Likelihood Inflating Sampling Algorithm

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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 in parallel on each subset using different processors. Each processor will be used to run an MCMC chain that samples sub-posterior distributions which are defined using an “inflated” likelihood function. We develop a strategy for combining the draws from different sub-posteriors to study the full posterior of the Bayesian Additive Regression Trees (BART) model. The performance of the method is tested using both simulated and real data.

Keywords: Bayesian Additive Regression Trees (BART), Bayesian Inference, Big data, Consensus Monte Carlo, Markov Chain Monte Carlo (MCMC).

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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 for some widely-used samplers 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 processing units, 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 partitioned into non-overlapping sub-sets, called shards, and each shard is analyzed by a different worker. For such strategies some essential MCMC-related questions are: 1) how to define the sub-posterior distributions for each shard, and 2) how to combine the MCMC samples obtained from each sub-posterior so that we can recover the same information that would have been obtained by sampling the full
posterior distribution. Existing communication-free parallel methods proposed by Scott et al. (2013), Neiswanger et al. (2013) and Wang and Dunson (2013) have in common the fact that the product of the unnormalized sub-posteriors is equal to the unnormalized full posterior distribution, but differ in the strategies used to combine the samples. Specifically, Neiswanger et al. (2013) approximate each sub-posterior using kernel density estimators, while Wang and Dunson (2013) use the Weierstrass transformation. The popular Consensus Monte Carlo (CMC) method (Scott et al., 2013) relies on a weighted averaging approach to combine sub-posterior samples. The CMC relies on theoretical derivations that guarantee its validity when the full-data posterior and all sub-posteriors are Gaussian or mixtures of Gaussian.

We introduce a new communication-free parallel method, the Likelihood Inflating Sampling Algorithm (LISA), that also relies on independent and parallel processing of the shards by different workers to sample the sub-posterior distributions. The latter are defined differently than in the competing approaches described above. In this paper, we develop techniques to combine the sub-posterior draws obtained for LISA in the case of Bayesian Additive Regression Trees (BART) (Chipman et al., 1998, 2010; Kapelner and Bleich, 2013) and compare the performance of our method with CMC.

Sections 2 and 3 contain a brief review of the CMC algorithm and the detailed description of LISA, respectively. 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 main application is introduced in Section 5 where the BART model is described, and we show the comparison between LISA and CMC when applied to this important model. We end the paper with a discussion of ideas for future work. The Appendix contains theoretical derivations and description of the steps used when running BART.
2 Review of Consensus Monte Carlo

In this paper we assume that of interest is to generate samples from \( \pi(\theta|\vec{Y}_N) \), the posterior distribution \( \theta \) given the iid sample \( \vec{Y}_N = \{Y_1, \ldots, Y_N\} \) of size \( N \). The assumption is that \( N \) is large enough to prohibit running a standard MCMC algorithm in which draws from \( \pi \) are obtained on a single computer. We use the notation \( \pi(\theta|\vec{Y}_N) \propto f(\vec{Y}_N|\theta)p(\theta) \), 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 for big data can be triggered because a) the data sample is too large to be stored on a single computer, or b) each chain update is too costly, e.g. if \( \pi \) is sampled via a Metropolis-Hastings type of algorithm each update requires \( N \) likelihood calculations.

In order to reduce the computational costs, the CMC method of Scott et al. (2013) partitions the sample into \( K \) batches (i.e. \( \vec{Y}_N = \bigcup_{j=1}^{K} Y^{(j)} \)) and uses the workers independently and in parallel to sample each sub-posterior. More precisely, the \( j \)-th worker (\( j = 1, ..., K \)) will generate samples from the \( j \)-th sub-posterior distribution defined as:

\[
\pi_{j,CMC}(\theta|Y^{(j)}) \propto f(Y^{(j)}|\theta)p(\theta)^{1/K}.
\]

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.

\[
\pi_{Full}(\theta|\vec{Y}_N) \propto \prod_{j=1}^{K} \pi_{j,CMC}(\theta|Y^{(j)}).
\]

When the full posterior is Gaussian, the weighted averages of the sub-samples from all batches can be used as full-data posterior draws. That is, assuming \( \theta^{(k)}_1, ..., \theta^{(k)}_S \) 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 \( \Sigma_k = \text{Var}(\theta|y^{(k)}) \).

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 also benefits from the random partition of the dataset followed by independently processing each batch on a different worker. Assuming that the data have been divided into \( K \) batches of approximately equal size \( n \), we define the 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:

\[
\pi_{j,LISA}(\theta|Y^{(j)}) \propto \left[ f(Y^{(j)}|\theta) \right]^K p(\theta).
\]

Since the data are assumed to be iid, inflating the likelihood function \( K \)-times is intuitive because the sub-posterior from each batch of data will be a closer representation of the whole data posterior. We thus expect that sub-posteriors sampled by each worker will be closer to the full posterior and thus improve the statistical efficiency of the Bayesian inference.

We indeed prove in a theorem below that under mild conditions, LISA’s sub-posterior distributions are asymptotically closer to the full posterior than those produced by the CMC-type approach.

The Taylor’s series expansion for a log-posterior density \( \log \pi(\theta|Y_N) \) around its poste-
prior mode $\hat{\theta}_N$ yields the approximation

$$\log \pi(\theta | \vec{Y}_N) \approx \log \pi(\hat{\theta}_N | \vec{Y}_N) - \frac{1}{2}(\theta - \hat{\theta}_N)^T \hat{I}_N (\theta - \hat{\theta}_N)$$

where $\hat{I}_N = -\frac{\partial^2 \log(\pi(\theta | \vec{Y}_N))}{\partial \theta \partial \theta^T}|_{\theta = \hat{\theta}_N}$. Exponentiating both sides will result in

$$\pi(\theta | \vec{Y}_N) \approx \pi(\hat{\theta}_N | \vec{Y}_N) \exp \left[ -\frac{1}{2}(\theta - \hat{\theta}_N)^T \hat{I}_N (\theta - \hat{\theta}_N) \right]$$

which shows asymptotic normality, i.e. $\hat{I}_N^{1/2}(\Theta - \hat{\theta}_N) \overset{D}{\to} N(0, I)$ as $N \to \infty$ where $\Theta \sim \pi(\cdot | \vec{Y}_N)$. Let $\hat{\theta}^{(j)}_{n,L}$ and $\hat{I}^{(j)}_{n,L}$ denote LISA’s sub-posterior mode and negative second derivative of its log sub-posterior at $\theta = \hat{\theta}^{(j)}_{n,L}$ for batch $j$, respectively (similarly $\hat{\theta}^{(j)}_{n,C}$ and $\hat{I}^{(j)}_{n,C}$ for CMC). Then consider the assumptions,

**A1**: There exists $M_1 > 0$ such that $\hat{\theta}_{n,L} = \hat{\theta}^{(j)}_{n,L}$ and $\hat{I}_{n,L} = \hat{I}^{(j)}_{n,L}$ \ $\forall \ j \in \{1, ..., K\}$ and all $n > M_1$ (i.e. sub-posterior distributions of LISA have the same mean and variance across all batches for a large enough $n$).

**A2**: There exists $M_2 > 0$ such that $\hat{\theta}_{n,C} = \hat{\theta}^{(j)}_{n,C}$ and $\hat{I}_{n,C} = \hat{I}^{(j)}_{n,C}$ \ $\forall \ j \in \{1, ..., K\}$ and all $n > M_2$ (i.e. sub-posterior distributions of CMC have the same mean and variance across all batches for a large enough $n$).

