<th>Method</th>
<th>Avg Time per iteration (Secs)</th>
<th>Speed-up</th>
</tr>
</thead>
<tbody>
<tr>
<td>CMC</td>
<td>11.99</td>
<td>31%</td>
</tr>
<tr>
<td>LISA</td>
<td>5.04</td>
<td>71%</td>
</tr>
<tr>
<td>modLISA</td>
<td>1.81</td>
<td>90%</td>
</tr>
<tr>
<td>SingleMachine</td>
<td>17.28</td>
<td>——</td>
</tr>
</tbody>
</table>

Table 3: Run Time Comparisons.

5.5 Real Data Analysis

The American Community Survey (ACS) is a growing survey from the US Census Bureau and the Public Use Microdata Sample (PUMS) is a sample of responses to ACS which consists of various variables related to people and housing units (see US Bureau of Census 2013). Considering the person-level data from PUMS 2013, we would like to predict a person’s total income based on variables such as sex, age, education, class of worker, living state, and citizenship status. We have collected information related to people who are employed and have total income of at least $5000 with education level of either Bachelor’s degree, Master’s degree, or a PhD which resulted in total number of observations of 437,297. We randomly divided the dataset into approximately 80% for training and 20% for testing with $K = 100$ batches considered in splitting the training set to apply modLISA. Computations were performed on the GPC supercomputer at the SciNet HPC Consortium (Loken et al. 2010) using 100 cores, each running on 3,500 observations. Considering the logarithm of total income for each person as the response variable, we have ran modLISA weighted avg BART on this dataset for 2000 iterations and discarded the first 1000 draws which resulted in 1000 posterior samples. Table 4 is showing the results of prediction RMSE for test data as well as average post burn-in $\sigma^2$ estimates and tree sizes. Note that "BayesTree" and "bartMachine" packages in R are extremely slow on such large datasets, thus we have only applied our modLISA to examine prediction error and tree sizes. As seen in Table 4, prediction RMSE of test data is very
Table 4: Results of 1000 posterior samples generated from modLISA weighted average BART with K=100 on PUMS 2013 data.

<table>
<thead>
<tr>
<th>Method</th>
<th>Pred.RMSE (test data)</th>
<th>Avg $\sigma^2$</th>
<th>Tree Nodes</th>
<th>Speed-up</th>
</tr>
</thead>
<tbody>
<tr>
<td>modLISA weighted avg</td>
<td>0.71</td>
<td>48.8</td>
<td>7</td>
<td>90%</td>
</tr>
</tbody>
</table>

small which indicates high prediction accuracy. In addition, by running SingleMachine BART for only one iteration, we have computed a 90% speed-up of modLISA with respect to SingleMachine which emphasizes its computational efficiency. Furthermore, trees grow at a reasonable size which can be justified from Table 5 that shows sufficient acceptance rates for each proposal. Overall, although modLISA weighted avg BART may not be the best fit for the ACS dataset but it performed well in terms of prediction and generating trees as small as SingleMachine BART which indicates how powerful this method can be in reducing computational costs while producing accurate predictions.

<table>
<thead>
<tr>
<th>Method</th>
<th>GROW</th>
<th>PRUNE</th>
<th>CHANGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>modLISA</td>
<td>9%</td>
<td>12%</td>
<td>13%</td>
</tr>
</tbody>
</table>

Table 5: Average acceptance rates of tree proposal moves.

6 Bayesian Logistic Regression

Recall the Logistic Regression model:

$$\log\left(\frac{F(x_i)}{1-F(x_i)}\right) = x_i^T \beta, \quad i = 1, ..., N$$

where $F(x_i) = P(y_i = 1|x_i)$. Consider a Bayesian framework for Logistic Regression such that the prior for $\beta$ is gaussian, i.e. $\beta \sim N(0, \gamma I_p)$. We will use the ”BayesLogit” package in R (Polson et al., 2013) to generate posterior samples from a Bayesian Logistic
Regression model. We are also able to use this package to apply LISA and CMC with only minor adjustments to input variables of the package.

We have simulated a dataset of size \( N = 30,000 \) with true parameters \( \beta = (\beta_0, \beta_1, \beta_2, \beta_3, \beta_4) = (2, -5, 1.5, -2.97, 10) \) and \( p = 5 \) predictors that follow a multivariate normal distribution, \( X_{p \times 1} \sim N(0, \Sigma) \), where diagonal and off-diagonal elements of \( \Sigma \) equal to 1 and 0.3, respectively. We have applied LISA and CMC on this dataset with \( K = 30 \) batches.

