Bayesian Additive Regression Trees for functional ANOVA model

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Abstract

Bayesian Additive Regression Trees (BART) is a powerful statistical model that leverages the strengths of Bayesian inference and regression trees. It has received significant attention for capturing complex non-linear relationships and interactions among predictors. However, the accuracy of BART often comes at the cost of interpretability. To address this limitation, we propose ANOVA Bayesian Additive Regression Trees (ANOVA-BART), a novel extension of BART based on the functional ANOVA decomposition, which is used to decompose the variability of a function into different interactions, each representing the contribution of a different set of covariates or factors. Our proposed ANOVA-BART enhances interpretability, preserves and extends the theoretical guarantees of BART, and achieves superior predictive performance. Specifically, we establish that the posterior concentration rate of ANOVA-BART is nearly minimax optimal, and further provides the same convergence rates for each interaction that are not available for BART. Moreover, comprehensive experiments confirm that ANOVA-BART surpasses BART in both accuracy and uncertainty quantification, while also demonstrating its effectiveness in component selection. These results suggest that ANOVA-BART offers a compelling alternative to BART by balancing predictive accuracy, interpretability, and theoretical consistency.

Keywords: Bayesian Additive Regression Trees, Functional ANOVA model.

1 Introduction

Bayesian trees and their ensembles have demonstrated significant success in statistics and machine learning ([3, 6, 4, 18, 29, 35, 36]). In particular, Bayesian Additive Regression Trees (BART, [4]), which put the prior mass on the space of ensembles of decision trees and obtain the posterior distribution, have received much attention for their superior prediction performance in various problems including causal inference ([19, 16]), variable selection ([32]), survival analysis ([49]), interaction detection ([7]), smooth function estimation ([33]),

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mean-variance function estimation ([42]), time series ([50]), monotone function estimation ([5]), to name just a few. The theoretical properties of BART ([46, 47, 26, 33]) has been actively explored.

A limitation of BART, however, is that it is a black-box approach in the sense that the relation between inputs and output is hard to be explained. This is because a linear combination of decision trees is not easily interpretable. Recently, interpretability is an important issue in statistics, machine learning and Artificial Intelligence (AI), and constructing interpretable models without hampering prediction performance becomes a critical mission.

Various methods to improve interpretability can be roughly categorized into two approaches - (1) post-processing approach and (2) interpretable model approach. The post-processing approach tries to interpret given black-box models. Representative examples are partial dependency plots ([9]), LIME ([45]) and SHAP ([34]). In contrast, interpretable model approach uses easily interpretable prediction models such as the linear model, generalized additive model ([17]) and more generally functional ANOVA model ([20]). In particular, the functional ANOVA model has a long history in statistics and received much attention recently in machine learning and AI ([20, 31, 22, 28, 24, 23, 8, 14, 21, 30, 25, 37, 40]).

The aim of this paper is to develop a Bayesian additive regression trees for the functional ANOVA model, which we call ANOVA-BART. The core idea of ANOVA-BART, which is an interpretable model approach, is to approximate each interaction of the given functional ANOVA model by a linear combination of decision trees. For interpretable modeling with the functional ANOVA model, identifiability must be ensured because explanations are derived from each interaction. Since ordinary decision trees do not satisfy the identifiability condition, we devise special decision trees to ensure the identifiability of each interaction,

and propose a prior which is computationally feasible and guarantees an (nearly) minimax optimal posterior concentration rate.

Approximations with ANOVA-BART and BART look similar in the sense that they approximate the true regression function by a linear combination of decision trees. However, the mechanisms of approximation of the two methods are quite different. For BART, the sizes of individual decision trees grow as the sample size increases while the number of trees used in the linear combination is fixed. On the other hand, in ANOVA-BART, the sizes of individual decision trees are fixed that are proportional to the interaction orders while the number of trees grows as the sample size increases. That is, BART approximates the true regression function by a linear combination of few large decision trees while ANOVA-BART does by a linear combination of large numbers of small trees. This qualitative difference makes the MCMC algorithm and technique to derive the posterior concentration rate of ANOVA-BART be much different from those of BART.

This paper is organized as follows. Section 2 reviews the functional ANOVA model and BART. The ANOVA-BART model is described in Section 3, and an MCMC algorithm for the posterior sampling of ANOVA-BART is developed in Section 4. Section 5 provides the posterior concentration rate of ANOVA-BART which is nearly minimax optimal. Section 6 demonstrates that ANOVA-BART outperforms other baseline models by analyzing simulation data as well as multiple benchmark datasets.

2 Preliminaries

We consider a standard nonparametric regression model given as

$$Y = f(\mathbf{x}) + \epsilon,$$

where $\mathbf{x} = (x_1, ..., x_p)^{\top} \in \mathcal{X} \subset \mathbb{R}^p$ and $Y \in \mathbb{R}$ are covariate vector and response variable, respectively, $f : \mathcal{X} \to \mathbb{R}$ is a regression function and $\epsilon \sim N(0, \sigma^2)$ is a noise. In this section, we review the functional ANOVA model and BART since our proposed method combines these two ideas.

2.1 Notation

For a real-valued function $f: \mathcal{X} \to \mathbb{R}$ and $1 \leq p < \infty$, we denote $||f||_{p,n} := (\sum_{i=1}^n f(\mathbf{x}_i)^p/n)^{1/p}$, where $\mathbf{x}_i = (x_{i,1}, ..., x_{i,p})^\top$, i = 1, ..., n, are given covariate vectors. We write $||f||_{p,\mu} := (\int_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x})^p \mu(d\mathbf{x}))^{1/p}$, where μ is a probability measure defined on \mathcal{X} . We define $[p] = \{1, ..., p\}$ to represent the set of integers from 1 to p. For two sequences a_n and b_n , we write $a_n = O(b_n)$ if there exist constants c > 0 and $n_0 \in \mathbb{N}$ such that $|a_n| \leq c|b_n|$ for all $n \geq n_0$. For $A = \{a_1, ..., a_m\}$ with natural numbers $a_1 < ... < a_m$, we write $(x_j, j \in A) := (x_{a_1}, ..., x_{a_m})^\top$.

2.2 Functional ANOVA model

We assume that $\mathcal{X} = \prod_{j=1}^p \mathcal{X}_j$, where \mathcal{X}_j is a subset of \mathbb{R} . For $\mathbf{x} \in \mathcal{X}$ and $S \subseteq [p]$, we write $\mathbf{x}_S := (x_j, j \in S)$ and $\mathcal{X}_S := \prod_{j \in S} \mathcal{X}_j$. For a given function f_S defined on \mathcal{X}_S and a probability measure μ on \mathcal{X} , we say that f_S satisfies the μ -identifiability condition ([21, 22]) if the following holds:

$$\forall j \in S \text{ and } \forall \mathbf{x}_{S \setminus \{j\}} \in \mathcal{X}_{S \setminus \{j\}}, \ \int_{\mathcal{X}_j} f_S(\mathbf{x}_S) \mu_j(dx_j) = 0,$$
 (1)

where μ_j is the marginal probability measure of μ on \mathcal{X}_j .

By the following theorem, any real-valued multivariate function f can be uniquely decomposed into a functional ANOVA model whose components satisfy the μ -identifiability condition. Let $\mu^{\text{ind}} = \prod_{j=1}^{p} \mu_j$.

Theorem 2.1 ([22, 39]). Any real-valued function f defined on \mathbb{R}^p can be uniquely decomposed as

$$f(\mathbf{x}) = \sum_{S \subseteq [p]} f_S(\mathbf{x}_S),\tag{2}$$

almost everywhere with respect to μ^{ind} , under the constraint that each interaction f_S satisfies the μ -identifiability condition.

Here, the low dimensional functions f_S s are called the |S|th-order interactions or components of f. Note that the functional ANOVA decomposition (2) of f depends on the choice of the measures μ used in the identifiability condition (1). In this paper, we use the empirical distribution μ_n of given covariate vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n$ for μ and we write simply 'the identifiability condition' whenever $\mu = \mu_n$. If μ is different from μ_n , we will explicitly specify it.

The functional ANOVA model with only the main effects is the generalized additive model (GAM, [17]) which is widely used in practice. For machine learning applications, [21, 30, 40] emphasize the usefulness of the functional ANOVA model as an interpretable AI tool. There are various algorithms to estimate the interactions in the functional ANOVA model including MARS ([8]), SSANOVA ([14]), COSSO ([31]), NAM ([1]), ANOVA-TPNN ([40]) and so on.

2.3 Bayesian Additive Regression Trees (BART)

BART ([4]) models the regression function f by the sum of random decision trees. That is, BART assumes a priori that $f(\cdot) = \beta_0 + \sum_{t=1}^T \mathbb{T}_t(\cdot)$, where \mathbb{T}_t s are random decision trees and obtains the posterior distribution of \mathbb{T}_t s. Each decision tree is represented by the three parameters at each node - (i) the binary indicator whether a node is internal or terminal, (ii) the pair of (split-variable, split-criterion) if the node is internal and (iii) the height (i.e the prediction value) if the node is terminal. BART puts a prior mass on these three parameters to generate independent random decision trees \mathbb{T}_t s while T is fixed in advance and not inferred. Then, BART samples from the posterior distribution $p(\mathbb{T}_1, \ldots, \mathbb{T}_T, \sigma^2 | \text{data})$ using the backfitting MCMC algorithm ([4]).

${f 3}$ ANOVA-BART : BART on the functional ANOVA model

In this section, we propose a version of BART for the functional ANOVA model which we call ANOVA-BART. The main idea of ANOVA-BART is to approximate each component of the functional ANOVA model (2) using a sum of decision trees that satisfy the identifiability condition. That is, we set

$$f_S(\mathbf{x}_S) = \sum_{t=1}^{T_S} \mathbb{T}_t^S(\mathbf{x}_S), \tag{3}$$

where \mathbb{T}_t^S s are specially designed decision trees defined on \mathcal{X}_S . Let \mathcal{T}^S be the class of decision trees where \mathbb{T}_t^S s belong. In the following subsections, we propose \mathcal{T}^S so that $f_S(\cdot)$ always satisfies the identifiability condition and devise a prior on \mathcal{T}^S for $S \subseteq [p]$ and the

other parameters including the numbers of decision trees T_S for each S as well as the variance σ^2 of noises. Note that ANOVA-BART treats the number of decision trees as random and also infers it while BART fixes it in advance, which makes ANOVA-BART differs theoretically as well as algorithmically from BART.

3.1 Choice of \mathcal{T}^S : Identifiable binary-product trees

A technical difficulty in choosing \mathcal{T}^S is that f_S should satisfy the identifiability condition (1). To ensure this restriction, we make each decision tree in \mathcal{T}^S satisfy the identifiability condition. Let $\mu_{n,S}$ be an empirical distribution of given $\mathbf{x}_{1,S},...,\mathbf{x}_{n,S}$, where $\mathbf{x}_{i,S} = (x_{i,j}, j \in S)$ for i = 1,...,n. When $S = \{\ell\}$, we write $\mu_{n,\ell}$ instead of $\mu_{n,\{\ell\}}$ for notational simplicity.

For the main effects (i.e. |S| = 1): We first consider decision trees for the main effect. For $\mathbb{T}^S \in \mathcal{T}^S$ with $S = \{\ell\}$, we consider a tree with one split by the covariate x_ℓ . That is, when x_ℓ is continuous covariate, any $\mathbb{T}^{\{\ell\}} \in \mathcal{T}^{\{\ell\}}$ is given as

$$\mathbb{T}^{\{\ell\}}(x_{\ell}) = \beta_{-1} \mathbb{I}(x_{\ell} \le s_{\ell}) + \beta_{1} \mathbb{I}(x_{\ell} > s_{\ell})$$

for $s_{\ell} \in \mathcal{A}_{\ell}$, where \mathcal{A}_{ℓ} is the set of all possible split values for x_{ℓ} which will be specified later on. To ensure the identifiability condition, we let β_{-1} and β_{1} satisfy

$$\beta_{-1}\mu_{n,\ell}\{x_{\ell} \le s_{\ell}\} + \beta_{1}\mu_{n,\ell}\{x_{\ell} > s_{\ell}\} = 0.$$

Note that only one of β_{-1} and β_1 is a free parameter and the other is determined automatically by the identifiability condition. Thus, the degree of freedom of (β_{-1}, β_1) is 1.

For categorical covariate x_{ℓ} , a decision tree with one split by the covariate x_{ℓ} is defined similarly by replacing $\mathbb{I}(x_{\ell} \leq s_{\ell})$ and $\mathbb{I}(x_{\ell} > s_{\ell})$ with $\mathbb{I}(x_{\ell} \in A)$ and $\mathbb{I}(x_{\ell} \in A^{c})$ for a subset A of supp (x_{ℓ}) , where supp (x_{ℓ}) is the support of x_{ℓ} . For notational convenience, we only consider continuous covariates in the followings, but all the arguments can be modified easily for categorical covariates.

For the second order interactions (i.e. |S| = 2): For the second order interaction, we consider the following form of a decision tree for $\mathbb{T}^{\{\ell,k\}} \in \mathcal{T}^{\{\ell,k\}}$:

$$\mathbb{T}^{\{\ell,k\}}(x_{\ell}, x_{k}) = \beta_{-1,-1} \mathbb{I}(x_{\ell} \leq s_{\ell}, x_{k} \leq s_{k}) + \beta_{-1,1} \mathbb{I}(x_{\ell} \leq s_{\ell}, x_{k} > s_{k})
+ \beta_{1,-1} \mathbb{I}(x_{\ell} > s_{\ell}, x_{k} \leq s_{k}) + \beta_{1,1} \mathbb{I}(x_{\ell} > s_{\ell}, x_{k} > s_{k}),$$
(4)

for $s_{\ell} \in \mathcal{A}_{\ell}$ and $s_k \in \mathcal{A}_k$. We consider this special decision tree structure to make it possible to choose β s that ensure the identifiability condition of $\mathbb{T}^{\{\ell,k\}}$. In fact, the identifiability condition holds when $\beta_{-1,-1}, \beta_{-1,1}, \beta_{1,-1}$ and $\beta_{1,1}$ satisfy the following conditions:

$$\mu_{n,\ell}\{X_{\ell} \leq s_{\ell}\}\beta_{-1,-1} + \mu_{n,\ell}\{X_{\ell} > s_{\ell}\}\beta_{1,-1} = 0,$$

$$\mu_{n,\ell}\{X_{\ell} \leq s_{\ell}\}\beta_{-1,1} + \mu_{n,\ell}\{X_{\ell} > s_{\ell}\}\beta_{1,1} = 0,$$

$$\mu_{n,k}\{X_{k} \leq s_{k}\}\beta_{-1,-1} + \mu_{n,k}\{X_{k} > s_{k}\}\beta_{-1,1} = 0,$$

$$\mu_{n,k}\{X_{k} \leq s_{k}\}\beta_{1,-1} + \mu_{n,k}\{X_{k} > s_{k}\}\beta_{1,1} = 0.$$

$$(5)$$

Similarly to the main effects, the degree of freedom of $(\beta_{-1,-1}, \beta_{-1,1}, \beta_{1,-1}, \beta_{1,1})$ is 1, that is, one of $\beta_{-1,-1}, \beta_{-1,1}, \beta_{1,-1}, \beta_{1,1}$ determines the other three. See Section A of Supplementary Material for details.