**Theorem 1.** Assume that **A1** and **A2** hold and $\hat{I}_N^{1/2}(\Theta_{Full} - \hat{\theta}_N) \overset{D}{\to} N(0, I)$ where $\Theta_{Full} \sim \pi_{Full}(\cdot | \vec{Y}_N)$. Then

$$\hat{I}_N^{1/2}(\Theta_{j,LISA} - \hat{\theta}_N) \overset{D}{\to} N(0, I) \quad \text{and} \quad \hat{I}_N^{1/2}(\Theta_{j,CMC} - \hat{\theta}_N) \overset{D}{\to} N(0, KI) \ \forall \ j \in \{1, ..., K\}$$

where $\Theta_{j,LISA} \sim \pi_{j,LISA}(\cdot | Y^{(j)})$ and $\Theta_{j,CMC} \sim \pi_{j,CMC}(\cdot | Y^{(j)})$.

**Proof.** See Appendix. \square

Theorem 1 states that LISA’s individual sub-posterior distributions are asymptotically
similar to the full posterior distribution, while CMC’s are over-dispersed by a factor of $K$.
Hence, we expect that LISA’s batch-specific sub-posteriors will be better approximations of the full posterior than the ones generated using the CMC’s design.

Thus, one straightforward strategy for combining LISA’s sub-samples is to uniformly sub-sample from the samples produced by each worker. However, we will see that this aggregation scheme for LISA can be exact in some cases, e.g. for a Bernoulli model with balanced batch samples, while in others it may require modifications to improve its performance.

In the next section we will illustrate LISA in some simple examples 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 $y_1, \ldots, y_N$ to be $N$ i.i.d. Bernoulli random variables with parameter $\theta$. Hence, we consider a prior $p(\theta) = \text{Beta}(a, b)$. Assuming that we know little about the size of $\theta$ we set $a = b = 1$ which corresponds to a $U(0, 1)$ prior. The resulting full-data posterior $\pi_{\text{Full}}(\theta|\vec{Y}_N)$ is $\text{Beta}(S + a, N - S + b)$ where $S = \sum_{i=1}^{N} y_i$ is the total number of ones.

Suppose we divide the data into $K$ batches with $S_j$ number of ones in batch $j$, such that $S_j = \frac{S}{K} \ \forall \ j \in \{1, \ldots, K\}$, i.e. the number of 1’s are divided equally between batches. Then the $j^{th}$ sub-posterior based on batch-data of size $n = \frac{N}{K}$ for each method will be:
• CMC:

\[ \pi_{j,CMC}(\theta|Y^{(j)}) = \text{Beta} \left( S_j + \frac{a-1}{K} + 1, n - S_j + \frac{b-1}{K} + 1 \right) \]
\[ = \text{Beta} \left( \frac{S}{K} + \frac{a-1}{K} + 1, \frac{N-S}{K} + \frac{b-1}{K} + 1 \right) \]

• LISA:

\[ \pi_{j,LISA}(\theta|Y^{(j)}) = \text{Beta}(S_jK + a, (n - S_j)K + b) \]
\[ = \text{Beta}(S + a, N - S + b) \]

which implies

\[ \pi_{j,LISA}(\theta|Y^{(j)}) = \pi_{Full}(\theta|\vec{Y}_N) \quad \forall \ j \in \{1, ..., K\}. \]

In this simple case any one of LISA’s sub-posterior distributions is equal to the full posterior distribution if the batches are balanced, i.e. the number of 1’s are equally split across all batches. Thus, LISA’s sub-samples from any batch will represent correctly the full posterior. On the other hand, the draws from the CMC sub-posterior distributions will need to be recombined to obtain a representative sample from the true full posterior \( \pi_{Full}(\theta|\vec{Y}_N) \).

However, when the number of ones is unequally distributed among the batches it is not clear the winner between CMC and LISA as both require a careful weighting of each batch sub-posterior samples.

In the remaining part of this paper, we will mainly focus on the performance of LISA when it is applied to the Bayesian Additive Regression Trees (BART) model. Interestingly, we discover that using a minor modification inspired by running LISA on the simpler Bayesian Linear Regression model we can approximate the full posterior. The idea behind
the modification is described in the next section.

### 4.2 Bayesian Linear Regression

Consider a standard linear regression model

\[
\vec{Y}_N = X\beta + \epsilon_N
\]

where \( \beta \in \mathbf{R}^p \), \( X \in \mathbf{R}^{N \times p} \) and \( \vec{Y}_N, \epsilon_N \in \mathbf{R}^N \) with \( \epsilon_N \sim \mathcal{N}_N(0, \sigma^2 I_N) \). We consider the conjugate priors

\[
p(\beta|\sigma^2) \sim \mathcal{N}_p(\mu_0, \sigma^2 \Omega_0^{-1}),
\]

\[
p(\sigma^2) \sim \text{Inv-Gamma}(a_0, b_0).
\]

Hence the full posterior distribution is

\[
\pi_{\text{Full}}(\beta, \sigma^2|\vec{Y}_N, X) \propto f(\vec{Y}_N|X, \beta, \sigma^2) \ p(\beta|\sigma^2) \ p(\sigma^2)
\]

\[
\propto (\sigma^2)^{-N/2} \exp\left(-\frac{1}{2\sigma^2}(\vec{Y}_N - X\beta)^T(\vec{Y}_N - X\beta)\right) \times
\]

\[
(\sigma^2)^{-p/2} \exp\left(-\frac{1}{2\sigma^2}(\beta - \mu_0)^T\Omega_0(\beta - \mu_0)\right) \times
\]

\[
(\sigma^2)^{-a_0-1} \exp\left(-\frac{b_0}{\sigma^2}\right)
\]

with conditional posterior distributions

\[
\pi_{\text{Full}}(\beta|\sigma^2, \vec{Y}_N, X) \sim \mathcal{N}_p(\mu_N, \sigma^2 \Omega_N^{-1})
\]

\[
\pi_{\text{Full}}(\sigma^2|\beta, \vec{Y}_N, X) \sim \text{Inv-Gamma}(a_N, b_N),
\]
where
\[
\begin{align*}
\Omega_N &= X^TX + \Omega_0 \\
\mu_N &= \Omega_N^{-1}(X^T\hat{\beta} + \Omega_0\mu_0) = \Omega_N^{-1}(X^TY_N + \Omega_0\mu_0)
\end{align*}
\] (4)

and
\[
\begin{align*}
a_N &= a_0 + \frac{N+p}{2} \\
b_N &= b_0 + \frac{1}{2} \left[ (Y_N - X\beta)^T(Y_N - X\beta) + (\beta - \mu_0)^T\Omega_0(\beta - \mu_0) \right].
\end{align*}
\] (5)