Figure 4 is comparing the marginal posterior distribution in SingleMachine to all 30 marginal sub-posterior distributions in LISA and CMC for \( \hat{\beta}_3 \) and \( \hat{\beta}_4 \). As it is seen, sub-posterior distributions in LISA capture the correct variance while CMC sub-posterior distributions have significantly larger variance compared to LISA which justifies our statement of over-dispersed sub-posterior distributions in CMC (Theorem 1).

In addition, Figure 5 is comparing SingleMachine to combined marginal posterior distributions of \( \hat{\beta}_3 \) and \( \hat{\beta}_4 \) in each method. As it is observed, combining LISA’s sub-samples using importance re-sampling weights generates over-dispersed posterior distributions while CMC generates posterior distributions with correct variances. However, LISA with importance re-sampling weights captures a more accurate and less biased mean compared to CMC and SingleMachine. On the other hand, Figure 4 showed that despite the fact that some sub-posterior distributions in both CMC and LISA have biased mean, but overall sub-posterior distributions in LISA are better approximations than in CMC as they capture the correct variance. This indicates that on average LISA may perform better and hence, we have also examined the performance of LISA by taking simple averages as well as weighted averages of all sub-samples (without theoretical justifications). Clearly from Figure 5, LISA weighted average and LISA simple average have significantly smaller variance compared to SingleMachine, CMC and LISA importance re-sampling while still capturing the correct mean.

In Table 6, we have calculated the Mean Squared Error (MSE) for each parameter that results from 1000 posterior draws in each method. Interestingly, LISA simple average has
the lowest MSE in all parameters which indicates higher estimation accuracy among all other methods (including SingleMachine). In addition, LISA simple average also has the least running time per processor as shown in Table 6 which specifies high computational
efficiency with 97% speed-up compared to SingleMachine.

Overall, LISA’s sub-posterior distributions generate the same variance as the full posterior distribution while CMC’s sub-posterior distributions are over-dispersed. However, although LISA simple average generated accurate estimations with under-dispersed posterior distributions, there is still an open question of specifying a better weighting scheme to combine LISA’s sub-samples in Bayesian Logistic Regression such that a similar variance is achieved as in the full posterior distribution.

Table 6: Mean Squared Errors (MSE) & Run times

<table>
<thead>
<tr>
<th>Algorithms</th>
<th>MSE($\hat{\beta}_0$)</th>
<th>MSE($\hat{\beta}_1$)</th>
<th>MSE($\hat{\beta}_2$)</th>
<th>MSE($\hat{\beta}_3$)</th>
<th>MSE($\hat{\beta}_4$)</th>
<th>Time/proc.</th>
</tr>
</thead>
<tbody>
<tr>
<td>CMC</td>
<td>0.0015</td>
<td>0.0094</td>
<td>0.0022</td>
<td>0.0045</td>
<td>0.0244</td>
<td>1.64</td>
</tr>
<tr>
<td>LISA (impt w.)</td>
<td>0.0261</td>
<td>0.1125</td>
<td>0.0420</td>
<td>0.0351</td>
<td>0.3973</td>
<td>3.91</td>
</tr>
<tr>
<td>LISA (wght avg)</td>
<td>0.0044</td>
<td>0.0037</td>
<td>0.0050</td>
<td>0.0017</td>
<td>0.0399</td>
<td>1.64</td>
</tr>
<tr>
<td>LISA (smpl avg)</td>
<td>0.0012</td>
<td>0.0003</td>
<td>0.0013</td>
<td>0.0002</td>
<td>0.0045</td>
<td>1.55</td>
</tr>
<tr>
<td>SingleMachine</td>
<td>0.0114</td>
<td>0.0285</td>
<td>0.0084</td>
<td>0.0115</td>
<td>0.1569</td>
<td>51.48</td>
</tr>
</tbody>
</table>
7 Discussion

In this paper, we introduce a new method for Bayesian posterior sampling for big data. The aim is to reduce the computational costs by randomly splitting the data into groups of approximately the same size and drawing sub-samples from each group independently and in parallel on different machines. The main goals are to specify the sub-posterior distributions for each machine as well as a method for combining all sub-samples to perform approximate full posterior draws. We demonstrated that LISA’s sub-posterior distributions are asymptotically a better choice in terms of closeness to the full posterior distribution compared to the ones from CMC. We showed that there exists models where LISA can perform better compared to CMC. However the main focus of this paper was to examine and improve LISA on a complex and widely used model, BART.

