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Scalable and Causal Bayesian Inference

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Dedicated to my wife Jarinya, son Phoenix and parents, Sonny and Violet
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Scalable and Causal Bayesian Inference

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This thesis will focus on two facets of Bayesian Estimation. Firstly, we propose methods that can improve parameter estimation in particle filtering when making use of a distributed computing environment by allowing for periodic communication between compute nodes. The periodic communication can improve the embarrassingly parallel version of our particle filter without dramatically increasing the computational costs. Our method is intended for use on data with large N or in streaming settings where latent parameters are changing over time. Secondly, we propose a method in estimating heterogeneous treatment effects in observational studies using transformed response variables via modification to Bayesian additive regression trees that incorporate a mixture model in the regression error terms thus avoiding model misspecification.

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Chapter 1

Overview

This thesis will focus on Bayesian methods in two areas. Firstly we introduce a new method based on almost embarrassingly parallel particle filtering. Secondly, we modify the Bayesian Additive Regression Trees algorithm in an application to estimating heterogeneous treatment effects.

The advent of High Performance (HPC) and parallel computing has opened the door to types of statistical analysis that were formerly unthinkable (Reumann et al., 2012), (Ko et al., 2021). This relatively new technology has always shown promise but with the acceptance of practitioners, the promise is coming into its own as an exciting new reality. Now that we are at or near the physical limitations for clock speeds of a computer’s central processing units, new ideas of how to make use of computation will need to be explored to advance statistical and scientific computation. Now, increases in compute power comes from the use of multiple cores within a computer processor chip. Modern HPC clusters or machines are equipped with more than one CPU that work on the same problem, thus enabling parallelism. Technology has also enabled other frontiers that are poised to propel statistics into the future.

The continuous generation of data has led to a world where more and more the catch phrase ”big data” is becoming more the norm than the exception. Organizations are having to make deliberate choices of what not to save as there is little ability to host in a data base, tempting as it may be to ”record everything”, all the observable events. Being as it is, there is tremendous value in understanding how to work with these new and now commonly available big data scenarios as they can deliver tremendous value to an organization. Models that that can process either large observational count data or large

parameter models that capture individual level effects have the capacity to significantly change an organizations bottom line.

In addition to advances in computation, there has also been an evolution in statistical thinking stemming from needs in sociology, economics, finance and practical industry needs to go beyond studying association to studying *causation*. Often, in observational settings, interventions are administered and need a *post-hoc* analysis to assess the effect of the intervention. Alternatively, a company may need to understand the effect of their product’s price on demand. These are examples of problems that are designed to be addressed with *causal inference* (CI). In CI settings there is generally the ability to infer population level effects which can be quite useful in assessing population level decision. There is also often the need to assess individual level effects which can help in such clinical settings as assessing the quality of an intervention on a specific subset of a population.

Chapter 3 explores how advances in distributed computing can leverage the ability to send messages over the network while learning from data to improve parameter estimation and statistical inference. We show for two separate models (2 different data generating processes) how allowing communication between compute nodes and/or processes, each having its own data partition, allows us to often improve model fit.

Chapter 4 explores applications in Causal Inference for observational data using a transformation of the response outcome that is a function of the response, an indicator variable designating treatment assignment, and the probability of treatment assignment. Our proposed model also makes use of a newly devised reparameterization of the error distribution proposed in (Zaidi and Mukherjee, 2018) allowing the model to better reflect the mixture nature of the transformed response variable (TRV). We accomplish this by modifying Bayesian Additive Regression Trees and adapting them to the causal setting. The modification is accomplished with BART by jointly modeling the unobserved treatment effect function and a second function that is also unobserved comprised of the response under the control and treatment conditions as well as the probability of treatment assignment. We show how our model is a preferred alternative to other competing models also using the TRV with respect

to reducing the error in heterogeneous treatment effect estimates. Additionally, we show how our model is competitive with other state of the art methods not using the TRV. We also discuss a shortcoming of the parameterization related to modeling the response functions which serve as a limiting factor in inference quality of the proposed method.

Chapter 2

Background

2.0.1 Bayesian Inference

Bayesian inference is a method of statistical inference reliant of Bayes' Theorem. Bayes theorem is a mathematical formulation of updating the probability of a hypothesis given information or evidence. Bayes theorem is particularly useful in the dynamic analysis of sequential data and in applying regularization for probabilistic models. Formally, given two events A and B , Bayes' Theorem simply states

$$P(B|A) = \frac{P(A|B)P(B)}{P(A)}$$

This formulation is very powerful and opens the door to interesting ways of interpreting both observed and unobserved phenomenon. Specifically, related to observed phenomenon, if we think of observed phenomenon as being represented by a set of data or records, X , θ as a set of parameters related to the mechanism by which the data is generated and $P(X)$ and $P(\theta)$ as probability distributions for the data and parameters, then

$$P(\theta|X) = \frac{P(X|\theta)P(\theta)}{P(X)} \tag{2.1}$$

which reflects the a posterior belief about θ given the evidence, X . This quantity is proportional to the likelihood $P(X|\theta)$ and the prior belief about θ , reflected in a prior distribution, $P(\theta)$, and is inversely proportional to a normalizing constant $P(X)$ reflecting the data generating mechanism.

Many approaches have been proposed in Bayesian Inference to estimate the posterior distribution, $P(\theta|X)$. Chapters 3 and 4 will both rely on Monte Carlo Sampling methods to estimate target distribution by producing samples intended to approximate the posterior conditional on evidence. Due to the high dimensional nature of our parameter space, θ , it can be intractable to produce samples of our parameter space at once. Because of this, methods that partition the parameter space have been devised and used with great success. As an example, consider a partition of $\theta = \{\theta_1, \theta_2\}$, where we then write equation 2.1 as

$$P(\theta_1|X, \theta_2) = \frac{P(X|\theta_1, \theta_2)P(\theta_1, \theta_2)}{P(X, \theta_2)} \quad (2.2)$$

Under this formulation, we are able to sample from the conditional distribution of θ_1 conditional on the other set of parameters and the data. Chapter 3 makes use of this technique, as it allows us to estimate parameters that are evolving in time as well as model data in streaming settings. Chapter 4 on the other hand does not have parameters that are evolving in time or deal with streaming data but still has a high dimensional parameter space. We therefore employ techniques such as Gibbs Sampling (Geman and Geman, 1984), Metropolis-Hastings (Metropolis et al., 1953) and Bayesian Backfitting (Hastie and Tibshirani, 2000), all of which rely on the framing provided by equation 2.2.

This formulation using Bayes theorem is also particularly useful in applying regularization to model parameters as depending on the specification for $P(\theta)$, this can have the effect of shrinking our estimates of θ towards our prior belief about θ . Models such as CART (Breiman et al., 1984a), BART (Chipman et al., 1998), and LASSO (Tibshirani, 1996) all make use of shrinkage to varying degrees to estimate model parameters. We make use of this technique in Chapter 4.

2.0.2 Sequential Monte Carlo (Particle Filtering)

Sequential Monte Carlo methods are a set of simulation based methods that provide a convenient way to approximate posterior distributions. One ad-

vantage of SMC methods is their ease of implementation and their ability to be parallelized, making them ideally suited to scalable solutions. To accomplish this, particle filtering uses a set of samples, also referred to as particles, to represent a posterior distribution of some parameter or set of parameters. Particle filters can be used to estimate the state of a signal that evolves through time by assigning to each particle a likelihood weight proportional to the probability of that particle being sample from a target distribution. As a simple example, consider a set of parameters θ and a set of observations $X = X_1, \dots, X_T$. SMC methods can formulate the problem of estimating the target distribution using a modification of equation 2.1,

$$\begin{aligned} P(\theta|X) &\propto P(X|\theta)P(\theta) \\ &= P(\theta)P(X_1|\theta)\dots P(X_T|\theta) \end{aligned}$$

And in so doing, we can think of $P(\theta)P(X_1|\theta)\dots P(X_{t-1}|\theta)$ as a prior on $P(X_t|\theta)$. Iterating on this idea we can sequentially learn the parameter θ from the data. This is one of the the foundational ideas of SMC and particle filtering which we use to great extent in Chapter 3.

2.0.3 Causal Inference

Causal Reasoning, the desire to understand cause and effect relationships, is known to at least date back to the fourth century BC with Aristotle's Physics (Falcon, 2015) where we find the first known protoscientific study of cause and effect. One of the primary types and applications of causal reasoning involves causal inference, with a primary focus being treatment effect estimation. A treatment effect is the effect a binary variable has on a response outcome of scientific or policy interest. In particular, the treatment effect measures the difference in outcomes between a unit(s) assigned to treatment vs a unit(s) assigned to the control condition. There have been two primary and heavily influential approaches to estimating treatment effects. The first termed do calculus based on graphical models introduced by (Pearl, 2009) and the other based on the potential outcomes framework (POF) introduced by (Rubin, 1978). In the POF, we are provided a set of sufficient conditions needed to define a causal effect or more specifically, a numeric quantity known

as the causal estimand that can be estimated from the data and who's effect on the response can be attributed to some intervention. For a hypothetical intervention, the causal effect for a unit is the difference that would be observed for a particular unit administered the intervention versus the same unit not administered the intervention. This is the fundamental problem of causal inference. That is, we are only capable of observing a single state of the unit. The unit administered the intervention or the unit not administered the intervention but never both. Consequently, unit level causal effects are not identifiable but under some standard assumptions discussed in Section 4.3, causal effects are identifiable. In this work, we develop a methodology that extends from the POF defined in (Rubin, 2005).

2.0.3.1 Transformed Response Variable for Causal Inference

In some sense, we can think of a unit or individual level treatment effect as a difference in two regression functions:

$$\tau(x) = E[Y|X = x, W = 1] - E[Y|X = x, W = 0] \quad (2.3)$$

where $\tau(x)$ is the unit level treatment effect, Y is a continuous outcome response, X is a set of observable covariates, and W is a binary indicator equal to 1 for units administered treatment and 0 otherwise. A consequential property of the unit level treatment effect is that it equals the population level average treatment effect after marginalizing over X . An alternative approach that avoids formulating the problem via two regression functions was popularized by (Athey and Imbens, 2015a) for estimating the unit level treatment effects. We discuss the potential upsides and downsides in more detail in chapter 4.

The alternative formulation termed the transformed response variable (TRV) is constructed as follows. If we denote our observed response value Y_i , our indicator variable indicating treatment assignment as W_i and the probability of treatment assignment (propensity score) as $P(W_i = 1) = p_i$ then the transformed response variable is defined as:

$$Y_i^* = \frac{Y_i(W_i - p_i)}{p_i(1 - p_i)} \quad (2.4)$$

This definition has the interesting characteristic such that

$$\tau(x) = E[Y_i^* | X_i = x]$$

We provide the proof in Appendix B.2.1 and in depth discussion and analysis in chapter 4.

2.0.3.2 Bayesian Additive Regression Trees

Decision trees have found vast popularity since their broad introduction with (Breiman et al., 1984a) which made their dissemination possible due to computers and available software. (Chipman et al., 1998) introduced a Bayesian version to probabilistically model a response variable conditional on the covariates by recursively partitioning the predictor space into subsets where the distribution of y is successively more homogeneous. Taking this idea further, (Chipman et al., 2010) extended CART into a boosting framework known as Bayesian Additive Regression Trees where the method fits a sequence of single trees, using each tree to fit residual data variation not explained by earlier trees in the sequence. BART has attained wide popularity due to its extensive flexibility to model response surfaces and its ability to produce full posterior inference including point and interval estimates of the unknown regression function. Owing to the flexibility of the method and its ease of modification, many have contributed to its expanded use. Modifications for BART for risk and survival analysis were proposed in (Sparapani et al., 2018) and (Sparapani et al., 2016). There are also adaptations to address function surface smoothness in (Linero and Yang, 2018) and (Starling et al., 2020a), estimating functions with heteroskedastic error (Pratola et al., 2020), adaptations that deal with sparsity and variable selection (Linero, 2018) and (Liu et al., 2021), categorical and count response outcomes (Murray, 2021), as well as adaptations for causal inference (Hahn et al., 2019); (Hill, 2011); (Starling et al., 2020b). For a full scale review of modeling developments regarding BART as of 2020, see (Hill et al., 2020).

At its core, BART is a semi-parametric regression model that estimates the conditional expectation of a response variable Y_i with a sum of weak learners, i.e., the trees. If one wishes to flexibly model a response function with

BART, we can do so with:

$$f(\mathbf{X}) = \sum_{j=1}^m g_j(\mathbf{X}, (T_j, \mathcal{M}_j)) \quad (2.5)$$

where m is the total number of trees in the model; the pair (T_j, \mathcal{M}_j) defines the structure of the j_{th} tree. Specifically, T_j defines the split rules and $\mathcal{M}_j = \eta_{j,1}, \dots, \eta_{j,b}$, the set of parameters associated with the b terminal nodes in tree j . The function $g(\cdot)$ is a single "weak" tree learner mapping the covariates X to a set of leaf nodes, \mathcal{M}_j which are determined by the set of splitting rules governed by T_j . The conditional mean function $f(\mathbf{X}) = E(Y_i|\mathbf{X})$ is computed by summing all the terminal nodes $\eta_{j,b}$ assigned to X by the functions $g_j(\cdot)$. There is extensive discussion about useful prior specifications for BART in (Chipman et al., 1998) and (Chipman et al., 2010). We go into further detail regarding prior specifications for our method in section 4.4.2

Chapter 3

Communal Monte Carlo Particle Filtering

3.1 Overview

In this chapter we explore how in a setting where we have streaming data and a parallel computing environment typically used for embarrassingly parallel model fitting, it is possible to significantly improve model fitting characteristics. We accomplish this by employing a relatively simple communication strategy between computational processes that typically would run to completion before sharing any parameter information. We validate our hypothesis with three separate trials. The first is with a dynamic linear regression model and the second is with a dynamic linear logistic regression model. Lastly, apply our logistic regression method to a real world data set of airline flight delay records.

3.2 Introduction

The recent methodologies for big data can be loosely grouped into three categories. They are resampling-based methods, divide and conquer methods, and methods that perform online updating. In this chapter we introduce Communal Monte Carlo which makes use of techniques typical of divide and conquer and online updating approaches. In particular, we employ at a base level Sequential Monte Carlo methods that can be characterized as the online updating portion but with an added resampling step to preserve particle diversity. Lastly, we also apply a divide and conquer strategy by partition our data which allows us to both improve computation time and potentially

respect memory constraints due to the machine’s capacity.

3.3 Background

The method presented in this work is a SMC method that makes use of particle resampling to preserve particle diversity and also runs on a distributed computing system where each computer process or node has its own shard of data where a batch model is trained. Our approach is unique in that it allows for intermittent communication between the processes/nodes allowing for potential improvement in inference quality.

The chapter is broken as follows: Sections 3.3 where we discuss relevant background including Sequential Monte Carlo (SMC). In section 3.4 where we briefly discuss previous parallel approaches relevant to our method. In section 3.5 we introduce Communal Monte Carlo and the necessary algorithms for the method. Finally we demonstrate the effectiveness of the approaches in sections 3.6 and in 3.7 we make concluding remarks and propose future work.

3.3.1 Sequential Monte Carlo

Sequential Monte Carlo (SMC) methods (Gordon et al., 1993), also known as Particle Filtering, are simulation-based Monte Carlo sampling methods used to solve filtering problems arising in Bayesian inference by represent a posterior distribution with a set of particles (samples). In the general setting, we assume that we have a sequence y_1, y_2, \dots of observations, each of which is associated with some (set of) latent parameters $\theta_0, \theta_1, \theta_2, \dots$. We assume the underlying stochastic process can be described in terms of some initial distribution $p(\theta_0)$, a Markovian transition distribution $p(\theta_t|\theta_{t-1})$ and some emission distribution $p(y_t|\theta_t)$ such that the observations y_t are conditionally independent given the θ_t . SMC methods use a swarm of P sequentially constructed “particles” $\{\theta_{0:T}^{(p)}, p = 1, \dots, P\}$, each associated with a weight $w_t^{(p)}$ to represent the posterior distribution over the $\theta_1, \dots, \theta_T$.

The simplest SMC algorithm, known as Sequential Importance Sampling (SIS), is a natural extension of importance sampling to the sequential

domain. At time t , each particle samples a value $\theta_t^{(p)}$ from some distribution $\pi(\theta_t|\theta_{0:t-1}, y_{1:t})$, and calculating the appropriate importance weights so that

$$w_t^{(p)} = w_{t-1}^{(p)} \frac{p(y_t|\theta_t^{(p)})p(\theta_t^{(p)}|\theta_{t-1}^{(p)})}{\pi(\theta_t^{(p)}|\theta_{0:t-1}^{(p)}, y_{0:t})}.$$

From the perspective of developing parallelizable algorithms, SIS is appealing, since each particle evolves independently from the rest of the swarm. However, as t increases, the particle weights become increasingly skewed, leading to a degenerate swarm that is dominated by a single particle. To avoid this, sequential importance resampling (SIR) periodically refreshes the samples, by sampling with replacement according to the normalized importance weights, resetting the importance weights to one. This allows us to propagate multiple copies of highly weighted particles, encouraging multiple particles to explore high-probability regions and reducing the degeneracy that plagues SIS. The Sequential Importance Resampling Algorithm introduced by (Kitagawa, 1996) and (Gordon et al., 1993) is detailed in Algorithm 1.

Algorithm 1 Sequential Importance Resampling (SIR)

Let N be number of observations in X , P be the number of particles, and $\theta_0 \sim P(\theta_0)$.

1. **for** $n = 1, \dots, N$ **do**:
 2. **for** $p = 1, \dots, P$ **do**:
 3. Sample $\theta_n^{(p)} \sim P(\theta_{n-1}^{(p)}|X_n)$
 4. Compute weight of particle $\xi_n^p = P(X_n|\theta_n^{(p)})$
 5. Normalize the weights ξ_n^p for $p \in (1, \dots, P)$
 6. Sample particles with replacement $\propto \xi_n^p$
 7. **return** $\theta_n^{(p)}$, the posterior estimate for $P(\theta|X) = \{\xi_n^p\}$
-

While SIR offers improved estimation over SIS, it is no longer easily parallelizable. Resampling must be performed at frequent intervals, and requires access to the entire swarm of particles. While more sophisticated SMC algorithms have been developed based on SIR (Whiteley et al., 2016), these

inherit the global dependency of SIR. In our work, we provide an approximate, parallelizable variant of SIR; while we focus on extending the basic SIR algorithm, our approach could easily be extended to most modern SMC algorithms.

3.3.2 Parallel Monte Carlo Methods and Related Work

As computers have become cheaper, faster and new technologies have facilitated communication between processes or compute nodes, there is a greater potential to take advantage of such "clusters" in a way that allows them to work together in a coordinated fashion. This ability allows for "divide and conquer" strategies. Conceptually, suppose we have observations X_1, \dots, X_N , the ability to run S separate compute processes in parallel allowing us to fit S separate models to the data. If we then divide the data into S sets, we can make use of all the available processes and fit f_1, \dots, f_s separate "mini" models to our S subsets of data. In the final step, we could combine our S models in an appropriate way so as to render an approximation representing a model fitting the full data set of N observations. Efforts to adapt and parallelize SMC algorithms to make use of more sophisticated computational resources and how the approaches differ from our own focus are detailed below.

Methods where the full data is split into a larger number of smaller datasets which may or may not overlap were introduced by Neiswanger et al. (2014), (Xiangyu Wang, David B. Dunson 2014) Wang and Dunson (2013), (Scott et al. 2013) Scott et al. (2016), Minsker et al. (2014) Inference is then performed on the data subsets and the model parameters are then combined in some reasonable manner. The Bag of Little Bootstraps (BLB) was proposed by Kleiner et al. (2012) which incorporates features of both the bootstrap and sub-sampling to obtain a robust, computationally efficient means of assessing estimator quality. Divide and conquer ideas previously used to design MCMC algorithms for big data with a sequential MCMC strategy have also been proposed by Casarin et al. (2015a). A stochastic gradient MCMC method that exploits distributed computation by using mini-batches of data greatly decreasing inference time was proposed by (Ahn et al., 2014) but is different

in that it is a fully distributed MCMC algorithm based on stochastic gradients rather than Particle Filtering.

Developing theory and methods of doing SMC in parallel, (Lee and Whiteley, 2016) focusing on controlling Effective Sample Size (ESS) through a method called α SMC. The approach does so in a way that minimizes communication between nodes using tree based graph structures which themselves are based on the structure of the computer cluster/network. The method does not partition the observed data amongst the S compute nodes but rather all the compute nodes see all the data, where as our approach focuses on the scalability in part through data partitioning. In addition their method in practice limits what nodes have access to what particles, where as we allow all nodes access to all particles at global communication points. Methodology proposed by (Nam et al., 2014) in which the number of underlying states, H , in a Hidden Markov Model (HMM) framework can be determined by the use of parallel sequential Monte Carlo samplers. However, the approach does not make use of data partitioning and network communication to improve overall performance or fit quality making the focus of how to leverage distributed computing very different than our own proposed method. A parallel version of SMC for optimization (PSMCO) by (Akyildiz et al., 2020) optimizes functions of the form

$\min_{\theta \in \Theta} f(\theta) = \sum_{i=1}^n f_i(\theta)$, by using partitioned subsets of the data on each worker node but then only keeps the particles from the best performing worker and disregards estimates found on other workers. In addition, PSMCO at each iteration will only use a subset of the f_i 's on each node; that is, each node will focus on optimizing only a subset of the global $f(\theta)$. Another key difference is that PSMCO transforms the function to be optimized from $\sum_{i=1}^n f_i(\theta)$ to one proportional to a probability measure of the form $\exp(-\sum_{i=1}^n f_i(\theta))$. Our method in turn does nothing of the sort since we use the same probability distribution on all nodes performing inference and in no way requires distributions of the form $c_0 \exp(-\sum_{i=1}^n f_i(\theta))$, where c_0 is a constant. Lastly, since PSMCO is a method designed for optimization, the particle with the highest density on the worker that has the highest marginal likelihood is used as the estimate for the global minimum of $f(\theta)$, where as our focus is on evaluating not only the MAP, but also all relevant moment's for any parameters of interest. A parallel SMC algorithm proposed by (Verge and Moulines, 2015), named the

island particle filter, allows for interaction between nodes, ie "particle islands", according to some resampling scheme. For example, an islands particle history can be replaced according to a draw from a multinomial distribution where each category represents another island's particle history and the likelihood of any one category being drawn is a function of the potential or likelihood function. The particles in each island are then jittered in a mutation step according to a Markov transition. In another proposal, (Verge and Moulines, 2015) also suggests saving the mutation step for situations where the effective sample size of the island falls below some threshold proportional to the number of particles in the island. And in a final proposal, the suggestion to perform the resampling of the islands only after the ESS falls below some threshold that is a function of the number of islands (ie. processors) and individuals (ie. particles) found on each island. These methods requires a global communication at every iteration to determine the ESS across the network, where as our approach relaxes the need for such frequent communication and also accomodates large datasets by partitioning the data across the compute nodes. There have also been contributions to the computational front, such as (Zhou, 2015) who provides a C++ template library that can be used to implement generic sequential Monte Carlo algorithms on parallel hardware using, most notably, MPI and (Casarin et al., 2015b) who developed a matlab package for efficient density combination making use of parallel GPU and multi-core CPU capabilities. (Lindsten et al., 2017) proposed a divide and conquer approach that accommodates paralleling but the the problem is broken up according to the graphical structure of the specified model with various compute nodes responsible for model inference specific to a portion of the graph. Again, our approach to leveraging distributed computing uses data partitioning and parallelization and particle swarms are kept local to each node until a global communication step. On the theoretical front, (Whiteley et al., 2016) were able to phrase sufficient conditions for time-uniform convergence in terms of algorithmic control of the ESS, in turn achievable by adaptive modulation of the interaction between particles. The results even concern the behavior of PF's run in parallel but fall short of addressing convergence properties in a data partitioned regime. (Míguez and Vázquez, 2016) and (Read et al., 2014) propose using parallel architecture for particle filtering where the particles are

partitioned amongst the compute nodes or elements but the observed data is not partitioned.

3.4 Parallel Methods and Consensus Monte Carlo

Increased computational resources has introduced some unique challenges in big data and there have been a variety of proposals in dealing with large datasets. Specifically, (Minsker et al., 2014), (Scott et al., 2016), (Srivastava et al., 2018) and (Neiswanger et al., 2014) to name a few have all suggested an approach reliant on partitioning a full data set into smaller subsets and distributing the data partitions into separate compute processes where separate MCMC chains can be run. The challenge comes with the final stage when the subset posteriors need to be combined in some sort of way so as to approximate the full posterior. Since our specific use case is focused on fast scalability, we found that of the aforementioned methods, the one most well suited to fast approximate inference was the Consensus Monte Carlo Method proposed by (Scott et al., 2016). Detailed derivation of the result for our specific use case can be found in Appendix A.1

3.5 Communal Monte Carlo

We now introduce our approximate, distributed online Sequential Monte Carlo algorithm, which we will refer to as Communal Monte Carlo (CMC). We assume that we have a model with time-evolving parameters θ_t , and that given N time-stamped data points (where n_t is the timestamp of the n th data point), we wish to approximate the posterior distribution $p(\theta_{t_n}|X_1, \dots, X_n)$, or $p(\theta_{t_0}, \dots, \theta_{t_n})$.