Using Gibbs sampling one can draw from the posterior of \( \beta \) and \( \sigma^2 \) using the conditional
distributions described in (2) and (3). Now assume the dataset has been randomly divided
into \( K \) batches, with data in the \( j \)th batch denoted by \( (X_j, Y^{(j)}) \). To simplify the notation
we assume that the sample size in each batch is \( n = \frac{N}{K} \). Thus, LISA’s conditional sub-
posterior distribution of \( \beta \) and \( \sigma^2 \) from batch \( j \) will be:
\[
\begin{align*}
\pi_{j,LISA}(\beta | \sigma^2, Y^{(j)}, X_j) &\sim N_p(\mu_{n,L}(j), \sigma^2\Omega_{n,L}(j)^{-1}) \\
\pi_{j,LISA}(\sigma^2 | \beta, Y^{(j)}, X_j) &\sim \text{Inv-Gamma}(a_{n,L}(j), b_{n,L}(j)),
\end{align*}
\] (6)

where, if we set \( \Omega_0^* = \Omega_0/K \) and \( b_0^* = b_0/K \), we have
\[
\begin{align*}
\Omega_{n,L}(j) &= KX_j^TX_j + \Omega_0 = K(X_j^TX_j + \Omega_0^*) \\
\mu_{n,L}(j) &= \Omega_{n,L}(j)^{-1}(KX_j^TY^{(j)} + \Omega_0\mu_0) \\
&= (X_j^TX_j + \Omega_0^*)^{-1}(X_j^TY^{(j)} + \Omega_0^*\mu_0)
\end{align*}
\] (8)

and
\[
\begin{aligned}
\left\{
\begin{array}{l}
\alpha_{n,L}(j) = \alpha_0 + \frac{nK+p}{2} = \alpha_0 + \frac{N+p}{2} \\
b_{n,L}(j) = b_0 + \frac{1}{2} \left[ K(Y^{(j)} - X_j\beta)^T(Y^{(j)} - X_j\beta) + (\beta - \mu_o)^T \Omega_0 (\beta - \mu_0) \right] \\
= K \left( b_0^* + \frac{1}{2} \left[ (Y^{(j)} - X_j\beta)^T(Y^{(j)} - X_j\beta) + (\beta - \mu_o)^T \Omega_0^* (\beta - \mu_0) \right] \right)
\end{array}
\right.
\] (9)

For the remaining part of the section we assume that the inferential focus is on prediction so we centre the discussion on the posterior samples for $\beta$. When comparing (4) to (8), we find similarities between LISA’s sub-posterior distributions and the original posterior distributions of each batch-data (which we call ”BatchSingleMachine”). Let $\mu_n(j)$ and $\Omega_n(j)$ denote the parameters for the conditional distribution of $\beta$ in BatchSingleMachine. Hence comparing to LISA, we have

\[
\left\{
\begin{array}{l}
\Omega_{n,L}(j) = K \Omega_n(j) \\
\mu_{n,L}(j) = \mu_n(j)
\end{array}
\right.
\]

implying

\[
\pi_{j,LISA} \left( \beta \bigg| \sigma^2, Y^{(j)}, X_j \right) = \mathcal{N}_p \left( \mu_n(j), \frac{\sigma^2}{K} \Omega_n(j)^{-1} \right). \tag{10}
\]

As it is clear from (10), 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 of $\beta$ by taking weighted averages of the sub-samples. For simplicity, denote $\mu_j = \mu_n(j)$ and $\Sigma_j = \frac{\sigma^2}{K} \Omega_n(j)^{-1}$ for $j \in \{1, \ldots, K\}$.

**Theorem 2.** Suppose that LISA is applied to the linear regression model (1). Suppose that each sub-posterior update for $\sigma^2$ is multiplied by $K$. Set weight $w_j = \Sigma_j^{-1}$.
Then, if $\hat{\beta}^{(j)}$ has pdf $\pi_{j,LISA}(\beta | \sigma^2, Y^{(j)})$ for any $1 \leq j \leq K$, then the weighted average

$$
\hat{\beta}_F = \frac{\sum_{j=1}^K w_j \hat{\beta}^{(j)}}{\sum_{j=1}^K w_j}
$$

has pdf $\pi_{Full}(\beta | \sigma^2, \bar{Y}_N)$.

Proof. Since in this model, LISA’s sub-posterior distributions of $\beta$ are normally distributed, taking weighted averages of sub-samples will also result in a normal distribution $\mathcal{N}_p(\mu^*, \Sigma^*)$, with mean and variance

$$
\Sigma^* = (\Sigma_1^{-1} + \cdots + \Sigma_K^{-1})^{-1} = \left( \frac{1}{\sigma^2} \Omega_{n,L}^{(1)} + \cdots + \frac{1}{\sigma^2} \Omega_{n,L}^{(K)} \right)^{-1} = \left( \frac{K}{\sigma^2} \Omega_n^{(1)} + \cdots + \frac{K}{\sigma^2} \Omega_n^{(K)} \right)^{-1} = \left[ \frac{K}{\sigma^2} (X_1^T X_1 + \Omega_0^*) + \cdots + \frac{K}{\sigma^2} (X_K^T X_K + \Omega_0^*) \right]^{-1} = \left[ \frac{K}{\sigma^2} (X^T X + K \Omega_0^*) \right]^{-1}.
$$

Thus

$$
\Sigma^* = (\Sigma_1^{-1} + \cdots + \Sigma_K^{-1})^{-1} = \frac{\sigma^2}{K} (X^T X + \Omega_0)^{-1} = \frac{\sigma^2}{K} \Omega_N^{-1},
$$

(11)
which implies

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

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

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

\[
= \Sigma^* \left[ K \sigma^2 (X_1 T \bar{Y}^{(1)} + \Omega_0 \mu_0) + \ldots + \frac{K}{\sigma^2} (X_K T \bar{Y}^{(K)} + \Omega_0 \mu_0) \right]
\]

\[
= \Sigma^* \left[ \frac{K}{\sigma^2} (X^T \bar{Y}_N + \Omega_0 \mu_0) \right]
\]

\[
= \frac{\sigma^2}{K} \Omega_N^{-1} \frac{K}{\sigma^2} (X^T \bar{Y}_N + \Omega_0 \mu_0) = \mu_N.
\]

Thus, LISA’s weighted samples are distributed \( \beta | \sigma^2, X, \bar{Y}_N \sim N_p(\mu_N, \sigma^2 \Omega_N^{-1}) \). Comparing this to the full posterior distribution, \( N_p(\mu_N, \sigma^2 \Omega_N^{-1}) \), 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, the adjustment of \( \sigma^2 \) into \( K \sigma^2 \), will restore the variance to the variance of the sub-posterior to that of the full posterior distribution. \( \square \)

In the next section, we will examine LISA’s performance on a more complex model, the Bayesian Additive Regression Trees (BART). We will see similarities between applying LISA to BART and the Bayesian Linear Regression model. Hence Theorem 2 will play an important role in LISA’s implementation for BART.

5 Bayesian Additive Regression Trees (BART)

Consider the nonparametric regression model:

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

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

Let \( \theta := ((T_1, M_1), ..., (T_m, M_m), \sigma^2) \) 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 \( p(M_j | T_j) = \prod_i p(\mu_{ij} | T_j) \).

- **Recommended number of trees:** \( m=200 \) (Chipman et al., 2010) and \( m=50 \) (Kapelner and Bleich, 2013)

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

  1. The probability that a node at depth \( d = 0, 1, ... \) 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 $N(\mu_\mu, \sigma_\mu^2)$ such that:

\[
\begin{align*}
& m\mu_\mu - k\sqrt{m}\sigma_\mu = y_{\text{min}} \\
& m\mu_\mu + k\sqrt{m}\sigma_\mu = y_{\text{max}}
\end{align*}
\]

with $k = 2$ recommended.