We applied LISA to BART on a simulated dataset and observed higher prediction accuracy compared to the CMC. In addition, LISA generated smaller trees in BART which resulted as a computationally more efficient algorithm. Despite LISA’s better performance, LISA and CMC both generated over-dispersed posterior distributions of BART. Guided by a correction that can be theoretically justified in the Bayesian Linear Regression model, we modify LISA for BART. The modLISA performed significantly better in terms of accuracy, speed-up and generating posterior draws that are essentially as accurate as those produced by SingleMachine, but at a fraction of the computational cost. At last, we applied modLISA for BART to a real dataset which also resulted in a high prediction accuracy. Overall, modLISA can be used as a powerful method to apply to BART on big datasets with large savings of computational time.

At the end, we also applied LISA to a Bayesian Logistic Regression model and we found LISA’s sub-posterior distributions to be better approximations compared to CMC. An open question left for future work and the inquisitive reader is whether there are better combination methods for LISA’s sub-samples.
8 Acknowledgement

This work has been supported by NSERC of Canada grants to RVC and JSR.

References


A Appendix

A.1 Proof of Theorem 1

For simplicity, assume \( n = N/K \) is the number of observations in each batch and consider \( \theta \) to be a one-dimensional parameter. Denote \( \hat{\theta}_{n,L} \) as LISA’s sub-posterior mode–asymptotic mean– that is assumed to be the same in all batches (similarly \( \hat{\theta}_{n,C} \) for CMC). We will derive asymptotic distributions of LISA and CMC in terms of the full posterior.

- For LISA:

  We know that \( (\pi_{Full}(\theta|\vec{y}_N))^K \propto \prod_{i=1}^{K} \pi_{i,LISA}(\theta|\vec{y}^{(i)}) \), hence:

  \[
  \log(\pi_{Full}(\theta|\vec{y}_N)) = \frac{1}{K} \sum_{i=1}^{K} \log(\pi_{i,LISA}(\theta|\vec{y}^{(i)})) + c \tag{11}
  \]

  where \( c \) is a constant. This implies that

  \[
  \left. \log(\pi_{Full}(\theta|\vec{y}_N)) \right|_{\theta = \hat{\theta}_N} = \frac{1}{K} \sum_{i=1}^{K} \log(\pi_{i,LISA}(\hat{\theta}_N|\vec{y}^{(i)})) + c
  \]

  and

  \[
  \frac{1}{K} \sum_{i=1}^{K} \log(\pi_{i,LISA}(\hat{\theta}_N|\vec{y}^{(i)})) \leq \frac{1}{K} \sum_{i=1}^{K} \log(\pi_{i,LISA}(\hat{\theta}_{n,L}|\vec{y}^{(i)})) \tag{12}
  \]

  Inequality \( \text{(12)} \) is true since \( \hat{\theta}_{n,L} \) is the mode of \( \log(\pi_{i,LISA}) \) for all \( i \in \{1, ..., K\} \).

  Now from \( \text{(11)} \) and \( \text{(12)} \), we have:

  \[
  \left. \log(\pi_{Full}(\theta|\vec{y}_N)) \right|_{\theta = \hat{\theta}_N} \leq \log(\pi_{Full}(\theta|\vec{y}_N)) \left|_{\theta = \hat{\theta}_{n,L}} \right.
  \]

  \[
  \tag{13}
  \]
But since $\hat{\theta}_N$ is the full posterior mode:

$$\log\left(\pi_{Full}(\theta|\vec{y}_N)\right)_{\theta=\hat{\theta}_N} \geq \log\left(\pi_{Full}(\theta|\vec{y}_N)\right)_{\theta=\hat{\theta}_{n,L}}$$  \hspace{1cm} (14)$$

Hence from (13) and (14) we get

$$\log\left(\pi_{Full}(\theta|\vec{y}_N)\right)_{\theta=\hat{\theta}_N} = \log\left(\pi_{Full}(\theta|\vec{y}_N)\right)_{\theta=\hat{\theta}_{n,L}}$$

which implies

$$\hat{\theta}_N = \hat{\theta}_{n,L}$$  \hspace{1cm} (15)$$

To compute the observed Fisher Information matrix, take the second derivative with respect to $\theta$ from both sides of (11):

$$\frac{\partial^2}{\partial \theta^2} \log\left(\pi_{Full}(\theta|\vec{y}_N)\right)_{\theta=\hat{\theta}_N} = \frac{1}{K} \sum_{i=1}^{K} \frac{\partial^2}{\partial \theta^2} \log\left(\pi_{i,LISA}(\theta|\vec{y}^{(i)})\right)_{\theta=\hat{\theta}_N}$$