We partition our data across S subsets and assign each dataset to a separate shard. We write $X^{(s)}$ to denote the data in the s th subset. We then run S independent SIR algorithms on the partitioned data up to time t_1 . The goal is to obtain S estimates of the posterior $p(\theta_{t_0}, \dots, \theta_{t_1}|\{X_n : n_t \leq t_1\})$. As discussed by (Minsker et al., 2014), naively approximating this posterior with $p(\theta_{t_0}, \dots, \theta_{t_1}|\{X_n^{(s)} : n_t \leq t_1\})$ overweights the contribution of the prior;

instead we use the stochastic approximation

$$\hat{p}(\theta|X) \propto p(\theta|X^{(s)})^S p(\theta)$$

where (Minsker et al., 2014) showed that while each of sub posterior might be “unstable”, in the aggregate, these random measures improve stability and yield smaller credible sets with good coverage properties.

At time t_1 , each shard s contains P particles, each representing a parameter value $\theta^{(s,p)}$. We replace each local swarm of particles with P particles sampled, uniformly with replacement, from the set of *all* particles across all S shards. Unlike the SIR steps, this requires global communication. We then propagate our local swarm of particles on the local observations up to the next global communication time t_2 . At the final communication time, we then approximate our target distribution with our set of particles using the Consensus Monte Carlo Algorithm proposed in (Scott et al., 2016). The algorithm is summarized in Algorithm 2.

Algorithm 2 Communal Monte Carlo (CMC)

Let X_{t_1}, \dots, X_{t_E} be a partition of the full data X , respecting the indexing t .

Let $\theta_{t_0}^{(s,p)}$ be our initial set of particles of size SP defined by our prior $P(\theta_0)$.

1. **for** $e = 1, \dots, E$ **do**
2. Sample w/o replacement from the set $\theta_{t_{e-1}}^{s,p}$ to S sub-sets of size P .
3. Distribute each partition of particles to each of the S shards.
4. In parallel run SIR Alg. for each shard $s \in 1, \dots, S$ with $X_{t_e}^{(s)}$.
5. Combine all S*P particles to form the set, $\theta_{t_e}^{(s,p)}$

return $\theta_{t_E}^{(s,p)}$, a sample from $\prod_{s=1}^S P(\theta_{s,E}|X_{s,E}) \approx P(\theta|X)$.

If we have a single global step, ie $t_1 = N_t$, then our algorithm can be seen as a variant of existing embarrassingly parallel algorithms such as those described in 3.3.2 but as we show in section 3.6 there is often advantage in allowing intermittent communication between the parallel processes.

We can think of the global steps as approximations to a global importance resampling operation. Since we have already locally resampled on

each shard, the appropriate resampling weights within a shard are uniform. While the relative weights for each shard are not uniform since each shard has a different normalizing constant equal to $\frac{1}{P(X)}$, calculating the true weights would be expensive due to the necessity of evaluating the likelihood for each SP particles on every shard. Therefore, we approximate the weights as equal.

3.6 Real Data and Simulation Studies

We hypothesize that, in scenarios where full SMC-based posterior inference is infeasible due to time, CMC allows us to obtain high-quality estimates of the posterior via parallelization. Further, we argue that where model parameters evolve over time, periodic communication allows for better posterior estimates than would be achieved using an "embarrassingly parallel" approach. To this end, we use our algorithm to perform posterior inference in two Bayesian models, using simulated data. We compare various number of shards (including one shard, ie standard SIR SMC) to explore the trade-off between inference time and estimate quality, and compare various communication frequencies (including an embarrassingly parallel scenario) to explore the benefit of periodic communication. We evaluate the effectiveness of our algorithm using two models including linear and logistic regression for our simulation studies. We also use a real world data set of airline flight delay data first used in (Hensman et al., 2013) as an example "big data" data set. It is worth noting, (Hensman et al., 2013) only used 4 months worth of data to validate their method but we in turn were easily able to incorporate an entire year of data, showcasing our methods ability to scale more effectively.

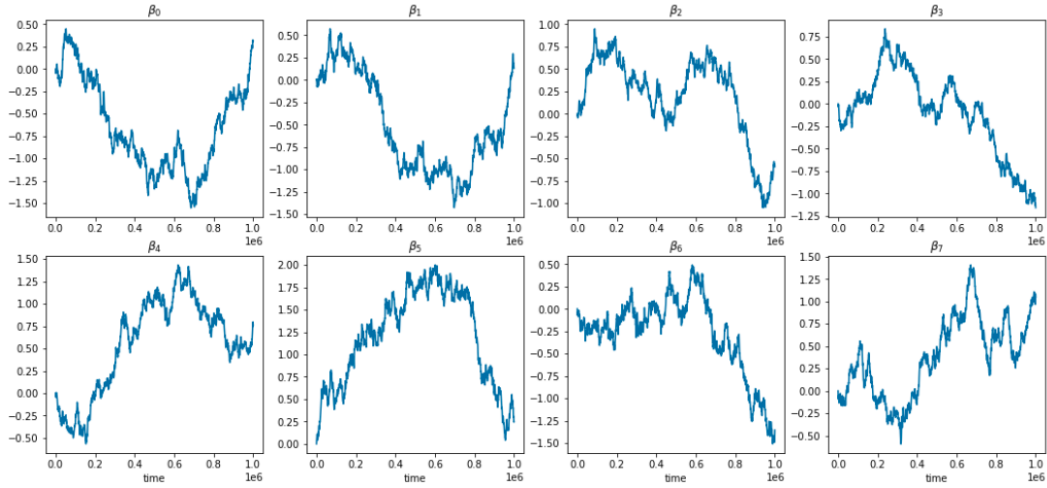
3.6.1 Models

We generate linear and logistic regression datasets where the true coefficients vary according to the Gaussian processes $\beta_k \sim GP(0, K)$, where K is a squared exponential kernel with unit bandwidth. Figure 3.1 shows some examples of how the β_k vary in time.

3.6.2 Data Sets

Regression: We simulated 20 datasets, each associated with a different set of $K = 32$ dynamically varying parameters β_k . Each dataset contained $N = 1000000$ observations, with one observation per unit-spaced time step, according to equations 3.1:

Figure 3.1: Plot showing 8 of the 32 time varying regression coefficients generated according to $\beta_k \sim GP(0, K)$



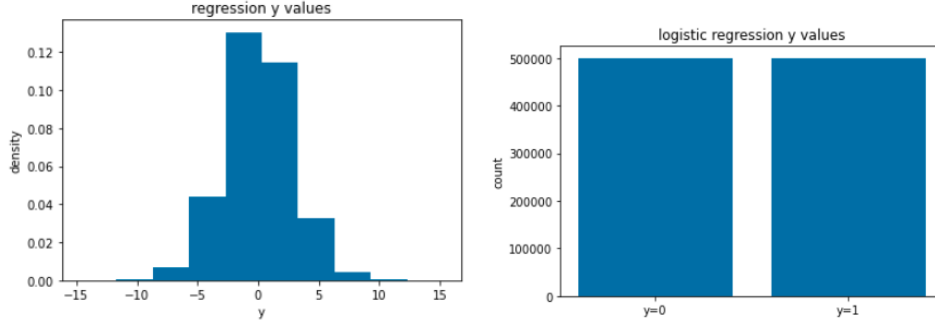
$$\begin{aligned}
 X_{k,t} &\sim \text{Uniform}(-1, 1); \quad k \in \{1, \dots, 32\} \\
 y_t &= \sum_{k=1}^{32} X_{k,t} \beta_{k,t} + \epsilon_t \\
 \epsilon_t &\sim N(0, 1)
 \end{aligned} \tag{3.1}$$

Figure 3.2 shows the range of y values take over all values of t

Show plots of regression coefficients and range of y values here

Logistic Regression (Classification): Our simulated data used in our logistic regression model is generated similarly to the regression data in that the regression coefficients and X follow the same DGP. However, our response

Figure 3.2: Histogram showing the distribution of y for an example regression data set on the left and distribution of y values for our logistic regression data on the right).



$y_t|X_t, \beta_t$ is drawn from a Bernoulli distribution, where we allowed for 10 observations per time step. We noticed there is some instability in the particle filters ability to learn the model when having only 1 observations per time stamp and so we elected to allow 10 observations per time stamp. This allows us to batch observations onto the same shard with the same timestamp. We allow for $t \in \{1, \dots, 100000\}$ where each time t has 10 corresponding observations $y_{i,t}$, where $i \in \{1, \dots, 10\}$ allowing for a total of $N = 1,000,000$ total observations.

We simulated 20 datasets, each associated with a different set of $K = 32$ dynamically varying parameters β_k . Each dataset contained $N = 100000$ observations, with 10 observation per unit-spaced time step, according to equations 3.2:

$$\begin{aligned}
 X_{i,k,t} &\sim \text{Uniform}(-1, 1); \quad k \in \{1, \dots, 32\}, \quad i \in \{1, \dots, 10\} \\
 \gamma_t &= \sum_{k=1}^{32} X_{k,t} \beta_{k,t} \\
 p_t &= \frac{1}{1 + \exp(-\gamma_t)} \\
 y_{i,t} &\sim \text{Bernoulli}(p_t); \quad i \in \{1, \dots, 10\}
 \end{aligned} \tag{3.2}$$

Figure 3.2 shows the range of y values take over all values of t .

3.6.3 Evaluation Metrics

We define the following evaluations metrics for our data sets.

Regression: After fitting a given model, we perform an out-of-sample (OOS) evaluation of the Mean Squared Error (MSE) between the fitted values, $Y_t|X\hat{\beta}_{N_t}$ and the true $E(Y_t|X\beta_{N_t})$, where β_{N_t} is our ground truth value of the regression coefficient determined at the last time value the data is simulated from the Gaussian Process regression coefficients and $\hat{\beta}_{N_t}$ is our estimate of β_{N_t} . We performed the evaluation on 20 separate data set replications to compute the expected Mean Squared Error (MSE), MSE_R , accross the $R = 20$ replications. We generated $N_{oos} = 1000000$ out of sample observations for our test set. Our out-of-sample MSE posterior estimate is therefore,

$$MSE = \frac{1}{N_{oos}} \sum_{n=1}^{N_{oos}} \frac{1}{P} \sum_{p=1}^P (X_n^* \beta_{N_t}^{(p)} - X_n^* \beta_{N_t})^2 \quad (3.3)$$

where P is our total number of particles and X^* is our out of sample data and N_t is the last time state. We report the mean and standard error of the MSE accross the 20 replications with

$$MSE_R = \sum_{r=1}^R \frac{MSE_r}{R} \quad (3.4)$$

Logistic Regression (Classification): After fitting a given model, we performan an OOS evaluation of the mean posterior log likelihood, $E[l(Y_t|X, \hat{\beta}_{N_t})]$, where $\hat{\beta}_{N_t}$ is our estimate of β_{N_t} . We performed the evaluation on 20 separate data set replications to compute the expected mean log likelihood ELL_R , accross the $R = 20$ replications. We generated $N_{oos} = 10000$ out of sample observations for our test set. Our out-of-sample $E[l(Y_t|X, \hat{\beta}_{N_t})]$ posterior estimate is therefore,

$$\begin{aligned}
\gamma_p &= \text{logit}^{-1}(X_n^* \beta_{N_t}^{(p)}) \\
E[l(Y_t|X, \hat{\beta}_{N_t})] &= \frac{1}{N_{oos}} \sum_{n=1}^{N_{oos}} \frac{1}{P} \sum_{p=1}^P y_n \log(\gamma_p) + (1 - y) \log(1 - \gamma_p)
\end{aligned}
\tag{3.5}$$

where P is our total number of particles and X^* is our out of sample data and N_t is the last time stamp. We report the mean and standard error of the expected mean log likelihood accross the 20 replications with

$$MLL_R = \sum_{r=1}^R \frac{E[l(Y_t|X, \hat{\beta}_{N_t})]_r}{R}
\tag{3.6}$$

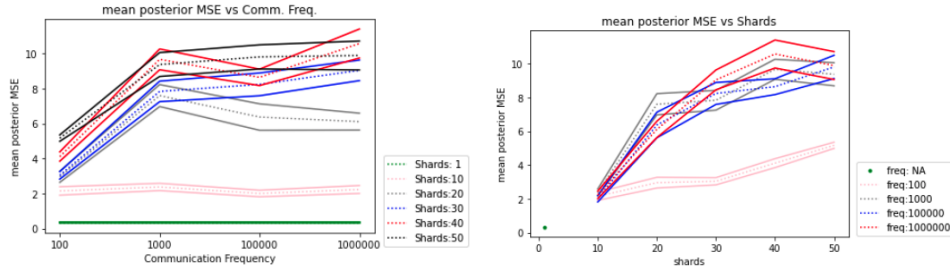
3.6.4 Regression Comparison of CMC vs. EPSMC

In our evaluations we compare the performance of Communal Monte Carlo with various communication frequencies vs the embarrassingly parallel (one communication at final time stamp) version. For our regression data, our primary comparison metric is out-of-sample Mean Squared Error.

In Figure 3.3 we can see comparisons between our CMC method vs its embarrassingly parallel counterparts with communication frequencies every 100, 1000, 100000, 1000000 and $S \in \{10, 20, 30, 40, 50\}$ shards and $P = 1000$ particles. Note that communication at 1000000 corresponds to an embarrassingly parallel version of our algorithm. We can see there is the most to gain with frequent communication over the embarrassingly parallel counterpart in this dynamic linear model example. In particular, for a fixed number of shards, we see that more frequent communication produces better fits as is evident with the increasing MSE as communication frequency increases from 100 onward. However, this is not the case for all shard counts. There appears to be little advantage to increased communication for 10 shards as compared to 20, 30, 40, and 50 shards. In this case, we believe this is because although we

lose inference quality with more partitions of the data, we are able to partially overcome this challenge by allowing the parallel processes to share parameter estimates. Additionally, for a fixed number of communication steps, we see that we obtain better performance with fewer shards. This makes sense because each compute node/process sees more data and therefore can produce a better fitting model. On the other hand, fewer shards means longer run times.

Figure 3.3: MSE_R (vertical axis) vs. communication frequency on the left and shards on the right (horizontal axis) . The non-solid lines are the estimated mean and solid bands are show ± 1 standard error. Our base line single machine comparisons are indicated in green



Next we consider the computational time. In figure 3.4 we can see the plot of MSE_R (y-axis) vs. total run time in seconds (x-axis). When it comes to run time, it is easy to see that for a fixed number of shards, increasing the communication frequency increases the run time. On the hand, communication comes at a cost that needs to be balanced with the number of shards used. For example, in the 30 shard runs, we see a decrease in computation time as compared to the 40 and 50 shard runs when communication frequency is 100. So, in this specific case, we get a better fit and *faster run time* with the 30 shard runs vs when we use 40 and 50 shards! This is due to the increased cost of communication for increasing numbers of shards. One key takeaway, is it is possible to improve model fit at the expense of some computational time as would be expected but even with frequent communication, we can sometimes get the benefits of both decreased computational time and improved fit.

Figure 3.4: MSE_R (y-axis) vs. run time in seconds (x-axis). The ± 1 standard error is indicated by the error bars. Note: the 1 shard run time was approximately 8500 seconds.

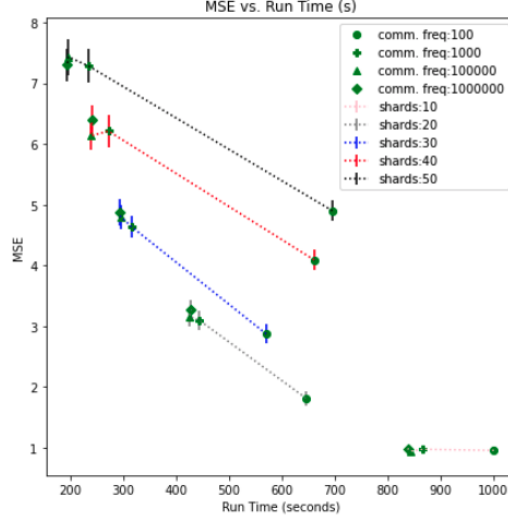
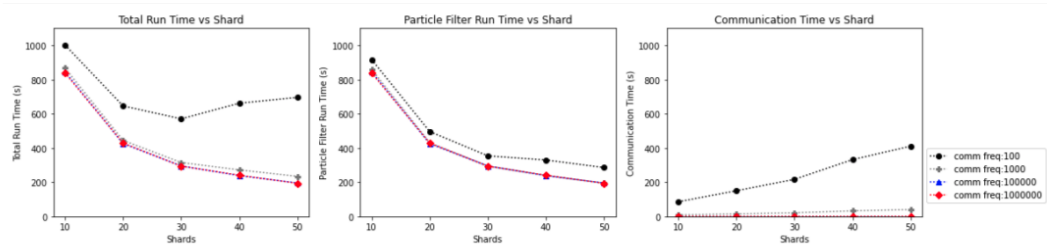


Figure 3.5 details the relationship between total run time, particle filter run time, and communication time for varying communication frequencies and shard counts. We can see in the plot of particle filter run time vs shards, the run time relationship is roughly proportional to $\frac{1}{s}$, where s is the shard count but in the plot of communication time vs shards, we see a relationship that is roughly linear. For a relatively frequent communication regime, a frequency of 100, in this case, the sum of particle filter run time and communication time will result in a smallest total run time that seems to occur around 30 shards which explains how we can get higher total run times for 40 and 50 shards even though each shard is processing less data than the 30 shard version.

Figure 3.5: time in seconds (y-axis) vs. shards (x-axis)



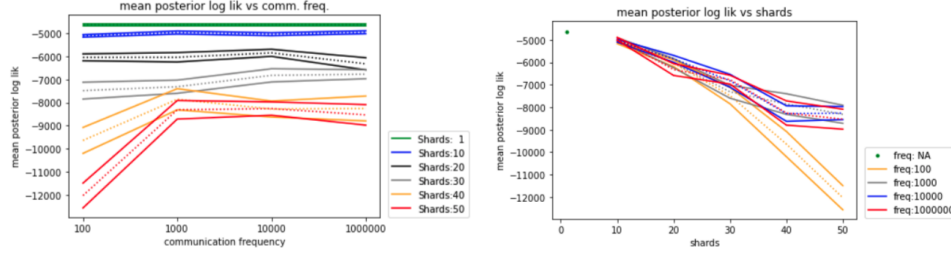
3.6.5 Logistic Regression Comparison of CMC vs. EPSMC

Next we show the results for our classification (logistic regression) model with 1000000 observations in total and where each time stamp has 10 observations for a total of $\frac{1000000}{10} = 100000$ unique time values. This allows us to batch our observations with one single machine getting all 10 observations with the same time stamp. It would be possible to distribute the observations with the same time stamp on separate machines but since our goal in part is to improve time efficiency, we elected to batch the observations with the same timestamp on the same machine.

In Figure 3.6 we can see comparisons between our CMC method vs its embarrassingly parallel counterparts with communication frequencies every 100, 1000, 10000, 100000 and $S \in \{10, 20, 30, 40, 50\}$ shards and $P = 1000$ particles. Note that communication at 1000000 corresponds to an embarrassingly parallel version of our algorithm. We can see there appears to be no improvement in log likelihood for the runs with 10, 20, and 30 shards. this implies to us the processes running in the embarrassingly parallel setting have enough data to learn model parameters and do not need the "advantage" of sharing information amongst themselves. Conversely, we see a collapse in the model fit for the 40 and 50 shard runs when allowing frequent communication. We suspect this is in part due to particle impoverishment but also due to dominant particles that have become "lost" in their parameter space exploration and yet managed to remain relatively dominant long enough to "pollute" the other processes leading the entire fitting process to perform poorly. A second compounding possibility is we were not able to select appropriate tuning parameters that would allow the separate processes to adapt to the fact that they are getting data that is more separated in time which coupled with the relatively weak signal from y values that are either 0 or 1 could also lead to the poor performance.

Next we consider the computational time. In Figure 3.7 we can see the plot of mean posterior log likelihood (y-axis) vs. run time in seconds(x-axis). When it comes to run time we see a similar patten to what we observed with the regression data but with run times occurring at roughly one tenth the time as would be expected since we are batching our observations in groups of 10 on each machine due to there being 10 observations per time stamp.

Figure 3.6: MLL_R (vertical axis) vs. communication frequency on the left and shards on the right (horizontal axis) . The non-solid lines are the estimated mean and solid bands are show ± 1 standard error. Our base line single machine comparisons are indicated in green



Additionally, even though the fit quality decreases as we increase the number of shards, we can dramatically reduce run time roughly proportional to $\frac{1}{s}$, where s is the number of shards. The practitioner, this is something to consider where execution time is critical. Lastly, in Figure 3.8, we see the same general patterns observed in the regression data with total run time, particle filter run time, and communication time. We see the particle filter run times roughly proportional to $\frac{1}{s}$, where s is the shard count but in the plot of communication time vs shards, we see a relationship that is roughly linear. For a relatively frequent communication regime (frequency of 100, in this case), the sum of particle filter run time and communication time will result in a minimum total run time that seems to occur around 30 shards which explains how we can get higher total run times for 40 and 50 shards even though each shard is processing less data than the 30 shard version.

Figure 3.7: MLL_R (y-axis) vs. run time in seconds (x-axis). The ± 1 standard error is indicated by the error bars. Note: the 1 shard run time was approximately 1500 seconds.

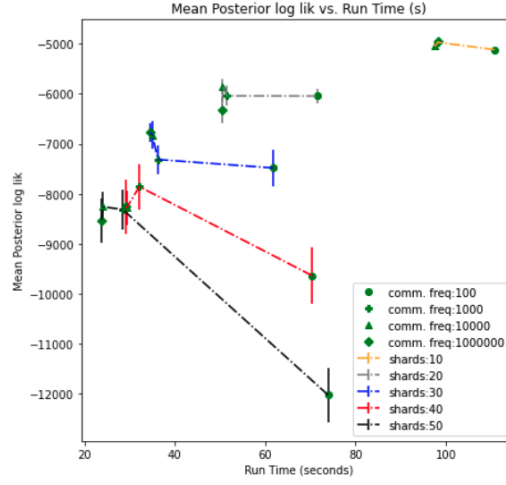
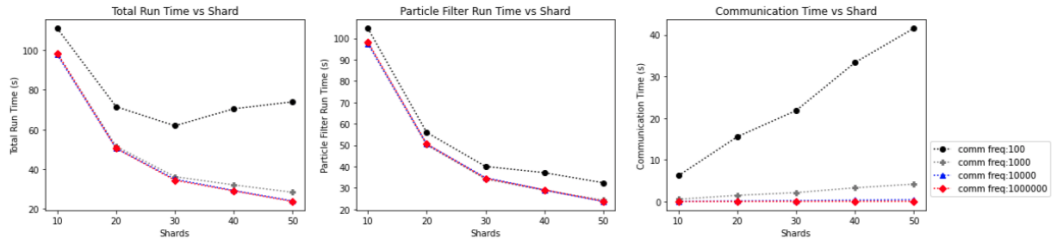


Figure 3.8: time in seconds (y-axis) vs. shards (x-axis)



3.6.6 Airline Flights Data

Our real world data set was first introduced in (Hensman et al., 2013) as a real world example of a data set that is relatively large in size and that is somewhat unwieldy for more advanced methods. There are many features available in this data set but we chose to include the following: age of the aircraft (number of years since deployment), distance that needs to be covered, airtime, scheduled departure time hour, scheduled arrival time hour, day of the week, day of the month and a time stamp. We chose to discretize with dummy variables scheduled arrival time hour, day of the week, day of the month which created a total of 76 regression parameters that would need be inferred from the data. The time stamp values start at 0 and increment every minute. Our training data begins with flights that departed beginning November 1st, 2012 and ending with September 30th, 2013. We use the flights from October 1st, 2013 to assess out of sample performance of our model. Our response variable y , is a binary indicator that is 1 if the flight arrival time is greater than 15 minutes past the scheduled arrival time and 0 otherwise. There were a total of $N = 6,331,671$ flight records and 480,960 unique time stamps in our training set and 11389 observations in our holdout set.

We performed our analysis with 10,20,30,40, and 50 shards as well with communication frequencies occurring every 100 and 1000 minutes and compare against the embarrassingly parallel versions. This analysis was repeated 20 times We also include as a baseline a single machine run (not in parallel) as a base line to assess best case model fit and worst case computational time performance. We report the mean and standard error of our analysis in a similar fashion to our simulation logistic regression analysis in 3.6.5.