For higher order interactions (i.e. |S| > 2): The decision tree in (4) for |S| = 2 can be

rewritten as

$$\mathbb{T}^{\{\ell,k\}}(x_{\ell},x_{k}) = \sum_{(v_{\ell},v_{k})\in\{-1,1\}^{2}} \beta_{v_{\ell},v_{k}} \mathbb{I}^{(v_{\ell})}(x_{\ell} - s_{\ell} > 0) \mathbb{I}^{(v_{k})}(x_{k} - s_{k} > 0)$$

with $\mathbb{I}^{(1)}(\cdot) := \mathbb{I}(\cdot)$ and $\mathbb{I}^{(-1)}(\cdot) := 1 - \mathbb{I}(\cdot)$. We generalize (4) for $S = \{\ell_1, \dots, \ell_d\}$ with d > 2 by

$$\mathbb{T}^{S}(\mathbf{x}_{S}) = \sum_{\mathbf{v} \in \{-1,1\}^{d}} \beta_{\mathbf{v}} \prod_{j=1}^{d} \mathbb{I}^{(v_{\ell_{j}})} (x_{\ell_{j}} - s_{\ell_{j}} > 0), \tag{6}$$

where $\mathbf{v} := (v_j, j \in S)$. We call a decision tree having the form of (6) a binary-product tree, which has been considered by [43, 41]. Binary means that the binary split is used for each covariate and product means that the split rules are produced by the product of the split rules of each covariate. Figure 1 draws the examples of binary-product trees for |S| = 1, 2 and 3.

Similar with (5), the binary-product tree in (6) satisfies the identifiability conditions if and only if the coefficients $\beta_{\mathbf{v}}$ for $\mathbf{v} \in \{-1,1\}^d$ satisfy the following conditions: for any $k = 1, \ldots, d$, and any $v_j \in \{-1,1\}$ for $j \in S \setminus \{\ell_k\}$,

$$\sum_{v_{\ell_k} \in \{-1,1\}} \beta_{\mathbf{v}} \mu_{n,\ell_k}^{(v_{\ell_k})} \{ X_{\ell_k} - s_{\ell_k} > 0 \} = 0, \tag{7}$$

where $\mu_{n,\ell_k}^{(1)} := \mu_{n,\ell_k}$ and $\mu_{n,\ell_k}^{(-1)} := 1 - \mu_{n,\ell_k}$. That is, Condition (7) extends Condition (5) to the case of general S. We refer to such a tree as an *identifiable binary-product* tree.

The degree of freedom of $(\beta_{\mathbf{v}}, \mathbf{v} \in \{-1, 1\}^d)$ is always 1 for every $d \in [p]$ (See Section A of Supplementary Material), and hence the heights of any identifiable binary-product tree are uniquely defined by choosing one of the heights. In this paper, we set $\beta_{-1,\dots,-1}$

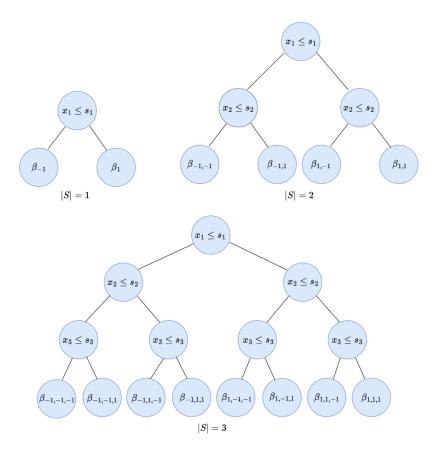


Figure 1: Binary-product trees for |S| being 1, 2, and 3, respectively. Nodes at the same depth share the same split rule, and an observation is assigned to the left child node whenever the rule is satisfied (otherwise, it goes to the right child)

as the free parameter. Then, any identifiable binary-product tree for the component S is parameterized by the vector of the split values $\mathbf{s} := (s_j, j \in S)$ corresponding to each covariate in S and the height $\beta_{-1,\dots,-1}$. Whenever needed, we write a given identifiable binary-product tree $\mathbb{T}^S(\mathbf{x}_S)$ as $\mathbb{T}(\mathbf{x}:S,\mathbf{s},\beta)$, where $\beta:=\beta_{-1,\dots,-1}$.

3.2 Prior distribution

ANOVA-BART assumes

$$f(\mathbf{x}) = \sum_{t=1}^{T} \mathbb{T}(\mathbf{x} : S_t, \mathbf{s}_t, \beta_t)$$
(8)

for $S_t \subseteq [p]$, $\mathbf{s}_t \in \prod_{i \in S_t} A_i$ and $\beta_t \in \mathbb{R}$.

The parameters that need to be inferred are $T, (S_1, \mathbf{s}_1, \beta_1), \dots, (S_T, \mathbf{s}_T, \beta_T)$ and σ^2 . First, we assume that prior of $(S_t, \mathbf{s}_t, \beta_t), t = 1, \dots, T$ are independent and identically distributed. In the following, we specify the prior distribution for $(S_t, \mathbf{s}_t, \beta_t), t = 1, \dots, T$ as well as T and σ^2 .

Prior for S. We let S follow the mixture distribution $\sum_{d=1}^{p} \omega_d$. Uniform {power([p], d)} for $\omega_d \geq 0$ and $\sum_{d=1}^{p} \omega_d = 1$, where power([p], d) is the collection of all subsets of [p] whose cardinality is d. The weights ω_d are defined recursively as in [4], as follows. For a given positive integer r, we let $p_{\text{split}}(d) = \alpha_{\text{split}}(1+d)^{-\gamma_{\text{split}}}$ for $\alpha_{\text{split}} \in (0,1)$ and $\gamma_{\text{split}} > 0$. Then, we set

$$\omega_d \propto (1 - p_{\text{split}}(d)) \prod_{l < d} p_{\text{split}}(l).$$
 (9)

Basically, ω_d is decreasing in d. The hyperparameters $\alpha_{\rm split}$ and $\gamma_{\rm split}$ control how fast ω_d decreases with d. That is, the probability $\Pr(|S| > d)$ increases as $\alpha_{\rm split}$ increases but decreases as $\gamma_{\rm split}$ increases.

Prior for s|S. Conditional on S, s_j , $j \in S$ are independent and uniformly distributed on \mathcal{A}_j , $j \in S$. In this paper, we set $\mathcal{A}_j = \{(x_{(i),j} + x_{(i-1),j})/2 : i = 2, ..., n\}$, where $x_{(i),j}$ s are the order statistics of given data $\{x_{i,j}, i = 1, ..., n\}$.

Prior for β . We use a diffuse Gaussian prior

$$\beta \sim N(0, \sigma_{\beta}^2)$$

for $\sigma_{\beta}^2 > 0$.

Prior for σ^2 . As usual, we set

$$\sigma^2 \sim IG\left(\frac{v}{2}, \frac{v\lambda}{2}\right)$$

for v > 0 and $\lambda > 0$, where IG(a, b) is the inverse gamma distribution with the shape parameter a and scale parameter b.

Prior for T. We use the following distribution for the prior of T:

$$\pi\{T = t\} \propto e^{-C_* t \log n}, \text{ for } t = 0, 1, \dots, T_{\text{max}},$$

where $C_* > 0$ and $T_{\text{max}} \in \mathbb{N}_+$ are hyperparameters.

4 Posterior Sampling

In this section, we develop an MCMC algorithm for posterior sampling of ANOVA-BART. We use a Gibbs sampling algorithm to generate the parameters $T, (S_1, \mathbf{s}_1, \beta_1), \ldots, (S_T, \mathbf{s}_T, \beta_T)$ and σ^2 from their conditional posterior distributions. For generating $(S_t, \mathbf{s}_t, \beta_t)$ others, we modify the Metropolis-Hastings (MH) algorithm of BART ([4]). We can generate σ^2 others easily since it is an inverse gamma distribution.

The hardest part is to generate T| others. In fact, others in T| others is even not well defined since $(S_1, \mathbf{s}_1, \beta_1), \ldots, (S_T, \mathbf{s}_T, \beta_T)$ depend on T. To resolve this problem and to make the convergence of the Gibbs sampler algorithm be faster, we rewrite f in (8) by introducing

the auxiliary binary randnom vector $\mathbf{z} = (z_1, \dots, z_{T_{\text{max}}})^{\top}$ as

$$f(\mathbf{x}) = \sum_{t=1}^{T_{\text{max}}} z_t \mathbb{T}(\mathbf{x} : S_t, \mathbf{s}_t, \beta_t).$$
 (10)

The prior distribution of $(z_1, \ldots, z_{T_{\text{max}}})|T$ is the uniform distribution on $\{0, 1\}^{T_{\text{max}}}$ subject to $\sum_{t=1}^{T_{\text{max}}} z_t = T$ (i.e. the hyper-geometric distribution). We develop a Gibbs sampling algorithm based on the model (10).

Let $\mathcal{D} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$ be given data which consist of n pairs of observed covariate vector and response variable. For the likelihood, we assume that y_i s are realizations of $Y_i = f(\mathbf{x}_i) + \epsilon_i$ conditional on f and σ^2 , where ϵ_i are independent Gaussian random noises with mean 0 and variance σ^2 .

4.1 Sampling $(S_t, \mathbf{s}_t, \beta_t)$ others

If $z_t = 0$, the conditional posterior distribution is equal to the prior distribution of $(S_t, \mathbf{s}_t, \beta_t)$. If $z_t = 1$, the conditional posterior distribution depends on solely through Resid_t, where

Resid_t =
$$\left\{ y_i - \sum_{k \neq t} z_k \mathbb{T}(\mathbf{x}_i : S_k, \mathbf{s}_k, \beta_k), i = 1, \dots, n \right\}$$

is the set of partial residuals derived from the current model that does not include the tth decision tree. Therefore, the sampling $(S_t, \mathbf{s}_t, \beta_t)$ from the conditional posterior distribution is equal to sampling from $(S_t, \mathbf{s}_t, \beta_t)|\text{Resid}_t, \sigma^2$. In turn, we decompose

$$\pi\{S_t, \mathbf{s}_t, \beta_t | \operatorname{Resid}_t, \sigma^2\} = \pi\{S_t, \mathbf{s}_t | \operatorname{Resid}_t, \sigma^2\} \pi\{\beta_t | \operatorname{Resid}_t, \sigma^2, S_t, \mathbf{s}_t\},$$

and we first generate (S_t, \mathbf{s}_t) and then generate β_t from the corresponding conditional posterior distributions.

For generating (S_t, \mathbf{s}_t) , we use a modification of the MH algorithm used in BART ([4]). We use a proposal distribution similar to one used in [27]. A key difference is that we consider only identifiable binary-product trees defined in Section 3.1. As a proposal distribution in the MH algorithm, we consider the following three possible alterations of (S_t, \mathbf{s}_t) :

- GROW: adding an element j^{new} selected randomly from S_t^c into S_t and choosing a split value for the newly selected element j^{new} by selecting it randomly from $\mathcal{A}_{j^{\text{new}}}$.
- PRUNE : deleting an element from S_t and the corresponding split value from \mathbf{s}_t .
- CHANGE: changing an element in S_t by one selected from S_t^c randomly and changing the split value accordingly.

The MH algorithm proposes $(S_t^{\text{new}}, \mathbf{s}_t^{\text{new}})$ using one of GROW, PRUNE, and CHANGE with probability 0.28, 0.28 and 0.44, respectively ([27]), and then accepts/rejects $(S_t^{\text{new}}, \mathbf{s}_t^{\text{new}})$ according to the acceptance probability given in Section B.1 of Supplementary Material.

Generating β_t from $\pi\{\beta_t|\text{Resid}_t, \sigma^2, S_t, \mathbf{s}_t\}$ can be done easily since the conditional posterior distribution is again Gaussian. The details of $\pi\{\beta_t|\text{Resid}_t, \sigma^2, S_t, \mathbf{s}_t\}$ are given in Section B.2 of Supplementary Material.

4.2 Sampling σ^2 others and z others

Generating σ^2 can be done easily since the conditional posterior distribution of σ^2 is an inverse Gamma distribution whose details are given in Section B.3 of Supplementary Material.

For generating \mathbf{z} others, we use a MH algorithm. For a proposal \mathbf{z}^{new} , we choose k randomly from $[T_{\text{max}}]$ and then let $z_k^{\text{new}} = 1 - z_k$ and $z_j^{\text{new}} = z_j$ for $j \neq k$. Then, we accept \mathbf{z}^{new} with the acceptance probability given in Section B.4 of Supplementary Material.

4.3 MCMC algorithm for ANOVA-BART

Algorithm 1 summarizes the proposed MCMC algorithm for ANOVA-BART. The MCMC algorithm is similar to that for BART([4]), but it has the additional sampling of \mathbf{z} . The sampling of \mathbf{z} is not needed for BART since the number of decision trees T is fixed.

Algorithm 1 MCMC algorithm for ANOVA-BART

Input: T_{max} : maximum number of decision trees, M: number of MCMC iteration

```
1: for i : 1 to M do
             for t : 1 to T_{max} do
  2:
                 if z_t = 1 then
  3:
                      (S_t, \mathbf{s}_t) \sim \mathrm{MH}_{S_t, \mathbf{s}_t}(\mathrm{Resid}_t, \sigma^2)
  4:
                      \beta_t \sim \pi\{\beta_t | \text{Resid}_t, \sigma^2, S_t, \mathbf{s}_t\}
  5:
  6:
                       (S_t, \mathbf{s}_t, \beta_t) \sim \pi\{S_t, \mathbf{s}_t, \beta_t\}
  7:
                 end if
  8:
             end for
  9:
            \mathbf{z} \sim \mathrm{MH}_{\mathbf{z}}(\mathcal{D}, \{(S_t, \mathbf{s}_t)\}_{t=1}^{T_{\mathrm{max}}}, \sigma^2)
10:
             \sigma^2 \sim \pi \{ \sigma^2 | \text{others} \}
11:
             return \{\mathbb{T}(\cdot: S_t, \mathbf{s}_t, \beta_t)\}_{t:z_t=1}, \sigma^2
12:
13: end for
```

Remark 4.1. In the algorithm, we do not need to generate $(S_t, \mathbf{s}_t, \beta_t)$ for $z_t = 0$ at every iteration. Instead, we generate $(S_t, \mathbf{s}_t, \beta_t)$ only when $z_t = 0$ but $z_t^{new} = 1$ to calculate $\pi\{\mathbf{z}^{new}|others\}$

5 Posterior concentration rate

In this section, we study theoretical properties of ANOVA-BART. In particular, we drive the posterior concentration rate of ANOVA-BART when the true model is smooth (i.e. Hölder smooth). Our posterior concentration rate is the same as the minimax optimal rate (up to a logarithm term) and adaptive to the smoothness of the true function. Moreover, we derive the posterior concentration rate of each interaction, which could be utilized to screen out unnecessary interactions out after posterior computation.