Since LISA’s asymptotic sub-posterior variances are assumed to be approximately equal in all batches, their observed Fisher Information matrices (at the mode) will also be equal. Hence using (15) we have:

$$\frac{1}{K} \sum_{i=1}^{K} \frac{\partial^2}{\partial \theta^2} \log\left(\pi_{i,LISA}(\theta|\vec{y}^{(i)})\right)_{\theta=\hat{\theta}_N} = \frac{1}{K} \sum_{i=1}^{K} \frac{\partial^2}{\partial \theta^2} \log\left(\pi_{i,LISA}(\theta|\vec{y}^{(i)})\right)_{\theta=\hat{\theta}_{n,L}} = \frac{1}{K} K \frac{\partial^2}{\partial \theta^2} \log\left(\pi_{i,LISA}(\theta|\vec{y}^{(i)})\right)_{\theta=\hat{\theta}_{n,L}} = \frac{\partial^2}{\partial \theta^2} \log\left(\pi_{i,LISA}(\theta|\vec{y}^{(i)})\right)_{\theta=\hat{\theta}_{n,L}} \forall \ i \in \{1, ..., K\}$$
Thus we get
\[
\frac{\partial^2}{\partial \theta^2} \log\left( \pi_{\text{Full}}(\theta|\bar{y}_N) \right) \bigg|_{\theta = \hat{\theta}_N} = \frac{\partial^2}{\partial \theta^2} \log\left( \pi_{\text{LISA}}(\theta|\bar{y}^{(i)}) \right) \bigg|_{\theta = \hat{\theta}_{n,L}} \quad \forall \ i \in \{1, ..., K\}
\]
which implies
\[
\hat{I}_{n,L}^{-1} = \hat{I}_N^{-1}, \quad (16)
\]
where \( \hat{I}_{n,L} \) is the observed Fisher Information in LISA.

• For CMC:

Since \( \pi_{\text{Full}}(\theta|\bar{y}_N) \propto \prod_{i=1}^{K} \pi_{i,\text{Cons}}(\theta|\bar{y}^{(i)}) \) we get
\[
\log\left( \pi_{\text{Full}}(\theta|\bar{y}_N) \right) = \sum_{i=1}^{K} \log\left( \pi_{i,\text{Cons}}(\theta|\bar{y}^{(i)}) \right) + c \quad (17)
\]
where \( c \) is a constant. Using an argument similar to the one in LISA derivations we obtain
\[
\log\left( \pi_{\text{Full}}(\theta|\bar{y}_N) \right) \bigg|_{\theta = \hat{\theta}_N} = \log\left( \pi_{\text{Full}}(\theta|\bar{y}_N) \right) \bigg|_{\theta = \hat{\theta}_{n,C}}
\]
which implies
\[
\hat{\theta}_N = \hat{\theta}_{n,C}. \quad (18)
\]

In addition, for comparing the observed Fisher Information matrices, we have:
\[
\frac{\partial^2}{\partial \theta^2} \log\left( \pi_{\text{Full}}(\theta|\bar{y}_N) \right) \bigg|_{\theta = \hat{\theta}_N} = \sum_{i=1}^{K} \frac{\partial^2}{\partial \theta^2} \log\left( \pi_{i,\text{Cons}}(\theta|\bar{y}^{(i)}) \right) \bigg|_{\theta = \hat{\theta}_N}
\]
and again since Consensus’s asymptotic sub-posterior variances are approximately equal in all batches, we can assume that their observed Fisher Information are also approximately equal (at the mode). Hence using (18):

\[
\sum_{i=1}^{K} \left. \frac{\partial^2}{\partial \theta^2} \log(\pi_{i,\text{Cons}}(\theta | \tilde{y}^{(i)})) \right|_{\theta = \hat{\theta}_N} = \sum_{i=1}^{K} \left. \frac{\partial^2}{\partial \theta^2} \log(\pi_{i,\text{Cons}}(\theta | \tilde{y}^{(i)})) \right|_{\theta = \hat{\theta}_{n,C}} = K \left. \frac{\partial^2}{\partial \theta^2} \log(\pi_{i,\text{Cons}}(\theta | \tilde{y}^{(i)})) \right|_{\theta = \hat{\theta}_{n,C}} \quad \forall \ i \in \{1, ..., K\}
\]

Then

\[
\left. \frac{\partial^2}{\partial \theta^2} \log(\pi_{\text{Full}}(\theta | \tilde{y}_N)) \right|_{\theta = \hat{\theta}_N} = K \left. \frac{\partial^2}{\partial \theta^2} \log(\pi_{i,\text{Cons}}(\theta | \tilde{y}^{(i)})) \right|_{\theta = \hat{\theta}_{n,C}} \quad \forall \ i \in \{1, ..., K\}
\]

implying

\[
\hat{I}^{-1}_{n,C} = K \hat{I}^{-1}_N
\]

where \(\hat{I}_{n,C}\) is the observed Fisher Information in CMC. Thus \(\forall \ i \in \{1, ..., K\}\):

\[
\pi_{i,\text{LISA}} \overset{D}{\rightarrow} N(\hat{\theta}_N, \hat{I}^{-1}_N)
\]
\[
\pi_{i,\text{Cons}} \overset{D}{\rightarrow} N(\hat{\theta}_N, K \hat{I}^{-1}_N).
\]

### A.2 BART

In this section we will use a similar explanation and notation given by Kapelner and Bleich (2013) to derive the acceptance ratios of the Metropolis-Hastings step in updating trees of BART. We will further extend these calculations for LISA and CMC.