RESULTS TO COME

3.6.7 Computational Resources

We fit our models to the simulated data using Stampede2, the flagship super computer of the National Science Foundation hosted by Texas Advanced Computing Center (TACC). It allows for massively parallel compute jobs and facilitates communication between compute nodes and up to 64 processes to

run in parallel per node. In our experiments, we allowed for up to 50 parallel jobs.

3.7 Discussion and Conclusion

WAITING FOR AIRLINE DATA RESULTS TO WRITE CONCLUSION

We have seen that Communal Monte Carlo has the capacity to improve the fit of models where pluralization is used. In particular where there are many parallel processes with partitioned data. We did not show in our analysis results where there was no benefit. We noticed that for small numbers of parallel processes consistent with what you have on a local laptop, such as 4 to 6 processes, there is no gain in fit performance. We also noticed that for the particular tuned settings we had chosen for our model fitting, above 50 shards for regression and 20 shards for classification, there also seemed to be a loss of advantageous performance with frequent communication doing as well as embarrassingly parallel. We have also seen in models that are less "hard" to learn, that increased communication does as well as the embarrassingly parallel counterpart.

The current work opens the possibility of improving model fitting with relatively simple communication strategies. We suspect that for more complex models such as ensemble tree methods where two functions are being fit, the models are sufficiently hard to learn that there is the possibility of improving tree ensemble methods by allowing communication between chains running in parallel. The objective obviously would be to "help" poor performing chains with trees that are stuck in a relatively low likelihood to find the part of the space with higher likelihood. Additionally, we have not shown any theoretical guarantees regarding under what circumstances specifically we can expect to see improvements in model performance. With a theoretical backdrop, we would have an illuminated road map of where to find opportunities for increased parallelization. Rather, what we have shown is it is possible to significantly improve model performance with little time cost with the use of very simple communication strategies in a parallel environment.

Next steps: learning comm frequency, gossip algos, see suggestions

Chapter 4

Bayesian Additive Regression Trees Mixture Model for Heterogeneous Causal Effects

4.1 Overview

In this section we propose a Bayesian semi-parametric model with a gaussian mixture distribution in the residual term to model heterogeneous treatment effects. The model revolves around the transformed response variable (TRV) from (Athey and Imbens, 2015a), which is a reformulation of the response variable used to model heterogeneous treatment effects. We aim to address 2 objectives.

1. Explicitly model heterogeneous treatment effects with a distribution implied by the TRV, thereby reducing the variance of the estimators.
2. Model both the treatment and control conditions jointly, thereby improving inference over models that do not model treatment and control conditions jointly.

4.2 Introduction

Population level treatment effects are typically estimated with the average treatment effect (ATE) which is a measure of the average difference between units assigned to treatment versus units assigned to control. The ATE is particularly useful when there is a lack of heterogeneity in the treatment effect but work from (Heckman et al., 2006); (Green and Kern, 2012); (Xie et al.,

2012) suggest this is less common than a population exhibiting heterogeneous treatment effects. An obvious downside to the ATE in the face of heterogeneity is the ATE will fail to estimate treatment effects in subgroups of the population should they exhibit heterogeneity. Importantly, we can deal with heterogeneity with a different approach and estimate the Conditional Average Treatment Effect (CATE) which is the average treatment effect conditional on the unit’s covariates. There have been both parametric and non-parametric methods proposed to estimate the CATE.

Among the parametric models of note used to estimate the conditional mean outcomes include linear and polynomial regression by (Pearl, 2009) and penalized regression approaches by (Tibshirani, 1996). Alternative non-parametric approaches have also been proposed to estimate heterogeneous treatment effects such as boosting (Powers et al., 2018), modified versions of Bayesian Additive Regression Trees (BART) (Hill, 2011); (Hahn et al., 2019); (Chipman et al., 2010) as well as more machine learning oriented regression tree methods by (Athey and Imbens, 2015a); (Breiman et al., 1984b) and ensemble methods by (Foster et al., 2011); (Wager and Athey, 2018); (Breiman, 2001); (Athey and Imbens, 2015b). The above methods have their strengths but are not without limitation which we discuss below. Estimating the CATE as proposed by (Wager and Athey, 2018) using random forest has sound theoretical justification due to the valid probabilistic statistical inference properties and tends to outperform other classical methods, particularly in the presence of irrelevant predictors. This approach, however has been outperformed by competing methods such as Bayesian Causal Forest by (Hahn et al., 2019). A second downfall of the random forest approach is due to the lack of a procedure to perform some regularization, random forests are a challenge to use for heterogeneous treatment effect estimation (Wendling et al., 2018). On the other hand BART based methods modified for estimating heterogeneous causal effects have been shown to perform quite well (Hahn et al., 2019); (Hill, 2011). The down side of the modified BART methods is the limited work related to their theoretical inferential properties related to CATE estimation when compared to (Wager and Athey, 2018). In particular, (Hill, 2011); (Hahn et al., 2019) lack theoretical support that the posterior concentrates around the true conditional mean function.

A second option for modeling the difference in conditional mean functions is to use the transformed response or outcome variables (TRV) (Dudík et al., 2014); (Beygelzimer and Langford, 2016) which has a similar flavor to inverse probability (propensity score) weighting (IPW) (Hirano et al., 2003). The TRV approach introduces a new response variable that is a function of the observed outcomes, Y , the binary treatment assignment variable, W , and the probability of treatment assignment (propensity score), p . Most importantly, the expected value of the TRV conditional on the covariates, X , is the CATE. This property in particular allows the TRV to be used with "off the shelf" machine learning and other regression related methods. Recent work by (Athey and Imbens, 2015a) with the TRV showed how one could model the CATE directly using the TRV as a function of the observed covariates with regression trees. This approach comes with a serious cost in that the estimation quality is poor due to the high variance resulting from modeling the TRV with the observed covariates without proper adjustment. (Zaidi and Mukherjee, 2018) then introduced a reparameterization that explicitly accounts for the properties of the TRV with a correctly specified model significantly reducing the variance previously associated with the TRV. We use the same reparameterization introduced by (Zaidi and Mukherjee, 2018) and a modified version of BART to introduce a new method, Conditional BART Mixture Model (CBARTMM), to estimate the CATE.

4.2.1 Notation and the Set Up

Our model is designed to address the scenario where we have data from an experiment where a binary variable, $W \in \{0, 1\}$, is assigned randomly with probability conditioned on the observed covariates, or in a quasi-experimental observational setting that satisfies the assumptions laid out in (Imbens and Rubin, 2015) which are required to make valid statistical inference of the CATE.

- **Assumption 1:** Individualistic and Probabilistic
- **Assumption 2:** Strong Ignorability:

$$Y(1), Y(0) \perp\!\!\!\perp W | X \quad (4.1)$$

$$0 < P(W = 1) < 1 \quad (4.2)$$

- **Assumption 3:** The Stable Unit Treatment Value Assumption (SUTVA):
The potential outcomes for any unit do not vary with the treatments assigned to other units, and, for each unit, there are no different forms or versions of each treatment level, which lead to different potential outcomes.

Assumption 1 is implied if all the units under study comprise a simple random sample from the target population, the units are independent and are identically distributed. Assumption 2 simply means the potential outcome of Y regardless of whether they were treated or not does not depend on whether they have been treated or not, ie. we can *ignore* how people ended up in the treatment group vs the control group and treat the potential outcomes as exchangeable. Assumption 3 assumes there is no interference between the units, and that there is only one version of the treatment.

Let N be the number of units in the data, indexed by $i \in \{1, \dots, N\}$. Let $W_i \in \{0, 1\}$, be the binary indicator for the treatment with $W_i = 0$ for units assigned to the control arm and $W_i = 1$ for units assigned to the treatment arm, and let X_i be a p -component vector of features, covariates or pre-treatment variables that are unaffected by treatment. Let $p = E[W_i] = P(W = 1)$ be the marginal probability of treatment assignment and $p_i = E[W_i|X_i] = P(W = 1|X_i)$ be the conditional probability of treatment assignment, also called the "propensity score".

We postulate, that there exists a pair of potential outcomes for each unit $(Y_i(0), Y_i(1))$, following the POF described in (Imbens and Rubin, 2015). We therefore define the unit-level causal effect as the difference in potential outcomes,

$$\tau_i = Y_i(1) - Y_i(0) \quad (4.3)$$

The observable outcome for unit i is the potential outcome linked to the outcome conditional on the treatment, W_i . That is,

$$Y_i = Y_i(W_i) = \begin{cases} Y_i(0), & \text{if } W_i = 0 \\ Y_i(1), & \text{if } W_i = 1 \end{cases} \quad (4.4)$$

The data consists of the triplet (Y_i, W_i, X_i) , for $i \in \{1, \dots, N\}$. We define the conditional average treatment effect (CATE), as

$$\tau(x)^{CATE} = E[Y_i(1) - Y_i(0)|X_i = x] \quad (4.5)$$

and the population average treatment effect as

$$\tau^{ATE} = E_X[E_Y[Y(1) - Y(0)|X]] = E[\tau^{CATE}] \quad (4.6)$$

4.3 Transformed Response Variable for Causal Inference

If we denote our observed response value Y_i , our indicator variable indicating treatment assignment as W_i and the probability of treatment assignment (propensity score) as $P(W_i = 1) = p_i$ then the transformed response variable is defined as:

$$Y_i^* = \frac{Y_i(W_i - p_i)}{p_i(1 - p_i)} \quad (4.7)$$

This definition has the quality such that $E[Y_i^*|X_i = x] = \tau^{CATE}$. We provide the proof in Appendix B.2.1

4.3.1 Advantages of the TRV

The TRV comes with a set of tree main advantages. First, modeling heterogeneous treatment effects with TRV as shown in (Athey and Imbens, 2015a);(Wager and Athey, 2018);(Powers et al., 2018) can be done with "off the shelf" machine learning (ML) techniques which is a major accomplishment since most ML regression models make use of an observed outcome and a set of covariates to which the modes are fit. Specifically, the TRV allows us to model the unobserved value, τ^{CATE} with a single regression, $E[Y_i^*|X_i = x]$. In the case of modeling treatment effects, we never observe the treatment effect directly making the TRV quite appealing in a very important way. Second, unlike most causal modeling approaches that focus on capturing $Y(1)|X - Y(0)|X$ by explicitly modeling $Y(0)|X$ and $Y(1)|X$ the TRV explicitly accounts for the

propensity score as defined in equation 4.7. Lastly, since we use a modeling approach that can flexibly adapt to the TRV’s implied mixture with correct model specification ((Zaidi and Mukherjee, 2018)), we are able to account for the complex relationship the covariates have with treatment heterogeneity.

4.3.2 Disadvantages of the TRV

As appealing as the TRV is described, it does not come without its significant downsides. Firstly, as shown in ((Athey and Imbens, 2015a); (Powers et al., 2018)), the TRV comes with a significantly high variance of the causal estimand. This is due to the fact that

$$Var(Y_i^*) = \frac{\sigma_1^2}{p_i} + \frac{\sigma_0^2}{1-p_i} + \frac{(1-p_i)\mu_1^2}{p_i} + \frac{p_i\mu_0^2}{1-p_i} - 2\mu_1\mu_0 \quad (4.8)$$

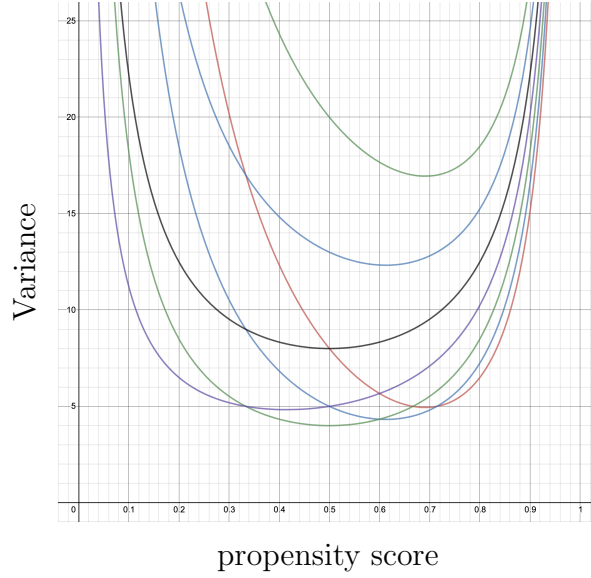
See B.2.2 for proof. We can clearly see the $Var(Y_i^*)$ has some unfavorable characteristics since variance of the estimator varies according to an inverse relationship with the propensity score and directly with the conditional means of $\mu_0 = Y(0)|X$ and $\mu_1 = Y(1)|X$. Figure 4.1 illustrates the relationships with a few examples.

A second downside until recently has been the lack of quantified uncertainty associated with the estimators using the inverse probability weighting schemes such as IPW and TRV. As can be seen in Figure 4.1, there is a dramatic increase in variability for propensity scores that are not unrealistically large or small which appears to be a limitation of the TRV. This limitation adds to the concern that the large variance can lead to poor interval estimation for the CATE as well as the ATE. Monte Carlo methods to estimate the uncertainty in the CATE have been demonstrated for use in (Knaus et al., 2020) but (Wager et al., 2014) has also shown that in some situations the Monte Carlo error can dominate the uncertainty quantification estimation. Because of this, in situations where the treatment effect is small, the conflation of the Monte Carlo error with the sampling error can lead to overstating the variance and hence lower the quality of the analysis. Additionally, (Powers et al., 2018) showed that the variance of the TRV grows with increasing sample size; hence,

Figure 4.1: An example of total variance,

$$Var(Y_i^*) = \frac{\sigma_1^2}{p_i} + \frac{\sigma_0^2}{1-p_i} + \frac{(1-p_i)\mu_1^2}{p_i} + \frac{p_i\mu_0^2}{1-p_i} - 2\mu_1\mu_0$$

where $\sigma_0 = \sigma_1 = 1$, $\mu_0 = -1$ and $\mu_1 \in (-3, -2, -1, 0, 1, 2, 3)$



working against methods like bootstrapping in situations when bootstrapping can do well.

It is because of the above limitations of the TRV that researchers such as (Zaidi and Mukherjee, 2018) have proposed a reparameterization of the model to estimate heterogeneous treatment effects by accounting for the implied mixture distribution of the TRV. We also used this same reparameterization to introduce a modified version of BART which comes with the benefits of estimated posterior distributions for the CATE at the unit level. Additionally, the model reparameterization allows us to greatly reduce the variance of our CATE estimates while still modeling the complex heterogeneous relationship of the covariates to the unit level treatment effect.

4.4 The Causal Bayesian Additive Regression Trees Mixture Model

In this section we introduce our model for Causal Bayesian Additive Regression trees with a mixture distribution in the residual term.

4.4.1 The Model

Let us consider two regression functions for a response for two different conditions under treatment and control

$$\begin{aligned} Y_i(1) &= f_1(x_i) + \epsilon_i(1), \text{ where } \epsilon_i(1) \sim N(0, \sigma^2) \\ Y_i(0) &= f_0(x_i) + \epsilon_i(0), \text{ where } \epsilon_i(0) \sim N(0, \sigma^2) \end{aligned} \quad (4.9)$$

Our estimand of interest is

$$\tau(x)^{CATE} = E[f_1(x_i) - f_0(x_i)] \quad (4.10)$$

If we substitute the regression functions under the treatment and control conditions into the definition of the TRV, we get the following mixture,

$$\begin{aligned} Y_i^* &= g(x) + \epsilon_i^* \\ \epsilon_i^* &\sim p_i N((1 - p_i)h(x_i), \frac{1}{p_i^2}\sigma^2) + (1 - p_i)N(-p_i h(x_i), \frac{1}{(1 - p_i)^2}\sigma^2) \\ g(x) &= f_1(x) - f_0(x) \\ h(x) &= \frac{f_1(x)}{p_i} + \frac{f_0(x)}{1 - p_i} \end{aligned} \quad (4.11)$$

Under this specification, $g(x)$ captures the unit level CATE, and $h(x)$ allows the model to adapt to the multi-modal nature of the TRV. A detailed derivation of the model in 4.11 is available in appendix B.3

According to (Zaidi and Mukherjee, 2018) the reason this formulation is superior to directly modeling f_1 and f_0 in equation 4.9, is because the conditional distributions of $Y_i|X_i, W = 0$ and $Y_i|X_i, W = 1$ may be hard to estimate due to lack of overlap in X for the two treatment levels. Additionally, (Powers et al., 2018) also argued that because f_0 and f_1 are never estimated

perfectly, ignoring the propensity score is a potential source of bias when estimating the CATE. In addition, (Hahn et al., 2019) points out that placing individual vague priors on the conditionals for Y_i make it a challenge for a model to capture the heterogeneity present in the data due to the implied priors on $(Y_i|X_i, W = 0) - (Y_i|X_i, W = 1)$ being potentially too vague.

4.4.2 Model Specification

We define our model as follows:

$$\begin{aligned}
Y_i^* &= g(x) + \epsilon_i^* \\
\epsilon_i^* &\sim p_i N((1 - p_i)h(x_i), \frac{1}{p_i^2}\sigma^2) + (1 - p_i)N(-p_i h(x_i), \frac{1}{(1 - p_i)^2}\sigma^2) \\
\mu_{j,b}^{(g)} &\sim N(\mu_0^{(g)}, \sigma_g^2) \\
\mu_{j,b}^{(h)} &\sim N(\mu_0^{(h)}, \sigma_h^2) \\
\sigma^2 &\sim \text{Inverse} - \text{Gamma}(a, b)
\end{aligned} \tag{4.12}$$

We estimate $g(x)$ and $h(x)$ using two BART models such that,

$$\begin{aligned}
g(x) &= \sum_{m=1}^{M_g} T_{g,m}(X) \\
h(x) &= \sum_{m=1}^{M_h} T_{h,m}(X)
\end{aligned} \tag{4.13}$$

where $T_{.,m}$ is a single binary tree in the sum of trees, M_g and M_h are the number of trees used to model $g(x)$ and $h(x)$, respectively. For each binary, $T_{.,m}$ there are an associated set of leaf nodes, $\mathcal{M}_m = \{\mu_{m,1}^{(\cdot)}, \dots, \mu_{m,b}^{(\cdot)}\}$ which denote a set of parameter values associated with each of the b terminal nodes of $T_{.,m}$. Following (Chipman et al., 2010), we also define our set of regularization priors in order to maintain the rich structure of 4.13 and prevent our trees from over fitting. We place a BART prior on the tree structures with equation 4.14 and

a prior on the leaf nodes with equation 4.15:

$$\begin{aligned}
& p((T_1^{(g)}, \mathcal{M}_1^{(g)}), \dots, (T_{M_g}^{(g)}, \mathcal{M}_{M_g}^{(g)}), (T_1^{(h)}, \mathcal{M}_1^{(h)}), \dots, (T_{M_h}^{(h)}, \mathcal{M}_{M_h}^{(h)}), \sigma) \\
&= \left[\prod_j p(T_j^{(g)}, \mathcal{M}_j^{(g)}) \right] \left[\prod_j p(T_j^{(h)}, \mathcal{M}_j^{(h)}) \right] p(\sigma) \\
&= \left[\prod_j p(\mathcal{M}_j^{(g)} | T_j^{(g)}) p(T_j^{(g)}) \right] \left[\prod_j p(\mathcal{M}_j^{(h)} | T_j^{(h)}) p(T_j^{(h)}) \right] p(\sigma)
\end{aligned} \tag{4.14}$$

where

$$\begin{aligned}
p(\mathcal{M}_j^{(g)} | T_j^{(g)}) &= \prod_i p(\mu_{i,j}^{(g)} | T_j^{(g)}) \\
p(\mathcal{M}_j^{(h)} | T_j^{(h)}) &= \prod_i p(\mu_{i,j}^{(h)} | T_j^{(h)})
\end{aligned} \tag{4.15}$$

where $\mu_{i,j}^{(g)} \in \mathcal{M}_j^{(g)}$ and $\mu_{i,j}^{(h)} \in \mathcal{M}_j^{(h)}$.

4.4.2.1 Priors on $\mu_{i,j}^*$ and σ^2

Unlike (Chipman et al., 2010), we do not scale the response variable Y_i^* to the interval $[-\frac{1}{2}, \frac{1}{2}]$ since doing so makes g and h unidentified. Rather, since we are not resealing the response, we make use of the data to select the hyperparameters. For a full discussion on selecting hyperparameters for the leaf node and variance parameters, see (Chipman et al., 2010). We followed the same approach in using data informed hyper-parameters related to $\mu_{i,j}^{(g)}$ and $\mu_{i,j}^{(h)}$:

$$\begin{aligned}
\mu_0^g &= \frac{\overline{Y_i^*}}{M_g} \\
\mu_0^h &= \frac{1}{M_h} \left(\frac{\sum_{i:W_i=1} \frac{Y_i}{p_i}}{\sum_i W_i} + \frac{\sum_{i:W_i=0} \frac{Y_i}{1-p_i}}{\sum_i (1-W_i)} \right) \\
\sigma_g &= \frac{0.5(\max(Y_i^*) - \min(Y_i^*))}{k\sqrt{M_g}} \\
\sigma_h &= \frac{0.5(\max(\frac{Y_i}{p_i}) - \min(\frac{Y_i}{p_i}))}{k\sqrt{M_h}}
\end{aligned} \tag{4.16}$$

Regarding the hyper-parameters for σ^2 , we used the same methodology suggested in (Chipman et al., 2010) and selected

$$a = 3$$

and

$$b \ni P(\sigma < \hat{\sigma}) = q = 0.99$$

4.4.2.2 Priors on $T_j^{(g)}$ and $T_j^{(h)}$

Our tree priors, $p(T_j^{(g)})$ and $p(T_j^{(h)})$ are governed by three parts.

1. The probability that a node at depth $d \in (0, 1, 2, \dots)$ is non-terminal given by

$$\frac{\alpha}{(1 + d)^\beta} \tag{4.17}$$

where $\alpha \in (0, 1)$, $\beta \in [0, \infty)$.

2. The distribution on the splitting variable assignments at each interior node.
3. The distribution on the splitting rule assignment in each interior node, conditional on the splitting variable.

Specifically, we use the uniform prior on available variables for the second item. and the uniform prior on the discrete set of available splitting values for the third item. As discussed in (Chipman et al., 2010) we want our sum of trees model to maintain relatively shallow trees and so we also set our $\alpha = 0.95$ and $\beta = 2$ in our examples. On the other hand, (Hahn et al., 2019) found good performance with their CBF in further regularizing tree depth and shrinking towards homogeneity for the function estimating the treatment effect ($g(x)$ in our case) with $\alpha = 0.25$ and $\beta = 3$. We also found there were some benefits to using $\alpha = 0.25$ and $\beta = 3$, although the benefits were not consistently better in our test cases.

4.4.2.3 The choice for M_g and M_h

Choosing M_g and M_h , the number of trees in the model for $g(x)$ and $h(x)$ respectively can be determined in several ways. First, treating M_g and M_h as unknown parameters and learning the correct values from the data would satisfy a fully Bayesian approach but would also serve to complicate the model more so. Having too few trees can lead to under fitting but does come with the advantage of lower computational costs and therefore faster model fitting time. On the other hand, allowing too many trees will cause a slight degradation in fit quality and result in significantly longer model fitting time. We found, for the example data sets we used to validate the model, $M_g = M_h = 25$ worked well consistently and did not require overly long periods of time to fit the model.

4.5 Posterior Sampling

Inference for our model involves sampling from the posterior distribution using Bayesian Back-fitting as specified in (Chipman et al., 2010) but with a few adjustments to accommodate the fact that we are fitting two functions rather than a single response function.

4.5.1 Basic outline of sampler

Since BART is an additive model and is fit via Bayesian back fitting, we begin by defining the residuals for the function $g(x)$ on the j^{th} tree. Let

$$\mathbf{R}_{-j}^{(g)} := Y_i^* - \sum_{m \neq j}^{M_g} T_m^{(g)}(X) - (w_i(1 - p_i)h(x_i) - (1 - w_i)p_i h(x_i)) \quad (4.18)$$

Similarly, we define the the residuals for the function $h(x)$ on the j^{th} tree. Let

$$\mathbf{R}_{-j}^{(h)} := Y_i^* - g(x_i) - \left(\mathbb{1}_{(w_i=1)}(1 - p_i) - \mathbb{1}_{(w_i=0)}p_i \right) \sum_{m \neq j}^{M_h} T_m^{(h)}(x_i) \quad (4.19)$$

And the residuals of the model using all trees is

$$\mathcal{E} := Y_i^* - g(x_i) - \left(\mathbb{1}_{(w_i=1)}(1 - p_i) - \mathbb{1}_{(w_i=0)}p_i \right) \sum_{m=1}^{M_h} \mathcal{T}_m^h(x_i) \quad (4.20)$$

The sampler

The sampler alternates between fitting the trees for g , followed by fitting the trees for h , followed by the draw for σ .