We consider the random-X design. That is, the input-output pairs $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)$ are assumed to be a realization of $(\mathbf{X}_1, Y_1), \dots, (\mathbf{X}_n, Y_n)$ that are independent copies of (\mathbf{X}, Y) whose distribution \mathbb{P}_0 is given as

$$\mathbf{X} \sim \mathbb{P}_{\mathbf{X}}$$
 and $Y|\mathbf{X} = \mathbf{x} \sim N(f_0(\mathbf{x}), \sigma_0^2)$.

Here, f_0 and σ_0^2 are the true regression function and the true variance, respectively. Let $\mathbf{X}^{(n)} = (\mathbf{X}_1, ..., \mathbf{X}_n)^{\top}$ and $Y^{(n)} = (Y_1, ..., Y_n)^{\top}$. The main reason of considering the random-X design rather than the fixed-X design is to apply the populational identifiability condition ($\mathbb{P}_{\mathbf{X}}$ -identifiability condition) to the functional ANOVA decomposition of f_0 . Discussions about the fixed-X design are given in Section G of Supplementary Material.

To derive the posterior concentration rate of ANOVA-BART, as usual, we will check the sufficient conditions given by [10]. The most technically difficult part is to study the approximation property of the sum of identifiable binary-product trees with bounded heights. Theorem C.1 in Section C.3 of Supplementary Material is the main approximation theorem for this purpose.

For technical reasons, we consider the truncated prior π_{ξ} for a large positive constant

 ξ defined as $\pi_{\xi}\{\cdot\} \propto \pi\{\cdot\}\mathbb{I}(\|f\|_{\infty} \leq \xi, 1/\xi \leq \sigma^2 \leq \xi)$, where $\pi\{\cdot\}$ is the prior introduced in Section 3.2. For posterior sampling with this prior, we generate samples of $(f(\cdot), \sigma^2)$ by the MCMC algorithm developed in Section 4 and only accept samples satisfying $\|f\|_{\infty} \leq \xi$ and $1/\xi \leq \sigma^2 \leq \xi$. We denote $\pi_{\xi}\{\cdot|\mathcal{D}\}$ the corresponding posterior.

5.1 Posterior Concentration Rate

For technical simplicity, we let $\mathcal{X}_j = [0, 1]$ for all $j \in [p]$. We consider the populationally identifiable ANOVA decomposition:

$$f_0(\mathbf{x}) = \sum_{S \subset [p]} f_{0,S}(\mathbf{x}_S),$$

where $f_{0,S}, S \subseteq [q]$ satisfy the populational identifiability condition ($\mathbb{P}_{\mathbf{X}}$ -identifiability condition). We assume the following regularity conditions.

- (J.1) There exists a density $p_{\mathbf{X}}$ of $\mathbb{P}_{\mathbf{X}}$ with respect to the Lebesgue measure on \mathbb{R}^p such that $0 < \inf_{\mathbf{x} \in \mathcal{X}} p_{\mathbf{X}}(\mathbf{x}) \le \sup_{\mathbf{x} \in \mathcal{X}} p_{\mathbf{X}}(\mathbf{x}) < \infty$.
- (J.2) Each $f_{0,S}$ is a Hölder smooth function with smoothness $\alpha \in (0,1]$, i.e.,

$$||f_{0,S}||_{\mathcal{H}^{\alpha}} := \sup_{\mathbf{x}, \mathbf{x}' \in [0,1]^{|S|}} \frac{|f_{0,S}(\mathbf{x}) - f_{0,S}(\mathbf{x}')|}{||\mathbf{x} - \mathbf{x}'||_2^{\alpha}} < \infty.$$

Additionally, we assume that $||f_{0,S}||_{\infty} \leq F$ for some positive constant F. For these assumptions, we write $f_{0,S} \in \mathcal{H}_F^{\alpha}$. Furthermore, we write $f_0 \in \mathcal{H}_{0,F}^{\alpha}$ if $f_{0,S} \in \mathcal{H}_F^{\alpha}$ for all $S \subseteq [p]$.

- (J.3) There exist $0 < \sigma_{\min}^2 < \sigma_{\max}^2 < \infty$ such that $\sigma_0^2 \in (\sigma_{\min}^2, \sigma_{\max}^2)$.
- (J.4) $T_{\text{max}} = O(n)$.

Theorem 5.1 (Posterior concentration of ANOVA-BART). Assume that (J.1), (J.2), (J.3) and (J.4) hold. Then, for given $\xi > \max\{2^p F, 1/\sigma_{\min}^2, \sigma_{\max}^2\}$, we have

$$\pi_{\xi} \Big\{ (f, \sigma^2) : \|f_0 - f\|_{2,n} + |\sigma_0^2 - \sigma^2| > B_n \epsilon_n \Big| \mathbf{X}^{(n)}, Y^{(n)} \Big\} \to 0,$$

for any $B_n \to \infty$ in \mathbb{P}_0^n as $n \to \infty$, where $\epsilon_n = n^{-\frac{\alpha}{2\alpha+p}} (\log n)^{\frac{1}{2}}$.

Note that our prior is assigned to satisfy the μ_n -identifiability condition. However, the posterior concentrate to the true function, which satisfies the $\mathbb{P}_{\mathbf{X}}$ -identifiability condition. This discrepancy constitutes one of the technically delicate points of the proofs of Theorem 5.1 and Theorem 5.2 that follows.

5.2 Comparison with BART

Posterior concentration rates of BART are derived in [47, 46, 26]. Even though ANOVA-BART is a special form of BART, the way of approximation f_0 is much different from BART. In particular, the number of decision trees increases as the sample size increases in ANOVA-BART while the sizes of each decision tree increase in BART.

ANOVA-BART approximates f_0 using a sum of many simple decision trees, whereas BART approximates f_0 using a finite number of large decision trees. That is, we have to prove that the sum of fixed size small identifiable binary-product trees can approximate a smooth function well. For this purpose, we first approximate a given function by a large decision tree as is done by [47]. Then, we prove that this large decision tree can be represented by the sum of many small identifiable binary-product trees, which is technically quite involved. See Section F of Supplementary Material.

An important practical advantage of ANOVA-BART compared to BART is Theorem 5.2 below, which derives the posterior concentration of each interaction. An obvious appli-

cations of Theorem 5.2 is to screen out unnecessary interactions a posteriori.

Theorem 5.2 (Posterior concentration of each interaction). Let $p_{\mathbf{X}}^{\text{ind}}(\mathbf{x}) = \prod_{j=1}^{p} p_{X_j}(x_j)$, where p_{X_j} is the density of X_j . In addition to Assumptions (J.1)-(J.4), we further assume that

$$0 < \inf_{\mathbf{x} \in \mathcal{X}} \frac{p_{\mathbf{X}}(\mathbf{x})}{p_{\mathbf{X}}^{\text{ind}}(\mathbf{x})} \le \sup_{\mathbf{x} \in \mathcal{X}} \frac{p_{\mathbf{X}}(\mathbf{x})}{p_{\mathbf{X}}^{\text{ind}}(\mathbf{x})} < \infty.$$

Then, for $S \subseteq [p]$ and $\xi > \max\{2^p F, 1/\sigma_{\min}^2, \sigma_{\max}^2\}$, we have

$$\pi_{\xi} \Big\{ f : \|f_{0,S} - f_S\|_{2,n} > B_n \epsilon_n \Big| \mathbf{X}^{(n)}, Y^{(n)} \Big\} \to 0,$$

for any $B_n \to \infty$ in \mathbb{P}_0^n , as $n \to \infty$.

The result of Theorem 5.2 can be fruitfully utilized to screen out unnecessary components after obtaining the posterior distribution. That is, we can delete f_S from the regression function when $||f_S||_{2,n}$ is small a posteriori. To be more specific, we delete f_S if

$$\pi\{\|f_S\|_{2,n} > \epsilon_n \log n | \mathcal{D}\} < \delta$$

for a given positive real number $\delta \in (0, 1/2)$. Theorem 5.2 implies that this post-hoc component selection procedure is selection-consistent (i.e. deleting all unnecessary components).

6 Experiments

This section presents the results of numerical experiments of ANOVA-BART. In Section 6.1, we conduct an analysis of synthetic data, while we focuse on real data analysis in Section 6.2.

We consider BART ([4]), SSANOVA ([14]), MARS ([8]) and NAM ([1]) as the baseline

methods. We use 'BayesTree' R package ([2]), 'gss' R package ([13]), 'earth' R package ([38]) and the official code in https://github.com/AmrMKayid/nam for implementing BART, SSANOVA, MARS and NAM, respectively. For NAM, we extend the code to implement NAMs to include the second order interactions. The detailed descriptions of the selection of hyperparameters in ANOVA-BART and baseline methods are presented in Section H of Supplementary Material. Note that while SSANOVA, MARS and NAM require specifying the maximum order of the components to be estimated, ANOVA-BART does not require the predefined maximum order.

6.1 Synthetic data analysis

We evaluate the performance of ANOVA-BART in view of prediction and component selection by analyzing synthetic data. To do this, we generate data using the Friedman's test function ([8, 4, 33]) defined as

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

where $\epsilon \sim N(0, \sigma_{\epsilon}^2)$. The error variance σ_{ϵ}^2 is set to make the signal-to-noise ratio be 5. For training data, we generate $\mathbf{x}_i = (x_{i1}, ..., x_{ip})^{\top}$, i = 1, ..., 1000 from the uniform distribution on $(0, 1)^p$ and then generate the output using only the first 5 covairates. This means that all covariates except the first five are noise.

6.1.1 Prediction performance

For all methods, hyperparameters are selected via 5-fold cross-validation on the training data. Independently generated test data of size 10,000 are used to compute the Root Mean Square Error (RMSE) as a measure of predictive performance. For ANOVA-BART and

BART, we use the Bayes estimators.

Table 1 presents the averages and standard errors of the RMSEs divided by the RMSE of ANOVA-BART based on 5 repetitions of the simulation. The optimal results are highlighted in **bold**. The results amply support that ANOVA-BART is favorably compared to the baseline emthods in prediction performance.

Table 1: Averages and standard errors of normalized RMSE on the synthetic data.

	ANOVA-BART	BART	SSANOVA	MARS	NAM
p=10	1.000 (—)	1.094 (0.02)	1.096 (0.03)	1.065 (0.01)	1.096 (0.03)
p = 50	1.000 (—)	1.065 (0.01)	1.200 (0.02)	1.015 (0.03)	1.327 (0.03)
p=100	1.000 ()	$1.051 \ (0.01)$	$1.142 \ (0.02)$	0.944 (0.02)	1.193 (0.01)

6.1.2 Component selection

To examine how effectively ANOVA-BART selects the true signal components, we conduct a simulation. We use the l_2 norm of each estimated component (i.e., $||f_S||_{2,n}$) as the important score, i.e., if $||f_S||_{2,n}$ large, we consider f_S to be important. We select the top 10 components based on the normalized important scores, which are presented in Figure 2 for various values of p. The red bars correspond to the signal components, while the blue bars are noisy ones. The results strongly indicate that ANOVA-BART can detect signal components very well.

6.2 Real data analysis

Table 2: Summaries of real data sets

Real data	Size	Dimension of covariates
BOSTON	506	13
ABALONE	4,177	10
BBB	208	134
SERVO	167	12
MPG	392	7

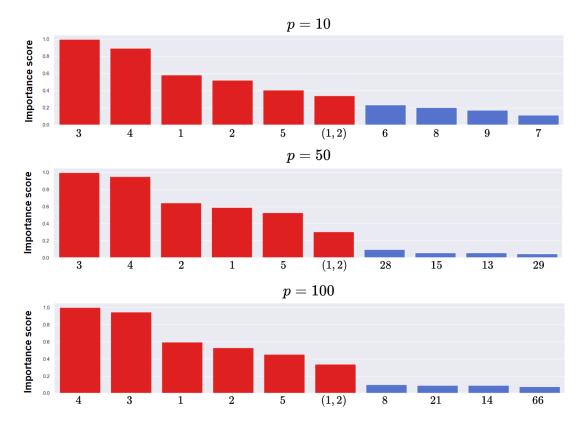


Figure 2: Importance scores of the estimated components by ANOVA-BART for p = 10, 50 and 100. The importance scores are normalized by dividing each score by the maximum importance score.

We analyze 5 real data sets including BOSTON, ABALONE, BBB, SERVO and MPG data sets. The four data sets except BBB are analyzed in [4] while BBB is examined in [33]. Table 2 summarizes the descriptions of the 5 datasets. We split each data into 80% training data and 20% test data, and repeat this random split 5 times to obtain 5 prediction measures.

6.2.1 Prediction performance

Table 3 presents the averages and standard errors of the RMSE values divided by the RMSE of ANOVA-BART for 5 datasets, where the best results are highlighted by **bold**. Similar to the synthetic data, ANOVA-BART is superior in prediction for real data.

Table 3: Averages and standard errors of normalized RMSE on real datasets.

Real data	ANOVA-BART	BART	SSANOVA	MARS	NAM
Boston	1.000 (—)	1.179 (0.11)	1.294 (0.10)	1.389 (0.09)	1.038 (0.05)
ABALONE	1.000 ()	1.022(0.03)	0.993 (0.03)	0.993(0.01)	0.917 (0.04)
BBB	1.000 (—)	1.053(0.01)	1.089(0.02)	1.396 (0.08)	1.112(0.03)
SERVO	1.000 ()	1.082(0.10)	2.595 (0.08)	1.393(0.14)	2.528 (0.08)
MPG	1.000 ()	$1.266 \ (0.15)$	1.447 (0.17)	$1.413 \ (0.18)$	$1.286 \ (0.14)$

6.2.2 Uncertainty quantification

An important advantage of Bayesian methods compared to frequentist's counterparts is superior performance of uncertainty quantification. We compare ANOVA-BART and BART in view of uncertainty quantification. As a measure of uncertainty quantification, we consider Continuous Ranked Probability Score (CRPS, [12]). For a given test sample (\mathbf{x}, y) , CRPS is defined as

$$CRPS(F_{\mathbf{x}}, y) := \int_{-\infty}^{\infty} (F_{\mathbf{x}}(z) - \mathbb{I}(y \le z))^2 dz,$$

where $F_{\mathbf{x}}$ is the predictive distribution of Y given $\mathbf{X} = \mathbf{x}$. Usually, we use the average of CRPS on test data. A smaller CRPS means better uncertainty quantification.