- The prior for $\sigma^2$ is Inv-Gamma(\(\frac{\nu}{2}, \frac{\nu}{2}\)) 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:

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

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

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

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

15
• $(T_j, M_j) \mid T_{(j)}, M_{(j)}, \sigma, Y, X$ 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:

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

The sampling of $(T_j, M_j)$ is performed in two steps:

1. $T_j \mid R_j, \sigma$ and
2. $M_j \mid T_j, R_j, \sigma$.

Step 2 involves sampling from each component of $M_j$ using

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

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

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

(13)

The Metropolis-Hastings (MH) algorithm is then applied to draw $T_j$ from (13) 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, "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 or CMC 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 reported in the Appendix.

As discussed by Scott et al. (2013), the approximation to the posterior produced by the CMC algorithm can be poor. Thus, for comparison reasons, we applied both LISA and CMC to BART using a simulated dataset (described further) with $K = 30$ batches. Given Theorem 1, since LISA’s sub-posterior distributions are asymptotically equivalent to the full posterior distribution, we examined its performance by uniformly taking sub-samples from all its batches as an approximation to full posterior samples. We will see further that LISA with uniform weights produces higher prediction accuracy compared to CMC. However, they both perform poorly in approximating the posterior samples as they generate larger trees and under-estimate $\sigma^2$, which results in over-dispersed posterior distributions.

The following sub-section discusses a modified version of LISA for BART which will have significant improvement in performance.
5.1 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 not 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 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 (13) 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 only the conditional distribution of the residuals, $R_j \mid M_j, T_j, \sigma$ is affected by the modifications brought by LISA. Note also that 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 affected by LISA. Consider the likelihood ratio for GROW proposal in LISA (full details are presented in the Appendix)

$$\frac{P(R \mid T_s, \sigma^2)}{P(R \mid T, \sigma^2)} = \sqrt{\frac{\sigma^2(\sigma^2 + Kn_l\sigma^2_\mu)}{(\sigma^2 + Kn_l\sigma^2_\mu)(\sigma^2 + Kn_l\sigma^2_\mu)}} \times$$

$$\exp \left\{ \frac{K^2\sigma^2_\mu}{2\sigma^2} \left[ \frac{(\sum_{i=1}^{n_l} R_{li,i})^2}{\sigma^2 + Kn_l\sigma^2_\mu} + \frac{(\sum_{i=1}^{n_R} R_{R,i})^2}{\sigma^2 + Kn_R\sigma^2_\mu} - \frac{(\sum_{i=1}^{n_l} R_{li,i})^2}{\sigma^2 + Kn_l\sigma^2_\mu} \right] \right\} \quad (14)$$

where $n_t$ is the total number of observations from batch-data that end up in terminal node...
The newly grown tree, $T_*$, splits terminal node $l$ into 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 (14), we can rewrite it as

$$
P(R | T_*, \sigma^2) = \sqrt{\frac{\frac{\sigma^2}{K} (\frac{\sigma^2}{K} + n_{l_L} \sigma^2) \mu}{(\frac{\sigma^2}{K} + n_{l_L} \sigma^2) (\frac{\sigma^2}{K} + n_{l_R} \sigma^2) \mu}} \times \exp \left\{ \frac{\sigma^2 \mu}{2K} \left[ \frac{(\sum_{i=1}^{n_{l_L}} R_{l,L,i})^2}{\frac{\sigma^2}{K} + n_{l_L} \sigma^2 \mu} + \frac{(\sum_{i=1}^{n_{l_R}} R_{l,R,i})^2}{\frac{\sigma^2}{K} + n_{l_R} \sigma^2 \mu} - \frac{(\sum_{i=1}^{n_l} R_{l,i})^2}{\frac{\sigma^2}{K} + n_l \sigma^2 \mu} \right] \right\}. \quad (15)$$

Expression (15) 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 $R_j | M_j, T_j, \sigma \sim \mathcal{N}(g(\cdot; M_j, T_j), \sigma^2)$. 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 modLISA, we don’t apply any changes in updating $\sigma^2$, i.e. we keep the same conditional distribution as in LISA:

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

where $\rho = \frac{\nu + Kn}{2}$ and $\gamma = \frac{1}{2} \left[ K \sum_{i=1}^{n} (y_i^{(k)} - \sum_{j=1}^{m} g(x_i^{(k)}; M_j, T_j))^2 + \lambda \nu \right]$. 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.
5.2 A Numerical Experiment – The Friedman’s function

We have simulated data of size $N = 20,000$ from Friedman’s test function (Friedman, 1991)

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

where the covariates $x = (x_1, \ldots, x_{10})$ are simulated independently from a $U(0, 1)$ and $y \sim \mathcal{N}(f(x), \sigma^2)$ with $\sigma^2 = 9$. Note that five of the ten covariates are unrelated to the response variable. We have also generated test data containing 5000 cases. 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 $x = (x_1, \ldots, x_{10})$. Since in this simulated data the true $f$ is known, one can compute the root mean squared error (RMSE) using average posterior draws of $\hat{f}(x)$ for each $x$ (i.e. $\bar{\hat{f}(x)}$), as an estimate to measure its performance, i.e. $\text{RMSE} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (f(x_i) - \bar{\hat{f}(x_i)})^2}$. It is known that SingleMachine BART may mix poorly when it is run on an extremely large dataset with small residual variance. However since the data simulated is of reasonable size and $\sigma$ is not very small the SingleMachine BART is expected to be a good benchmark for comparison (see discussion in Pratola et al., 2016).

5.2.1 Comparison of modLISA with Competing Methods

We have implemented modLISA, LISA, and CMC for BART with $K = 30$ batches on the simulated data for 5000 iterations with a total of 1000 posterior draws. Table 1 shows results from all methods including the SingleMachine which runs BART on the full dataset using only one machine. Results are averaged over three different realizations of train and test data, and are reporting the Train and Test RMSE for each method, along with average post burn-in $\sigma^2$ estimates and tree sizes. In addition, Table 1 also includes the average Train and Test coverage of 95% prediction intervals, i.e. the proportion of 1000 newly simulated $y$ at a given train or test $x$ that is covered by its corresponding
95% prediction interval. As it is seen from Table 1, LISA does a terrible job at estimating \( \sigma^2 \), its estimate being orders of magnitude smaller than the one produced by CMC. And although LISA has better prediction performance compared to CMC, we also observe much higher coverage probabilities for CMC. On the other hand, CMC and LISA both generate larger trees compared to SingleMachine, with CMC generating trees that are ten times larger than LISA’s. Overall, it is clear that neither CMC nor LISA exhibit desirable properties for BART. The story changes with modLISA with weighted average which dominates both CMC and LISA across all performance indicators since it has the lowest RMSE, the highest coverage, the lowest tree sizes, and less biased \( \sigma^2 \) estimates and produces results that are the closest to the ones produced by SingleMachine.