Sampling the trees and nodes for $g(x)$, we iterate through all $j = 1, \dots, M_g$ trees

- $T_j^{(g)} | \mathbf{R}_{-j}^{(g)}, \sigma^2, h(x)$
- $\mathcal{M}_j^{(g)} | T_j^{(g)}, \mathbf{R}_{-j}^{(g)}, \sigma^2, h(x)$

Sampling the trees and nodes for $h(x)$, we iterate through all $j = 1, \dots, M_h$ trees

- $T_j^{(h)} | \mathbf{R}_{-j}^{(h)}, \sigma^2, g(x)$
- $\mathcal{M}_j^{(h)} | T_j^{(h)}, \mathbf{R}_{-j}^{(h)}, \sigma^2, g(x)$

Finally, we sample σ^2

- $\sigma^2 | T_1^{(g)}, \dots, T_M^{(g)}, T_1^{(h)}, \dots, T_M^{(h)}, \mathcal{E}$

4.5.2 $\mu_{ij}^{(g)}$, $\mu_{ij}^{(h)}$, and σ conditionals:

In this subsection we show the resulting distributions used in posterior sampling but detailed derivations are available in appendix B.4.

Leaf Nodes of $g(x)$: The conditional distribution of the leaf nodes of $g(x)$ are given by

$$\mu_{i,j}^{(g)} | \sigma^2, T_j^{(g)}, y, \sim N \left(\frac{\sum_{i=1}^{n_{j,b}^{(g)}} \frac{y_{j,i \in \eta_{j,b,g}}}{\sigma_{g,i}^2} + \frac{\mu_0^{(g)}}{\sigma_g^2}}{\frac{1}{\sigma_g^2} + \sum_{i=1}^n \frac{1}{\sigma_{g,i}^2}}, \left[\frac{1}{\sigma_g^2} + \sum_{i=1}^n \frac{1}{\sigma_{g,i}^2} \right]^{-1} \right) \quad (4.21)$$

Where $\eta_{j,b,g}$ is node b in $T_j^{(g)}$, $n_{j,b}^{(g)}$ is the number of observations in $\eta_{j,b,g}$ and $y_{j,i}^{(g)} \in \eta_{j,b,g}$.

$$\begin{aligned} y_{j,i}^{(g)} &= \mathbf{R}_{-j}^{(g)} \\ \sigma_{g,i}^2 &= w_i \frac{\sigma^2}{p_i^2} + (1 - w_i) \frac{\sigma^2}{(1 - p_i)^2} \end{aligned} \quad (4.22)$$

Leaf Nodes of $h(x)$: The conditional distribution of the leaf nodes of $h(x)$ are given by

$$\mu_{i,j}^{(h)} | \sigma^2, T_j^{(h)}, y, \sim N \left(\frac{\sum_{i=1}^{n_{j,b}^{(h)}} \frac{y_{j,i \in \eta_{j,b,h}}}{\sigma_{h,i}^2} + \frac{\mu_0^{(h)}}{\sigma_h^2}}{\frac{1}{\sigma_h^2} + \sum_{i=1}^n \frac{1}{\sigma_{h,i}^2}}, \left[\frac{1}{\sigma_h^2} + \sum_{i=1}^n \frac{1}{\sigma_{h,i}^2} \right]^{-1} \right) \quad (4.23)$$

where $\eta_{j,b,h}$ is node b in $T_j^{(h)}$, $n_{j,b}^{(h)}$ is the number of observations in $\eta_{j,b,h}$ and $y_{j,i}^{(h)} \in \eta_{j,b,h}$.

$$\begin{aligned} y_{j,i}^{(h)} &= \left(\mathbb{1}_{(w_i=1)}(1 - p_i) - \mathbb{1}_{(w_i=0)}p_i \right)^{-1} \mathbf{R}_{-j}^{(h)} \\ \sigma_{h,i}^2 &= \frac{\sigma^2}{p_i^2(1 - p_i)^2} \end{aligned} \quad (4.24)$$

and finally we have, The conditional distribution of σ given by

$$\sigma^2 \sim IG \left(\frac{n}{2} + a, b + \frac{1}{2} \sum_{i=1}^n p_{a,w}^2 \mathcal{E}^2 \right) \quad (4.25)$$

where $p_{a,w}^2 = \mathbb{1}_{(w_i=1)}p_i^2 + \mathbb{1}_{(w_i=0)}(1 - p_i)^2$.

4.5.3 Sampling the Tree Structures

We adapt the "grow" and "prune" steps in (Chipman et al., 2010) to use the appropriate likelihood, which is described below. Marginalizing the portion of the likelihood associated with $\eta_{j,b}^{(g)}$ can be accomplished with the following integral:

$$\begin{aligned}
L(\eta_{j,b}^{(g)} | \sigma^2, T_{j \notin M}^{(g)}, T^{(h)}, y) &= \int_{-\infty}^{\infty} L(\eta_{j,b}^{(g)} | \mu_{j,b}^{(g)}, \sigma^2, T_{j \notin M_g}^{(g)}, T^{(h)}, y) \pi(\mu_{j,b}^{(g)}) d\mu_{j,b}^{(g)} \\
&= \left(\sigma_{\mu}^{-2} + \sum_{i=1}^{n_{j,b}^{(g)}} \sigma_{g,i}^{-2} \right)^{-1/2} (2\pi)^{-n_{j,b}^{(g)}/2} \sigma_{\mu}^{-1} \prod_{i=1}^{n_{j,b}^{(g)}} \sigma_{g,i}^{-1} \\
&\quad \exp \left(-\frac{1}{2} \left[\sum_{i=1}^{n_{j,b}^{(g)}} \frac{y_{j,i}^{(g)2}}{\sigma_{g,i}^2} + \frac{\mu_0^2}{\sigma_{\mu}^2} \right] + \frac{1}{2} \left(\sigma_{\mu}^{-2} + \sum_{i=1}^{n_{j,b}^{(g)}} \sigma_{g,i}^{-2} \right)^{-1} \left(\sum_{i=1}^{n_{j,b}^{(g)}} \frac{y_{j,i}^{(g)}}{\sigma_{g,i}^2} + \frac{\mu_0}{\sigma_{\mu}^2} \right)^2 \right)
\end{aligned} \tag{4.26}$$

where $T_{j \notin M_g}^{(g)}$ denotes the set of trees comprising $g(x)$, not including the j^{th} tree. Similarly, we can do the same for the portion of the likelihood associated with $\eta_{j,b}^{(h)}$

$$\begin{aligned}
L(\eta_{j,b}^{(h)} | \sigma^2, T_{j \notin M}^{(h)}, T^{(g)}, y) &= \int_{-\infty}^{\infty} L(\eta_{j,b}^{(h)} | \mu_{j,b}^{(h)}, \sigma^2, T_{j \notin M_g}^{(h)}, T^{(g)}, y) \pi(\mu_{j,b}^{(h)}) d\mu_{j,b}^{(h)} \\
&= \left(\sigma_{\mu}^{-2} + \sum_{i=1}^{n_{j,b}^{(h)}} \sigma_{h,i}^{-2} \right)^{-1/2} (2\pi)^{-n_{j,b}^{(h)}/2} \sigma_{\mu}^{-1} \prod_{i=1}^{n_{j,b}^{(h)}} \sigma_{h,i}^{-1} \\
&\quad \exp \left(-\frac{1}{2} \left[\sum_{i=1}^{n_{j,b}^{(h)}} \frac{y_{j,i}^{(h)2}}{\sigma_{h,i}^2} + \frac{\mu_0^2}{\sigma_{\mu}^2} \right] + \frac{1}{2} \left(\sigma_{\mu}^{-2} + \sum_{i=1}^{n_{j,b}^{(h)}} \sigma_{h,i}^{-2} \right)^{-1} \left(\sum_{i=1}^{n_{j,b}^{(h)}} \frac{y_{j,i}^{(h)}}{\sigma_{h,i}^2} + \frac{\mu_0}{\sigma_{\mu}^2} \right)^2 \right)
\end{aligned} \tag{4.27}$$

where $T_{j \notin M_h}^{(h)}$ denotes the set of trees comprising $h(x)$, not including the j^{th} tree.

With the marginal likelihood associated with the leaf node parameters, we can propose growth move in the way described in Section 2.0.3.2. After generating a proposal T' , we accept with probability

$$\alpha = \min \left[1, \frac{\pi(T' | \sigma^2, \mathbf{y}) q(T | T')}{\pi(T | \sigma^2, \mathbf{y}) q(T' | T)} \right] \tag{4.28}$$

where The expression for the ratio of likelihoods is

$$\begin{aligned}
\frac{\pi(T'|\sigma^2, \mathbf{y})}{\pi(T|\sigma^2, \mathbf{y})} &= \frac{\left(\sigma_\mu^{-2} + \sum_{i=1}^{n_{j,b_{combined}}^*} \sigma_i^{-2}\right)^{1/2}}{\sigma_\mu \left(\sigma_\mu^{-2} + \sum_{i=1}^{n_{j,b_{left}}^*} \sigma_i^{-2}\right)^{1/2} \left(\sigma_\mu^{-2} + \sum_{i=1}^{n_{j,b_{right}}^*} \sigma_i^{-2}\right)^{1/2}} \\
&\quad \exp\left(\frac{1}{2}\left(\sigma_\mu^{-2} + \sum_{i=1}^{n_{j,b_{left}}^*} \sigma_i^{-2}\right)^{-1} \left(\sum_{i=1}^{n_{j,b_{left}}^*} \frac{\tilde{y}_i}{\sigma_i^2} + \frac{\mu_0}{\sigma_\mu^2}\right)^2\right) \\
&\quad \exp\left(\frac{1}{2}\left(\sigma_\mu^{-2} + \sum_{i=1}^{n_{j,b_{right}}^*} \sigma_i^{-2}\right)^{-1} \left(\sum_{i=1}^{n_{j,b_{right}}^*} \frac{\tilde{y}_i}{\sigma_i^2} + \frac{\mu_0}{\sigma_\mu^2}\right)^2\right) \\
&\quad \exp\left(-\frac{1}{2}\left(\sigma_\mu^{-2} + \sum_{i=1}^{n_{j,b_{combined}}^*} \sigma_i^{-2}\right)^{-1} \left(\sum_{i=1}^{n_{j,b_{combined}}^*} \frac{\tilde{y}_i}{\sigma_i^2} + \frac{\mu_0}{\sigma_\mu^2}\right)^2\right)
\end{aligned} \tag{4.29}$$

where $\sigma_i = \sigma_{g,i}$ as defined in equation 4.22 when sampling tree proposals for $g(x)$ and $\sigma_i = \sigma_{h,i}$ as defined in 4.24 when sampling tree proposals for h .

Detailed derivations for the Metropolis-Hastings step are available in appendix B.5

4.6 Experimental Evaluation

In this section we validate our TRV BART based model on multiple simulated data sets each with varying characteristics. We use the simulations to show that our method performs better when compared to the other TRV based methods when evaluating the CATE and discuss how ATE estimation is affected by the unique properties of our model. We also compare against other Bayesian and non-Bayesian tree based ensemble methods and show that although our method is not the top performing method, it is a significant improvement over previous standard methods used to estimate CATE's.

4.6.1 Experimental Evaluation Metrics

In this section we will introduce the evaluation metrics we used to evaluate our method. We also state how we compute the relevant metrics for competing metrics when there is not direct counterpart as is the case for the non-Bayesian approaches. We will consider performance for both CATE as well as ATE.

Causal BART mixture model: We first specify the method used to estimate the CATE. The model is trained on data (X_1, \dots, X_N) and the two estimated functions produce estimates

$$\begin{aligned}\mathbf{g} &= (g(X_1), \dots, g(X_n)) \\ \mathbf{h} &= (h(X_1), \dots, h(X_n))\end{aligned}$$

We therefore have posterior samples $(\mathbf{g}^j, \mathbf{h}^j)_{j=1}^K$, assuming we have K samples from the posterior. These samples are then used to compute our evaluation metrics for the CATE for each X_i for $i \in 1, \dots, N$ as

$$\tau_i^{CATE(j)}(X_i) = g^{(j)}(X_i)$$

Given the posterior samples we can compute a point estimate using the posterior mean

$$\begin{aligned}RMSE_{CATE} &= \left(\frac{1}{N} \sum_{i=1}^N (\tau_i^{CATE} - \widehat{\tau_i^{CATE}})^2 \right)^{1/2} \\ B_{CATE} &= \frac{1}{N} \sum_{i=1}^N (\tau_i^{CATE} - \widehat{\tau_i^{CATE}}) \\ C_{CATE} &= \frac{1}{N} \sum_{i=1}^N \mathbb{1}(\tau_i^{CATE} \in [\tau_i^{CATE, lwr}, \tau_i^{CATE, upr}]) \\ MIL_{CATE} &= \frac{1}{N} \sum_{i=1}^N \tau_i^{CATE, upr} - \tau_i^{CATE, lwr}\end{aligned}\tag{4.30}$$

Similarly, regarding the ATE, we can define similar metrics. Let N_{iter} be the number of MCMC samples or bootstrap samples depending on the method type we are comparing, then

$$\begin{aligned}
RMSE_{ATE} &= \left(\frac{1}{N_{iter}} \sum_{i=1}^{N_{iter}} (\tau_i^{ATE} - \widehat{\tau_i^{ATE}})^2 \right)^{1/2} \\
B_{ATE} &= \frac{1}{N_{iter}} \sum_{i=1}^{N_{iter}} (\tau_i^{ATE} - \widehat{\tau_i^{ATE}}) \\
C_{ATE} &= \frac{1}{N_{iter}} \sum_{i=1}^{N_{iter}} \mathbb{1}(\tau_i^{ATE} \in [\tau_i^{ATE, lwr}, \tau_i^{ATE, upr}]) \\
MIL_{ATE} &= \frac{1}{N_{iter}} \sum_{i=1}^{N_{iter}} \tau_i^{ATE, upr} - \tau_i^{ATE, lwr}
\end{aligned} \tag{4.31}$$

Summary of alternative methods used: We will compare our method to other tree based methods on both the ATE and CATE. We have selected as comparison methods non-TRV methods including Bayesian Causal Forests developed by (Hahn et al., 2019), causalBART developed by (Hill, 2011), and Causal Random Forest developed by (Wager and Athey, 2018). To compare against other TRV based methods, we compare the BART and Random Forest "off the shelf" using the TRV. We also compare other TRV tree based methods proposed in (Athey and Imbens, 2015a). In all our experimental runs, we use the true propensity score to assess the quality of the estimation of the CATE and ATE.

4.6.2 Data Sets

In order to evaluate the performance of our model, we consider 4 simulated data sets. The first two are the simulated data sets found in (Zaidi and Mukherjee, 2018), however we add noise to the system and set the variance parameter $\sigma^2 = 25$ in both models. One is a high dimensional case with 40 predictors we will call Case A, the other is of a lower dimensional case with 5 predictors we will call Case B. We also consider two of the simulated data

sets from (Hahn et al., 2019) each with 5 predictors. The first is with a non-linear mean response function and heterogeneous treatment effect which we will call Case NLHet. Additionally, we consider the non-linear mean response function and homogeneous treatment which we will refer to as Case NLHom. All data sets have a total of 250 observations. We also performed 200 replications of our analysis per data set for our method as well as comparison methods.

Case A: We begin with the data set with 40 predictors. The Data Generating Process (DGP) is as follows:

$$\begin{aligned} X_k &\sim \text{Normal}(0, 1); \quad k = 1, \dots, 15, \\ X_k &\sim \text{Uniform}(0, 1); \quad k = 16, \dots, 30, \\ X_k &\sim \text{Bernoulli}(q_k); \quad q_k = \text{logit}^{-1}(X_{k-30}X_{k-15}); \quad k = 31, \dots, 35, \\ X_k &\sim \text{Poisson}(\lambda_k); \quad \lambda_k = 5 + 0.75X_{k-35}(X_{k-20} + X_{k-5}); \quad k = 36, \dots, 40. \end{aligned}$$

Next we simulate the propensity scores and the corresponding treatment assignments.

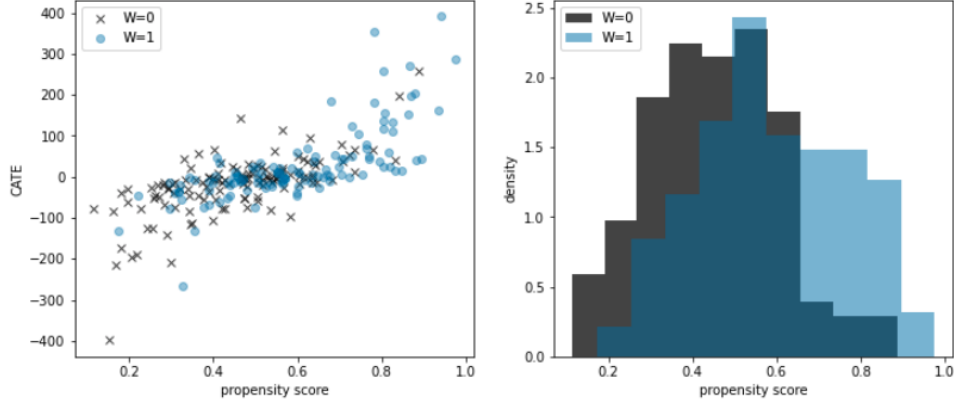
$$\begin{aligned} p_i &= \text{logit}^{-1}\left(0.3 \sum_{k=1}^5 X_k - 0.5 \sum_{k=21}^2 5X_k - 0.0001 \sum_{k=26}^3 5X_k + 0.055 \sum_{k=36}^4 0X_k\right), \\ W &\sim \text{Bernoulli}(p_i). \end{aligned}$$

And here we will generate the potential outcomes along with the observed outcomes.

$$\begin{aligned} f(\mathbf{X}) &= \frac{\sum_{k=16}^{19} X_k \exp(X_{k+14})}{1 + \sum_{k=16}^{19} X_k \exp(X_{k+14})}, \\ Y(0) &= 0.15 \sum_{k=1}^5 X_k + 1.5 \exp(1 + 1.5f(\mathbf{X})) + \epsilon_i, \\ Y(1) &= \sum_{k=1}^5 (2.15X_k + 2.75X_k^2 + 10X_k^3) + 1.25 \left(0.5 + 1.5 \sum_{k=36}^4 0X_k\right)^{1/2} + \epsilon_i, \\ &= WY(1) + (1 - W)Y(0); \quad \epsilon_i \stackrel{i.i.d.}{\sim} \text{Normal}(0, 25) \end{aligned}$$

Figure 4.2 shows some summary distributions along with the relationship of the propensity score and the CATE.

Figure 4.2: Summary plots of Case A. On the left we have CATE on the y-axis vs propensity score on the x-axis broken up by treatment assignment. On the right we have the histogram of the propensity scores broken up by each level of treatment.



Case B: Next we define the DGP for Case B which is similar to the one proposed in (Zaidi and Mukherjee, 2018) but again rather than have a near deterministic outcome we adapt the DGP to include a non-trivial amount of noise in the variance term with $\sigma^2 = 25$. The DGP is as follows:

$$\begin{aligned} X_k &\sim \text{Normal}(0, 1); \quad k = 1, \dots, 3, \\ X_4 &\sim \text{Bernoulli}(p = 0.25), \\ X_5 &\sim \text{Binomial}(n = 2, p = 0.5). \end{aligned}$$

Next we generate the propensity scores.

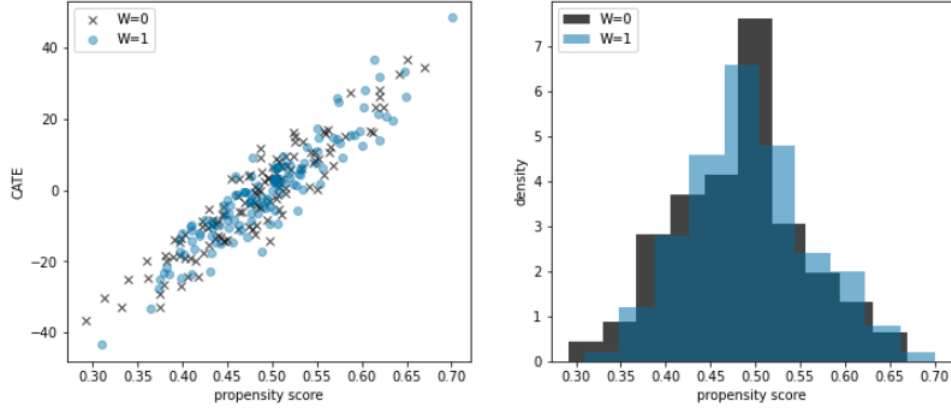
$$\begin{aligned} p_i &= \text{logit}^{-1}(0.1X_1 + 0.001X_2 + .275X_3 + 0.03X_4), \\ W &\sim \text{Bernoulli}(p_i) \end{aligned}$$

Finally we generate the potential and observed outcomes.

$$\begin{aligned}
t(x) &= -2x + 5, \\
f(X) &= -6 + t(X_5) + |X_3 - 1|, \\
Y(0) &= f(X) - 15X_3 + \epsilon_i, \\
Y(1) &= f(X) + (1 + 2X_2X_3) + \epsilon_i, \\
Y &= WY(1) + (1W)Y(0); \quad \epsilon_i \stackrel{i.i.d.}{\sim} \text{Normal}(0, 25).
\end{aligned}$$

Figure 4.3 shows some summary distributions along with the relationship of the propensity score and the CATE.

Figure 4.3: Summary plots of Case B. On the left we have CATE on the y-axis vs propensity score on the x-axis broken up by treatment level. On the right we have the histogram of the propensity scores broken up by treatment level.



Case NLHet: Next we consider the DGP from (Hahn et al., 2019) with a non-linear mean function, $f_0(x)$ and Heterogeneous treatment effect $\tau(x)$. Our

data is generated as follows

$$\begin{aligned} X_1 &\sim \text{Normal}(0, 1), \\ X_2 &\sim \text{Normal}(0, 1), \\ X_3 &\sim \text{Normal}(0, 1), \\ X_4 &\sim \text{DiscreteUniform}(\{1, 2, 3\}) \\ X_5 &\sim \text{Binomial}(n = 1, p = .5) \end{aligned}$$

Next we generate the non linear mean function and CATE.

$$\begin{aligned} t(x) &= -2x + 5, \\ f_0(X) &= -6 + t(X_4) + 6|X_3 - 1|, \\ \tau(x) &= 1 + 2X_2X_5. \end{aligned}$$

Finally, we generate the propensity score.

$$\pi(x_i) = 0.8\Phi\left(\frac{3f_0(x_i)}{s - 0.5X_1} + 0.05 + \frac{u_i}{10}\right),$$

where $s = \text{std}(\hat{\mu})$ is computed from the sample and $u_i \sim \text{Uniform}(0, 1)$. Figure 4.4 shows some summary distributions along with the relationship of the propensity score and the CATE.

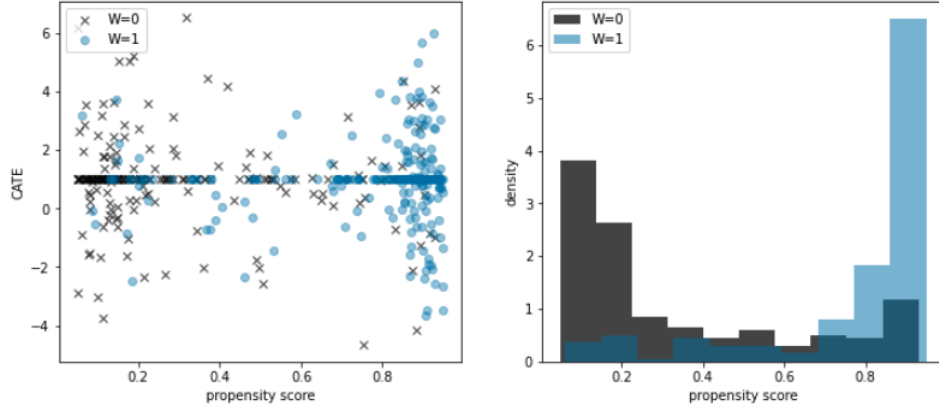
Case NLHom: . Next we consider the DGP from (Hahn et al., 2019) with a non-linear mean function, $f_0(x)$ and Homogeneous treatment effect $\tau(x)$. Our data is generated as follows.

$$\begin{aligned} X_1 &\sim \text{Normal}(0, 1), \\ X_2 &\sim \text{Normal}(0, 1), \\ X_3 &\sim \text{Normal}(0, 1), \\ X_4 &\sim \text{DiscreteUniform}(\{1, 2, 3\}) \\ X_5 &\sim \text{Binomial}(n = 1, p = .5) \end{aligned}$$

Next we generate the non linear mean function and treatment effects.

$$\begin{aligned} t(1) &= 2, \quad t(2) = -1, \quad t(3) = -4, \\ f_0(X) &= -6 + t(X_4) + 6|X_3 - 1|, \\ \tau(x) &= 3. \end{aligned}$$

Figure 4.4: Summary plots of non-linear $f_0(x)$ and heterogeneous treatment effect. On the left we have CATE on the y-axis vs propensity score on the x-axis broken up by treatment level. On the right we have the histogram of the propensity scores broken up by treatment level.