Table 4 presents the average and standard errors of 5 CRPS values normalized by the CRPS of ANOVA-BART obtained by 5 random splits of training and test data with the best results highlighted in **bold**. The results suggest that ANOVA-BART is better than BART in uncertainty quantification, too.

Table 4: Averages and standard errors of normalized CRPS on real datasets.

Real data	ANOVA-BART	BART
Boston	1.000 (—)	1.087 (0.04)
ABALONE	1.000 ()	0.859 (0.04)
BBB	1.000 (—)	1.025 (0.03)
SERVO	1.000 (—)	1.220(0.02)
MPG	1.000 (—)	$1.006 \ (0.04)$

7 Conclusion

ANOVA-BART can be considered as an interpretable modification of BART and shows superior performance to BART as well as other competitors on multiple benchmark datasets. Theoretically, ANOVA-BART achieves not only a (near) minimax posterior concentration rate and but also selection consistency.

There are several possible future works. First, we only consider regression problems but ANOVA-BART can be extended easily for classification problems by employing the logistic regression model. Second, theoretical results are obtained for a fixed dimension p of covariates. It would be interesting to modify ANOVA-BART for high-dimensional cases where p diverges also. Componentwise sparse priors would be needed for this purpose. Third, it would be useful to exploring a new MCMC algorithm for improving the scalability of ANOVA-BART.

Supplementary Material for

'Bayesian Additive Regression Trees for Functional ANOVA Model'

A Degree of freedom of the height vector of a binaryproduct tree

In this section, we explain how the height vector $\boldsymbol{\beta} = (\beta_{\mathbf{v}}, \mathbf{v} \in \{-1, 1\}^{|S|})$ of a binary-product tree is derived from the parameters (S, \mathbf{s}, β) and the μ -identifiability condition. Proposition A.1 reveals that the degrees of freedom of $\boldsymbol{\beta}$ is 1. We also establish the boundedness of the constant associated with the heights, under the identifiability condition, as shown in Proposition A.2.

Proposition A.1. For $S = \{\ell_1, ..., \ell_d\} \subseteq [p]$, $\mathbf{s} = (s_j, j \in S)$ and $\boldsymbol{\beta}$, consider a μ -identifiable binary-product tree

$$\mathbb{T}^{S}(\mathbf{x}_{S}) = \sum_{\mathbf{v} \in \{-1,1\}^{d}} \beta_{\mathbf{v}} \prod_{j=1}^{d} \mathbb{I}^{(v_{\ell_{j}})} (x_{\ell_{j}} - s_{\ell_{j}} > 0),$$

where $\mathbf{v} = (v_j, j \in S)$ and $d \leq p$. Then, the degree of freedom of $\boldsymbol{\beta}$ is 1. Furthermore, for any $\beta \in \mathbb{R}$, we have $\beta_{\mathbf{v}} = \beta \times \mathfrak{a}_{\mathbf{v}}$, where $\mathfrak{a}_{\mathbf{v}} = \prod_{j=1}^{d} \mathfrak{a}_{\ell_j}^{\mathbb{I}(v_{\ell_j}=1)}$ and $\mathfrak{a}_{\ell_j} = -\frac{\mu_{\ell_j}\{X_{\ell_j} - s_{\ell_j} \leq 0\}}{\mu_{\ell_j}\{X_{\ell_j} - s_{\ell_j} > 0\}}$.

Proof. Without loss of generality, we let $S = \{1, ..., d\}$. For \mathbb{T}^S , the μ -identifiability condition can be rewritten as (A.1).

$$\sum_{v_j \in \{-1,1\}^d} \beta_{v_1,\dots,v_d} \mu_j^{(v_j)} \{ X_j - s_j > 0 \} = 0$$
(A.1)

for all $(v_k, k \neq j) \in \{-1, 1\}^{d-1}$ and all $j = 1, \dots, d$.

Let $\mathcal{V}_+ = \{j \in [d] : v_j = 1\}$ for a given $\mathbf{v} \in \{-1, 1\}^d$, and for given $W \subseteq \{1, \dots, d\}$, let $\mathfrak{p}_W \in \{-1, 1\}^d$ be the vector whose *i*th element is 1 if $i \in W$ and -1 otherwise. For $\mathbf{v} = (-1, \dots, -1)$, let $\beta_{\mathbf{v}} = \beta \in \mathbb{R}$, and for $\mathbf{v} \neq (-1, \dots, -1)$, let $\beta_{\mathbf{v}} = \beta a_{\mathbf{v}}$, and we are going to calculate $\mathfrak{a}_{\mathbf{v}}$.

Case (1): $|\mathcal{V}_{+}| = 1$. Suppose that $v_{j} = 1$ for $j \in [d]$. The μ -identifiability condition requires that

$$\beta \mu_j \{ X_j - s_j \le 0 \} + \beta \mathfrak{a}_{\mathfrak{p}_j} \mu_j \{ X_j - s_j > 0 \} = 0, \tag{A.2}$$

where μ_j is the marginal probability measure defined in (1). Therefore, we have $\mathfrak{a}_{\mathfrak{p}_{\{j\}}} = -\frac{\mu_j\{X_j-s_j\leq 0\}}{\mu_j\{X_j-s_j>0\}}$ and denote it as \mathfrak{a}_j .

Case (2): $|\mathcal{V}_+| = 2$. Suppose that $v_j = v_k = 1$ for $j, k \in [d]$ with $j \neq k$. The μ -identifiability condition implies

$$\beta \mathfrak{a}_j \mu_k \{ X_k - s_k > 0 \} + \beta \mathfrak{a}_{\mathfrak{p}_{\{j,k\}}} \mu_k \{ X_k - s_k \le 0 \} = 0,$$

and thus we have

$$\mathfrak{a}_{\mathfrak{p}_{\{j,k\}}} = -\mathfrak{a}_j \frac{\mu_k \{X_k - s_k \le 0\}}{\mu_k \{X_k - s_k > 0\}} = \mathfrak{a}_j \mathfrak{a}_k.$$

Case (3): $|\mathcal{V}_+| > 2$. Repeating the above computation, we conclude $\mathfrak{a}_{\mathbf{v}} = \prod_{j=1}^d \mathfrak{a}_j^{\mathbb{I}(v_j=1)}$ for general \mathbf{v} .

Proposition A.2. If μ is the empirical distribution μ_n , it holds that $\max_{\mathbf{v}} |\mathfrak{a}_{\mathbf{v}}| \leq n^d$.

Proof. Since $1/n \le \mu_{n,j}^{(v_j)} \{X_j - s_j > 0\} \le 1$ for $v_j \in \{-1,1\}$, we have $|\mathfrak{a}_{\mathbf{v}}| \le n^d$ for any

 $s_j \in \mathcal{A}_j$, where \mathcal{A}_j is defined in Section 3.2.

B Posterior Sampling

In this section, we provide details of the conditional posteriors and the acceptance probabilities of the proposed MH algorithm within the MCMC algorithm in Section 4.

B.1 Acceptance probability for (S_t, \mathbf{s}_t) when $z_t = 1$

B.1.1 Transition probability

Note that the proposal distribution q of $(S_t^{\mathrm{new}}, \mathbf{s}_t^{\mathrm{new}})$ is given as

$$q(S_t^{\text{new}}, \mathbf{s}_t^{\text{new}} | S_t, \mathbf{s}_t, \text{GROW})$$

= $\Pr(\text{Selecting a new input variable } j^{\text{new}} \text{ from } S^c_t \text{ and the corresponding split value})$

$$= \frac{1}{|S_t^c|} \frac{1}{|\mathcal{A}_{j^{\text{new}}}|},$$

where j^{new} is the index of a newly selected input variable,

$$q(S_t^{\text{new}}, \mathbf{s}_t^{\text{new}} | S_t, \mathbf{s}_t, \text{CHANGE})$$

= Pr(Deleting one from S_t , and selecting j^{new} from S_t^c , and choosing one from $\mathcal{A}_{j^{\text{new}}}$)

$$= \frac{1}{|S_t|} \frac{1}{|S_t^c|} \frac{1}{|\mathcal{A}_{j^{\text{new}}}|},$$

and

$$q(S_t^{\text{new}}, \mathbf{s}_t^{\text{new}} | S_t, \mathbf{s}_t, \text{PRUNE})$$

= $\Pr(\text{Selecting an input variable in } S_t \text{ to be deleted})$

$$=\frac{1}{|S_t|}.$$

To sum up, we have

$$q(S_t^{\text{new}}, \mathbf{s}_t^{\text{new}}|S_t, \mathbf{s}_t) = \frac{1}{|S_t^c|} \frac{1}{|\mathcal{A}_{j^{\text{new}}}|} \Pr(\text{GROW}) \mathbb{I}(|S_t^{\text{new}}| = |S_t| + 1)$$

$$+ \frac{1}{|S_t|} \frac{1}{|S_t^c|} \frac{1}{|\mathcal{A}_{j^{\text{new}}}|} \Pr(\text{CHANGE}) \mathbb{I}(|S_t^{\text{new}}| = |S_t|)$$

$$+ \frac{1}{|S_t|} \Pr(\text{PRUNE}) \mathbb{I}(|S_t^{\text{new}}| = |S_t| - 1).$$

B.1.2 Posterior ratio

Let $r_{t,i} = y_i - \sum_{k \neq t} z_k \mathbb{T}(\mathbf{x}_i : S_k, \mathbf{s}_k, \beta_k)$ for i = 1, ..., n. Then, conditional on $S_t, \mathbf{s}_t, \beta_t$ and others, $r_{t,1}, \ldots, r_{t,n}$ are independent and

$$r_{t,i}|S_t, \mathbf{s}_t, \beta_t, \text{ others } \sim N(\mathfrak{a}_{\mathbf{v}_{t,i}}\beta_t, \sigma^2)$$

where $\mathbf{v}_{t,i} = (v_{t,i,j}, j \in S_t) \in \{-1,1\}^{|S_t|}$ such that $\prod_{j \in S_t} \mathbb{I}^{(v_{t,i,j})}(x_{i,j} - s_j > 0) = 1$. Since $\pi(\beta_t) = N(0, \sigma_{\beta}^2)$, a straightforward calculation after integrating out β_t yields that

$$\pi(S_t, \mathbf{s}_t | r_1, \dots, r_n, \text{ others}) \propto \frac{1}{\sqrt{A}} \exp\left(\frac{B^2}{2A}\right) \pi(S_t, \mathbf{s}_t),$$

where

$$A = \frac{1}{\sigma^2} \left(\sum_{i=1}^n \mathfrak{a}_{\mathbf{v}_{t,i}}^2 \right) + \frac{1}{\sigma_\beta^2}$$

and

$$B = \frac{1}{\sigma^2} \left(\sum_{i=1}^n \mathfrak{a}_{\mathbf{v}_{t,i}} r_{t,i} \right).$$

Thus, the ratio of the posterior of $(S_t^{\text{new}}, \mathbf{s}_t^{\text{new}})$ and that of (S_t, \mathbf{s}_t) is

$$\frac{\pi(S_t^{\text{new}}, \mathbf{s}_t^{\text{new}} | r_{t,1}, \dots, r_{t,n}, \text{ others})}{\pi(S_t, \mathbf{s}_t | r_{t,1}, \dots, r_{t,n}, \text{ others})} = \sqrt{\frac{A}{A^{\text{new}}}} \exp\left(\frac{(B^{\text{new}})^2}{2A^{\text{new}}} - \frac{B^2}{2A}\right) \frac{\pi(S_t^{\text{new}}, \mathbf{s}_t^{\text{new}})}{\pi(S_t, \mathbf{s}_t)}$$

where A^{new} and B^{new} are defined similarly to A and B. Moreover, the ratio of the priors is given as follows.

For GROW, we have

$$\frac{\pi(S_t^{\text{new}}, \mathbf{s}_t^{\text{new}})}{\pi(S_t, \mathbf{s}_t)} = \frac{\alpha_{\text{split}}(1 - \alpha_{\text{split}}(2 + d)^{-\gamma_{\text{split}}})}{((1 + d)^{\gamma_{\text{split}}} - \alpha_{\text{split}}) \times (p - d)\eta},$$

where $d = |S_t|$, and $\eta = |\mathcal{A}_{j^{\text{new}}}|$, where j^{new} is the index of a newly selected input variable.

For PRUNE, we have

$$\frac{\pi(S_t^{\text{new}}, \mathbf{s}_t^{\text{new}})}{\pi(S_t, \mathbf{s}_t)} = \frac{(d^{\gamma_{\text{split}}} - \alpha_{\text{split}}) \times (p - d + 1)\eta}{\alpha_{\text{split}} \times (1 - \alpha_{\text{split}}(1 + d)^{-\gamma_{\text{split}}})}$$

where $d = |S_t|$, and $\eta = |\mathcal{A}_{j^{\text{new}}}|$ where j^{new} is the index of a deleted input variable.

For CHANGE, we have

$$\frac{\pi(S_t^{\text{new}}, \mathbf{s}_t^{\text{new}})}{\pi(S_t, \mathbf{s}_t)} \times \frac{q(S_t, \mathbf{s}_t | S_t^{\text{new}}, \mathbf{s}_t^{\text{new}})}{q(S_t^{\text{new}}, \mathbf{s}_t^{\text{new}} | S_t, \mathbf{s}_t)} = 1.$$

Therefore, in the case of CHANGE, the prior ratio is not required.