<table>
<thead>
<tr>
<th>Method</th>
<th>TrainRMSE</th>
<th>TestRMSE</th>
<th>TrainCov</th>
<th>TestCov</th>
<th>Avg ( \hat{\sigma}^2 )</th>
<th>Tree Nodes</th>
</tr>
</thead>
<tbody>
<tr>
<td>CMC</td>
<td>2.73</td>
<td>2.94</td>
<td>45.71 %</td>
<td>47.83 %</td>
<td>1.91</td>
<td>602</td>
</tr>
<tr>
<td>LISA (unif wgh)</td>
<td>1.18</td>
<td>1.19</td>
<td>1.54 %</td>
<td>1.54 %</td>
<td>0.001</td>
<td>55</td>
</tr>
<tr>
<td>modLISA (wgh avg)</td>
<td>0.57</td>
<td>0.59</td>
<td>92.93 %</td>
<td>92.91 %</td>
<td>7.97</td>
<td>7</td>
</tr>
<tr>
<td>SingleMachine</td>
<td>0.55</td>
<td>0.56</td>
<td>94.67 %</td>
<td>94.65 %</td>
<td>9.04</td>
<td>7</td>
</tr>
</tbody>
</table>

Table 1: Comparing Train & Test RMSE, average Train & Test coverage of 95% prediction intervals, average post burn-in \( \hat{\sigma}^2 \), and tree sizes in each method for \( K = 30 \) to SingleMachine BART (all results are averaged over three different realizations of data).

<table>
<thead>
<tr>
<th>Method</th>
<th>GROW</th>
<th>PRUNE</th>
<th>CHANGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>CMC</td>
<td>21%</td>
<td>0.03%</td>
<td>34%</td>
</tr>
<tr>
<td>LISA</td>
<td>1.8%</td>
<td>0.5%</td>
<td>1.6%</td>
</tr>
<tr>
<td>modLISA</td>
<td>20%</td>
<td>26%</td>
<td>19%</td>
</tr>
<tr>
<td>SingleMachine</td>
<td>9%</td>
<td>10%</td>
<td>6%</td>
</tr>
</tbody>
</table>

Table 2: Average acceptance rates of tree proposal moves.

The size of trees produced by each method is in sync with the average acceptance rates of each tree proposal move shown in Table 2. It is noticeable the difference between CMC and LISA ’s average acceptance rates between growing a tree and pruning one. On the other hand, modLISA has overall larger acceptance rates with the smallest relative
absolute difference between growing and pruning probabilities compared to LISA and CMC (6/20 = 23.1% for modLISA, 98.6% for CMC, and 72.2% for LISA) and is closest to SingleMachine (10%). 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.

Figure 1: Comparing empirical distribution functions of $\hat{f}(x)$ obtained via modLISA, LISA, and CMC with $K = 30$, to the one produced by SingleMachine BART for two different pairs of train and test data.
5.2.2 Comparison with SingleMachine BART

In order to investigate the closeness of posterior samples in each method to the SingleMachine BART, we have plotted in Figure 1 the empirical distribution functions of $\hat{f}(x)$ generated from each algorithm for two pairs of observations in the train and test dataset. One can see that the empirical distribution functions in LISA and CMC don’t match the ones from SingleMachine (in both train and test data), and look over-dispersed as they cover a larger range of $x$ values within $F_n(x) \in (0, 1)$. However, the empirical distribution functions in modLISA weighted average look much closer to SingleMachine with a similar dispersion but a slight shift in location.

In order to assess the performance of the sampling procedures considered, we use the Cramér-von Mises distance to assess the difference between 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 $F(x) = F_{BART}(x)$ to be the empirical distribution function generated from posterior samples in SingleMachine BART and $F_n(x)$ is similarly computed for the alternative method that is considered for comparison.

Using a set of $T = 1000$ equispaced points, we compute the average squared difference between the single machine and all other alternative methods for each observation in the dataset. To illustrate, for LISA we estimate $\omega$ using $\hat{\omega}^2_{LISA} = \frac{1}{T} \sum_{j=1}^{T} (F_{LISA}(t_j) - F_{BART}(t_j))^2$.

Figure 2 is comparing the fitted polynomial trends of $\hat{\omega}^2$ (in each method) versus mean predicted $\hat{f}(x)$ in SingleMachine with their corresponding 95% credible regions (for both train and test data). Clearly in LISA and modLISA, there are small variations around the trends with no significant changes in values of $\hat{\omega}^2$ among different mean predicted $\hat{f}(x)$, which specifies consistency within different train or test observations. In addition, the gap between trends from train and test data indicate that the average distance between LISA/modLISA and SingleMachine’s distributions are smaller for test data compared to
Figure 2: Blue lines: Fitted polynomial trends (for both train and test data) of average squared difference between empirical distribution functions of SingleMachine and the following: (a) CMC, (b) LISA with uniform weights and (c) 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.

train data. Furthermore, there are still small variations seen around CMC’s trends, but with slight changes in values of \( \hat{\omega}^2 \) among different mean predicted \( \hat{f}(x) \), especially for the test dataset which indicates inconsistency within different observations.
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 (for both train and test data).

To emphasize the difference in performance between modLISA and its competitors, Figure 3 shows all the fitted polynomial trends without their credible regions for the train and test data. One can see that there is a large gap between $\hat{\omega}^2$ values in modLISA weighted average and other alternative methods (for both train and test data), with modLISA having the lowest value. Thus 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 train observations for each trend which is calculated to be 0.013 for modLISA that is significantly smaller than 0.059, 0.048 for CMC, and LISA, respectively. Similarly, the average $\hat{\omega}^2$ over test data are 0.008, 0.047, and 0.031 for modLISA, CMC, and LISA respectively, which again the smallest value is seen in modLISA. Hence we conclude that modLISA weighted average generate closest to true posterior draws of BART and has the best performance among its alternative methods.

At last we compare run time per iteration for each method so we can draw some
conclusions regarding the overall efficiency.

5.2.3 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.

<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.

As it is seen in Table 3, modLISA, LISA and CMC with $K = 30$ 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 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.

5.3 Additional Considerations

5.3.1 Effect of $N$ (number of training data) on Posterior Accuracy

To see how the number of training data ($N$) can effect the posterior accuracy, we have examined the performance of all methods when $N$ is increased to 60,000 while we keep the same number of batches $K = 30$. Tables 4 shows the results of 1000 posterior samples
generated from fitting the BART model to the training set with additional 5000 data considered as test cases.

<table>
<thead>
<tr>
<th>Method</th>
<th>TrainRMSE</th>
<th>TestRMSE</th>
<th>TrainCov</th>
<th>TestCov</th>
<th>Avg $\hat{\sigma}^2$</th>
<th>Tree Nodes</th>
</tr>
</thead>
<tbody>
<tr>
<td>CMC</td>
<td>2.85</td>
<td>5.56</td>
<td>25.74 %</td>
<td>17.28 %</td>
<td>0.48</td>
<td>983</td>
</tr>
<tr>
<td>LISA (unif wgh)</td>
<td>1.17</td>
<td>1.19</td>
<td>0.84 %</td>
<td>0.84 %</td>
<td>0.0003</td>
<td>125</td>
</tr>
<tr>
<td>modLISA (wgh avg)</td>
<td>0.41</td>
<td>0.42</td>
<td>94.54 %</td>
<td>94.53 %</td>
<td>8.82</td>
<td>7</td>
</tr>
<tr>
<td>SingleMachine</td>
<td>0.41</td>
<td>0.41</td>
<td>94.83 %</td>
<td>94.84 %</td>
<td>9.04</td>
<td>11</td>
</tr>
</tbody>
</table>

Table 4: Results from a 60,000 training dataset with $K = 30$. Reporting Train & Test RMSE, average Train & Test coverage of 95 % prediction intervals, average post burn-in $\hat{\sigma}^2$, and tree sizes in each method.