Finally, we generate the propensity score.

$$\pi(x_i) = 0.8\Phi\left(\frac{3f_0(x_i)}{s - 0.5X_1} + 0.05 + \frac{u_i}{10}\right),$$

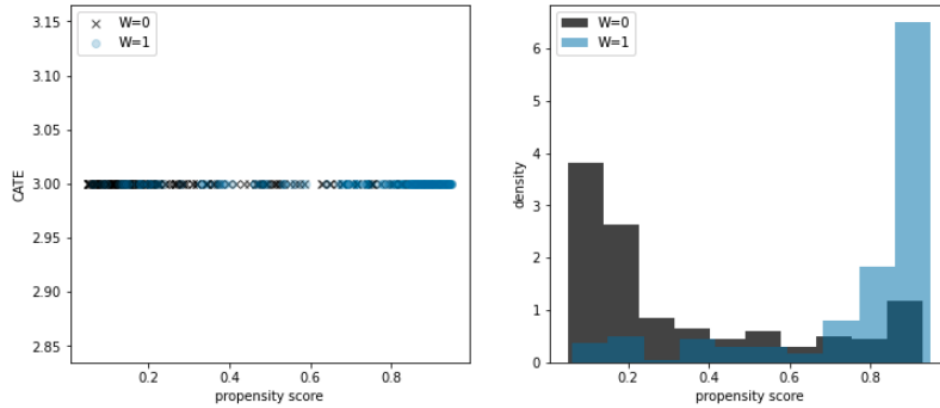
where $s = std(f_0)$ is computed from the sample and $u_i \sim Uniform(0, 1)$. Figure 4.5 shows some summary distributions along with the relationship of the propensity score and the CATE.

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4.6.3 Comparison Methods

In this section we discuss the results when comparing our method against competing models. Our comparisons include Bayesian Causal Forest introduced in (Hahn et al., 2019) and available in the bcf package in R, the method introduced in (Hill, 2011) and is available in the bartCause package in R, the method introduced in (Athey and Imbens, 2015a) and is available in the R package, causalTree and available for installation from

Figure 4.5: Summary plots of non-linear $f_0(x)$ and homogeneous treatment effect. On the left we have homogeneous effect on the y-axis vs propensity score on the x-axis broken up by treatment level. On the right we have the histogram of the propensity scores broken up by treatment level.



<https://github.com/susanathey/causalTree>, finally we compare against the "off the shelf" version of the TRV with a standard implementation of BART from the `bartMachine` library in R. In the case of the Bayesian methods, we used the default settings of the methods to collect posterior summaries. For non-Bayesian methods, we relied on bootstrapping to generate uncertainty estimates. Our own Causal BART Mixture Model was run with 2000 burn-in and 2000 sample iterations. Each method was run with 200 replications. Results of the analysis are summarized with a collection of histograms laid out in a tabular format allowing a qualitative evaluation of the summary distributional characteristics as well as the quantitative mean.

One key consideration in the results we are showing is that we tried numerous combinations of tree counts ranging from 2 to 250 for both g and h and found that 25 trees for both g and h was sufficient to produce comparable results to high tree count version of g and h .

We use the following labels for ours and competing methods.

- **cbartmm25** - our Causal BART Mixture Model with 25 trees in g and

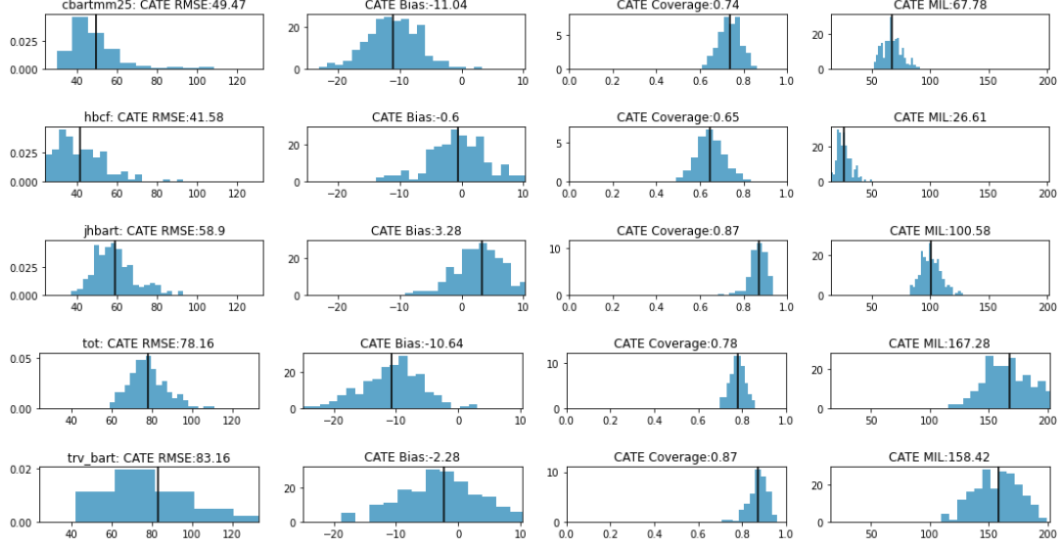
h , tree depth priors for g and h with $\alpha = 0.0.95$ and $k = 2.0$, standard regularization priors for $\mu_{i,j}^*$ defined in equations 4.16, hyper parameters for σ had $a = 3.0$ and $q = 0.99$.

- **cbartmm50200** - Our Causal BART Mixture Model with 50 trees in g and 200 in h , tree depth priors for g with $\alpha = 0.0.25$ and $k = 3.0$ and h with $\alpha = 0.0.95$ and $k = 2.0$, standard regularization priors for $\mu_{i,j}^*$ defined in equations 4.16, hyper parameters for σ had $a = 3.0$ and $q = 0.99$. The tree regularization priors found in this model are the same regularization tree depth priors suggested in (Hahn et al., 2019).
- **hbcf** - The Bayesian Causal Forest introduced in (Hahn et al., 2019) with default settings, the same covariates X used in $\mu(x)$ and $\tau(x)$. The propensity score is also used as a predictor in this example.
- **jhbart** - The model introduced in (Hill, 2011).
- **tot** - the Adaptive Transformed Outcome Tree introduced in (Athey and Imbens, 2015a).
- **trv_bart** - regular BART with the TRV used as the response. This is the particular comparison allows us to gauge the "off-the-shelf" performance of modeling $\tau(x)$ directly with the TRV.

Case A: Summarizing results for the CATE, we can see in in Figure 4.6 resulting summary distributions for ours and competing methods. Although hbcf is the top model in terms of MSE, cbartmm25 comes in second compared to all other competing comparisons. Most importantly, we see a significant improvement over the TRV methods tot and trv_bart. We do see decreases in CATE coverage over the other TRV methods, however sot he picture is not all positive. Additionally, we also notice the MIL of cbartmm25 is significantly decreased as compared to tot and trv_bart.

Next we consider the results for the ATE. Figure 4.7 summarizes these results. We can see in terms of RMSE and Coverage, cbartmm25 is almost uniformly outperformed by all other competing methods. Additionally, for cbartmm25 we see that RMSE and Bias are very close. We hypothesise and

Figure 4.6: Case A CATE

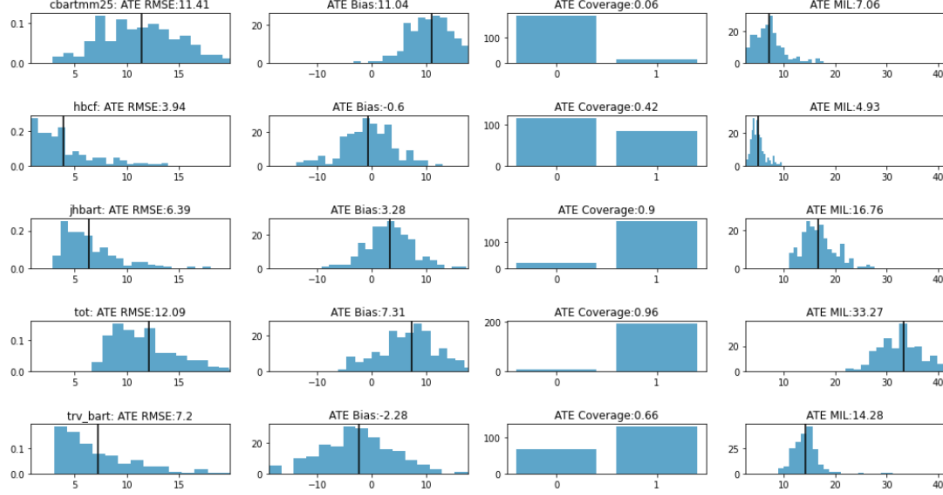


show evidence for why we believe we are seeing such poor performance in section 4.6.4.

Case B: Summarizing results for the CATE, we can see in in Figure 4.8 resulting summary distributions for ours and competing methods. Although hbcf is the top model in terms of MSE, cbartmm25 comes in second compared to all other competing comparisons. Most importantly, we see a significant improvement over the TRV methods tot and trv_bart. We do see decreases in CATE coverage over the other TRV methods, however sot he picture is not all positive. Additionally, we also notice the MIL of cbartmm25 is significantly decreased as compared to tot and trv_bart.

Next we consider the results for the ATE. Figure 4.9 summarizes these results. We can see in terms of RMSE cbartmm25 has the lowest RMSE. Regarding Coverage, cbartmm25 is uniformly outperformed by all other competing methods. We hypothesise and show evidence for why we believe we are seeing such poor performance in section 4.6.4.

Figure 4.7: Case A ATE

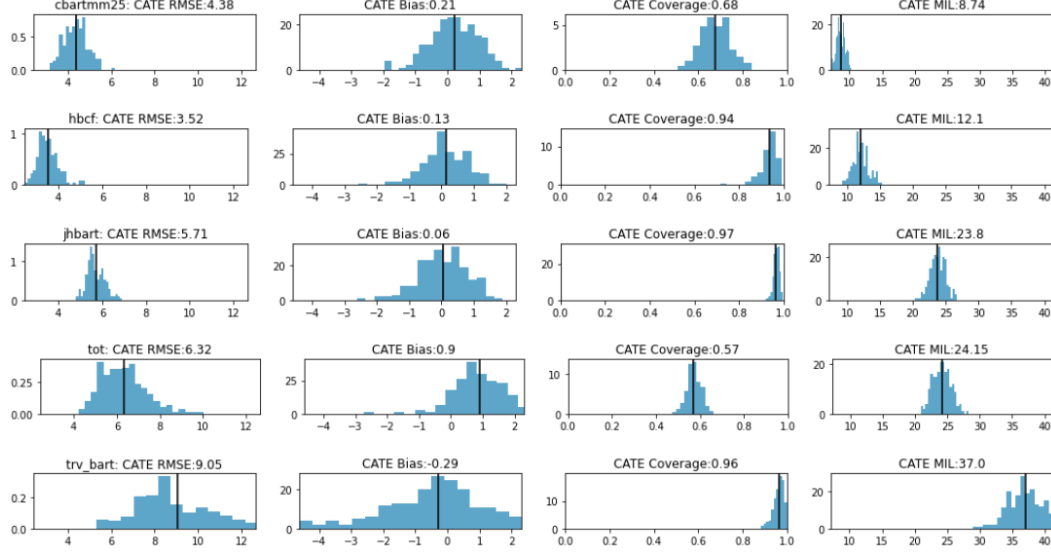


Case NLHet: Summarizing results for the CATE, we can see in in Figure 4.10 resulting summary distributions for ours and competing methods. Although hbcf and jhbart outperform both our versions of our Causal BART Mixture Model on RMSE, we again outperform on tot and trv_bart. We do see decreases in CATE coverage over the other TRV methods however. Additionally, we also notice the MIL of cbartmm25 is significantly decreased as compared to tot and trv_bart.

Next we consider the results for the ATE. Figure 4.11 summarizes these results. We can see in terms of RMSE and Coverage, cbartmm25 is outperformed by all other non-TRV competing methods. Additionally, for cbartmm25 we see that RMSE and Bias are very close. We hypothesise and show evidence for why we believe we are seeing such poor performance in section 4.6.4.

Case NLHom: Summarizing results for the CATE, we can see in in Figure 4.12 resulting summary distributions for ours and competing methods. Although hbcf and jhbart outperform both our versions of our Causal BART Mixture Model on RMSE, we again outperform compared to tot and trv_bart. We do see decreases in CATE coverage over the other TRV methods however.

Figure 4.8: Case B CATE



Additionally, we also notice the MIL of cbartmm25 is significantly decreased as compared to tot and trv_bart.

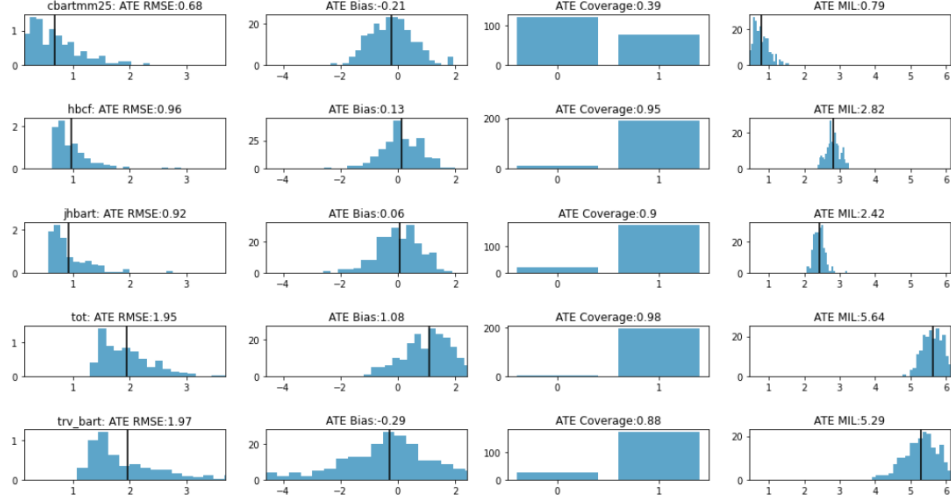
Next we consider the results for the ATE. Figure 4.13 summarizes these results. We can see in terms of RMSE and Coverage, cbartmm25 is outperformed by all other non-TRV competing methods. Additionally, for cbartmm25 we see that RMSE and Bias are very close. We hypothesise and show evidence for why we believe we are seeing such poor performance in section 4.6.4.

4.6.4 Problems with $h(x)$:

In this section we discuss the a major draw back with the Causal BART Mixture Model. In particular, as it relates to the models ability to estimate the ATE.

We suspect the primary driver in creating a poor ATE estimator is

Figure 4.9: Case B ATE

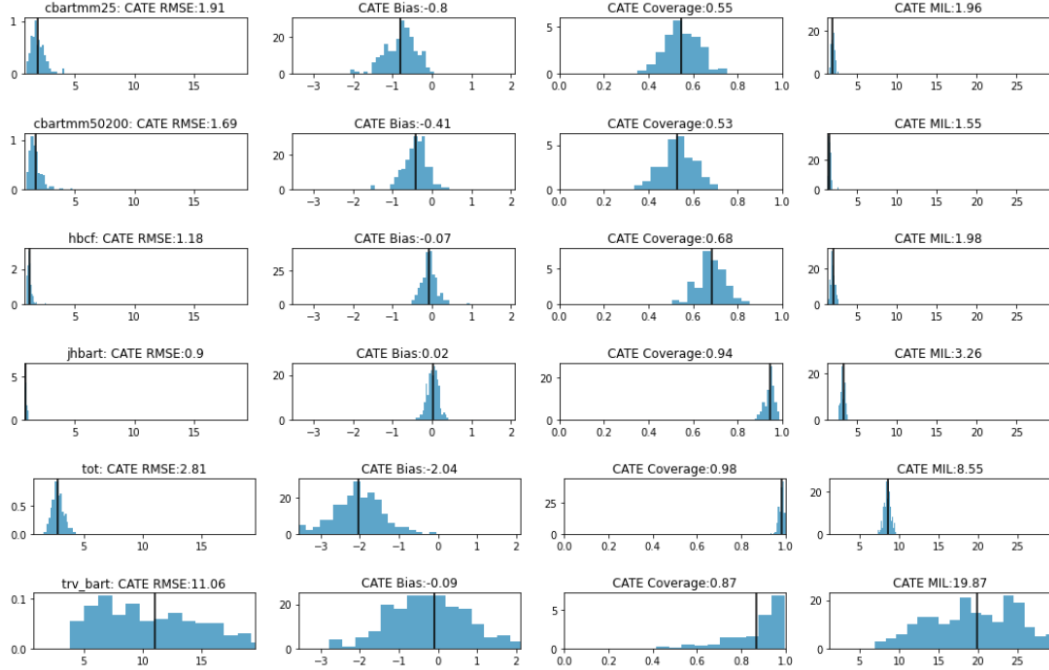


related to values of $h(x)$ that are sufficiently far from the rest of the population resulting in poor estimation for the CATE and consequently resulting in an outlier effect when marginalizing over X . Recall from equations ??, large values can result for multiple reasons including values of pi close to 0 or 1 or relatively large magnitude values of f_0 or f_1 . We attempted to adjust for this by using various forms of trimming but were unsuccessful in doing so when using estimated values of h or values of the propensity score but rather found that using the true h was where we found meaningful impact. This is clearly a major drawback as h is an unobserved quantity and hence difficult to properly or well estimate creating a serious limitation for the method. We discuss in section 4.7 how if the TRV is to become a viable causal inference approach, this detail will need to be resolved.

We estimate the coverage probability for the CATE via a gaussian process using the true values of $h(x)$ as the only predictor. It is easy to see in the tails of the distribution of h , we have a drop off in coverage of the CATE. Figures 4.14, 4.15, 4.16, 4.17 illustrate the issues with coverage and values of $h(x)$

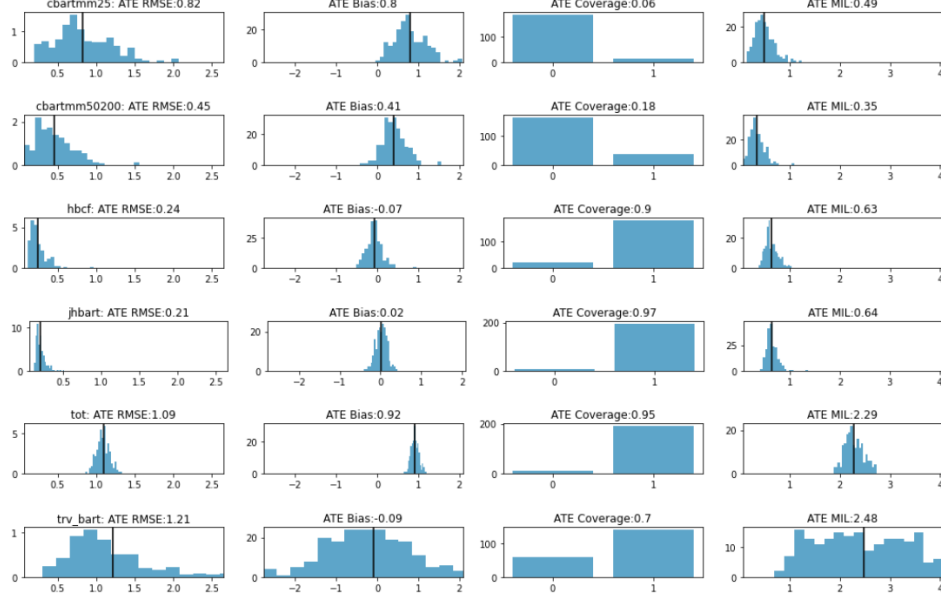
Figures 4.18, 4.19, 4.20, 4.21, 4.20, 4.23 show the results for 3 separate analysis where we systematically remove the observations that have the upper

Figure 4.10: Case NLHet CATE



and lower 5% of observations in `cbartmm_tth0590`, upper and lower 10% of observations in `cbartmm_tth1090`, and upper and lower 15% of observations in `cbartmm_tth1585`. We can see the dramatic improvement in RMSE for our CATE estimates as we trim observations with relatively large values of $h(x)$. Perhaps more dramatically, the coverage in the ATE becomes quite competitive with the other models when we focus on the central portions of the observations as it relates to h . It is also worth noting the relationship between the ATE RMSE and Bias become more desirable as we remove the observations found in the tails of the distribution of h . Finally, key to note that selecting observations based on "outlierness" with respect to g or p_i did not yield consistent results in the other example data sets considered, suggesting the main driver for poor performance is h .

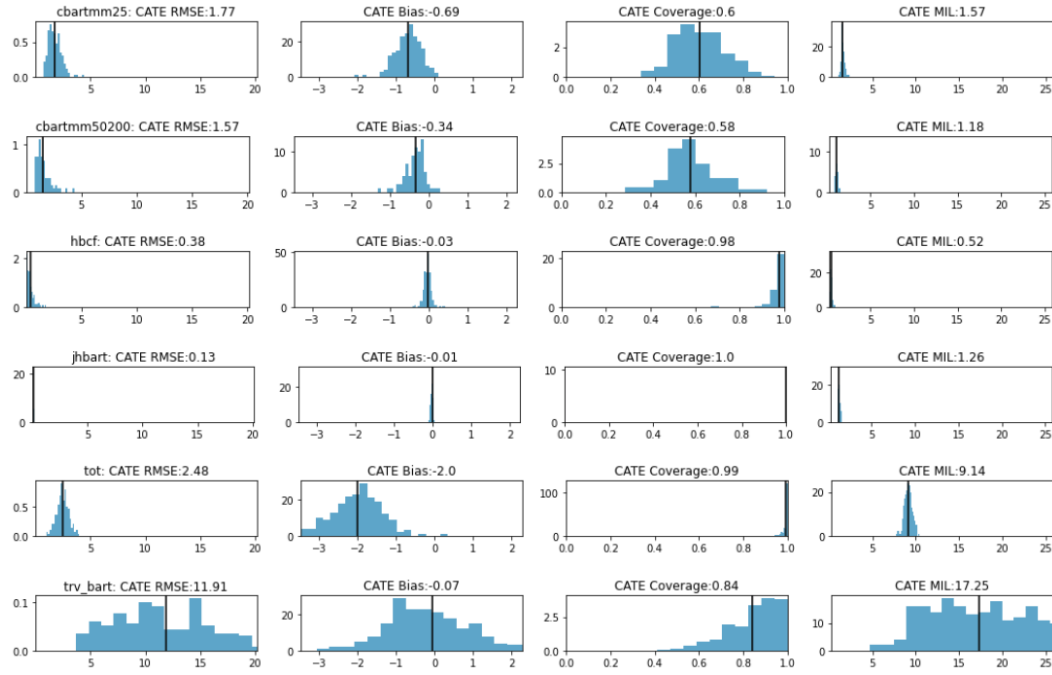
Figure 4.11: Case NLHet ATE



4.7 Discussion and Future Work

In this chapter we introduced the Causal BART Mixture Model and showed how accounting for the mixture implied by the TRV improves CATE estimates significantly over existing methods using the TRV. Additionally, we also showed that our method is often competitive with other state of the art methods in estimating CATE's. We also noted that our proposed model has issues when estimating the ATE. We proposed a hypothesis involving $h(x)$ that seems to be at the core of the poor estimation related to the ATE and the effect of marginalizing over X has on the estimation. That that end, moving forward, if TRV causal models are to be competitive against other state of the art methods, learning to deal with $h(x)$ should be the top a researchers mind when proposing methods related to the TRV. Another avenue in future work worth considering would be to modify priors in the model to impose in effect a variable selection sparsity inducing prior of predictor variables. Priors proposed in (Linero, 2018) provide a relatively easy to follow blue print to do so, making for a relatively easy to achieve extension to the Causal BART

Figure 4.12: Case NLHom CATE



Mixture Model.