B.1.3 Acceptance probability

In summary, we accept $(S_t^{\text{new}}, \mathbf{s}_t^{\text{new}})$ with probability p_{accept} , where

$$p_{\text{accept}} = \min \left\{ 1, \frac{\pi(S_t^{\text{new}}, \mathbf{s}_t^{\text{new}} | r_{t,1}, \dots, r_{t,n}, \text{ others})}{\pi(S_t, \mathbf{s}_t | r_{t,1}, \dots, r_{t,n}, \text{ others})} \frac{q(S_t, \mathbf{s}_t | S_t^{\text{new}}, \mathbf{s}_t^{\text{new}})}{q(S_t^{\text{new}}, \mathbf{s}_t^{\text{new}} | S_t, \mathbf{s}_t)} \right\}.$$

B.2 $\beta_t \sim \pi(\beta_t | S_t, \mathbf{s}_t, \text{ others})$ when $z_t = 1$

Note that the distribution of $r_{t,1}, \ldots, r_{t,n}$ conditional on $\beta_t, S_t, \mathbf{s}_t$, others are independent and

$$r_{t,i}|S_t, \mathbf{s}_t, \beta_t, \text{ others } \sim N(\mathfrak{a}_{\mathbf{v}_{t,i}}\beta_t, \sigma^2).$$

Since a priori $\beta_t \sim N(0, \sigma_{\beta}^2)$, which is conjugate, it is not difficult to show that

$$\beta_t | S_t, \mathbf{s}_t, \text{ others } \sim N\left(\frac{B}{A}, \frac{1}{A}\right),$$

where
$$A = \frac{1}{\sigma^2} \left(\sum_{i=1}^n \mathfrak{a}_{\mathbf{v}_{t,i}}^2 \right) + \frac{1}{\sigma_\beta^2}$$
 and $B = \frac{1}{\sigma^2} \left(\sum_{i=1}^n \mathfrak{a}_{\mathbf{v}_{t,i}} r_{t,i} \right)$.

B.3 Sampling σ^2 others

Let $r_i = y_i - \sum_{t=1}^{T_{\text{max}}} z_t \mathbb{T}(\mathbf{x}_i : S_t, \mathbf{s}_t, \beta_t)$ for i = 1, ..., n. Since $\sigma^2 \sim IG\left(\frac{v}{2}, \frac{v\lambda}{2}\right)$, it follows that

$$\sigma^2$$
 others $\sim IG\left(\frac{v+n}{2}, \frac{v\lambda + \sum_{i=1}^n r_i^2}{2}\right)$.

B.4 Sampling z others

First, we choose an index k randomly from $\{1, ..., T_{\text{max}}\}$, and then let $\mathbf{z}^{\text{new}} = (z_1^{\text{new}},, z_{T_{\text{max}}}^{\text{new}})$, where $z_k^{\text{new}} = 1 - z_k$ and $z_t^{\text{new}} = z_t$ for $t \neq k$. Since

$$y_i | \mathbf{z}^{\text{new}}, \text{ others} \sim N \left(\sum_{t=1}^{T_{\text{max}}} z_t^{\text{new}} \mathfrak{a}_{\mathbf{v}_{t,i}} \beta_t, \sigma^2 \right)$$

and

$$\pi\{\mathbf{z}^{\text{new}}\} = \pi \left\{ T = \sum_{t=1}^{T_{\text{max}}} z_t^{\text{new}} \right\} \operatorname{pr} \left\{ \text{Choose } \sum_{t=1}^{T_{\text{max}}} z_t^{\text{new}} \text{ elements from } T_{\text{max}} \text{ elements} \right\}$$

$$\propto \exp\left(-C_* \sum_{t=1}^{T_{\text{max}}} z_t^{\text{new}} \log n \right) / \binom{T_{\text{max}}}{\sum_{t=1}^{T_{\text{max}}} z_t^{\text{new}}},$$

we have

$$\pi\{\mathbf{z}^{\text{new}}|y_1,, y_n, \text{ others}\}$$

$$\propto \exp\bigg(-\frac{1}{2\sigma^2}\sum_{i=1}^n \bigg(y_i - \sum_{t=1}^{T_{\text{max}}} z_t^{\text{new}} \mathfrak{a}_{\mathbf{v}_{t,i}} \beta_t\bigg)^2 - C_* \sum_{t=1}^{T_{\text{max}}} z_t^{\text{new}} \log n\bigg) \bigg/ \bigg(\sum_{t=1}^{T_{\text{max}}} z_t^{\text{new}} \bigg).$$

Similarly, we can calculate $\pi\{\mathbf{z}|y_1,....,y_n,\text{others}\}$. Therefore, the posterior ratio is calculated as:

$$\begin{split} &\frac{\pi\{\mathbf{z}^{\text{new}}|y_1,....,y_n,\text{others}\}}{\pi\{\mathbf{z}|y_1,....,y_n,\text{others}\}} \\ &= \exp\bigg(-\frac{1}{2\sigma^2}\sum_{i=1}^n \bigg(\mathfrak{a}_{\mathbf{v}_{k,i}}\beta_k(z_k-z_k^{\text{new}})\bigg(2y_i-\sum_{t=1}^{T_{\text{max}}}z_t\mathfrak{a}_{\mathbf{v}_{t,i}}\beta_t-\sum_{t=1}^{T_{\text{max}}}z_t^{\text{new}}\mathfrak{a}_{\mathbf{v}_{t,i}}\beta_t\bigg)\bigg)\bigg) \times \frac{\left(\sum_{t=1}^{T_{\text{max}}}z_t\right)}{\left(\sum_{t=1}^{T_{\text{max}}}z_t^{\text{new}}\right)}. \end{split}$$

Finally, we accept \mathbf{z}^{new} with a acceptance probability $\tau_{\text{accept}},$ where

$$\tau_{\text{accept}} = \min \left(1, \frac{\pi \{ \mathbf{z}^{\text{new}} | y_1, ..., y_n, \text{others} \} q(\mathbf{z} | \mathbf{z}^{\text{new}})}{\pi \{ \mathbf{z} | y_1, ..., y_n, \text{others} \} q(\mathbf{z}^{\text{new}} | \mathbf{z})} \right).$$

C Proofs of Theorem 5.1

C.1 Additional notations

For two positive sequences $\{a_n\}$ and $\{b_n\}$, we use the notation $a_n \lesssim b_n$ to indicate that there exists a positive constant c > 0 such that $a_n \leq cb_n$ for all $n \in \mathbb{N}$. We use the little o notation, writing $a_n = o(b_n)$ to mean that $\lim_{n \to \infty} a_n/b_n = 0$. We denote $N(\varepsilon, \mathcal{F}, d)$ as the ε -covering number of \mathcal{F} with respect to a semimetric d. Let $\mathbb{P}^n_{\mathbf{X}} = \prod_{i=1}^n \mathbb{P}_{\mathbf{X}_i}$, where $\mathbb{P}_{\mathbf{X}_i}$ is the probability distribution of \mathbf{X}_i , for i = 1, ..., n. We denote $\|\cdot\|_1$ as a ℓ_1 norm for a vector, i.e., for a given vector $\mathbf{e} = (e_1, \ldots, e_n)$, $\|\mathbf{e}\|_1 := \sum_{i=1}^n |e_i|$. For a real-valued function $f: \mathcal{X} \to \mathbb{R}$, we denote $\|f\|_{\infty} := \sup_{\mathbf{x} \in \mathcal{X}} |f(\mathbf{x})|$.

C.2 Overall strategy

For a given identifiable binary-product tree with the parameters S, \mathbf{s}, β , we define the corresponding binary-product partition \mathcal{R} of \mathcal{X} as

$$\mathcal{R} := \left\{ \bigcap_{j \in S} \{ \mathbf{x} : x_j \le s_j \}^{(v_j)} : v_j \in \{-1, 1\}, j \in S \right\}.$$

Here, we let $A^{(1)} = A$ and $A^{(-1)} = A^c$ for a given set A. For a given binary-product partition \mathcal{R} , let $var(\mathcal{R})$ and $sval(\mathcal{R})$ be the set of split variables and the set of split values used in constructing \mathcal{R} , respectively. Since there is an one-to-one relation between (S, \mathbf{s}) and \mathcal{R} , we parameterize a given identifiable binary-product tree by \mathcal{R} , β instead of S, \mathbf{s} , β . We will use these two parameterizations interchangeably unless there is any confusion.

Let f be an ensemble of T many identifiable binary-product trees. Then, it can be parameterized by $T, \mathcal{E} = (\mathcal{R}_1, \dots, \mathcal{R}_T)$ and $\mathcal{B} = (\beta_1, \dots, \beta_T)$, where (\mathcal{R}_t, β_t) is the parameter of the tth identifiable binary-product tree used in f. Whenever we want to emphasize the

parameters of a given ensemble f, we write $f_{T,\mathcal{E},\mathcal{B}}$ or $f_{\mathcal{E},\mathcal{B}}$. We refer to $\mathcal{E} = (\mathcal{R}_1, \dots, \mathcal{R}_T)$ as an ensemble partition of length T. For a given T, let $\mathcal{E}(T)$ be the set of all possible ensemble partitions \mathcal{E} of length T. Finally, we let

$$\mathcal{F} := \left\{ f_{T,\mathcal{E},\mathcal{B}} : T \in [T_{\text{max}}], \mathcal{E} \in \mathcal{E}(T), \mathcal{B} \in \mathbb{R}^T \right\},\,$$

which is the support of the prior π (before truncation).

Note that our goal is to show that for any $\delta > 0$,

$$\lim_{n \to \infty} \mathbb{P}_0^n \left\{ \pi_{\xi} \{ \|f - f_0\|_{2,n} + |\sigma^2 - \sigma_0^2| > B_n \epsilon_n | \mathbf{X}^{(n)}, Y^{(n)} \} > \delta \right\} = 0.$$
 (C.1)

We prove (C.1) as follows. We first specify a subset A_n of \mathcal{X}^n such that $\mathbb{P}^n_{\mathbf{X}}\{A_n\} \to 1$ as $n \to \infty$, and for any $\mathbf{x}^{(n)} \in A_n$ we have

$$\mathbb{P}_{Y^{(n)}} \left\{ \left\{ \pi_{\xi} \{ \|f - f_0\|_{2,n} + |\sigma^2 - \sigma_0^2| > B_n \epsilon_n | \mathbf{X}^{(n)}, Y^{(n)} \} > \delta \right\} \middle| \mathbf{X}^{(n)} = \mathbf{x}^{(n)} \right\} \to 0 \quad (C.2)$$

as $n \to \infty$, where $\mathbb{P}_{Y^{(n)}}\{\cdot | \mathbf{X}^{(n)}\}$ is the conditional distribution of $Y^{(n)}$ given $\mathbf{X}^{(n)}$. Then, we complete the proof easily since for any $\delta > 0$,

$$\mathbb{P}_{0}^{n} \left\{ \left\{ \pi_{\xi} \{ \| f - f_{0} \|_{2,n} + |\sigma^{2} - \sigma_{0}^{2}| > B_{n} \epsilon_{n} | \mathbf{X}^{(n)}, Y^{(n)} \} > \delta \right\} \right\} \\
\leq \mathbb{P}_{0}^{n} \left\{ \left\{ \pi_{\xi} \{ \| f - f_{0} \|_{2,n} + |\sigma^{2} - \sigma_{0}^{2}| > B_{n} \epsilon_{n} | \mathbf{X}^{(n)}, Y^{(n)} \} > \delta \right\} \cap A_{n} \right\} + \mathbb{P}_{\mathbf{X}}^{n} (A_{n}^{c}) \\
\to 0$$

as $n \to \infty$.

Let $C_{\mathbb{B}}$ and d_{σ} be positive constants to be determined later (Section C.7 of Supplemen-

tary Material). To prove (C.2), we verify the following three conditions for $\mathbf{x}^{(n)} \in A_n$: there exists $\mathcal{F}^n \subset \mathcal{F}$ depending on $\mathbf{x}^{(n)}$ such that

$$\log N\left(\frac{\epsilon_n}{72}, \mathcal{F}^n, \|\cdot\|_{\infty}\right) \le n\epsilon_n^2 \tag{C.3}$$

$$\pi \left\{ f \in \mathcal{F} : \|f - f_0\|_{\infty} \le C_{\mathbb{B}} \epsilon_n \right\} \ge e^{-d_1 n \epsilon_n^2} \tag{C.4}$$

$$\pi\{\mathcal{F}\backslash\mathcal{F}^n\} \le e^{-(2d_1+d_\sigma+2)n\epsilon_n^2} \tag{C.5}$$

for some constant $d_1 > 0$. In turn, we show that these three conditions imply the posterior convergence rate in (C.2) by checking the conditions in Theorem 4 of [11].

C.3 Construction of A_n

For constructing A_n , we need the following theorem which shows that any populationally identifiable smooth function can be approximated by a sum of identifiable binary-product trees whose heights are bounded. This theorem is technically involved, and its proof is given in Section F of Supplementary Material.

Theorem C.1. For $\alpha \in (0,1]$, suppose g_S be a populationally identifiable S-component function in \mathcal{H}_F^{α} . Then, there exist positive constants m and C such that for any $T_S \in \mathbb{N}_+$, there exist T_S many binary-product partitions $\mathcal{R}_1, \ldots, \mathcal{R}_{T_S}$ with $var(\mathcal{R}_t) = S$ for all $t \in [T_S]$ and T_S many real numbers $\beta_1, \ldots, \beta_{T_S}$ depending on $\mathbf{x}^{(n)}$ such that $\sup_j |\beta_j| \leq C$ and

$$\left\| g_S(\cdot) - \sum_{t=1}^{T_S} \mathbb{T}(\cdot : \mathcal{R}_t, \beta_t) \right\|_{\infty} \le \|g_S\|_{\mathcal{H}^{\alpha}} \frac{m^{\alpha}}{(T_S^{\frac{1}{|S|}} + 1)^{\alpha}} + \Phi_{n,S}(\mathbf{x}^{(n)}, T_S), \tag{C.6}$$

where

$$\mathbb{P}_{\mathbf{X}}^{n} \left\{ \Phi_{n,S}(\mathbf{X}^{(n)}, T_{S}) \leq (24F + 1)2^{|S|} \sqrt{(T_{S}^{\frac{1}{|S|}} + 1)^{|S|}} \sqrt{\frac{\log n}{n}} \right\}$$

$$\geq 1 - 2^{|S| + 1} |S| (T_{S}^{\frac{1}{|S|}} + 1)^{|S|^{2}} \exp\left(-\frac{(T_{S}^{\frac{1}{|S|}} + 1)^{|S|} \log n}{4F^{2}}\right)$$

for all sufficiently large n.