Comparing Table 4 to 1, it is not surprising that the Train and Test RMSEs in modLISA, LISA, and SingleMachine decrease as $N$ increases. While LISA and CMC estimates for $\sigma^2$ get worse, modLISA generates more accurate estimates of $\sigma^2$ with a larger $N$. Trees have consistent size in modLISA, but tend to grow larger in CMC and LISA (as $N$ rises). Empirical coverages decrease in CMC and LISA, while they increase in modLISA and SingleMachine for larger training data (specifically, modLISA competes with SingleMachine for larger $N$). Overall, as $N$ increases, modLISA seems to be a more reliable method as it has a better performance compared to all other alternatives.

5.3.2 Effect of $K$ (number of batches) on Posterior Accuracy

To examine the effect of $K$ on posterior accuracy, we have generated 1000 posterior draws from fitting the 20,000 dataset to each method with $K = 10$ (except SingleMachine). The results are shown in Table 5.

Comparing Table 1 with $K = 30$ to Table 5, we see that as $K$ decreases, the performance of LISA and CMC drops while modLISA generates stronger results, which is what we intuitively expect as each batch has more information when $K$ is smaller. We also note the promising advantage that modLISA exhibits over the SingleMachine when $K = 10$ in terms of RMSE.
Table 5: Results from a 20,000 training dataset with $K = 10$. Reporting Train & Test RMSE, average Train & Test coverage of 95% prediction intervals, average post burn-in $\hat{\sigma}^2$, and tree sizes in each method.

5.4 Varying the Underlying Model – Different $f(x)$

Consistency in performance of modLISA can also be seen when the underlying model is changed. For instance, we also considered a sample of size 20,000 using

$$f(x) = 3\sqrt{x_1} - 2x_2^2 + 5x_3x_4,$$

where $x = (x_1, \ldots, x_4)$ is a four-dimensional input vector that is simulated independently from a $U(0, 1)$ and $y \sim \mathcal{N}(f(x), \sigma^2)$ with $\sigma^2 = 1$. Additional 5000 data have also been simulated as test cases. Similarly, by fitting this newly simulated dataset to each method with $K = 30$, we have generated 1000 posterior samples with results averaged across three different realizations of data shown in Table 6.

Table 6: Results from a 20,000 training dataset with a different underlying model with $K = 30$. Reporting Train & Test RMSE, average Train & Test coverage of 95% prediction intervals, average post burn-in $\hat{\sigma}^2$, and tree sizes in each method (the results are averaged over three different realizations of data).

Again modLISA has the best performance among its alternatives, and its performance is closest to SingleMachine. This confirms the previous simulation results and we conclude
that modLISA is a more reliable method for BART models with large datasets.

In the next section we will apply modLISA weighted average BART to a big real data.

### 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 437,297 observations. We randomly divided the dataset into approximately 80% training and 20% testing sets, with \( K = 100 \) batches considered for splitting the training data 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 with weighted average and SingleMachine BART on this dataset for 1500 iterations (since SingleMachine is very slow) and discarded the first 1000 draws which resulted in 500 posterior samples. Table 7 is showing the results of Test RMSE as well as average post burn-in \( \sigma^2 \) estimates and tree sizes. As seen in Table 7, Test RMSE

<table>
<thead>
<tr>
<th>Method</th>
<th>TestRMSE</th>
<th>Avg ( \hat{\sigma}^2 )</th>
<th>Tree Nodes</th>
<th>Speed-up</th>
</tr>
</thead>
<tbody>
<tr>
<td>modLISA (wgh avg)</td>
<td>0.71</td>
<td>0.488</td>
<td>7</td>
<td>90%</td>
</tr>
<tr>
<td>SingleMachine</td>
<td>0.70</td>
<td>0.485</td>
<td>23</td>
<td>–</td>
</tr>
</tbody>
</table>

Table 7: Results of 1000 posterior samples generated from modLISA with \( K = 100 \) and SingleMachine BART on PUMS 2013 test data.
in modLISA is similar to the one from SingleMachine which indicates high prediction accuracy. However, modLISA shows significant advantage as it has 90% speed-up with respect to SingleMachine.

<table>
<thead>
<tr>
<th>Method</th>
<th>GROW</th>
<th>PRUNE</th>
<th>CHANGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>modLISA</td>
<td>10 %</td>
<td>11 %</td>
<td>14 %</td>
</tr>
<tr>
<td>SingleMachine</td>
<td>8%</td>
<td>7%</td>
<td>7%</td>
</tr>
</tbody>
</table>

Table 8: Average acceptance rates of tree proposal moves.

This can be justified from Table 8 that shows overall higher acceptance rates for each proposal in modLISA compared to SingleMachine. The 90% speedup is in this case important as it takes more than a day to simulate from the posterior using SingleMachine. The result indicate the potential of this method for reducing computational costs while producing accurate predictions.

6 Discussion

The challenge of using MCMC algorithms to sample posterior distributions obtained from a massive sample of observations is a serious one.

In this paper, we introduced a new method based on the idea of randomly dividing the data into batches and drawing samples from each of the resulting sub-posteriors independently and parallel on different machines. We propose a novel way to define the sub-posteriors and we develop a strategy to combine the samples produced by each batch analysis for the important class of Bayesian Additive Regression Trees Models. For this model, the proposed methodology performs very well and shows reduction in computation time that are as high as 90%.

In future work we would like to find a procedure for combining the sub-posterior samples that will make LISA easy to adapt to a wide variety of models. We also hope
that our paper will stimulate the research into this type of divide-and-conquer approaches for Big Data MCMC and will expand the research on how to construct the batch-specific sub-posteriors along with novel strategies of combining or weighting the samples obtained from each batch analysis.

7 Acknowledgement

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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. Given assumptions A1 and A2, we assume \( n > M_1 \) for LISA and \( n > M_2 \) for CMC to derive their asymptotic distributions in terms of the full posterior.

- For LISA:
  
  We know that \( \left( \pi_{\text{Full}}(\theta|Y_N) \right)^K \propto \prod_{j=1}^{K} \pi_{j,\text{LISA}}(\theta|Y^{(j)}) \), hence:

  \[
  \log \left( \pi_{\text{Full}}(\theta|Y_N) \right) = \frac{1}{K} \sum_{j=1}^{K} \log \left( \pi_{j,\text{LISA}}(\theta|Y^{(j)}) \right) + c \tag{1}
  \]

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

  \[
  \log \left( \pi_{\text{Full}}(\theta|Y_N) \right) \bigg|_{\theta = \hat{\theta}_N} = \frac{1}{K} \sum_{j=1}^{K} \log \left( \pi_{j,\text{LISA}}(\hat{\theta}_N|Y^{(j)}) \right) + c
  \]

  and

  \[
  \frac{1}{K} \sum_{j=1}^{K} \log \left( \pi_{j,\text{LISA}}(\hat{\theta}_N|Y^{(j)}) \right) \leq \frac{1}{K} \sum_{j=1}^{K} \log \left( \pi_{j,\text{LISA}}(\hat{\theta}_{n,L}|Y^{(j)}) \right) \tag{2}
  \]

  Inequality (2) is true since \( \hat{\theta}_{n,L} \) is the mode of \( \log(\pi_{j,\text{LISA}}) \) for all \( j \in \{1, \ldots, K\} \).