Figure 4.13: Case NLHom ATE

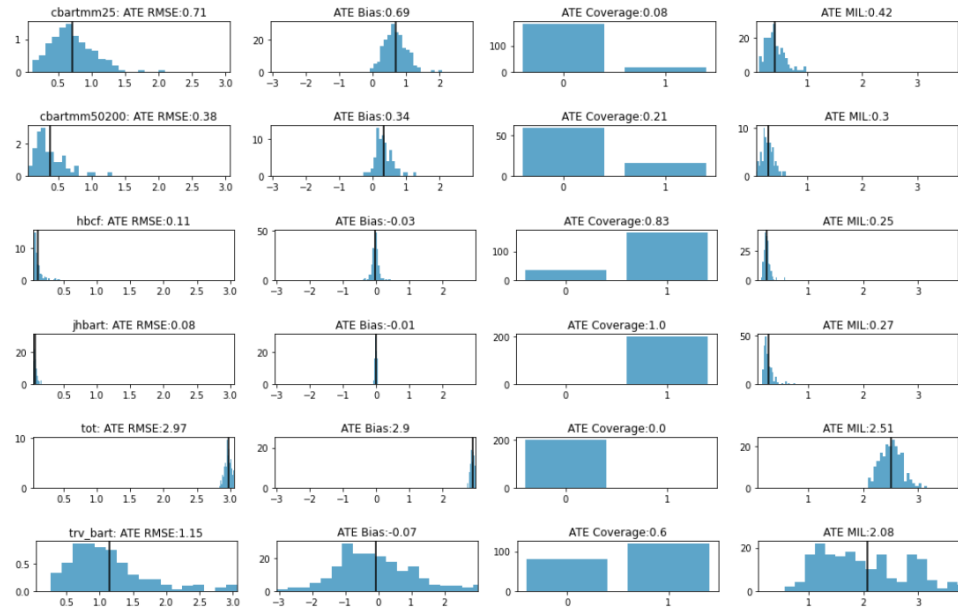


Figure 4.14: Case A CATE coverage probability as a function of $h(x)$ in the top image and below we show the distribution of $h(x)$. Vertical marks 'I' indicate for the example data which observation with specific value of h are either covered indicated by value of 1 vs not covered indicated with a value of 0. Coverage is calculated for the 95% credible interval.

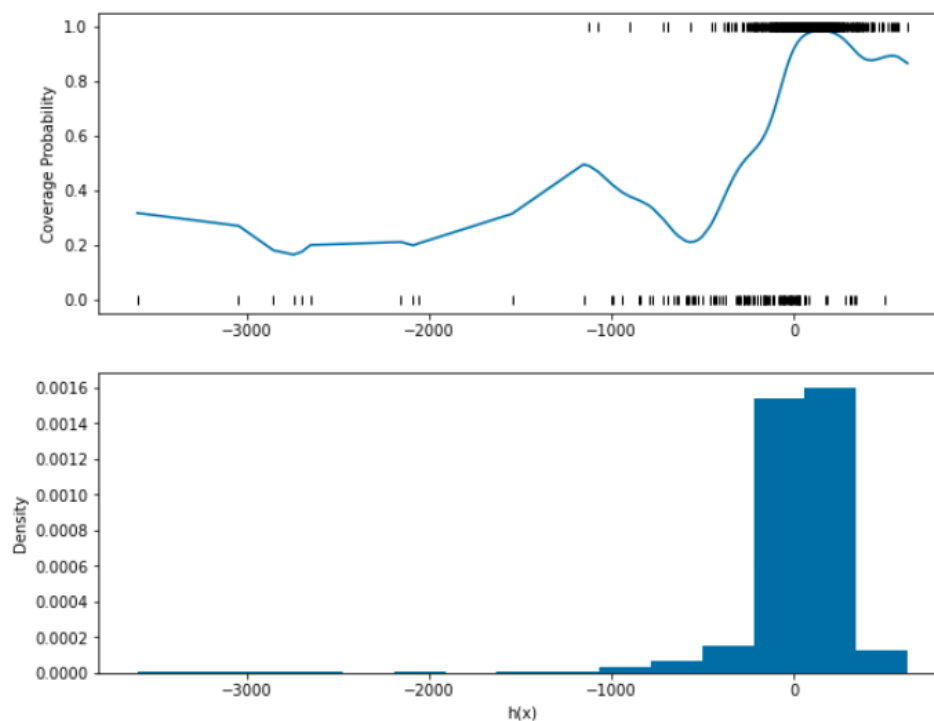


Figure 4.15: Case B CATE coverage probability as a function of $h(x)$ in the top image and below we show the distribution of $h(x)$. Vertical marks 'I' indicate for the example data which observation with specific value of h are either covered indicated by value of 1 vs not covered indicated with a value of 0. Coverage is calculated for the 95% credible interval.

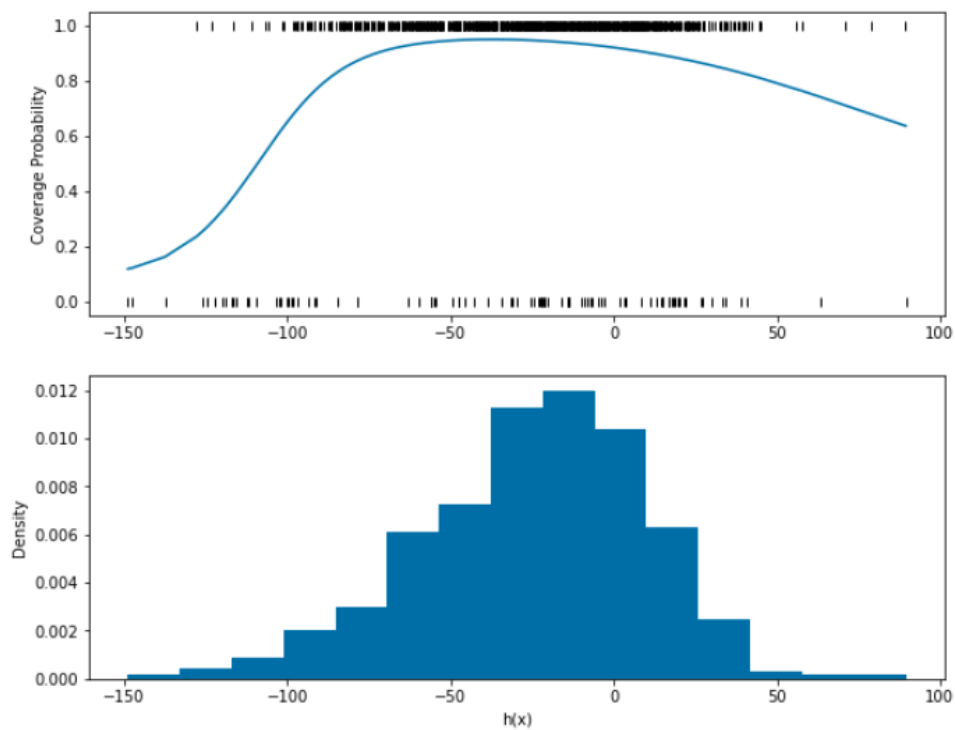


Figure 4.16: Case NLHet CATE coverage probability as a function of $h(x)$ in the top image and below we show the distribution of $h(x)$. Vertical marks 'I' indicate for the example data which observation with specific value of h are either covered indicated by value of 1 vs not covered indicated with a value of 0. Coverage is calculated for the 95% credible interval.

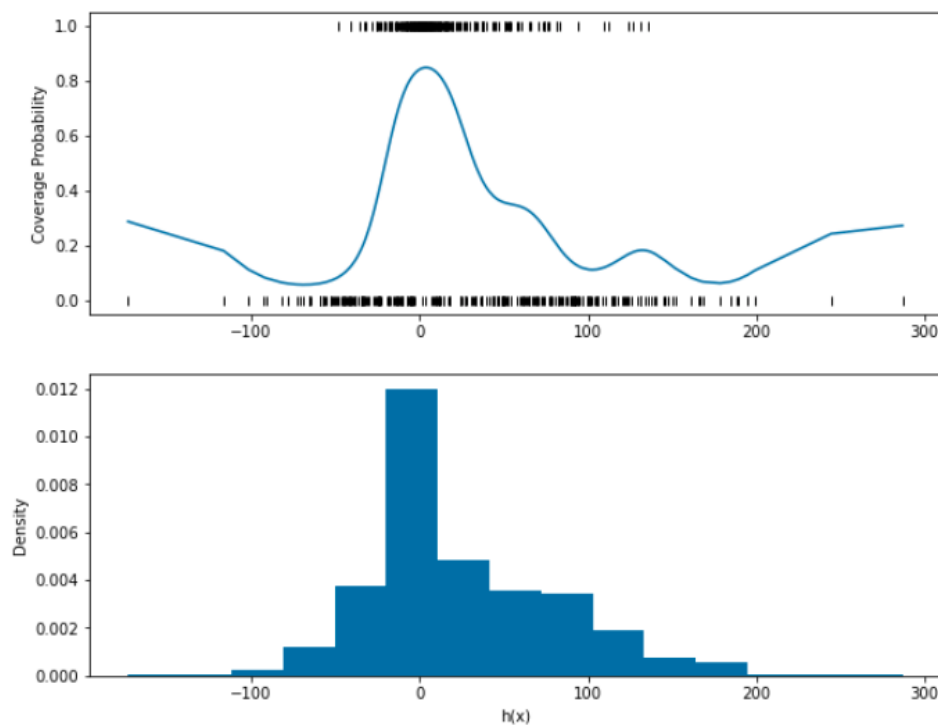


Figure 4.17: Case NLHom CATE coverage probability as a function of $h(x)$ in the top image and below we show the distribution of $h(x)$. Vertical marks 'I' indicate for the example data which observation with specific value of h are either covered indicated by value of 1 vs not covered indicated with a value of 0. Coverage is calculated for the 95% credible interval.

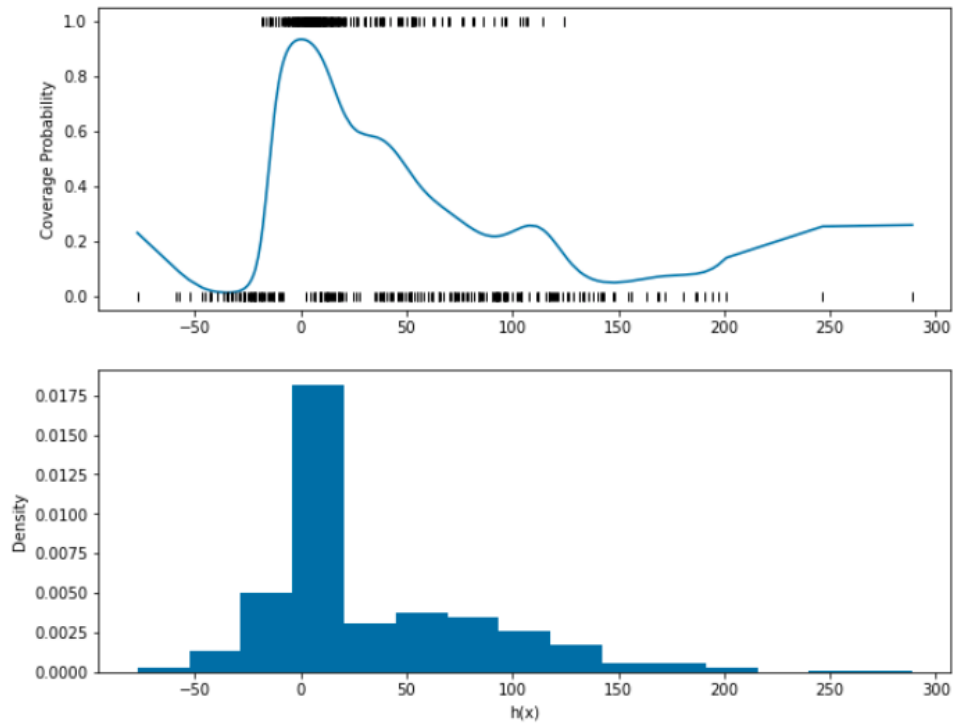


Figure 4.18: Case A CATE: When trimming true h

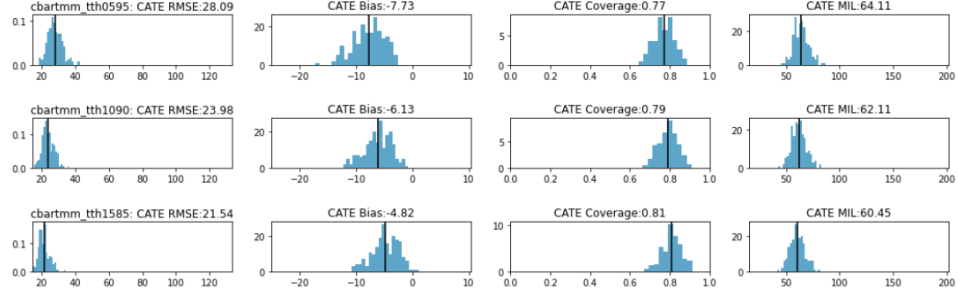


Figure 4.19: Case A ATE: When trimming true h .

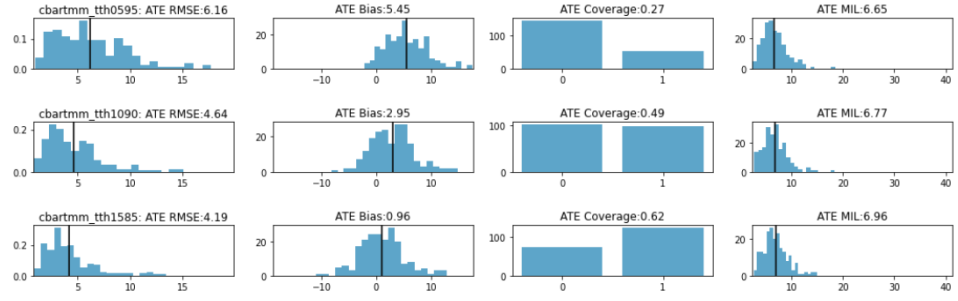


Figure 4.20: Case NLHet CATE: When trimming true h

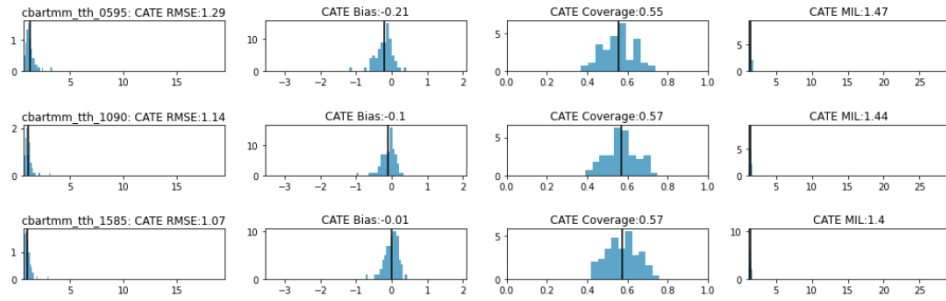


Figure 4.21: Case NLHet ATE: When trimming true h.

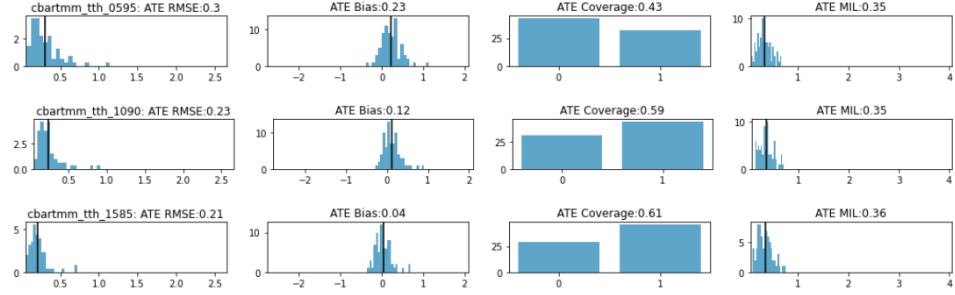


Figure 4.22: Case NLHom CATE: When trimming true h

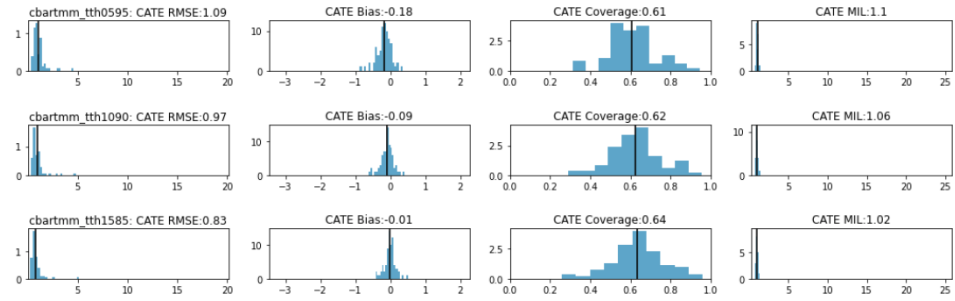
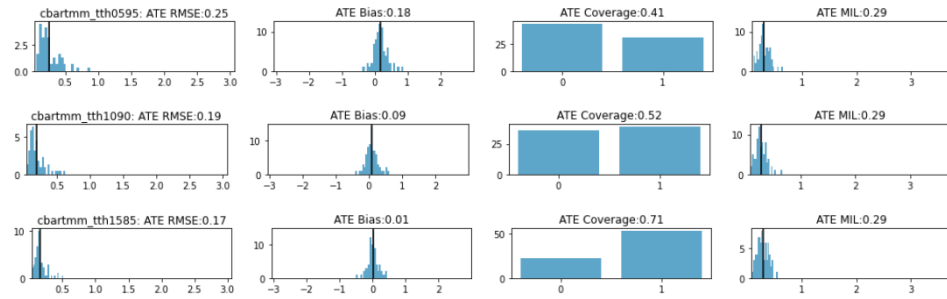


Figure 4.23: Case NLHom ATE: When trimming true h.



Chapter 5

Conclusion

In this work, we have extended existing approaches to big data with distributed compute as well as provided evidence for scalable communication strategies. We also introduced CBARTMM...

In Chapter 3, we explored communication strategies in distributed computing environments for models that perform on-line learning via particle filtering genetic algorithms. We showed that allowing communication between the compute processes has the capacity to significantly improve model fit. We also showed from our experiments the potential downside is limited to increased compute time but does not adversely affect the model fit quality, implying a possible avenue for improving model performance where parameter learning is performed in a distributed computing environment.

In Chapter 4 we introduced a reparameterization for a causal inference model using the TRV. We used applied a modification to BART which allowed us to expand the set of methods in estimating CATE's as well as outline what we believe are some inherent challenges in using the TRV for modeling CATE and ATE. Regardless, were able to explicitly model heterogeneous treatment effects with a distribution implied by the TRV, thereby reducing the variance of the estimators. Finally, we also introduced a method that models both the treatment and control conditions in an observational setting jointly, thereby improving inference over some models that do not model treatment and control conditions jointly.

Appendices

Appendix A

Appendix: Sequential Monte Carlo Particle Filtering

A.1 Consensus Monte Carlo Stochastic Approximation Covariance Adjustment

The Consensus Monte Carlo method, originally proposed by (Scott et al., 2016) posits an approximation to a target distribution can be estimated with the simplifying assumption our posterior distribution is drawn from a *MVN* distribution when our samples or particles come from a collection of sub-posteriors. Let $\tilde{P}(\theta)_s \propto P(\theta)P(y_s|\theta)^s$, and assume that this is well approximated by a Gaussian with mean $\tilde{\mu}_s$, covariance $\tilde{\Sigma}_s$.

$$\begin{aligned} P(\theta|y)^s &\propto \prod_i \tilde{P}(\theta)_i \\ &\propto \prod_{i=1}^S \exp\left(\frac{-1}{2}(\theta - \tilde{\mu}_i)^T \tilde{\Sigma}_i^{-1}(\theta - \tilde{\mu}_i)\right) \end{aligned} \quad (\text{A.1})$$

so,

$$P(\theta|y) \propto \left(\prod_{i=1}^S \exp\left(\frac{-1}{2}(\theta - \tilde{\mu}_i)^T \tilde{\Sigma}_i^{-1}(\theta - \tilde{\mu}_i)\right) \right)^{1/s} \quad (\text{A.2})$$

If

$$P(X) \propto \exp\left(-\frac{1}{2}(X - \mu)^T \Sigma^{-1}(X - \mu)\right)$$

then if $P'(X) \propto P(X)^{1/s}$, we have

$$\begin{aligned}
p'(X) &\propto \left(\exp \left\{ -\frac{1}{2}(X - \mu)^T \Sigma^{-1}(X - \mu) \right\} \right)^{1/s} \\
&= \left(\exp \left\{ -\frac{1}{2s}(X - \mu)^T \Sigma^{-1}(X - \mu) \right\} \right) \\
&\propto N(X; \mu, s\Sigma)
\end{aligned}$$

and

$$P(\theta|y) \propto \prod_{i=1}^S \exp \left(-\frac{1}{2}(\theta - \tilde{\mu}_i)^T (s\tilde{\Sigma}_i)^{-1}(\theta - \tilde{\mu}_i) \right)$$

Which implies we have mean and covariance with

$$\begin{aligned}
\tilde{V}^{-1} &= \sum_{i=1}^S \tilde{\Sigma}_i^{-1} S^{-1} \\
&= S^{-1} \sum_{i=1}^S \tilde{\Sigma}_i^{-1}
\end{aligned} \tag{A.3}$$

$$\begin{aligned}
\tilde{\mu} &= \tilde{V} \sum_{i=1}^S S^{-1} \tilde{\Sigma}_i^{-1} \tilde{\mu}_i \\
&= S \left(\sum_{i=1}^S \tilde{\Sigma}_i^{-1} \right)^{-1} S^{-1} \sum_{i=1}^S \tilde{\Sigma}_i^{-1} \tilde{\mu}_i \\
&= \left(\sum_{i=1}^S \tilde{\Sigma}_i^{-1} \right)^{-1} \sum_{i=1}^S \tilde{\Sigma}_i^{-1} \tilde{\mu}_i
\end{aligned} \tag{A.4}$$

From this we see that, $\mu = \tilde{\mu}$. Or in other words, the mean of our stochastic approximated sub-posteriors are the same as the Consensus Monte Carlo Mean. Additionally, we can see $S\tilde{V} = V$. Therefore,

$$P(\theta|\mathbf{y}) \propto N(\tilde{\mu}, S\tilde{V}) \tag{A.5}$$

Appendix B

Appendix: Causal BART Mixture Model

In this supplement, we provide proofs and derivations for the theoretical underpinnings of the Causal BART Mixture Model.

B.1 Theorems

In this section we have various proofs used through out this document.

Multi-Variance Theorem: Let y_1, \dots, y_n be a sequence of size n of independent random variables with $y_i \sim N(\mu, \sigma_i^2)$, then

$$\mu \sim N \left(\frac{\sum_{i=1}^n \frac{y_i}{\sigma_i^2}}{\sum_{i=1}^n \frac{1}{\sigma_i^2}}, \left[\sum_{i=1}^n \frac{1}{\sigma_i^2} \right]^{-1} \right) \quad (\text{B.1})$$

Proof: Our likelihood for $\mu|Y$ is

$$\begin{aligned}
L(\mu|y, \sigma_1^2, \dots, \sigma_n^2) &\propto \\
&\prod_{i=1}^n \exp\left(-\frac{1}{2} \frac{(y_i - \mu)^2}{\sigma_i^2}\right) \\
&= \exp\left(\sum_{i=1}^n -\frac{1}{2} \frac{(y_i - \mu)^2}{\sigma_i^2}\right) \\
&= \exp\left(-\frac{1}{2} \sum_{i=1}^n \frac{(\mu - y_i)^2}{\sigma_i^2}\right) \\
&= \exp\left(-\frac{1}{2} \sum_{i=1}^n \frac{\mu^2 - 2y_i\mu + y_i^2}{\sigma_i^2}\right) \tag{B.2} \\
&= \exp\left(-\frac{1}{2} \left(\sum_{i=1}^n \frac{\mu^2}{\sigma_i^2} - 2\left(\sum_{i=1}^n \frac{y_i}{\sigma_i^2}\right)\mu + \dots\right)\right) \\
&= \exp\left(-\frac{1}{2} \left(\sum_{i=1}^n \frac{1}{\sigma_i^2}\right) \left(\mu^2 - 2\left(\sum_{i=1}^n \frac{1}{\sigma_i^2}\right)^{-1} \left(\sum_{i=1}^n \frac{y_i}{\sigma_i^2}\right)\mu + \dots\right)\right) \\
&= \exp\left(-\frac{1}{2} \left(\sum_{i=1}^n \frac{1}{\sigma_i^2}\right) \left(\mu^2 - 2\left(\sum_{i=1}^n \frac{1}{\sigma_i^2}\right)^{-1} \left(\sum_{i=1}^n \frac{y_i}{\sigma_i^2}\right)\mu + \dots\right)\right)
\end{aligned}$$

Completing the square with μ as our variable of interest yields

$$L(\mu|y, \sigma_1^2, \dots, \sigma_n^2) \propto \exp\left(-\frac{1}{2} \frac{\left(\mu - \left[\sum_{i=1}^n \frac{1}{\sigma_i^2}\right]^{-1} \left[\sum_{i=1}^n \frac{y_i}{\sigma_i^2}\right]\right)^2}{\left[\sum_{i=1}^n \frac{1}{\sigma_i^2}\right]^{-1}}\right) \tag{B.3}$$

Therefore,

$$\mu \sim N\left(\left[\sum_{i=1}^n \frac{1}{\sigma_i^2}\right]^{-1} \left[\sum_{i=1}^n \frac{y_i}{\sigma_i^2}\right], \left[\sum_{i=1}^n \frac{1}{\sigma_i^2}\right]^{-1}\right) \tag{B.4}$$

as desired.