Recall expression (8) which presents the target distribution that we are interested to
draw samples from, using the Metropolis-Hastings algorithm:

\[
p(T \mid R, \sigma) \propto p(T) \int p(R \mid M, T, \sigma) p(M \mid T, \sigma) \, dM
\]

Assume we propose \( T_* \), then the acceptance ratio will be:

\[
\begin{align*}
r &= \frac{P(T_* \rightarrow T)}{P(T \rightarrow T_*)} \times \frac{P(R \mid T_*, \sigma^2)}{P(R \mid T, \sigma^2)} \times \frac{P(T_*)}{P(T)}
\end{align*}
\]

We will calculate \( r \) for each possible proposal:

**GROW Proposal:**

- **Transition ratio:** Consider growing one of the \( b \) terminal nodes of tree \( T \), say node \( \eta \), to two children nodes. Then we will have:

\[
P(T \rightarrow T_*) = P(GROW) \, P(\text{choosing } \eta) \, P(\text{choosing a predictor to split on}) \cdot P(\text{choosing a splitting value})
\]

\[
= P(GROW) \frac{1}{b} \frac{1}{p(\eta)} \frac{1}{n_p(\eta)}
\]

where \( p(\eta) \) denotes the number of predictors left available to split on at node \( \eta \) (there must be at least two unique values in each predictor to consider), and \( n_p(\eta) \) denotes the number of unique splitting values left in the chosen \( p \)th attribute.

In addition, we have:

\[
P(T_* \rightarrow T) = P(PRUNE) \, P(\text{choosing } \eta \text{ to prune}) = P(PRUNE) \frac{1}{w_*}
\]

where \( w_* \) is the number of nodes with two terminal nodes in the new tree \( T_* \). Hence
the transition ratio will be:

\[
P(T_x \to T) \frac{P({\text{PRUNE}})}{w_*} = \frac{P(T \to T_*)}{P({\text{GROW}})} \frac{b \rho(\eta) n_{\eta}(\eta)}{w_*}
\]

- **Likelihood ratio:** For computing the likelihood ratio, we have:

\[
P(R_1, ..., R_n \mid T, \sigma^2) = \prod_{l=1}^{b} P(R_{l1}, ..., R_{ln_l} \mid \sigma^2)
\]

since the data are partitioned across all \(b\) terminal nodes of tree \(T\). \(R_{lj}\) denotes the \(j\)-th data (residual) in the \(l\)-th terminal node and \(n_l\) is the number of observations in the \(l\)-th terminal node. From BART we know that \(\mu_l \sim N(0, \sigma_\mu^2)\), hence we will have:

\[
P(R_{l1}, ..., R_{ln_l} \mid \sigma^2) = \int_{\mathbb{R}} P(R_{l1}, ..., R_{ln_l} \mid \mu_l, \sigma^2) P(\mu_l; \sigma_\mu^2) d\mu_l
\]

by completion of the square this will equal to:

\[
P(R_{l1}, ..., R_{ln_l} \mid \sigma^2) =
\]

\[
\frac{1}{(2\pi \sigma^2)^{n_l/2}} \sqrt{\frac{\sigma^2}{\sigma^2 + n_l \sigma_\mu^2}} \exp\left(-\frac{1}{2\sigma^2} \left[ \sum_{i=1}^{n_l} (R_{li} - \bar{R}_l)^2 - \frac{\bar{R}_l^2 n_l^2}{n_l + \sigma^2 / \sigma_\mu^2} + n_l \bar{R}_l^2 \right]\right) (20)
\]

where \(\bar{R}_l\) is the average residual at terminal node \(l\). Note that the likelihood is specified by all terminal nodes, and since \(T\) differs from \(T_x\) only at its \(l\)-th terminal node which splits into two terminal children \(l_L\) and \(l_R\), the probability terms from other terminal nodes will be canceled in the likelihood ratio which results in (using
\[
\frac{P(R | T_*, \sigma^2)}{P(R | T, \sigma^2)} = \sqrt{\frac{\sigma^2 (\sigma^2 + n_l \sigma^2)}{(\sigma^2 + n_l \sigma^2 \mu^2)} \times \exp \left( \frac{\sigma^2 \mu^2}{2\sigma^2} \left[ \frac{\left( \sum_{i=1}^{n_l} R_{L,i} \right)^2}{\sigma^2 + n_l \sigma^2 \mu^2} + \frac{\left( \sum_{i=1}^{n_R} R_{R,i} \right)^2}{\sigma^2 + n_R \sigma^2 \mu^2} - \frac{\left( \sum_{i=1}^{n_l} R_{i} \right)^2}{\sigma^2 + n_l \sigma^2 \mu^2} \right] \right) \}
\]