Let $t_{n,S}$ be the smallest positive integer satisfying

$$||f_{0,S}||_{\mathcal{H}^{\alpha}} \frac{m^{\alpha}}{(t_{n,S}^{\frac{1}{|S|}} + 1)^{\alpha}} + (24F + 1)2^{|S|} \sqrt{(t_{n,S}^{\frac{1}{|S|}} + 1)^{|S|}} \sqrt{\frac{\log n}{n}} \le \frac{C_{\mathbb{B}} \epsilon_n}{2^{p+1}}.$$
 (C.7)

Note that $t_{n,S} \lesssim n\epsilon_n^2/\log n$. Now, we let

$$A_n := \left\{ \mathbf{x}^{(n)} : \Phi_{n,S}(\mathbf{x}^{(n)}, t_{n,S}) \le (24F + 1)2^{|S|} \sqrt{(t_{n,S}^{\frac{1}{|S|}} + 1)^{|S|}} \sqrt{\frac{\log n}{n}} \text{ for all } S \subseteq [p] \right\}.$$
 (C.8)

By Theorem C.1, $\mathbb{P}^n_{\mathbf{X}}(A_n) \to 1$ as $n \to \infty$.

C.4 Proof of Condition (C.3)

We consider the sieve

$$\mathcal{F}^n := \{ f_{T,\mathcal{E},\mathcal{B}} : T \in [M_n], \mathcal{E} \in \mathcal{E}(T), \mathcal{B} \in [-n,n]^T \}.$$

for some positive integer $M_n \leq T_{\text{max}}$, and will choose M_n so that \mathcal{F}^n satisfies Condition (C.3) with $\epsilon_n^2 = n^{-\frac{2\alpha}{2\alpha+p}} \log n$. For this purpose, we need the following lemma.

Lemma C.2. For given $T \in \mathbb{N}_+$ and $\mathcal{E} \in \mathcal{E}(T)$, let

$$\mathcal{F}^n(T,\mathcal{E}) := \{ f_{T,\mathcal{E},\mathcal{B}} : \mathcal{B} \in [-n,n]^T \}.$$

Then, we have $N(\epsilon, \mathcal{F}^n(T, \mathcal{E}), \|\cdot\|_{\infty}) \leq \left(1 + \frac{2n^{p+1}T}{\epsilon}\right)^T$

Proof. For the T-dimensional hypercube $[-n, n]^T$, We have

$$N(\epsilon_1, [-n, n]^T, \|\cdot\|_1) \le \left(1 + \frac{2nT}{\epsilon_1}\right)^T \tag{C.9}$$

for any $\epsilon > 0$. Let $\{\mathcal{B}^1, ..., \mathcal{B}^{N(\epsilon_1, [-n,n], \|\cdot\|_1)}\}$ be an ϵ_1 -cover of $[-n, n]^T$, and for given $\mathcal{B} \in [-n, n]^T$, let $\tilde{\mathcal{B}}$ be an element in the ϵ_1 -cover such that $\|\mathcal{B} - \tilde{\mathcal{B}}\|_1 \leq \epsilon_1$. Then, for any $f_{\mathcal{E}, \mathcal{B}} \in \mathcal{F}^n(T, \mathcal{E})$, we have

$$\sup_{\mathbf{x}} |f_{\mathcal{E},\mathcal{B}}(\mathbf{x}) - f_{\mathcal{E},\tilde{\mathcal{B}}}(\mathbf{x})| \leq \sup_{\mathbf{x}} \sum_{t=1}^{T} |\mathbb{T}(\mathbf{x} : \mathcal{R}_{t}, \beta_{t}) - \mathbb{T}(\mathbf{x} : \mathcal{R}_{t}, \tilde{\beta}_{t})|$$

$$\leq \sum_{t=1}^{T} \sup_{\mathbf{v} \in \{-1,1\}^{|S_{t}|}} |\beta_{t}, \mathbf{v} - \tilde{\beta}_{t}, \mathbf{v}|$$

$$= \sum_{t=1}^{T} \sup_{\mathbf{v} \in \{-1,1\}^{|S_{t}|}} |\mathfrak{a}_{t}, \mathbf{v}| |\beta_{t} - \tilde{\beta}_{t}|$$

$$\leq \sum_{t=1}^{T} n^{|S_{t}|} |\beta_{t} - \tilde{\beta}_{t}|$$

$$\leq n^{p} \epsilon_{1},$$

where we use the inequality that $\sup_{\mathbf{v}\in\{-1,1\}^{|S_t|}} |\mathfrak{a}_{t,\mathbf{v}}| \leq n^{|S_t|}$ obtained in Proposition A.2. By letting $\epsilon_1 = \epsilon/n^p$ in (C.9), we have

$$N(\epsilon, \mathcal{F}^n(T, \mathcal{E}), \|\cdot\|_{\infty}) \le \left(1 + \frac{2n^{p+1}T}{\epsilon}\right)^T,$$
 (C.10)

which completes the proof.

An upper bound of the covering number of \mathcal{F}^n is given as

$$N\left(\frac{\epsilon_{n}}{72}, \mathcal{F}^{n}, \|\cdot\|_{\infty}\right) \leq \sum_{T=1}^{M_{n}} \sum_{\mathcal{E} \in \mathcal{E}(T)} N\left(\frac{\epsilon_{n}}{72}, \mathcal{F}^{n}(T, \mathcal{E}), \|\cdot\|_{\infty}\right)$$

$$\leq \sum_{T=1}^{M_{n}} \left(1 + \frac{72n^{p+1}T}{\epsilon_{n}}\right)^{T} \sum_{\mathcal{E} \in \mathcal{E}(T)} 1$$

$$\lesssim \sum_{T=1}^{M_{n}} \left(1 + \frac{72n^{p+1}T}{\epsilon_{n}}\right)^{T} n^{Tp}$$

$$\leq M_{n} n^{M_{n}p} \left(1 + \frac{72n^{p+1}M_{n}}{\epsilon_{n}}\right)^{M_{n}},$$
(C.11)

where the inequality in (C.11) is due to

$$\sum_{\mathcal{E} \in \mathcal{E}(T)} 1 \lesssim n^{Tp}.$$

Therefore, we have the following upper bound of the log covering number:

$$\log N\left(\epsilon_n^2, \mathcal{F}^n, \|\cdot\|_{\infty}\right) \lesssim \log M_n + M_n p \log n + M_n \log\left(1 + \frac{72n^{p+1}M_n}{\epsilon_n}\right)$$

With $M_n = \lfloor C_1 \frac{n\epsilon_n^2}{\log n} \rfloor$ for some large enough constant $C_1 > 0$ (will be determined later), Condition (C.3) is satisfied.

C.5 Proof of Condition (C.4)

For given $\mathbf{x}^{(n)} \in A_n$, let \hat{f}_S be an ensemble of $t_{n,S}$ many identifiable binary-product trees satisfying $||f_{0,S} - \hat{f}_S||_{\infty} \le C_{\mathbb{B}} \epsilon_n/2^{p+1}$, whose existence is guaranteed by Theorem C.1, and

let $\hat{f} = \sum_{S \subseteq [p]} \hat{f}_S$. Let $\hat{\mathcal{E}}_S$ and $\hat{\mathcal{B}}_S$ be the ensemble partitions and height vector for \hat{f}_S and let $\hat{\mathcal{E}}$ and $\hat{\mathcal{B}}$ be the ensemble partition and height vector for \hat{f} . Let $t_n = \sum_{S \subseteq [p]} t_{n,S}$.

Note that for any $\mathcal{B} \in \mathbb{R}^{t_n}$,

$$||f_{t_n,\hat{\mathcal{E}},\mathcal{B}} - f_{t_n,\hat{\mathcal{E}},\hat{\mathcal{B}}}||_{\infty} \leq \sum_{t=1}^{t_n} ||\mathbb{T}(\cdot : \hat{\mathcal{R}}_t, \beta_t) - \mathbb{T}(\cdot : \hat{\mathcal{R}}_t, \hat{\beta}_t)||_{\infty}$$

$$\leq \sum_{t=1}^{t_n} n^p |\beta_t - \hat{\beta}_t|$$

$$\leq n^p \sqrt{t_n} ||\mathcal{B} - \hat{\mathcal{B}}||_2,$$

where the second inequality follows from Proposition A.2. Hence, if $\|\mathcal{B} - \hat{\mathcal{B}}\|_2 \leq (n^p \sqrt{t_n})^{-1} C_{\mathbb{B}} \epsilon_n / 2$, we have

$$||f_0 - f_{t_n,\hat{\mathcal{E}},\mathcal{B}}||_{\infty} \le ||f_0 - f_{t_n,\hat{\mathcal{E}},\hat{\mathcal{B}}}||_{\infty} + ||f_{t_n,\hat{\mathcal{E}},\mathcal{B}} - f_{t_n,\hat{\mathcal{E}},\hat{\mathcal{B}}}||_{\infty} \le C_{\mathbb{B}}\epsilon_n.$$

Thus, to prove Condition (C.4), it suffices to show that

$$\pi \left\{ T = t_n, \mathcal{E} = \hat{\mathcal{E}}, \|\mathcal{B} - \hat{\mathcal{B}}\|_2 \le (n^p \sqrt{t_n})^{-1} C_{\mathbb{B}} \epsilon_n / 2 \right\}$$
 (C.12)

is sufficiently large. We decompose (C.12) as

$$\pi \left\{ T = t_n, \mathcal{E} = \hat{\mathcal{E}}, \|\mathcal{B} - \hat{\mathcal{B}}\|_2 \le (n^p \sqrt{t_n})^{-1} C_{\mathbb{B}} \epsilon_n / 2 \right\}$$

$$= \pi \left\{ T = t_n \right\} \pi \left\{ \mathcal{E} = \hat{\mathcal{E}} | T = t_n \right\} \pi \left\{ \|\mathcal{B} - \hat{\mathcal{B}}\|_2 \le (n^p \sqrt{t_n})^{-1} C_{\mathbb{B}} \epsilon_n / 2 | \mathcal{E} = \hat{\mathcal{E}}, T = t_n \right\}.$$

We will show that these three prior probabilities on the right hand side of the above equality are sufficiently large.

C-(a). A lower bound of $\pi\{T=t_n\}$: Since $t_n \lesssim n\epsilon_n^2/\log n$, there exists a constant $d_2>0$

such that

$$\pi\{T = t_n\} = \frac{\exp(-C_* t_n \log n)}{\sum_{t=0}^{T_{\text{max}}} \exp(-C_* t_n \log n)}$$
$$\geq (1 - n^{-C_*}) \exp(-C_* t_n \log n)$$
$$\geq \exp(-d_2 n \epsilon_n^2)$$

for all sufficiently large n.

C-(b). A lower bound of $\pi\{\mathcal{E} = \hat{\mathcal{E}}|T=t_n\}$: Let $\mathcal{E} = (\mathcal{R}_t, t=1, \ldots, t_n)$ and $\hat{\mathcal{E}} = (\hat{\mathcal{R}}_t, t=1, \ldots, t_n)$. Note that conditional on $T=t_n$, $\mathcal{R}_t, t \in [t_n]$ are independent a priori and thus we have

$$\pi\{\mathcal{E} = \hat{\mathcal{E}}|T = t_n\} = \prod_{t=1}^{t_n} \pi\{\mathcal{R}_t = \hat{\mathcal{R}}_t\}.$$

In turn,

$$\pi\{\mathcal{R}_t = \hat{\mathcal{R}}_t\} = \pi \left\{ |\operatorname{var}(\mathcal{R}_t)| = |\operatorname{var}(\hat{\mathcal{R}}_t)| \right\}$$

$$\times \pi \left\{ \operatorname{var}(\mathcal{R}_t) = \operatorname{var}(\hat{\mathcal{R}}_t) \middle| |\operatorname{var}(\mathcal{R}_t)| = |\operatorname{var}(\hat{\mathcal{R}}_t)| \right\}$$

$$\times \pi \left\{ \operatorname{sval}(\mathcal{R}_t) = \operatorname{sval}(\hat{\mathcal{R}}_t) \middle| \operatorname{var}(\mathcal{R}_t) = \operatorname{var}(\hat{\mathcal{R}}_t) \right\},$$

where

$$\pi \left\{ |\operatorname{var}(\mathcal{R}_t)| = |\operatorname{var}(\hat{\mathcal{R}}_t)| \right\} = \frac{\omega_{|\operatorname{var}(\hat{\mathcal{R}}_t)|}}{\sum_{d=0}^p \omega_d} \ge \frac{\omega_p}{2},$$

$$\pi \left\{ \operatorname{var}(\mathcal{R}_t) = \operatorname{var}(\hat{\mathcal{R}}_t) \middle| |\operatorname{var}(\mathcal{R}_t)| = |\operatorname{var}(\hat{\mathcal{R}}_t)| \right\} = 1 \middle/ \binom{p}{|\operatorname{var}(\hat{\mathcal{R}}_t)|}$$

and

$$\pi \left\{ \operatorname{sval}(\mathcal{R}_t) = \operatorname{sval}(\hat{\mathcal{R}}_t) \middle| \operatorname{var}(\mathcal{R}_t) = \operatorname{var}(\hat{\mathcal{R}}_t) \right\} = \prod_{j \in \operatorname{var}(\hat{\mathcal{R}}_t)} \frac{1}{|\mathcal{A}_j|} \ge n^{-p}.$$

Thus we have

$$\pi \left\{ \mathcal{E} = \hat{\mathcal{E}} | T = t_n \right\} \ge \left(\frac{\omega_p}{2 \binom{p}{|\operatorname{var}(\hat{\mathcal{R}}_t)|}} n^{-p} \right)^{t_n} \ge \exp(-d_3 n \epsilon_n^2)$$

for a certain constant $d_3 > 0$.