B.2 Proofs

B.2.1

Here we prove $E[Y_i^*|X_i = x] = \tau^{CATE}$

proof:

$$\begin{aligned} E[Y_i^*|X_i = x] &= E[Y_i \frac{W_i - p_i}{p(1 - p_i)} | X_i = x] \\ &= E[W_i Y_i \frac{W_i - p_i}{p_i(1 - p_i)} + (1 - W_i) Y_i \frac{W_i - p_i}{p_i(1 - p_i)} | X_i = x] \end{aligned} \quad (B.5)$$

Because $W_i Y_i = W_i(1)$ and $(1 - W_i) Y_i = (1 - W_i) Y_i(0)$, we can re-write the expression as

$$\begin{aligned} E[Y_i^*|X_i = x] &= E[W_i Y_i(1) \frac{W_i - p_i}{p_i(1 - p_i)} + (1 - W_i) Y_i(0) \frac{W_i - p_i}{p_i(1 - p_i)} | X_i = x] \\ &= E[Y_i(1) \frac{W_i(1 - p_i)}{p_i(1 - p_i)}] - E[Y_i(0) \frac{(1 - W_i)p_i}{p_i(1 - p_i)} | X_i = x] \end{aligned}$$

Because of unconfoundedness, we have

$$\begin{aligned} E[Y_i^*|X_i = x] &= E[Y_i(1)|X_i = x] E[W_i|X_i = x] \frac{1}{p_i} \\ &\quad - E[Y_i(0)|X_i = x] E[1 - W_i|X_i = x] \frac{1}{1 - p_i} \\ &= f_1(x) - f_0(x) = \tau^{CATE} \end{aligned}$$

B.2.2

Derivation for $Var[Y_i^*|X_i = x]$ Let

$$E[y_i(1)|X_i = x] = \mu_1$$

$$E[y_i(0)|X_i = x] = \mu_0$$

$$w_i|X_i = x \sim \text{Bernoulli}(p_i)$$

,

$$Var[y_i(1)|X_i = x] = \sigma_1^2$$

$$\text{Var}[y_i(0)|X_i = x] = \sigma_0^2$$

$$Y_i^* = \frac{y_i(w_i - p_i)}{p_i(1 - p_i)}$$

$$E[Y_i^*|X_i = x] = \tau_i$$

$$\text{then, } \text{Var}[Y_i^*|X_i = x] = \frac{\sigma_1^2 + \mu_1^2}{p_i} + \frac{\sigma_0^2 + \mu_0^2}{1 - p_i} - \tau_i^2 = \frac{\sigma_1^2}{p_i} + \frac{\sigma_0^2}{1 - p_i} + \frac{(1 - p_i)\mu_1^2}{p_i} + \frac{p_i\mu_0^2}{1 - p_i} - 2\mu_1\mu_0$$

Proof:

We will need the following expectation results to complete our derivation for $\text{Var}[Y_i^*|X_i = x]$. Conditioning on $X_i = x$, the following functions of w_i and p_i have the following expectations:

$$E[w_i(w_i - p_i)^2|X_i = x] = \sum_{w_i=0}^1 w_i(w_i - p_i)^2 p_i^{w_i} (1 - p_i)^{1-w_i} = p_i(1 - p_i)^2$$

(B.6)

$$E[(1 - w_i)(w_i - p_i)^2|X_i = x] = \sum_{w_i=0}^1 (1 - w_i)(w_i - p_i)^2 p_i^{w_i} (1 - p_i)^{1-w_i} = p_i^2(1 - p_i)$$

(B.7)

$$E[w_i(w_i - p_i)|X_i = x] = \sum_{w_i=0}^1 w_i(w_i - p_i) p_i^{w_i} (1 - p_i)^{1-w_i} = p_i(1 - p_i)$$

(B.8)

$$E[(1 - w_i)(w_i - p_i)|X_i = x] = \sum_{w_i=0}^1 (1 - w_i)(w_i - p_i) p_i^{w_i} (1 - p_i)^{1-w_i} = -p_i(1 - p_i)$$

(B.9)

$$\begin{aligned}
Var[Y_i^*|X_i = x] &= E[(Y_i^* - \tau_i)^2|X_i = x] \\
&= E[(\frac{y_i(w_i - p_i)}{p_i(1 - p_i)} - \tau_i)^2|X_i = x] \\
&= E[\frac{y_i^2(w_i - p_i)^2}{p_i^2(1 - p_i)^2} - 2\frac{y_i(w_i - p_i)}{p_i(1 - p_i)}\tau_i + \tau_i^2|X_i = x] \\
&= E[w_i\frac{y_i(1)^2(w_i - p_i)^2}{p_i^2(1 - p_i)^2} + (1 - w_i)\frac{y_i(0)^2(w_i - p_i)^2}{p_i^2(1 - p_i)^2} \\
&\quad - 2w_i\frac{y_i(1)(w_i - p_i)}{p_i(1 - p_i)}\tau_i - \\
&\quad 2(1 - w_i)\frac{y_i(0)(w_i - p_i)}{p_i(1 - p_i)}\tau_i + \tau_i^2|X_i = x]
\end{aligned} \tag{B.10}$$

Because of unconfoundedness we have

$$\begin{aligned}
Var(Y_i^*) &= \frac{E[y_i(1)^2|X_i = x]E[w_i(w_i - p_i)^2|X_i = x]}{p_i^2(1 - p_i)^2} \\
&\quad + \frac{E[y_i(0)^2|X_i = x]E[(1 - w_i)(w_i - p_i)^2|X_i = x]}{p_i^2(1 - p_i)^2} \\
&\quad - 2\frac{E[y_i(1)|X_i = x]E[w_i(w_i - p_i)|X_i = x]}{p_i(1 - p_i)}\tau_i \\
&\quad - 2\frac{E[y_i(0)|X_i = x]E[(1 - w_i)(w_i - p_i)|X_i = x]}{p_i(1 - p_i)}\tau_i \\
&\quad + \tau_i^2
\end{aligned} \tag{B.11}$$

Using the expectations listed above and that

$\tau_i = E[y_i(1)|X_i = x] - E[y_i(0)|X_i = x]$, we have

$$\begin{aligned}
Var(Y_i^*) &= \frac{E[y_i(1)^2|X_i = x]p_i(1-p_i)^2|X_i = x]}{p_i^2(1-p_i)^2} \\
&\quad + \frac{E[y_i(0)^2|X_i = x]p_i^2(1-p_i)|X_i = x]}{p_i^2(1-p_i)^2} \\
&\quad - 2\frac{E[y_i(1)|X_i = x]p_i(1-p_i)}{p_i(1-p_i)}\tau_i \\
&\quad - 2\frac{E[y_i(0)|X_i = x]p_i(1-p_i)}{p_i(1-p_i)}\tau_i + \\
&\quad \tau_i^2 \\
&= \frac{E[y_i(1)^2|X_i = x]}{p_i} + \frac{E[y_i(0)^2|X_i = x]}{1-p_i} \\
&\quad - 2\tau_i(E[y_i(1)|X_i = x] - E[y_i(0)|X_i = x]) + \tau_i^2 \\
&= \frac{E[y_i(1)^2|X_i = x]}{p_i} + \frac{E[y_i(0)^2|X_i = x]}{1-p_i} - 2\tau_i^2 + \tau_i^2 \\
&= \frac{E[y_i(1)^2|X_i = x]}{p_i} + \frac{E[y_i(0)^2|X_i = x]}{1-p_i} - \tau_i^2
\end{aligned} \tag{B.12}$$

Next, we use the fact that $E[x^2|X_i = x] = \sigma^2 + \mu^2$ and apply new notation for $\sigma_0^2 = Var[y_i(0)|X_i = x]$, $\sigma_1^2 = Var[y_i(1)|X_i = x]$, $\mu_0 = E[y_i(0)|X_i = x]$, and $\mu_1 = E[y_i(1)|X_i = x]$, so we have

$$\begin{aligned}
Var(Y_i^*) &= \frac{\sigma_1^2 + \mu_1^2}{p_i} + \frac{\sigma_0^2 + \mu_0^2}{1-p_i} - \tau_i^2
\end{aligned} \tag{B.13}$$

At this stage we can use what we know about τ_i to reduce further.

Namely, $\tau_i = \mu_1 - \mu_0$ and so, we have

$$\begin{aligned}
Var(Y_i^*) &= \frac{\sigma_1^2 + \mu_1^2}{p_i} + \frac{\sigma_0^2 + \mu_0^2}{1 - p_i} - (\mu_1 - \mu_0)^2 \\
&= \frac{\sigma_1^2 + \mu_1^2}{p_i} + \frac{\sigma_0^2 + \mu_0^2}{1 - p_i} + \mu_1^2 + \mu_0^2 - 2\mu_1\mu_0 \\
&= \frac{\sigma_1^2}{p_i} + \frac{\sigma_0^2}{1 - p_i} + \frac{\mu_1^2}{p_i} - \frac{p_i\mu_1^2}{p_i} + \frac{\mu_0^2}{1 - p_i} - \frac{(1 - p_i)\mu_0^2}{1 - p_i} - 2\mu_1\mu_0
\end{aligned} \tag{B.14}$$

So, finally we have

$$Var(Y_i^*) = \frac{\sigma_1^2}{p_i} + \frac{\sigma_0^2}{1 - p_i} + \frac{(1 - p_i)\mu_1^2}{p_i} + \frac{p_i\mu_0^2}{1 - p_i} - 2\mu_1\mu_0 \tag{B.15}$$

as desired.

B.3 Derivation of Mixture Model for Y_i^*

Since $Y_i^* = Y_{i,obs} \frac{W_i - p_i}{p_i(1 - p_i)}$, either we have $W_i = 0$ or $W_i = 1$, we can write the expression as a mixture with

$$\begin{aligned}
E[Y_i^*] &= Y_i^* P(W = 1) + Y_i^* P(W = 0) \\
&= Y_{i,obs} \frac{1 - p_i}{p_i(1 - p_i)} P(W = 1) + Y_{i,obs} \frac{0 - p_i}{p_i(1 - p_i)} P(W = 0) \\
&= Y_i(1) \frac{1 - p_i}{p_i(1 - p_i)} p_i - Y_i(0) \frac{p_i}{p_i(1 - p_i)} (1 - p_i) \\
&= Y_i(1) - Y_i(0)
\end{aligned} \tag{B.16}$$

We therefore define

$$\begin{aligned}
Y_i(1) &= f_1(x_i) + \epsilon_i(1), \text{ where } \epsilon_i(1) \sim (0, \sigma^2) \\
Y_i(0) &= f_0(x_i) + \epsilon_i(0), \text{ where } \epsilon_i(0) \sim (0, \sigma^2)
\end{aligned} \tag{B.17}$$

$$h(x) = \frac{f_1(x)}{p_i} + \frac{f_0(x)}{1 - p_i} \tag{B.18}$$

$$g(x) = f_1(x) - f_0(x) \quad (\text{B.19})$$

Now, notice that

$$\begin{aligned} E[Y_i^*] &= E[Y_i(1) - Y_i(0)] \\ &= E[f_1(x_i) + \epsilon_i(1) - (f_0(x_i) + \epsilon_i(0))] \\ &= E[f_1(x_i)] + E[\epsilon_i(1)] - E[f_0(x_i)] - E[\epsilon_i(0)] \\ &= E[f_1(x_i)] - E[f_0(x_i)] \\ &= E[f_1(x_i) - f_0(x_i)] \\ &= E[g(x_i)] \end{aligned} \quad (\text{B.20})$$

which implies $E[g(x_i)] = \tau(x_i)$. Now, substituting $Y_i(1) = f_1(x) + \epsilon_i(1)$ and $Y_i(0) = f_0(x) + \epsilon_i(0)$ under the treatment and control cases in the definition of the Transformed Response yields the following mixture model,

$$\begin{aligned} Y_i^* &= g(x) + \epsilon_i^*, \\ \epsilon_i^* &\sim p_i N((1 - p_i)h(x_i), \frac{1}{p_i^2}\sigma^2) + (1 - p_i)N(-p_i h(x_i), \frac{1}{(1 - p_i)^2}\sigma^2) \end{aligned} \quad (\text{B.21})$$

Proof:

First consider, $(Y_i^*|W_i = 1)$:

$$\begin{aligned} (Y_i^*|W_i = 1) &= Y_i(1) \frac{1 - p_i}{p_i(1 - p_i)} \\ &= (f_1(x_i) + \epsilon_i(1)) \frac{1}{p_i} \\ &= \frac{f_1(x_i)}{p_i} + \frac{\epsilon_i(1)}{p_i} + f_1(x_i) - f_1(x_i) + f_0(x_i) - f_0(x_i) \\ &= f_1(x_i) - f_0(x_i) + \frac{f_1(x_i)}{p_i} + \frac{\epsilon_i(1)}{p_i} - f_1(x_i) + f_0(x_i) \\ &= g(x_i) + \frac{1 - p_i}{p_i} f_1(x_i) + \frac{1 - p_i}{1 - p_i} f_0(x_i) + \frac{\epsilon_i(1)}{p_i} \\ &= g(x_i) + (1 - p_i) \left(\frac{1}{p_i} f_1(x_i) + \frac{1}{1 - p_i} f_0(x_i) \right) + \frac{\epsilon_i(1)}{p_i} \\ &= g(x_i) + (1 - p_i)h(x_i) + \frac{\epsilon_i(1)}{p_i} \end{aligned} \quad (\text{B.22})$$

Next, consider $(Y_i^*|W_i = 0)$:

$$\begin{aligned}
(Y_i^*|W_i = 0) &= Y_i(0) \frac{0 - p_i}{p_i(1 - p_i)} \\
&= (f_0(x_i) + \epsilon_i(0)) \frac{-1}{1 - p_i} \\
&= \frac{-f_0(x_i)}{1 - p_i} + \frac{-\epsilon_i(0)}{1 - p_i} + f_1(x_i) - f_1(x_i) + f_0(x_i) - f_0(x_i) \\
&= f_1(x_i) - f_0(x_i) \\
&\quad - \frac{p_i}{p_i} f_1(x_i) + \frac{1 - p_i}{1 - p_i} f_0(x_i) - \frac{1}{1 - p_i} f_0(x_i) - \frac{\epsilon_i(0)}{1 - p_i} \quad (\text{B.23}) \\
&= g(x_i) + \frac{-p_i}{p_i} f_1(x_i) + \frac{-p_i}{1 - p_i} f_0(x_i) - \frac{\epsilon_i(0)}{1 - p_i} \\
&= g(x_i) - p_i \left(\frac{1}{p_i} f_1(x_i) + \frac{1}{1 - p_i} f_0(x_i) \right) + \frac{\epsilon_i(0)}{p_i - 1} \\
&= g(x_i) - p_i h(x_i) + \frac{\epsilon(0)}{p - 1}
\end{aligned}$$

since our errors, $\epsilon_i(1)$ and $\epsilon_i(0) \sim N(0, \sigma^2)$, we have that Y_i^* is drawn from a Gaussian mixture with

$$\begin{aligned}
Y_i^* &= g(x_i) + \epsilon_i^*, \\
\epsilon_i^* &\sim p_i N((1 - p_i)h(x_i), \frac{1}{p_i^2} \sigma^2) + (1 - p_i) N(-p_i h(x_i), \frac{1}{(1 - p_i)^2} \sigma^2) \quad (\text{B.24})
\end{aligned}$$

as desired.

B.4 Posterior Derivations

B.4.1 Derivation of $g|X, W, Y, p, h, (T^h, \mathcal{M}^h), (T^g, \mathcal{M}^g), \sigma^2$

$$\begin{aligned}
Y_i^* &= g(x) + \epsilon_i^* \\
&= \sum_{m=1}^M T_m(X) + \epsilon_i^* \quad (\text{B.25})
\end{aligned}$$

So, for Tree j , we are fitting

$$Y_i^* - \sum_{m \neq j}^M T_m(X) - (w_i(1 - p_i)h(x_i) - (1 - w_i)p_i h(x_i)) = T_j + \epsilon_i^* \quad (\text{B.26})$$

Conditional on our stochastic tree process, our likelihood is

$$\prod_{i=1}^n \left[p_i \frac{1}{\sqrt{2\pi}} \frac{1}{\frac{\sigma}{p_i}} \exp \left(-\frac{1}{2} \frac{Y_{j,i}^2}{\frac{\sigma^2}{p_i^2}} \right) + (1 - p_i) \frac{1}{\sqrt{2\pi}} \frac{1}{\frac{\sigma}{1-p_i}} \exp \left(-\frac{1}{2} \frac{Y_{j,i}^2}{\frac{\sigma^2}{(1-p_i)^2}} \right) \right] \quad (\text{B.27})$$

where

$$Y_{j,i} = \left(Y_i^* - \sum_{m \neq j}^M T_m(X) - (w_i(1 - p_i)h(x_i) - (1 - w_i)p_i h(x_i)) \right)$$

$T_j(x_i)$ is the value of the mean function for x_i for the j^{th} tree.

which is the y value after subtracting out the rest of the residuals explained by all other trees not including the j^{th} tree as well as the mixture means.

$$\begin{aligned} L(\sigma, T, \mathcal{M}|Y_j) = & \prod_{i=1}^n \left(p_i \frac{1}{\sqrt{2\pi}} \frac{p_i}{\sigma} \exp \left(-\frac{1}{2} \frac{(y_{j,i} - T_j(x_i))^2}{\frac{\sigma^2}{p_i^2}} \right) \right. \\ & \left. + (1 - p_i) \frac{1}{\sqrt{2\pi}} \frac{1 - p_i}{\sigma} \exp \left(-\frac{1}{2} \frac{(y_{j,i} - T_j(x_i))^2}{\frac{\sigma^2}{(1-p_i)^2}} \right) \right) \end{aligned} \quad (\text{B.28})$$

Suppose there are B_j nodes in our j^{th} tree, then we can factor the above expression as

$$\begin{aligned} L(\sigma, T, \mathcal{M}|Y_j) = & \prod_{b=1}^{B_j} \prod_{i=1}^{n_{j,b}} \left(p_i \frac{1}{\sqrt{2\pi}} \frac{p_i}{\sigma} \exp \left(-\frac{1}{2} \frac{(y_{j,i \in \eta_{j,b}} - \mu_{j,b})^2}{\frac{\sigma^2}{p_i^2}} \right) \right. \\ & \left. + (1 - p_i) \frac{1}{\sqrt{2\pi}} \frac{1 - p_i}{\sigma} \exp \left(-\frac{1}{2} \frac{(y_{j,i \in \eta_{j,b}} - \mu_{j,b})^2}{\frac{\sigma^2}{(1-p_i)^2}} \right) \right) \end{aligned} \quad (\text{B.29})$$

Because of unconfoundedness, we have

$$L(\sigma, T, \mathcal{M}|Y_j) = \prod_{b=1}^{B_j} \prod_{i=1}^{n_{j,b}} \left(\mathbb{1}_{(w_i=1)} \frac{1}{\sqrt{2\pi}} \frac{p_i}{\sigma} \exp \left(-\frac{1}{2} \frac{(y_{j,i \in \eta_{j,b}} - \mu_{j,b})^2}{\frac{\sigma^2}{p_i^2}} \right) + \mathbb{1}_{(w_i=0)} \frac{1}{\sqrt{2\pi}} \frac{1-p_i}{\sigma} \exp \left(-\frac{1}{2} \frac{(y_{j,i \in \eta_{j,b}} - \mu_{j,b})^2}{\frac{\sigma^2}{(1-p_i)^2}} \right) \right) \quad (\text{B.30})$$

$$L(\sigma, T, \mathcal{M}|Y_j) = \prod_{b=1}^{B_j} \left[\prod_{i=1}^{n_{j,b;w_i=1}} \frac{1}{\sqrt{2\pi}} \frac{p_i}{\sigma} \exp \left(-\frac{1}{2} \frac{(y_{j,i \in \eta_{j,b}} - \mu_{j,b})^2}{\frac{\sigma^2}{p_i^2}} \right) \prod_{i=1}^{n_{j,b;w_i=0}} \frac{1}{\sqrt{2\pi}} \frac{1-p_i}{\sigma} \exp \left(-\frac{1}{2} \frac{(y_{j,i \in \eta_{j,b}} - \mu_{j,b})^2}{\frac{\sigma^2}{(1-p_i)^2}} \right) \right] \quad (\text{B.31})$$

Here we introduce another change of notation to simplify our conditional likelihood with $\sigma_i^2 = w_i \frac{\sigma^2}{p_i^2} + (1-w_i) \frac{\sigma^2}{(1-p_i)^2}$

$$L(\sigma, T, \mathcal{M}|Y_j) = \prod_{b=1}^{B_j} \prod_{i=1}^{n_{j,b}} \left(\frac{1}{\sqrt{2\pi\sigma_i^2}} \exp \left(-\frac{1}{2} \frac{(y_{j,i \in \eta_{j,b}} - \mu_{j,b})^2}{\sigma_i^2} \right) \right) \quad (\text{B.32})$$

So, conditional on all the trees, including tree j and the scalar terminal node parameters, the leaf node parameters are independent. Below is the full conditional for each $\mu_{j,b}$ which can be drawn sequentially using a Gibbs step. If assume the following prior for $\mu_{j,b}$'s

$$\mu_{j,b} \sim N(\mu_{g,0}, \sigma_{g,\mu}^2) \quad (\text{B.33})$$

then by Multi-Variance Theorem (Theorem B.1),

$$\mu_{j,b} | \sigma^2, T, y, \sim N \left(\frac{\sum_{i=1}^{n_{j,b}} \frac{y_{j,i \in \eta_{j,b}}}{\sigma_i^2} + \frac{\mu_{g,0}}{\sigma_{g,\mu}^2}}{\frac{1}{\sigma_\mu^2} + \sum_{i=1}^n \frac{1}{\sigma_i^2}}, \left[\frac{1}{\sigma_\mu^2} + \sum_{i=1}^n \frac{1}{\sigma_i^2} \right]^{-1} \right) \quad (\text{B.34})$$

Where η_j^b is node b or T_j , $n_{j,b}$ is the number of observations in η_j^b and $y_{j,i} \in \eta_j^b$.