(21)

where \( R_{lL} \) and \( R_{lR} \) are residuals in the left and right child (respectively) with corresponding number of observations \( n_{lL} \) and \( n_{lR} \).

- **Tree Structure ratio:** Recall the descriptions given in BART related to the probability that node \( \eta \) at depth \( d_\eta \) is non-terminal:

\[
P_{\text{Split}}(\eta) = \frac{\alpha}{(1 + d_\eta)^\beta}
\]

with probability of assigning a rule given as:

\[
P_{\text{Rule}}(\eta) = \frac{1}{p(\eta) n_p(\eta)}
\]

Hence, the prior on each tree will be:

\[
P(T) = \prod_{\eta \in \text{non-terminal nodes}} P_{\text{Split}}(\eta) P_{\text{Rule}}(\eta) \times \prod_{\eta \in \text{terminal nodes}} (1 - P_{\text{Split}}(\eta))
\]

which will result in the following tree structure ratio:

\[
\frac{P(T_*)}{P(T)} = \alpha \frac{(1 - \frac{\alpha}{(2 + d_\eta)^\beta})^2}{((1 + d_\eta)^\beta - \alpha) p(\eta) n_p(\eta)}
\]

(22)
**PRUNE Proposal:**

- **Transition ratio:** A similar description as in the GROW step will lead to:

\[
\frac{P(T_* \rightarrow T)}{P(T \rightarrow T_*)} = \frac{P(GROW)}{P(PRUNE)} \frac{w}{(b-1) p(\eta^*) n_p(\eta^*)}
\]

where \(w\) is the number of nodes with two terminal nodes in tree \(T\). Note that tree \(T_*\) has one less terminal nodes \((b - 1)\).

- **Likelihood ratio:** This is the inverse of the likelihood ratio in the GROW proposal.

- **Tree Structure ratio:** This is also the inverse of the tree structure in the GROW proposal.

**CHANGE Proposal:**

- **Transition ratio:** As described by Kapelner and Bleich (2013), for simplicity, we will only change the rule assignments for nodes with two terminal children. Hence:

\[
P(T \rightarrow T_*) = P(CHANGE) P(\text{choosing } \eta) P(\text{choosing a predictor to split on}) \times P(\text{choosing a splitting value})
\]

with the first three terms canceling in the transition ratio given as:

\[
\frac{P(T_* \rightarrow T)}{P(T \rightarrow T_*)} = \frac{n_p(\eta^*)}{n_p(\eta)}
\]

- **Likelihood ratio:** \(T_*\) differs from \(T\) only from the two terminal children effected by the changed rules from their parents. Hence, by canceling the probabilities from
other terminal nodes, we will achieve the likelihood ratio:

\[
\frac{P(R \mid T_*, \sigma^2)}{P(R \mid T, \sigma^2)} = \sqrt{\frac{(\frac{\sigma^2}{\sigma_1^2} + n_1)(\frac{\sigma^2}{\sigma_2^2} + n_2)}{(\frac{\sigma^2}{\sigma_1^2} + n_1^*)((\frac{\sigma^2}{\sigma_2^2} + n_2^*)}} \times
\exp\left(\frac{1}{2\sigma^2} \left[ \left(\sum_{i=1}^{n_1^*} R_{1,i}^*\right)^2 - \left(\sum_{i=1}^{n_1} R_{1,i}\right)^2 \right] - \left(\sum_{i=1}^{n_2^*} R_{2,i}^*\right)^2 - \left(\sum_{i=1}^{n_2} R_{2,i}\right)^2 \right) \right)
\]

(23)

where subscripts 1 and 2 denote the two terminal children, while the asterisk refers to the proposed tree \(T_*\).