  Now from (1) and (2), we have:

  \[
  \log \left( \pi_{\text{Full}}(\theta|Y_N) \right) \bigg|_{\theta = \hat{\theta}_N} \leq \log \left( \pi_{\text{Full}}(\theta|Y_N) \right) \bigg|_{\theta = \hat{\theta}_{n,L}} \tag{3}
  \]
But since $\hat{\theta}_N$ is the full posterior mode:

$$\log\left(\pi_{\text{Full}}(\theta|Y_N)\right)\bigg|_{\theta=\hat{\theta}_N} \geq \log\left(\pi_{\text{Full}}(\theta|Y_N)\right)\bigg|_{\theta=\hat{\theta}_{n,L}} \quad (4)$$

Hence from (3) and (4) we get

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

which implies

$$\hat{\theta}_N = \hat{\theta}_{n,L} \quad (5)$$

To calculate the variance, take the second derivative with respect to $\theta$ from both sides of (1) evaluated at $\theta = \hat{\theta}_N$:

$$\frac{\partial^2}{\partial \theta^2} \log\left(\pi_{\text{Full}}(\theta|Y_N)\right)\bigg|_{\theta=\hat{\theta}_N} = \frac{1}{K} \sum_{j=1}^{K} \frac{\partial^2}{\partial \theta^2} \log\left(\pi_{j,\text{LISA}}(\theta|Y^{(j)})\right)\bigg|_{\theta=\hat{\theta}_N}$$

Since $\hat{I}_{n,L} = \hat{I}_{n,L}^{(j)} \quad \forall \ j \in \{1, ..., K\}$, and that equation (5) holds, we will have:

$$\frac{1}{K} \sum_{j=1}^{K} \frac{\partial^2}{\partial \theta^2} \log\left(\pi_{j,\text{LISA}}(\theta|Y^{(j)})\right)\bigg|_{\theta=\hat{\theta}_N} = \frac{1}{K} \sum_{j=1}^{K} \frac{\partial^2}{\partial \theta^2} \log\left(\pi_{j,\text{LISA}}(\theta|Y^{(j)})\right)\bigg|_{\theta=\hat{\theta}_{n,L}}$$

which implies

$$\hat{I}_{n,L} = \hat{I}_{n,L}$$

which implies

$$\hat{I}_{n,L} = \hat{I}_N,$$
• For CMC:

Since $\pi_{Full}(\theta|Y_N) \propto \prod_{j=1}^{K} \pi_{j,CMC}(\theta|Y^{(j)})$ we get

$$\log (\pi_{Full}(\theta|Y_N)) = \sum_{j=1}^{K} \log (\pi_{j,CMC}(\theta|Y^{(j)})) + c$$  \hspace{1cm} (6)

where $c$ is a constant. Using an argument similar to the one in LISA derivations we obtain

$$\log (\pi_{Full}(\theta|Y_N))|_{\theta = \hat{\theta}_N} = \log (\pi_{Full}(\theta|Y_N))|_{\theta = \hat{\theta}_{n,C}}$$

which implies

$$\hat{\theta}_N = \hat{\theta}_{n,C}.$$  \hspace{1cm} (7)

In addition, taking the second derivatives with respect to $\theta$ from equation (6) will result in:

$$\frac{\partial^2}{\partial \theta^2} \log (\pi_{Full}(\theta|Y_N))|_{\theta = \hat{\theta}_N} = \sum_{j=1}^{K} \frac{\partial^2}{\partial \theta^2} \log (\pi_{j,CMC}(\theta|Y^{(j)}))|_{\theta = \hat{\theta}_N}$$

which again using the fact that $\hat{I}_{n,C} = \hat{I}_{n,C}^{(j)} \quad \forall \quad j \in \{1, ..., K\}$ and that (7) holds, will give us:

$$\sum_{j=1}^{K} \frac{\partial^2}{\partial \theta^2} \log (\pi_{j,CMC}(\theta|Y^{(j)}))|_{\theta = \hat{\theta}_N} = \sum_{j=1}^{K} \frac{\partial^2}{\partial \theta^2} \log (\pi_{j,CMC}(\theta|Y^{(j)}))|_{\theta = \hat{\theta}_{n,C}} = K(-\hat{I}_{n,C})$$
implying

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

(8)

Thus \( \forall \ j \in \{1, ..., K\} \):

\[ \hat{I}^{1/2}_N (\Theta_{j,LISA} - \hat{\theta}_N) \overset{D}{\rightarrow} N(0, I) \]

& \[ \hat{I}^{1/2}_N (\Theta_{j,CMC} - \hat{\theta}_N) \overset{D}{\rightarrow} N(0, KI) \]

where \( \Theta_{j,LISA} \sim \pi_{j,LISA}(.,|Y^{(j)}) \) and \( \Theta_{j,CMC} \sim \pi_{j,CMC}(.,|Y^{(j)}) \)

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

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

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

\[ r = \frac{P(T_* \rightarrow T)}{P(T \rightarrow T_*)} \times \frac{P(R | T_*, \sigma^2)}{P(R | T, \sigma^2)} \times \frac{P(T_*)}{P(T)} \]

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:

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

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

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:

\[
P(T^* \rightarrow T) = P(PRUNE) \cdot P(\text{choosing } \eta \text{ to prune}) = P(PRUNE) \frac{1}{w^*}
\]

where $w^*$ is the number of nodes with two terminal nodes in the new tree $T^*$. Hence the transition ratio will be:

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

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

\[
P(R_1, \ldots, R_n \mid T, \sigma^2) = \prod_{l=1}^{b} P(R_{t_1}, \ldots, R_{nt_l} \mid \sigma^2)
\]

since the data are partitioned across all $b$ terminal nodes of tree $T$. $R_{t}$ 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 $\mu_l \sim N(0, \sigma^2_{\mu})$, hence we will
have:

\[ P(R_{l_1}, ..., R_{l_n} \mid \sigma^2) = \int_{\mathbb{R}} P(R_{l_1}, ..., R_{l_n} \mid \mu_l, \sigma^2) P(\mu_l; \sigma^2_{\mu}) \, d\mu_l \]

by completion of the square this will equal to:

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

\[ \frac{1}{(2\pi\sigma^2)^{n_l/2}} \exp\left( -\frac{1}{2\sigma^2} \left[ \sum_{i=1}^{n_l} (R_{l_i} - \bar{R}_l)^2 - \frac{\bar{R}_l^2 n_l^2}{n_l + \sigma^2_{\mu}^2} + n_l \bar{R}_l^2 \right] \right) \quad (9) \]

where \( R_l \) is the average residual at terminal node \( l \). Note that the likelihood is specified by all terminal nodes, and since \( T \) differs from \( T^* \) 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 (9)):

\[ \frac{P(R \mid T^*, \sigma^2)}{P(R \mid T, \sigma^2)} = \frac{\sigma^2 (\sigma^2 + n_l \sigma^2_{\mu})}{(\sigma^2 + n_{lL} \sigma^2_{\mu}) (\sigma^2 + n_{lR} \sigma^2_{\mu})} \times \]

\[ \exp\left( \frac{\sigma^2_{\mu}}{2\sigma^2} \left[ \frac{(\sum_{i=1}^{n_{lL}} R_{l_L,i})^2}{\sigma^2 + n_{lL} \sigma^2_{\mu}} + \frac{(\sum_{i=1}^{n_{lR}} R_{l_R,i})^2}{\sigma^2 + n_{lR} \sigma^2_{\mu}} - \frac{(\sum_{i=1}^{n_l} R_{l,i})^2}{\sigma^2 + n_l \sigma^2_{\mu}} \right] \right) \quad (10) \]