B.4.2 Derivation of $h|X, W, Y, p, h, (T^h, \mathcal{M}^h), (T^g, \mathcal{M}^g), \sigma^2$

We begin with our expression for Y_i^* :

$$\begin{aligned} Y_i^* &= g(x_i) + \epsilon_i^* \\ &= g(x_i) + w_i(1 - p_i)h(x_i) - (1 - w_i)p_i h(x_i) + \epsilon_i, \\ &= g(x_i) + \mathbb{1}_{(w_i=1)}(1 - p_i) \sum_{m=1}^{M_h} T_m^h(x_i) - \mathbb{1}_{(w_i=0)}p_i \sum_{m=1}^{M_h} T_m^h(x_i) + \epsilon_i \end{aligned} \tag{B.35}$$

Where $\epsilon_i \sim p_i N(0, \frac{\sigma^2}{p_i^2}) + (1 - p_i)N(0, \frac{\sigma^2}{(1-p_i)^2})$. So, for the j^{th} tree, we are fitting

$$\begin{aligned} Y_i^* - g(x_i) - \left(\mathbb{1}_{(w_i=1)}(1 - p_i) - \mathbb{1}_{(w_i=0)}p_i \right) \sum_{m \neq j}^{M_h} T_m^h(x_i) = \\ \left(\mathbb{1}_{(w_i=1)}(1 - p_i) - \mathbb{1}_{(w_i=0)}p_i \right) T_j^h(x_i) + \epsilon_i \end{aligned} \tag{B.36}$$

Conditional on our stochastic tree process, our likelihood is

$$\begin{aligned} \mathcal{L}(\text{parameters} | \text{Data}) = & \left(Y_i^* - g(x_i) - w_i(p_i) \sum_{m \neq j}^{M_h} T_m^h(x_i) \right. \\ & \left. - w_i(p_i) T_j^h(x_i) \right)^2 \\ \prod_{i=1}^n \left[p_i \frac{1}{\sqrt{2\pi}} \frac{1}{\frac{\sigma}{p_i}} \exp \left(- \frac{1}{2} \frac{\left(Y_i^* - g(x_i) - w_i(p_i) \sum_{m \neq j}^{M_h} T_m^h(x_i) \right. \right.}{\frac{\sigma^2}{p_i^2}} \right. \\ & \left. \left. - w_i(p_i) T_j^h(x_i) \right)^2}{\frac{\sigma^2}{p_i^2}} \right] \\ & + \\ & \left(Y_i^* - g(x_i) - w_i(p_i) \sum_{m \neq j}^{M_h} T_m^h(x_i) \right. \\ & \left. - w_i(p_i) T_j^h(x_i) \right)^2 \\ (1 - p_i) \frac{1}{\sqrt{2\pi}} \frac{1}{\frac{\sigma}{1-p_i}} \exp \left(- \frac{1}{2} \frac{\left(Y_i^* - g(x_i) - w_i(p_i) \sum_{m \neq j}^{M_h} T_m^h(x_i) \right. \right.}{\frac{\sigma^2}{(1-p_i)^2}} \right. \\ & \left. \left. - w_i(p_i) T_j^h(x_i) \right)^2}{\frac{\sigma^2}{(1-p_i)^2}} \right) \\ & \left. \right] \end{aligned} \tag{B.37}$$

where $w_i(p_i) = \left(\mathbb{1}_{(w_i=1)}(1-p_i) - \mathbb{1}_{(w_i=0)}p_i \right)$. Factoring out $w_i(p_i)$ and applying $w_i = 0$ or 1 consistent with the mixture term, we have

$$\begin{aligned} \mathcal{L}(\text{parameters}|\text{Data}) = & \\ & \prod_{i=1}^n \left[p_i \frac{1}{\sqrt{2\pi}} \frac{1}{\frac{\sigma}{p_i}} \exp \left(-\frac{1}{2} \frac{\left(\frac{Y_i^* - g(x_i)}{1-p_i} - \sum_{m \neq j}^{M_h} T_m^h(x_i) - T_j^h(x_i) \right)^2}{\frac{\sigma^2}{p_i^2(1-p_i)^2}} \right) \right. \\ & + \\ & \left. (1-p_i) \frac{1}{\sqrt{2\pi}} \frac{1}{\frac{\sigma}{1-p_i}} \exp \left(-\frac{1}{2} \frac{\left(\frac{Y_i^* - g(x_i)}{-p_i} - \sum_{m \neq j}^{M_h} T_m^h(x_i) - T_j^h(x_i) \right)^2}{\frac{\sigma^2}{p_i^2(1-p_i)^2}} \right) \right] \end{aligned} \quad (\text{B.38})$$

Then, further simplifying, we have

$$\begin{aligned} \mathcal{L}(\text{parameters}|\text{Data}) = & \\ & \prod_{i=1}^n \left[p_i \frac{1}{\sqrt{2\pi}} \frac{1}{\frac{\sigma}{p_i}} \exp \left(-\frac{1}{2} \frac{\left(-\frac{Y_i^* - g(x_i)}{1-p_i} + \sum_{m \neq j}^{M_h} T_m^h(x_i) + T_j^h(x_i) \right)^2}{\frac{\sigma^2}{p_i^2(1-p_i)^2}} \right) \right. \\ & + \\ & \left. (1-p_i) \frac{1}{\sqrt{2\pi}} \frac{1}{\frac{\sigma}{1-p_i}} \exp \left(-\frac{1}{2} \frac{\left(\frac{Y_i^* - g(x_i)}{p_i} + \sum_{m \neq j}^{M_h} T_m^h(x_i) + T_j^h(x_i) \right)^2}{\frac{\sigma^2}{p_i^2(1-p_i)^2}} \right) \right] \end{aligned} \quad (\text{B.39})$$

$$\begin{aligned}
\mathcal{L}(\text{parameters}|\text{Data}) = & \\
& \prod_{i=1}^n \left[p_i \frac{1}{\sqrt{2\pi}} \frac{1}{\frac{\sigma}{p_i}} \exp \left(-\frac{1}{2} \frac{\left(T_j^h(x_i) - \left(\frac{Y_i^* - g(x_i)}{1-p_i} - \sum_{m \neq j}^{M_h} T_m^h(x_i) \right) \right)^2}{\frac{\sigma^2}{p_i^2(1-p_i)^2}} \right) \right. \\
& + \\
& \left. (1-p_i) \frac{1}{\sqrt{2\pi}} \frac{1}{\frac{\sigma}{1-p_i}} \exp \left(-\frac{1}{2} \frac{\left(T_j^h(x_i) - \left(\frac{g(x_i) - Y_i^*}{p_i} - \sum_{m \neq j}^{M_h} T_m^h(x_i) \right) \right)^2}{\frac{\sigma^2}{p_i^2(1-p_i)^2}} \right) \right]
\end{aligned} \tag{B.40}$$

where $T_j^h(x_i)$ is the value of the mean function for x_i for the j^{th} tree for the function h . Next, we will introduce a change in notation for simplicity

$$Y_{j,i}^h = w_i \left(\frac{Y_i^* - g(x_i)}{1-p_i} - \sum_{m \neq j}^{M_h} T_m^h(x_i) \right) + (1-w_i) \left(\frac{g(x_i) - Y_i^*}{p_i} - \sum_{m \neq j}^{M_h} T_m^h(x_i) \right) \tag{B.41}$$

$$\sigma_{h,i}^2 = \frac{\sigma^2}{p_i^2(1-p_i)^2} \tag{B.42}$$

Inserting our change of variables and making the change in how we factor our expression, we have

$$\begin{aligned}
L(\sigma, T^h, \mathcal{M}^h | Y_j) = & \\
& \prod_{b=1}^{B_j^h} \prod_{i=1}^{n_{j,b}^h} \left[p_i \frac{1}{\sqrt{2\pi}} \frac{1}{\frac{\sigma}{p_i}} \exp \left(-\frac{1}{2} \frac{\left(\mu_{j,b}^h - Y_{j,i \in \eta_{j,b}^h}^h \right)^2}{\sigma_{h,i}^2} \right) \right. \\
& + (1-p_i) \frac{1}{\sqrt{2\pi}} \frac{1}{\frac{\sigma}{1-p_i}} \exp \left(-\frac{1}{2} \frac{\left(\mu_{j,b}^h - Y_{j,i \in \eta_{j,b}^h}^h \right)^2}{\sigma_{h,i}^2} \right) \left. \right]
\end{aligned} \tag{B.43}$$

Again, taking advantage of unconfoundedness, we have

$$\begin{aligned}
L(\sigma, T^h, \mathcal{M}^h | Y_j) = & \prod_{b=1}^{B_j^h} \prod_{i=1}^{n_{j,b}^h} \left[\mathbb{1}_{(w_i=1)} \frac{1}{\sqrt{2\pi}} \frac{1}{\frac{\sigma}{p_i}} \exp \left(-\frac{1}{2} \frac{\left(\mu_{j,b}^h - Y_{j,i \in \eta_{j,b}^h}^h \right)^2}{\sigma_{h,i}^2} \right) \right. \\
& \left. + \mathbb{1}_{(w_i=0)} \frac{1}{\sqrt{2\pi}} \frac{1}{\frac{\sigma}{1-p_i}} \exp \left(-\frac{1}{2} \frac{\left(\mu_{j,b}^h - Y_{j,i \in \eta_{j,b}^h}^h \right)^2}{\sigma_{h,i}^2} \right) \right] \quad (\text{B.44})
\end{aligned}$$

$$L(\sigma, T^h, \mathcal{M}^h | Y_j) \propto \prod_{b=1}^{B_j^h} \prod_{i=1}^{n_{j,b}^h} \left[\frac{1}{\sqrt{2\pi}} \frac{1}{\sigma_{h,i}} \exp \left(-\frac{1}{2} \frac{\left(\mu_{j,b}^h - Y_{j,i \in \eta_{j,b}^h}^h \right)^2}{\sigma_{h,i}^2} \right) \right] \quad (\text{B.45})$$

So, conditional on all the trees, including tree j and the scalar terminal node parameters, the leaf node parameters are independent. Below is the full conditional for each $\mu_{j,b}^h$ which can be drawn sequentially using a Gibbs step. If we assume the following prior for the $\mu_{j,b}^h$'s

$$\mu_{j,b}^h \sim N(\mu_{h,0}, \sigma_{h,\mu}^2) \quad (\text{B.46})$$

then by the Multi-Variance Theorem (Theorem B.1),

$$\mu_{j,b}^h | \sigma^2, T, y, \sim N \left(\frac{\sum_{i=1}^{n_{j,b}} \frac{Y_{j,i \in \eta_{j,b}^h}^h}{\sigma_{h,i}^2} + \frac{\mu_{h,0}}{\sigma_{h,\mu}^2}}{\frac{1}{\sigma_{h,\mu}^2} + \sum_{i=1}^n \frac{1}{\sigma_{h,i}^2}}, \left[\frac{1}{\sigma_{h,\mu}^2} + \sum_{i=1}^n \frac{1}{\sigma_{h,i}^2} \right]^{-1} \right) \quad (\text{B.47})$$

B.4.3 Derivation of $\sigma^2|X, W, Y, p, h, g, (T^h, \mathcal{M}^h), (T^g, \mathcal{M}^g)$

Again, we use the same likelihood as before

$$\begin{aligned} \mathcal{L}(\text{parameters}|\text{data}) = & \prod_{i=1}^n \left[p_i \frac{1}{\sqrt{2\pi}} \frac{1}{\frac{\sigma}{p_i}} \exp \left(-\frac{1}{2} \frac{\left(Y_i^* - g(x_i) - w_i(p_i)h(x_i) \right)^2}{\frac{\sigma^2}{p_i^2}} \right) \right. \\ & + \\ & \left. (1 - p_i) \frac{1}{\sqrt{2\pi}} \frac{1}{\frac{\sigma}{1-p_i}} \exp \left(-\frac{1}{2} \frac{\left(Y_i^* - g(x_i) - w_i(p_i)h(x_i) \right)^2}{\frac{\sigma^2}{(1-p_i)^2}} \right) \right] \end{aligned} \quad (\text{B.48})$$

and assume a prior on σ^2 of the form

$$\sigma^2 \sim IG(a, b) \quad (\text{B.49})$$

Applying the same approach as in the derivations for g and h , we have

$$\begin{aligned}
& \mathcal{L}(\sigma^2 | data, params) \propto \\
& \prod_{i=1}^n \left[p_i \frac{1}{\sqrt{2\pi}} \frac{1}{p_i} \exp \left(-\frac{1}{2} \frac{\left(Y_i^* - g(x_i) - w_i(pI)h(x_i) \right)^2}{\frac{\sigma^2}{p_i^2}} \right) \right. \\
& \quad + \\
& \quad (1-p_i) \frac{1}{\sqrt{2\pi}} \frac{1}{1-p_i} \exp \left(-\frac{1}{2} \frac{\left(Y_i^* - g(x_i) - w_i(pI)h(x_i) \right)^2}{\frac{\sigma^2}{(1-p_i)^2}} \right) \\
& \quad \left. \right] \left[\frac{b^a}{\Gamma(a)} (\sigma^{-2})^{-a-1} \exp \left(\frac{-b}{\sigma^2} \right) \right] \\
& = \prod_{i=1}^n \left[\mathbb{1}_{(w_i=1)} p_i \frac{1}{\sqrt{2\pi}} \frac{1}{p_i} \exp \left(-\frac{1}{2} \frac{\left(Y_i^* - g(x_i) - w_i(pI)h(x_i) \right)^2}{\frac{\sigma^2}{p_i^2}} \right) \right. \\
& \quad + \\
& \quad \mathbb{1}_{(w_i=0)} (1-p_i) \frac{1}{\sqrt{2\pi}} \frac{1}{1-p_i} \exp \left(-\frac{1}{2} \frac{\left(Y_i^* - g(x_i) - w_i(pI)h(x_i) \right)^2}{\frac{\sigma^2}{(1-p_i)^2}} \right) \\
& \quad \left. \right] \left[\frac{b^a}{\Gamma(a)} (\sigma^{-2})^{-a-1} \exp \left(\frac{-b}{\sigma^2} \right) \right] \\
& = \left(\frac{1}{\sqrt{2\pi}} \right)^n \left[\prod_{i=1}^n (\mathbb{1}_{(w_i=1)} p_i^2 + \mathbb{1}_{(w_i=0)} (1-p_i)^2) \right] \\
& \quad \left[(\sigma^2)^{-\frac{n}{2}-1} \exp \left(-\frac{b + \frac{1}{2} \sum_{i=1}^n p_{a,w} \left(Y_i^* - g(x_i) - p_{b,w} h(x_i) \right)^2}{\sigma^2} \right) \right]
\end{aligned} \tag{B.50}$$

If we define

$$p_{a,w}^2 = \mathbb{1}_{(w_i=1)} p_i^2 + \mathbb{1}_{(w_i=0)} (1-p_i)^2$$

then σ^2 has posterior of the form

$$\sigma^2 \sim IG\left(\frac{n}{2} + a, b + \frac{1}{2} \sum_{i=1}^n p_{a,w}^2 \left(Y_i^* - g(x_i) - w_i(p_i)h(x_i)\right)^2\right) \quad (\text{B.51})$$

B.5 Metropolis-Hastings Step Derivations

B.5.1 Marginalizing the portion of the likelihood associated with

$$\eta_{j,b}^*$$

We begin with our factorized likelihood where it is easy to see the leaf nodes are independent

$$L(\eta_{j,b}^* | \sigma^2, T_{j \notin M}^*, T^{\notin*}, y) = \int_{-\infty}^{\infty} L(\eta_{j,b}^* | \mu_{j,b}^*, \sigma^2, T_{j \notin M}^*, T^{\notin*}, y) \pi(\mu_{j,b}^*) d\mu_{j,b}^* \quad (\text{B.52})$$

=

$$\begin{aligned} & \int_{-\infty}^{\infty} \prod_{i=1}^{n_{j,b}^*} \left(\mathbb{1}_{(w_i=1)} \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma_i} \exp\left(-\frac{1}{2} \frac{(\tilde{y}_i - \mu_{j,b}^*)^2}{\sigma_i^2}\right) + \right. \\ & \quad \left. \mathbb{1}_{(w_i=0)} \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma_i} \exp\left(-\frac{1}{2} \frac{(\tilde{y}_i - \mu_{j,b}^*)^2}{\sigma_i^2}\right) \right) \\ & \quad \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma_\mu} \exp\left(-\frac{1}{2} \frac{(\mu_{j,b}^* - \mu_0)^2}{\sigma_\mu^2}\right) d\mu_{j,b}^* \end{aligned} \quad (\text{B.53})$$

=

$$\begin{aligned} & \int_{-\infty}^{\infty} \prod_{i=1}^{n_{j,b}^*} \left(\frac{1}{\sqrt{2\pi}} \frac{1}{\sigma_i} \exp\left(-\frac{1}{2} \frac{(\tilde{y}_i - \mu_{j,b}^*)^2}{\sigma_i^2}\right) \right) \\ & \quad \frac{1}{\sqrt{2\pi}} \frac{1}{\sigma_\mu} \exp\left(-\frac{1}{2} \frac{(\mu_{j,b}^* - \mu_0)^2}{\sigma_\mu^2}\right) d\mu_{j,b}^* \end{aligned}$$

$$\begin{aligned}
&= \\
&\int_{-\infty}^{\infty} (2\pi)^{-n/2} \left(\prod_{i=1}^{n_{j,b}^*} \sigma_i^{-1} \right) \exp \left(\frac{-1}{2} \sum_{i=1}^{n_{j,b}^*} \frac{(\tilde{y}_i - \mu_{j,b}^*)^2}{\sigma_i^2} \right) \\
&\quad (2\pi)^{-1/2} \sigma_{\mu}^{-1} \exp \left(\frac{-1}{2} \frac{(\mu_{j,b}^* - \mu_0)^2}{\sigma_{\mu}^2} \right) d\mu_{j,b}^* \\
&= \\
&\int_{-\infty}^{\infty} (2\pi)^{-(n+1)/2} \sigma_{\mu}^{-1} \left(\prod_{i=1}^{n_{j,b}^*} \sigma_i^{-1} \right) \\
&\quad \exp \left(\frac{-1}{2} \left(\sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i^2}{\sigma_i^2} - 2\mu_{j,b}^* \sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i}{\sigma_i^2} + \sum_{i=1}^{n_{j,b}^*} \frac{\mu_{j,b}^{*2}}{\sigma_i^2} \right. \right. \\
&\quad \left. \left. + \frac{\mu_{j,b}^{*2} - 2\mu_{j,b}^* \mu_0 + \mu_0^2}{\sigma_{\mu}^2} \right) \right) d\mu_{j,b}^* \\
&= \\
&\int_{-\infty}^{\infty} (2\pi)^{-(n+1)/2} \sigma_{\mu}^{-1} \left(\prod_{i=1}^{n_{j,b}^*} \sigma_i^{-1} \right) \exp \left(\frac{-1}{2} \left[\sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i^2}{\sigma_i^2} + \frac{\mu_0^2}{\sigma_{\mu}^2} \right] \right) \\
&\quad \exp \left(\frac{-1}{2} \left[\left(\sigma_{\mu}^{-2} + \sum_{i=1}^{n_{j,b}^*} \sigma_i^{-2} \right) \mu_{j,b}^{*2} - 2 \left(\sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i}{\sigma_i^2} + \frac{\mu_0}{\sigma_{\mu}^2} \right) \mu_{j,b}^* \right] \right) d\mu_{j,b}^* \\
&\hspace{15em} (\text{B.54})
\end{aligned}$$

=

$$\begin{aligned}
& \int_{-\infty}^{\infty} (2\pi)^{-(n+1)/2} \sigma_{\mu}^{-1} \left(\prod_{i=1}^{n_{j,b}^*} \sigma_i^{-1} \right) \exp \left(\frac{-1}{2} \left[\sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i^2}{\sigma_i^2} + \frac{\mu_0^2}{\sigma_{\mu}^2} \right] \right) \\
& \exp \left(\frac{-1}{2} \left[\left(\sigma_{\mu}^{-2} + \sum_{i=1}^{n_{j,b}^*} \sigma_i^{-2} \right) \right. \right. \\
& \quad \left(\mu_{j,b}^{*2} - 2 \left(\sigma_{\mu}^{-2} + \sum_{i=1}^{n_{j,b}^*} \sigma_i^{-2} \right)^{-1} \left(\sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i}{\sigma_i^2} + \frac{\mu_0}{\sigma_{\mu}^2} \right) \mu_{j,b}^* \right. \\
& \quad \left. \left. + \left(\sigma_{\mu}^{-2} + \sum_{i=1}^{n_{j,b}^*} \sigma_i^{-2} \right)^{-2} \left(\sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i}{\sigma_i^2} + \frac{\mu_0}{\sigma_{\mu}^2} \right)^2 \right. \right. \\
& \quad \left. \left. - \left(\sigma_{\mu}^{-2} + \sum_{i=1}^{n_{j,b}^*} \sigma_i^{-2} \right)^{-2} \left(\sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i}{\sigma_i^2} + \frac{\mu_0}{\sigma_{\mu}^2} \right)^2 \right] \right) d\mu_{j,b}^*
\end{aligned}$$

=

$$\begin{aligned}
& \int_{-\infty}^{\infty} (2\pi)^{-(n+1)/2} \sigma_{\mu}^{-1} \left(\prod_{i=1}^{n_{j,b}^*} \sigma_i^{-1} \right) \exp \left(\frac{-1}{2} \left[\sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i^2}{\sigma_i^2} + \frac{\mu_0^2}{\sigma_{\mu}^2} \right] \right) \\
& \exp \left(\frac{1}{2} \left(\sigma_{\mu}^{-2} + \sum_{i=1}^{n_{j,b}^*} \sigma_i^{-2} \right) \left(\sigma_{\mu}^{-2} + \sum_{i=1}^{n_{j,b}^*} \sigma_i^{-2} \right)^{-2} \left(\sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i}{\sigma_i^2} + \frac{\mu_0}{\sigma_{\mu}^2} \right)^2 \right) \\
& \exp \left(\frac{-1}{2} \left[\left(\sigma_{\mu}^{-2} + \sum_{i=1}^{n_{j,b}^*} \sigma_i^{-2} \right) \right. \right. \\
& \quad \left(\mu_{j,b}^{*2} - 2 \left(\sigma_{\mu}^{-2} + \sum_{i=1}^{n_{j,b}^*} \sigma_i^{-2} \right)^{-1} \left(\sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i}{\sigma_i^2} + \frac{\mu_0}{\sigma_{\mu}^2} \right) \mu_{j,b}^* + \right. \\
& \quad \left. \left. \left(\sigma_{\mu}^{-2} + \sum_{i=1}^{n_{j,b}^*} \sigma_i^{-2} \right)^{-2} \left(\sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i}{\sigma_i^2} + \frac{\mu_0}{\sigma_{\mu}^2} \right)^2 \right] \right) d\mu_{j,b}^*
\end{aligned}$$

(B.55)

=

$$\begin{aligned}
& (2\pi)^{-(n+1)/2} \sigma_\mu^{-1} \left(\prod_{i=1}^{n_{j,b}^*} \sigma_i^{-1} \right) \exp \left(\frac{-1}{2} \left[\sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i^2}{\sigma_i^2} + \frac{\mu_0^2}{\sigma_\mu^2} \right] \right) \\
& \exp \left(\frac{1}{2} \left(\sigma_\mu^{-2} + \sum_{i=1}^{n_{j,b}^*} \sigma_i^{-2} \right)^{-1} \left(\sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i}{\sigma_i^2} + \frac{\mu_0}{\sigma_\mu^2} \right)^2 \right) \\
& \int_{-\infty}^{\infty} \exp \left(\frac{-1}{2} \left[\left(\sigma_\mu^{-2} + \sum_{i=1}^{n_{j,b}^*} \sigma_i^{-2} \right) \right. \right. \\
& \quad \left. \left(\mu_{j,b}^{*2} - 2 \left(\sigma_\mu^{-2} + \sum_{i=1}^{n_{j,b}^*} \sigma_i^{-2} \right)^{-1} \left(\sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i}{\sigma_i^2} + \frac{\mu_0}{\sigma_\mu^2} \right) \mu_{j,b}^* + \right. \right. \\
& \quad \left. \left. \left. \left(\sigma_\mu^{-2} + \sum_{i=1}^{n_{j,b}^*} \sigma_i^{-2} \right)^{-2} \left(\sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i}{\sigma_i^2} + \frac{\mu_0}{\sigma_\mu^2} \right)^2 \right] \right] \right) d\mu_{j,b}^*
\end{aligned} \tag{B.56}$$

=

$$\begin{aligned}
& (2\pi)^{-(n+1)/2} \sigma_\mu^{-1} \left(\prod_{i=1}^{n_{j,b}^*} \sigma_i^{-1} \right) \exp \left(\frac{-1}{2} \left[\sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i^2}{\sigma_i^2} + \frac{\mu_0^2}{\sigma_\mu^2} \right] \right) \\
& \exp \left(\frac{1}{2} \left(\sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i}{\sigma_i^2} + \frac{\mu_0}{\sigma_\mu^2} \right)^2 \right) \\
& (2\pi)^{1/2} \left(\sigma_\mu^{-2} + \sum_{i=1}^{n_{j,b}^*} \sigma_i^{-2} \right)^{-1/2}
\end{aligned}$$

$$\begin{aligned}
&= \\
&\left(\sigma_\mu^{-2} + \sum_{i=1}^{n_{j,b}^*} \sigma_i^{-2} \right)^{-1/2} (2\pi)^{-n_{j,b}^*/2} \sigma_\mu^{-1} \prod_{i=1}^{n_{j,b}^*} \sigma_i^{-1} \\
&\exp \left(-\frac{1}{2} \left[\sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i^2}{\sigma_i^2} + \frac{\mu_0^2}{\sigma_\mu^2} \right] \right. \\
&\quad \left. + \frac{1}{2} \left(\sigma_\mu^{-2} + \sum_{i=1}^{n_{j,b}^*} \sigma_i^{-2} \right)^{-1} \left(\sum_{i=1}^{n_{j,b}^*} \frac{\tilde{y}_i}{\sigma_i^2} + \frac{\mu_0}{\sigma_\mu^2} \right)^2 \right)
\end{aligned}$$

Leaving us with the marginalized portion of the likelihood associated with $\eta_{j,b}^*$

B.5.2 Marginalized leaf node parameters for $g(x)$

Let

$$\tilde{y}_i = Y_{j,i} = \left(Y_i^* - \sum_{m \neq j}^M \mathcal{T}_m^g(X) - (w_i(1-p_i)h(x_i) - (1-w_i)p_i h(x_i)) \right) \quad (\text{B.57})$$

and

$$\sigma_i^2 = w_i \frac{\sigma^2}{p_i^2} + (1-w_i) \frac{\sigma^2}{(1-p_i)^2} \quad (\text{B.58})$$

then we can simply use the derivation in B.5.1 to get the marginalized likelihood associated with the leaf node parameters for $g(x)$

B.5.3 Marginalized leaf node parameters for $h(x)$

Let

$$\begin{aligned}
\tilde{y}_i = Y_{j,i}^h &= w_i \left(\frac{Y_i^* - g(x_i)}{1-p_i} - \sum_{m \neq j}^{M_h} \mathcal{T}_m^h(x_i) \right) \\
&\quad + (1-w_i) \left(\frac{g(x_i) - Y_i^*}{p_i} - \sum_{m \neq j}^{M_h} \mathcal{T}_m^h(x_i) \right)
\end{aligned} \quad (\text{B.59})$$

and

$$\sigma_i^2 = \sigma_{h,i}^2 = \frac{\sigma^2}{p_i^2(1-p_i)^2} \quad (\text{B.60})$$

then we can simply use the derivation in B.5.1 to get the marginalized likelihood associated with the leaf node parameters for $h(x)$

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