- **Tree Structure ratio:** Following the definition of \(P(T)\), we will have:

\[
\frac{P(T_*)}{P(T)} = \frac{n_p(\eta)}{n_{p^*}(\eta^*)}
\]

Note that:

\[
\frac{P(T_* \rightarrow T)}{P(T \rightarrow T_*)} \times \frac{P(T_*)}{P(T)} = 1
\]

### A.3 LISA for BART

**GROW Proposal:**

- **Transition ratio:** No change.
Likelihood ratio: Equation (20) changes to:

\[
P(R_{l_1}, ..., R_{l_n} \mid \sigma^2) =
\]

\[
\frac{1}{(2\pi \sigma^2)^{n_l/2}} \sqrt{\frac{\sigma^2}{\sigma^2 + K n_l \sigma^2_\mu}} \exp\left(-\frac{K}{2\sigma^2} \left[ \sum_{i=1}^{n_l} (R_{l_i} - \bar{R}_l)^2 - \frac{K \bar{R}_l^2}{Kn_l + \frac{\sigma^2}{\sigma^2_\mu}} + n_l \bar{R}_l^2 \right]\right)
\]

Thus the likelihood ratio will change to:

\[
\frac{P(R \mid T_*, \sigma^2)}{P(R \mid T, \sigma^2)} = \sqrt{\frac{\sigma^2(\sigma^2 + K n_l \sigma^2_\mu)}{(\sigma^2 + K n_{L_l} \sigma^2_\mu)(\sigma^2 + K n_{R_l} \sigma^2_\mu)}} \times
\]

\[
\exp\left(\frac{K^2 \sigma^2_\mu}{2\sigma^2} \left[ \frac{(\sum_{i=1}^{n_{L_l}} R_{l_{L_i,i}})^2}{\sigma^2 + K n_{L_l} \sigma^2_\mu} + \frac{(\sum_{i=1}^{n_{R_l}} R_{l_{R,i},i})^2}{\sigma^2 + K n_{R_l} \sigma^2_\mu} - \frac{(\sum_{i=1}^{n_l} R_{l,i})^2}{\sigma^2 + K n_l \sigma^2_\mu} \right]\right)
\]

Tree Structure ratio: No change.

PRUNE Proposal:

• Transition ratio: No change.

• Likelihood ratio: This is the inverse of the likelihood ratio in the GROW proposal.

• Tree Structure ratio: No change.

CHANGE Proposal:

• Transition ratio: No change.
• Likelihood ratio:

\[
\frac{P(R \mid T^\star, \sigma^2)}{P(R \mid T, \sigma^2)} = \sqrt{\frac{(\frac{\sigma^2}{\sigma^2} + Kn_1)(\frac{\sigma^2}{\sigma^2} + Kn_2)}{(\frac{\sigma^2}{\sigma^2} + Kn_1^\star)(\frac{\sigma^2}{\sigma^2} + Kn_2^\star)}} \times
\exp\left(\frac{K^2}{2\sigma^2} \left[ \frac{\sum_{i=1}^{n_1^\star} R_{1,i}^2}{\frac{\sigma^2}{\sigma^2} + Kn_1^\star} + \frac{\sum_{i=1}^{n_2^\star} R_{2,i}^2}{\frac{\sigma^2}{\sigma^2} + Kn_2^\star} - \frac{\sum_{i=1}^{n_1^\star} R_{1,i}^2}{\frac{\sigma^2}{\sigma^2} + Kn_1} - \frac{\sum_{i=1}^{n_2^\star} R_{2,i}^2}{\frac{\sigma^2}{\sigma^2} + Kn_2} \right] \right)
\]

(26)

• Tree Structure ratio: No change.

The conditional posterior of \( \sigma^2 \) and \( M_j \) changes to:

• \( \sigma^2 \mid (T_1, M_1), \ldots, (T_m, M_m), Y, X \propto Inv - Gamma(\rho, \gamma) \)

where \( \rho = \nu + Kn \) and \( \gamma = \frac{1}{2} \left[ K \sum_{i=1}^{n} (y_i - \sum_{j=1}^{m} g(x_i; M_j, T_j))^2 + \lambda \nu \right] \).

• For the conditional posterior \( M_j \mid T_j, R_j, \sigma \), we have:

\[
\mu_{ij} \mid T_j, R_j, \sigma \sim N\left(\frac{\sigma^2}{\sigma^2} + Kn_i \bar{R}_{j(i)} + K_n \mu, \frac{\sigma^2}{\sigma^2} + Kn_i \right)
\]

where \( \bar{R}_{j(i)} \) denotes the average residual (computed without tree \( j \)) at terminal node \( i \) with total number of data \( n_i \). Note that we can consider \( \mu_\mu = 0 \).