C-(c). A lower bound of $\pi\{\|\mathcal{B} - \hat{\mathcal{B}}\|_2 \le (n^p \sqrt{t_n})^{-1} C_{\mathbb{B}} \epsilon_n / 2 | \mathcal{E} = \hat{\mathcal{E}}, T = t_n\}$:

$$\pi \left\{ \mathcal{B} \in \mathbb{R}^{t_n} : \|\hat{\mathcal{B}} - \mathcal{B}\|_2 \le \frac{C_{\mathbb{B}}}{n^p \sqrt{t_n}} \times \frac{\epsilon_n}{2} \right\}$$

$$\geq 2^{-t_n} \left(\frac{t_n}{2}\right)^{-\frac{t_n}{2} - 1} \exp\left(-\frac{\|\hat{\mathcal{B}}\|_2^2}{\sigma_{\beta}^2} - \frac{(C_{\mathbb{B}}\epsilon_n)^2}{8n^{2p}t_n\sigma_{\beta}^2}\right) \left(\frac{(C_{\mathbb{B}}\epsilon_n)^2}{4n^{2p}t_n\sigma_{\beta}^2}\right)^{\frac{t_n}{2}}$$

$$\geq 2^{-t_n} \left(\frac{t_n}{2}\right)^{-\frac{t_n}{2} - 1} \exp\left(-\frac{t_nC^2}{\sigma_{\beta}^2} - \frac{(C_{\mathbb{B}}\epsilon_n)^2}{8n^{2p}t_n\sigma_{\beta}^2}\right) \left(\frac{(C_{\mathbb{B}}\epsilon_n)^2}{4n^{2p}t_n\sigma_{\beta}^2}\right)^{\frac{t_n}{2}},$$
(C.13)

where (C.13) is derived from equation (8.9) in ([47]) and (C.14) is derived from Theorem C.1. Finally, the three terms in (C.14) are bounded below by

$$2^{-t_n} \left(\frac{t_n}{2}\right)^{-\frac{t_n}{2} - 1} = 2^{-t_n} \exp\left(-\left(1 + \frac{t_n}{2}\right) \log \frac{t_n}{2}\right) \ge \exp(-d_4 n \epsilon_n^2)$$

for some constant $d_4 > 0$,

$$\exp\left(-\frac{t_n C^2}{\sigma_{\beta}^2} - \frac{(C_{\mathbb{B}}\epsilon_n)^2}{8n^{2p}t_n\sigma_{\beta}^2}\right) \ge \exp(-d_5n\epsilon_n^2) \tag{C.15}$$

for some constant $d_5 > 0$ and

$$\left(\frac{(C_{\mathbb{B}}\epsilon_n)^2}{4n^{2p}t_n\sigma_{\beta}^2}\right)^{\frac{t_n}{2}} \ge \exp(-d_6n\epsilon_n^2)$$

for some constant $d_6 > 0$. The proof is done by letting $d_1 = \sum_{i=2}^6 d_i$.

C.6 Proof of Condition (C.5)

We will check Condition (C.5) with the choice $C_1 > (2d_1 + d_{\sigma} + 2)/C_*$, where d_1 is the constant satisfying Condition (C.4). Note that we have

$$\mathcal{F} \backslash \mathcal{F}^n = \left\{ T > M_n \right\} \bigcup \left\{ \left\{ T \le M_n \right\} \cap \left\{ \exists t \in [T] \text{ s.t } |\beta_t| > n \right\} \right\}.$$

Therefore, $\pi\{\mathcal{F}\backslash\mathcal{F}^n\}$ is upper bounded by

$$\pi\{\mathcal{F}\backslash\mathcal{F}^n\} \le \pi\{T > M_n\} + \pi\{T \le M_n\}\pi\{\exists t \in [T] \text{ s.t } |\beta_t| > n|T \le M_n\}$$
$$\le \pi\{T > M_n\} + \pi\{\exists t \in [T] \text{ s.t } |\beta_t| > n|T \le M_n\}.$$

Case 1. Upper bound of $\pi\{T > M_n\}$. We will show that $\pi\{T > M_n\}e^{(2d_1+d_\sigma+2)n\epsilon_n^2} \to 0$ as $n \to \infty$, where $M_n = \lfloor C_1 \frac{n\epsilon_n^2}{\log n} \rfloor$, which holds because

$$\pi\{T > M_n\} = \frac{\sum_{t=M_n+1}^{T_{\text{max}}} \exp(-C_* t \log n)}{\sum_{t=0}^{T_{\text{max}}} \exp(-C_* t \log n)}$$

$$= \frac{\frac{1}{n^{(M_n+1)C_*}} \left(1 - \frac{1}{n^{(T_{\text{max}}+1)C_*}}\right)}{1 - \frac{1}{n}} \times \frac{1 - \frac{1}{n}}{\left(1 - \frac{1}{n^{(T_{\text{max}}+1)C_*}}\right)}$$

$$= \exp(-(M_n + 1)C_* \log n).$$

Hence, $\pi\{T > M_n\}e^{(2d_1+d_\sigma+2)n\epsilon_n^2} \to 0$ as $n \to \infty$.

Case 2. Upper bound of $\pi\{\exists t \in [T] \text{ s.t } |\beta_t| > n|T \leq M_n\}$. We have

$$\pi\{\exists i \in [T] \text{ s.t } |\beta_t| > n | T \le M_n\} \le M_n \pi\{|\beta_1| > n\}$$

$$\le 2M_n \exp\left(-\frac{n^2}{2\sigma_\beta^2}\right),$$

where $\beta_1 \sim N(0, \sigma_{\beta}^2)$ and $\sigma_{\beta}^2 > 0$ is a constant. Hence, $\pi\{\exists t \in [T] \text{ s.t } |\beta_t| > n|T \le M_n\}e^{(2d_1+d_{\sigma}+2)n\epsilon_n^2} \to 0$ as $n \to \infty$.

C.7 Verification of the conditions in Theorem 4 of [11]

For given $f \in \mathcal{F}$ and $\sigma^2 \in \mathbb{R}_+$, consider the probability model $Y|\mathbf{X} = f(\mathbf{X}) + \epsilon$ with $\epsilon \sim N(0, \sigma^2)$ and $\mathbf{X} \sim \mathbb{P}_{\mathbf{X}}$. Let $\theta = (f, \sigma^2)$ and let p_{θ} be the density of (\mathbf{X}, Y) with parameter θ . For given data $\mathbf{x}^{(n)}$ and $\theta = (f, \sigma^2)$, let $p_{\theta,i}$ be the density of Gaussian distribution $N(f(\mathbf{x}_i), \sigma^2)$ for i = 1, ..., n.

For given two densities $p_{\theta_1}, p_{\theta_2}$, let $K(p_{\theta_1}, p_{\theta_2})$ be a Kullback-Leibler (KL) divergence defined as $K(p_{\theta_1}, p_{\theta_2}) = \int \log(p_{\theta_1}(\mathbf{v})/p_{\theta_2}(\mathbf{v}))p_{\theta_1}(\mathbf{v})d\mathbf{v}$, where $\mathbf{v} \in \mathcal{X} \times \mathbb{R}$. Let $V(p_{\theta_1}, p_{\theta_2}) = \int |\log(p_{\theta_1}(\mathbf{v})/p_{\theta_2}(\mathbf{v})) - K(p_{\theta_1}, p_{\theta_2})|^2 p_{\theta_1}(\mathbf{v})d\mathbf{v}$.

Let $\mathcal{F}_{\xi} = \{f \in \mathcal{F} : ||f||_{\infty} \leq \xi\}$ and let $\Theta_{\xi} = \mathcal{F}_{\xi} \times \mathbb{R}_{+}$. Similarly, we define $\mathcal{F}_{\xi}^{n} = \{f \in \mathcal{F}^{n} : ||f||_{\infty} \leq \xi\}$ and $\Theta_{\xi}^{n} = \mathcal{F}_{\xi}^{n} \times (1/\xi, \xi)$. Following Theorem 4 of [11], to show the posterior concentration rate in (C.2), it suffices to verify that for all $f_{0} \in \mathcal{H}_{0,F}^{\alpha}$ and $\mathbf{x}^{(n)} \in A_{n}$, there exists a sieve Θ_{ξ}^{n} and a constant $d_{*} > 0$ such that the following three conditions are satisfied.

$$\log N\left(\frac{\epsilon_n}{36}, \Theta_{\xi}^n, \|\cdot\|_{2,n}\right) \le n\epsilon_n^2 \tag{C.16}$$

$$\pi_{\xi}\{\mathbb{B}_n\} \ge e^{-d_* n\epsilon_n^2} \tag{C.17}$$

$$\pi_{\xi}\{\Theta_{\xi}\backslash\Theta_{\xi}^{n}\} \le e^{-(d_{*}+2)n\epsilon_{n}^{2}},$$
(C.18)

where

$$\mathbb{B}_n := \left\{ \theta \in \Theta_{\xi} : \frac{1}{n} \sum_{i=1}^n K(p_{\theta_0,i}, p_{\theta,i}) \le \epsilon_n^2, \frac{1}{n} \sum_{i=1}^n V(p_{\theta_{0,i}}, p_{\theta,i}) \le \epsilon_n^2 \right\}.$$

We will show that the above three conditions are satisfied to complete the proof of Theorem 5.1.

Verification of Condition (C.16). Note that

$$N\left(\frac{\epsilon_n}{36}, \Theta_{\xi}^n, \|\cdot\|_{2,n}\right) \leq N\left(\epsilon_n/72, \mathcal{F}_{\xi}^n, \|\cdot\|_{\infty}\right) N\left(\epsilon_n/72, (1/\xi, \xi), |\cdot|\right).$$

Since $N\left(\epsilon_n/72, (1/\xi, \xi), |\cdot|\right) \leq \left(1 + \frac{72 \max(1/\xi, \xi)}{\epsilon_n}\right)$, Condition (C.3) implies

$$\log N\left(\frac{\epsilon_n}{36}, \Theta_{\xi}^n, \|\cdot\|_{2,n}\right) \lesssim n\epsilon_n^2.$$

Verification of Condition (C.17). Direct calculation yields,

$$\frac{1}{n} \sum_{i=1}^{n} K(p_{\theta_0,i}, p_{\theta,i}) = \frac{1}{2} \log \left(\frac{\sigma^2}{\sigma_0^2} \right) - \frac{1}{2} \left(1 - \frac{\sigma_0^2}{\sigma^2} \right) + \frac{\|f - f_0\|_{2,n}^2}{2\sigma^2},$$

$$\frac{1}{n} \sum_{i=1}^{n} V(p_{\theta_0,i}, p_{\theta,i}) = \frac{1}{2} \left(1 - \frac{\sigma_0^2}{\sigma^2} \right)^2 + \frac{\sigma_0^2 \|f - f_0\|_{2,n}^2}{\sigma^2}.$$

As in the proof of Theorem 2 in [26], by using Taylor expansion, there exist a positive constant $C_{\mathbb{B}}$ such that

$$\mathbb{B}_n \supseteq \{ \theta \in \Theta_{\xi} : ||f - f_0||_{2,n} \le C_{\mathbb{B}} \epsilon_n, |\sigma^2 - \sigma_0^2| \le C_{\mathbb{B}} \epsilon_n \}.$$

Additionally, we have

$$\pi_{\xi} \{ \theta \in \Theta_{\xi} : \|f - f_0\|_{2,n} \le C_{\mathbb{B}} \epsilon_n, |\sigma^2 - \sigma_0^2| \le C_{\mathbb{B}} \epsilon_n \}$$
$$\ge \pi_{\xi} \{ \theta \in \Theta_{\xi} : \|f - f_0\|_{\infty} \le C_{\mathbb{B}} \epsilon_n, |\sigma^2 - \sigma_0^2| \le C_{\mathbb{B}} \epsilon_n \}.$$

In turn, since $\xi \ge \max\{2^p F, 1/\sigma_{\min}^2, \sigma_{\max}^2\} + C_{\mathbb{B}} \epsilon_n$ for sufficiently large n, we have

$$\pi_{\xi} \{ \theta \in \Theta_{\xi} : \|f - f_0\|_{\infty} \le C_{\mathbb{B}} \epsilon_n, |\sigma^2 - \sigma_0^2| \le C_{\mathbb{B}} \epsilon_n \}$$
$$\ge \pi \{ f : \|f - f_0\|_{\infty} \le C_{\mathbb{B}} \epsilon_n \} \pi \{ \sigma^2 : |\sigma^2 - \sigma_0^2| \le C_{\mathbb{B}} \epsilon_n \},$$

and from the proof of Theorem 2 in [26], we have $\pi\{\sigma^2 : |\sigma^2 - \sigma_0^2| \le C_{\mathbb{B}}\epsilon_n\} \gtrsim \frac{1}{n}$. Let d_{σ} be a positive constant such that $\pi\{\sigma^2 : |\sigma^2 - \sigma_0^2| \le C_{\mathbb{B}}\epsilon_n\} \ge \exp(-d_{\sigma}n\epsilon_n^2)$. Thus, Condition (C.4) implies

$$\pi_{\xi} \left\{ \theta \in \Theta_{\xi} : \frac{1}{n} \sum_{i=1}^{n} K(p_{\theta_{0},i}, p_{\theta,i}) \le \epsilon_{n}^{2}, \frac{1}{n} \sum_{i=1}^{n} V(p_{\theta_{0},i}, p_{\theta,i}) \le \epsilon_{n}^{2} \right\} \ge e^{-(d_{1} + d_{\sigma})n\epsilon_{n}^{2}}.$$

Verification of Condition (C.18). Note that $\pi_{\xi}\{\Theta_{\xi}\backslash\Theta_{\xi}^{n}\} \leq \pi_{\xi}\{\mathcal{F}\backslash\mathcal{F}^{n}\}$. In turn,

$$\pi_{\xi}\{\mathcal{F}\backslash\mathcal{F}^n\} \leq \frac{\pi\{\mathcal{F}\backslash\mathcal{F}^n\}}{\pi\{\|f\|_{\infty} \leq \xi\}} \leq \frac{\pi\{\mathcal{F}\backslash\mathcal{F}^n\}}{\pi\{\|f - f_0\|_{\infty} \leq \epsilon_n\}},$$

which is less than $e^{-(d_1+d_{\sigma}+2)n\epsilon_n^2}$ by Condition (C.4) and Condition (C.5) whenever $2^pF + C_{\mathbb{B}}\epsilon_n \leq \xi$. The proof is completed by letting $d_* = d_1 + d_{\sigma}$.

D Bridging the empirical and populational identifiabilities for multinary-product trees

For any component $S \subseteq [p]$, we first define a multinary-product tree, which is an extension of a binary-product tree, as follows. Recall that $\mathcal{X}_j = [0,1]$ for all $j \in [p]$. A partition \mathcal{P}_j of \mathcal{X}_j is called an interval partition if any element in \mathcal{P}_j is an interval. For example, $\{[0,1/3),[1/3,2/3),[2/3,1]\}$ is an interval partition. In the followings, we only consider interval partitions and we simply write them as 'partitions' unless there is any confusion. Let \mathcal{P}_j be a given partition of \mathcal{X}_j for each $j \in S$, where $\phi_j := |\mathcal{P}_j| \geq 2$. Let $\mathcal{P} = \prod_{j \in S} \mathcal{P}_j$. Then, the multinary-product tree defined on the product partition \mathcal{P} with the height vector $\mathbf{\gamma} = (\gamma_{\ell}, \ell \in \prod_{j \in S} \{1, \dots, \phi_j\})$ is defined as

$$f_{S,\mathcal{P},\gamma}(\mathbf{x}) = \sum_{\ell} \gamma_{\ell} \mathbb{I}(\mathbf{x}_S \in I_{\ell}),$$

where $I_{\ell} = \prod_{j \in S} I_{j,\ell_j}, I_{j,\ell_j} \in \mathcal{P}_j$. Note that a binary-product tree is a special case of a multinary-product tree with $\phi_j = 2$ for all $j \in S$. Figure D.3 compares binary-product tree and multinary-product tree.