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:

\[ P_{\text{split}}(\eta) = \frac{\alpha}{(1 + d_{\eta})^3} \]
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:

\[ \frac{P(T_*)}{P(T)} = \alpha \frac{(1 - \frac{\alpha}{(2 + d_{\eta})^2})^2}{((1 + d_{\eta})^\beta - \alpha) p(\eta) n_p(\eta)} \] (11)

**PRUNE Proposal:**

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

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

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:

\[
\frac{P(R \mid T_*, \sigma^2)}{P(R \mid T, \sigma^2)} = \sqrt{\frac{\left(\frac{\sigma^2}{\sigma_{p^*}^2} + n_1\right)\left(\frac{\sigma^2}{\sigma_{p^*}^2} + n_2\right)}{\left(\frac{\sigma^2}{\sigma_p^2} + n_1^*\right)\left(\frac{\sigma^2}{\sigma_p^2} + n_2^*\right)}} \times
\exp\left(\frac{1}{2\sigma^2} \left[\sum_{i=1}^{n_1^*} R_{1^*,i}^2 + \sum_{i=1}^{n_2^*} R_{2^*,i}^2 - \left(\sum_{i=1}^{n_1} R_{1,i}^2\right)^2 - \left(\sum_{i=1}^{n_2} R_{2,i}^2\right)^2\right]\right) \tag{12}
\]

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 (9) changes to:

\[
P(R_{l_1}, ..., R_{l_{nl}} \mid \sigma^2) = \frac{1}{(2\pi \sigma^2)^{n_l/2}} \sqrt{\frac{\sigma^2}{\sigma^2 + Kn_l \sigma_\mu^2}} \exp \left( - \frac{K}{2\sigma^2} \left[ \sum_{i=1}^{n_l} (R_{l_i} - \bar{R}_{l_i})^2 - \frac{K \bar{R}_{l_i} n_i^2}{Kn_l + \sigma_\mu^2} + n_i \bar{R}_{l_i}^2 \right] \right)
\]

Thus the likelihood ratio will change to:

\[
\frac{P(R \mid T_*, \sigma^2)}{P(R \mid T, \sigma^2)} = \sqrt{\frac{\sigma^2(\sigma^2 + Kn_l \sigma_\mu^2)}{(\sigma^2 + Kn_{lL} \sigma_\mu^2)(\sigma^2 + Kn_{lR} \sigma_\mu^2)}} \times \exp \left( \frac{K^2 \sigma_\mu^2}{2\sigma^2} \left[ \frac{\left( \sum_{i=1}^{n_{lL}} R_{lL,i} \right)^2}{\sigma^2 + Kn_{lL} \sigma_\mu^2} + \frac{\left( \sum_{i=1}^{n_{lR}} R_{lR,i} \right)^2}{\sigma^2 + Kn_{lR} \sigma_\mu^2} - \frac{(\sum_{i=1}^{n_l} R_{l,i})^2}{\sigma^2 + Kn_l \sigma_\mu^2} \right] \right)
\]

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:

\[
P(R \mid T_*, \sigma^2) = \frac{\begin{vmatrix} \left(\frac{\sigma^2}{\sigma_\mu^2} + K n_1\right) \left(\frac{\sigma^2}{\sigma_\mu^2} + K n_2\right) \\ \left(\frac{\sigma^2}{\sigma_\mu^2} + K n_1^*\right) \left(\frac{\sigma^2}{\sigma_\mu^2} + K n_2^*\right) \end{vmatrix}}{P(R \mid T, \sigma^2)} \times \\
\exp \left( \frac{K^2}{2\sigma^2} \left[ \sum_{i=1}^{n_1^*} R_{1^*,i}^2 + \sum_{i=1}^{n_2^*} R_{2^*,i}^2 - \sum_{i=1}^{n_1^*} R_{1*,i}^2 - \sum_{i=1}^{n_2^*} R_{2*,i}^2 \right] \right) \tag{15} \]

• 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 \( \rho = \frac{\nu + Kn_2}{2} \) 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:

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

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 \( \mu_\mu = 0 \).
A.4 CMC for BART

GROW Proposal:

- **Transition ratio**: No change.

- **Likelihood ratio**: Equation (9) changes to:

\[
P(R_{l1}, \ldots, R_{lnl} \mid \sigma^2) = \frac{1}{(2\pi \sigma^2)^{n_l/2}} \left(\sqrt{2\pi \sigma^2}\right)^{1-K} \sqrt{\frac{\sigma^2}{\alpha^2} + n_l \sigma^2_{\mu}} \times \\
\exp \left(- \frac{1}{2\sigma^2} \sum_{i=1}^{n_l} (R_{li} - \bar{R}_l)^2 - \frac{\bar{R}_l^2 n_l^2}{n_l + \frac{\sigma^2}{K \sigma^2_{\mu}}} + n_l \bar{R}_l^2 \right) \tag{16}
\]

Thus the likelihood ratio will change to:

\[
\frac{P(R \mid T^*_s, \sigma^2)}{P(R \mid T, \sigma^2)} = \left(\sqrt{2\pi \sigma^2}\right)^{1-K} \sqrt{\frac{\sigma^2}{\alpha^2} + n_l \sigma^2_{\mu}} \times \\
\exp \left(\frac{\sigma^2_{\mu}}{2\sigma^2} \left[\frac{\left(\sum_{i=1}^{n_l} R_{lL,i}\right)^2}{\alpha^2 + n_l \sigma^2_{\mu}} + \frac{\left(\sum_{i=1}^{n_R} R_{lR,i}\right)^2}{\alpha^2 + n_R \sigma^2_{\mu}} - \frac{\left(\sum_{i=1}^{n_l} R_{li}\right)^2}{\alpha^2 + n_l \sigma^2_{\mu}}\right]\right) \tag{17}
\]

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

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

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:**

\[
\frac{P(R \mid T_\ast, \sigma^2)}{P(R \mid T, \sigma^2)} = \sqrt{\frac{\left(\frac{\sigma^2}{K\sigma^2_K} + n_1\right)\left(\frac{\sigma^2}{K\sigma^2_K} + n_2\right)}{\left(\frac{\sigma^2}{K\sigma^2_K} + n_1^\ast\right)\left(\frac{\sigma^2}{K\sigma^2_K} + n_2^\ast\right)}} \times
\]

\[
\exp\left(\frac{1}{2\sigma^2} \left[ \left(\sum_{i=1}^{n_1^\ast} R_{1\ast,i}\right)^2 + \left(\sum_{i=1}^{n_2^\ast} R_{2\ast,i}\right)^2 - \left(\sum_{i=1}^{n_1} R_{1,i}\right)^2 - \left(\sum_{i=1}^{n_2} R_{2,i}\right)^2 \right] \right) \quad (18)
\]

• **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:

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

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

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

where \(\rho = \frac{\nu + 2 + K(n-2)}{2K}\) and \(\gamma = \frac{1}{2} \left[ \sum_{i=1}^{n} (y_i - \sum_{j=1}^{m} g(x_i; M_j, T_j))^2 + \frac{\lambda_w}{K} \right].\)
For the conditional posterior $M_j \mid T_j, R_j, \sigma$, we have:

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

where we can consider $\mu_\mu = 0$.

References