\section*{A.4 CMC for BART}

\textbf{GROW Proposal:}

• Transition ratio: No change.
• **Likelihood ratio:** Equation (20) changes to:

\[
P(R_{l_1}, ..., R_{l_n} \mid \sigma^2) = \frac{1}{(2\pi\sigma^2)^{n/2}} \left( \sqrt{2\pi\sigma^2} \right)^{-\frac{k}{2}} \sqrt{\frac{\sigma^2}{\frac{k}{K} + n_l\sigma^2}} \times \\
\exp\left( -\frac{1}{2\sigma^2} \left[ \sum_{i=1}^{n_l} (R_{l_i} - \bar{R}_l)^2 - \frac{\bar{R}_l^2}{n_l + \frac{\sigma^2}{K\sigma^2}} + n_l\bar{R}_l^2 \right] \right) \tag{27}
\]

Thus the likelihood ratio will change to:

\[
\frac{P(R \mid T^*, \sigma^2)}{P(R \mid T, \sigma^2)} = \left( \sqrt{2\pi\sigma^2} \right)^{-\frac{k}{2}} \sqrt{\frac{\sigma^2}{\frac{k}{K} + n_{lL}\sigma^2}} \times \\
\exp\left( \frac{\sigma^2}{2\sigma^2} \left[ \frac{(\sum_{i=1}^{n_{lL}} R_{lL,i})^2}{\frac{k}{K} + n_{lL}\sigma^2} + \frac{(\sum_{i=1}^{n_{lR}} R_{lR,i})^2}{\frac{k}{K} + n_{lR}\sigma^2} - \frac{(\sum_{i=1}^{n_l} R_{l_i})^2}{\frac{k}{K} + n_l\sigma^2} \right] \right) \tag{28}
\]

• **Tree Structure ratio:** The tree structure ratio will be raised to the power \(1/K\):

\[
\left( \frac{P(T^*)}{P(T)} \right)^{\frac{1}{K}}
\]

**PRUNE Proposal:**

• **Transition ratio:** No change.

• **Likelihood ratio:** This is the inverse of the likelihood ratio in the GROW proposal.

• **Tree Structure ratio:** This is also the inverse of the tree structure ratio in the GROW proposal.
CHANGE Proposal:

- **Transition ratio:** No change.

- **Likelihood ratio:**

\[
\frac{P(R \mid T^*, \sigma^2)}{P(R \mid T, \sigma^2)} = \sqrt{\frac{(\frac{a^2}{K \sigma^2} + n_1)(\frac{a^2}{K \sigma^2} + n_2)}{(\frac{a^2}{K \sigma^2} + n_1^*)(\frac{a^2}{K \sigma^2} + n_2^*)}} \times \exp \left( \frac{1}{2\sigma^2} \left[ \frac{(\sum_{i=1}^{n_1} R_{1,i})^2}{\frac{\sigma^2}{K \sigma^2} + n_1} + \frac{(\sum_{i=1}^{n_2} R_{2,i})^2}{\frac{\sigma^2}{K \sigma^2} + n_2} - \frac{(\sum_{i=1}^{n_1} R_{1,i})^2}{\frac{\sigma^2}{K \sigma^2} + n_1^*} - \frac{(\sum_{i=1}^{n_2} R_{2,i})^2}{\frac{\sigma^2}{K \sigma^2} + n_2^*} \right] \right) \quad (29)
\]

- **Tree Structure ratio:** The tree structure ratio will be raised to the power $1/K$.

Now the product of transition ratio and tree structure ratio is not 1 anymore:

\[
\frac{P(T^* \rightarrow T)}{P(T \rightarrow T^*)} \times \frac{P(T^*)}{P(T)} = n_p(\eta)^{\frac{1}{K} - 1} n_p^*(\eta^*)^{1 - \frac{1}{K}}
\]

The conditional posterior of $\sigma^2$ and $M_j$ changes to:

- $\sigma^2 \mid (T_1, M_1), \ldots, (T_m, M_m), Y, X \propto \text{Inv-Gamma}(\rho, \gamma)$

where $\rho = \frac{\nu + 2 + K(n-2)}{2K}$ and $\gamma = \frac{1}{2} \left[ \sum_{i=1}^{n} (y_i - \sum_{j=1}^{m} g(x_i; M_j, T_j))^2 + \frac{\lambda}{K} \right]$.

- For the conditional posterior $M_j \mid T_j, R_j, \sigma$, we have:

\[
\mu_{ij} \mid T_j, R_j, \sigma \sim N\left( \frac{\frac{\sigma^2}{K \sigma^2} \mu_{ij} + n_i \bar{R}_{j(i)}}{\frac{\sigma^2}{K \sigma^2} + n_i}, \frac{\sigma^2}{K \sigma^2} + n_i \right)
\]

where we can consider $\mu_{ij} = 0$. 

46