D.1 Identifiable transformation of multinary-product tree

For a given probability measure ν on $[0,1]^{|S|}$, we explain how we transform any multinary-product tree to a ν -identifiable multinary-product tree. Let f_S be a multinary-product tree f_S defined as

$$f_S(\mathbf{x}_S) = \sum_{\ell} \gamma_{\ell} \mathbb{I}(\mathbf{x}_S \in I_{\ell}).$$

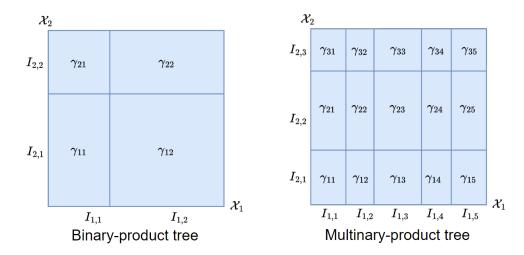


Figure D.3: Examples of binary-product tree and multinary-product tree. The left panel is a binary-product tree, while the right panel illustrates the partition and cell heights of a multinary-product tree with $\phi_1 = 5$ and $\phi_2 = 3$.

We modify γ_{ℓ} so that the resulting function satisfies the ν -identifiability condition. That is, the resulting function is a ν -identifiable multinary-product tree.

For $W \subseteq S$, let $\ell_W = (\ell_j, j \in W)$ and let $W^c = S - W$. For the modification of γ_{ℓ} , we let

$$\tilde{\gamma}_{\boldsymbol{\ell}} = \gamma_{\boldsymbol{\ell}} + \sum_{k=1}^{|S|} (-1)^k \left(\sum_{W:|W|=k,W\subseteq S} \mathbb{E}_{\nu,W}(\gamma_{\boldsymbol{\ell}}) \right),$$

where

$$\mathbb{E}_{\nu,W}(\gamma_{\ell}) := \sum_{\ell_W \in \prod_{t \in W} [\phi_t]} \gamma_{(\ell_{W^c},\ell_W)} \nu_W^{\text{ind}} \{ I_{\ell_W} \}. \tag{D.1}$$

Here, $\nu_W^{\text{ind}} = \prod_{j \in W} \nu_j$ and $I_{\ell_W} = \prod_{j \in W} I_{j,\ell_j}$. Note that ν_j is the marginal probability measure for $j \in S$. When $W = \{j\}$, we write $\mathbb{E}_{\nu,j}$ instead of $\mathbb{E}_{\nu,\{j\}}$ for notational simplicity.

For given $j \in S$, we can rewrite $\tilde{\gamma}_{\ell}$ as

$$\begin{split} \tilde{\gamma}_{\boldsymbol{\ell}} = & \gamma_{\boldsymbol{\ell}} + \sum_{k=1}^{|S|} (-1)^k \left(\sum_{W:|W|=k,j \in W,W \subseteq S} \mathbb{E}_{\nu.W}(\gamma_{\boldsymbol{\ell}}) \right) \\ & + \sum_{k=1}^{|S|-1} (-1)^k \left(\sum_{W:|W|=k,j \notin W,W \subseteq S} \mathbb{E}_{\nu,W}(\gamma_{\boldsymbol{\ell}}) \right) \\ = & \gamma_{\boldsymbol{\ell}} - \mathbb{E}_{\nu,j}(\gamma_{\boldsymbol{\ell}}) + \sum_{k=2}^{|S|} (-1)^k \left(\sum_{W:|W|=k,j \in W,W \subseteq S} \mathbb{E}_{\nu,W}(\gamma_{\boldsymbol{\ell}}) \right) \\ & + \sum_{k=1}^{|S|-1} (-1)^k \left(\sum_{W:|W|=k,j \notin W,W \subseteq S} \mathbb{E}_{\nu,W}(\gamma_{\boldsymbol{\ell}}) \right) \end{split}$$

Thus, we have

$$\mathbb{E}_{\nu,j}(\tilde{\gamma}_{\boldsymbol{\ell}}) = \sum_{k=2}^{|S|} (-1)^k \left(\sum_{W:|W|=k,j\in W,W\subseteq S} \mathbb{E}_{\nu,W}(\gamma_{\boldsymbol{\ell}}) \right) \\
+ \sum_{k=1}^{|S|-1} (-1)^k \left(\sum_{W:|W|=k,j\notin W,W\subseteq S} \mathbb{E}_{\nu,W\cup\{j\}}(\gamma_{\boldsymbol{\ell}}) \right) \\
= \sum_{k=1}^{|S|-1} (-1)^k \left(\sum_{W:|W|=k,j\notin W,W\subseteq S} (-\mathbb{E}_{\nu,W\cup\{j\}}(\gamma_{\boldsymbol{\ell}}) + \mathbb{E}_{\nu,W\cup\{j\}}(\gamma_{\boldsymbol{\ell}})) \right) \\
= 0$$

for $j \in S$. Therefore, $\tilde{\gamma}_{\ell}$ satisfies the ν -identifiability condition.

We denote the resulting function by f_{ν,f_S} , i.e.,

$$f_{\nu,f_S}(\mathbf{x}_S) = \sum_{\ell} \tilde{\gamma}_{\ell} \mathbb{I}(\mathbf{x}_S \in I_{\ell}). \tag{D.2}$$

D.2 Approximation error between the empirically and populationally identifiable multinary-product trees

We first investigate the approximation error between a given empirically identifiable multinaryproduct tree and its populationally identifiable version obtained by the formula (D.2), whose result is given in the following theorem. For $S \subseteq [p]$, let \mathbb{P}_S be the distribution of \mathbf{X}_S and $\mathbb{P}_S^{\text{ind}} = \prod_{j \in S} \mathbb{P}_j$, where \mathbb{P}_j is the probability distribution of \mathbf{X}_j .

Theorem D.1. Let $\mathcal{F}_{S,K,\xi}^{E}$ be the set of all empirically identifiable S-component multinaryproduct trees f_S with $\max_{j\in S} |\mathcal{P}_j| \leq K$ and $||f_S||_{\infty} \leq \xi$. Then, we have

$$\mathbb{P}_{\mathbf{X}}^{n} \left\{ \sup_{f_{S} \in \mathcal{F}_{S,K,\xi}^{E}} \|f_{S} - f_{\mathbb{P}_{S},f_{S}}\|_{\infty} \le (24\xi + 1)2^{|S|} \sqrt{\frac{K \log n}{n}} \right\} \\
\ge 1 - 2^{|S|+1} |S| K^{|S|} \exp\left(-\frac{K \log n}{4\xi^{2}}\right).$$

Proof. Consider an identifiable multinary-product tree f_S given as

$$f_S(\mathbf{x}_S) = \sum_{\ell} \gamma_{\ell} \mathbb{I}(\mathbf{x}_S \in I_{\ell}).$$

Note that γ_{ℓ} s depend on the data $\mathbf{X}^{(n)}$ because of the identifiability condition.

We will show that $\mathbb{E}_{\mathbb{P}_S,W}(\gamma_{\ell})$ is small for all $W \subseteq S$. Let $\phi_j = |\mathcal{P}_j|$ for $j \in S$. Note that

for all $W \subseteq S$, we have

$$\begin{split} \left| \mathbb{E}_{\mathbb{P}_{S},W}(\gamma_{\boldsymbol{\ell}}) \right| &= \left| \sum_{\boldsymbol{\ell}_{W} \in \prod_{t \in W} [\phi_{t}]} \gamma_{(\boldsymbol{\ell}_{W^{c}},\boldsymbol{\ell}_{W})} \mathbb{P}_{W}^{\text{ind}} \left\{ I_{\boldsymbol{\ell}_{W}} \right\} \right| \\ &\leq \sum_{\boldsymbol{\ell}_{W \setminus \{j\}} \in \prod_{t \in W \setminus \{j\}} [\phi_{t}]} \left| \sum_{\ell_{j} \in [\phi_{j}]} \gamma_{(\boldsymbol{\ell}_{j^{c}},\ell_{j})} \prod_{i \in W} \mathbb{P}_{i} \left\{ I_{i,\ell_{i}} \right\} \right| \\ &= \sum_{\boldsymbol{\ell}_{W \setminus \{j\}} \in \prod_{t \in W \setminus \{j\}} [\phi_{t}]} \left(\prod_{i \in W \setminus \{j\}} \mathbb{P}_{i} \left\{ I_{i,\ell_{i}} \right\} \right) \left| \sum_{\ell_{j} \in [\phi_{j}]} \gamma_{(\boldsymbol{\ell}_{j^{c}},\ell_{j})} \mathbb{P}_{j} \left\{ I_{j,\ell_{j}} \right\} \right| \\ &\leq \max_{\boldsymbol{\ell}_{j^{c}} \in \prod_{t \in S \setminus \{j\}} [\phi_{t}]} \left| \sum_{\ell_{j} \in [\phi_{j}]} \gamma_{(\boldsymbol{\ell}_{j^{c}},\ell_{j})} \mathbb{P}_{j} \left\{ I_{j,\ell_{j}} \right\} \right| \\ &= \max_{\boldsymbol{\ell}_{j^{c}} \in \prod_{t \in S \setminus \{j\}} [\phi_{t}]} \left| \mathbb{E}_{\mathbb{P}_{S},j}(\gamma_{\boldsymbol{\ell}}) \right|. \end{split}$$

In turn, since $\mathbb{E}_{\mu_{n,S},j}(\gamma_{\ell}) = 0$ for any $j \in W$, we have

$$\mathbb{E}_{\mathbb{P}_{S},j}(\gamma_{\boldsymbol{\ell}}) = \mathbb{E}_{\mathbb{P}_{S},j}(\gamma_{\boldsymbol{\ell}}) - \mathbb{E}_{\mu_{n,S},j}(\gamma_{\boldsymbol{\ell}})$$

$$= \sum_{\ell_{j} \in [\phi_{j}]} \gamma_{(\boldsymbol{\ell}_{j^{c}},\ell_{j})} (\mathbb{P}_{j}\{I_{j,\ell_{j}}\} - \mu_{n,j}\{I_{j,\ell_{j}})\}$$

$$= \sum_{\ell_{j} \in [\phi_{j}]} \gamma_{(\boldsymbol{\ell}_{j^{c}},\ell_{j})} \left(\mathbb{P}_{j}\{I_{j,\ell_{j}}\} - \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}(X_{i,j} \in I_{j,\ell_{j}})\right). \tag{D.3}$$

In the following, we will show that (D.3) is small.

For a given interval partition $\mathcal{P} = \{I_1, \dots, I_{\phi_j}\}$ of [0,1] with $\phi_j \leq K$ and a vector $\boldsymbol{\gamma} \in [-\xi, \xi]^{\phi_j}$, define a function $q_{\mathcal{P}, \boldsymbol{\gamma}}$ as $q_{\mathcal{P}, \boldsymbol{\gamma}}(x) = \sum_{\ell=1}^{\phi_j} \gamma_\ell \mathbb{I}(x \in I_\ell)$. The proof would be complete if we show

$$\mathbb{P}_{\mathbf{X}}^{n} \left\{ \sup_{q \in \mathcal{Q}_{K,\xi}} \left| \frac{1}{n} \sum_{i=1}^{n} q(X_{i,j}) - \mathbb{E}_{j}[q(X_{j})] \right| > (24\xi + 1) \sqrt{\frac{K \log n}{n}} \right\} \le 2 \exp\left(-\frac{K \log n}{4\xi^{2}}\right), \tag{D.4}$$

where $Q_{K,\xi}$ is the set of all $q_{\mathcal{P},\gamma}$ with $\phi_j \leq K$ and $\gamma \in [-\xi,\xi]^{\phi_j}$, and \mathbb{E}_j denotes the

expectation under \mathbb{P}_j .

For Rademacher random variables $\boldsymbol{\vartheta} = \{\vartheta_1, ..., \vartheta_n\}$, we define the empirical and populational Rademacher complexities as

$$\mathbf{R}_{j}(\mathbf{x}_{1},...,\mathbf{x}_{n}) = \mathbb{E}_{\boldsymbol{\vartheta}} \left[\sup_{q \in \mathcal{Q}_{K,\xi}} \left| \frac{1}{n} \sum_{i=1}^{n} \vartheta_{i} q(x_{i,j}) \right| \right] \quad \text{and} \quad \mathbf{R}_{j}(\mathcal{Q}_{K,\xi}) = \mathbb{E}_{\mathbf{X}}^{n} [\mathbf{R}_{j}(\mathbf{X}_{1},...,\mathbf{X}_{n})].$$

For $k \in [n]$, let $\mathbf{X}^{(n),\text{new}}$ denote the data obtained by replacing the kth observation with a new one (independent with the data), i.e.,

$$\mathbf{X}^{(n),\text{new}} = (\mathbf{X}_1,...,\mathbf{X}_{k-1},\mathbf{X}_k^{\text{new}},\mathbf{X}_{k+1},...,\mathbf{X}_n).$$

Then, we have

$$\left| \sup_{q \in \mathcal{Q}_{K,\xi}} \triangle_{\mathbf{X}^{(n)}}(q) - \sup_{q \in \mathcal{Q}_{K,\xi}} \triangle_{\mathbf{X}^{(n),\text{new}}}(q) \right|$$

$$\leq \sup_{q \in \mathcal{Q}_{K,\xi}} \left| \triangle_{\mathbf{X}^{(n)}}(q) - \triangle_{\mathbf{X}^{(n),\text{new}}}(q) \right|$$

$$\leq \sup_{q \in \mathcal{Q}_{K,\xi}} \left| \frac{1}{n} \left(q(X_{k,j}) - q(X_{k,j}^{\text{new}}) \right) \right|$$

$$\leq \frac{2\xi}{n},$$

where

$$\triangle_{\mathbf{X}^{(n)}}(q) = \left| \frac{1}{n} \sum_{i=1}^{n} q(X_{i,j}) - \mathbb{E}_j[q(X_j)] \right|.$$

Therefore, using McDiarmid's inequality ([48]), we have

$$\mathbb{P}_{\mathbf{X}}^{n} \left\{ \left| \sup_{q \in \mathcal{Q}_{K,\xi}} \triangle_{\mathbf{X}^{(n)}}(q) - \mathbb{E}_{\mathbf{X}}^{n} \left[\sup_{q \in \mathcal{Q}_{K,\xi}} \triangle_{\mathbf{X}^{(n)}}(q) \right] \right| \geq \sqrt{\frac{K \log n}{n}} \right\} \leq 2 \exp\left(-\frac{K \log n}{4\xi^{2}} \right).$$

The covering number of $Q_{K,\xi}$ can be easily derived using a similar approach used in Section C.4 of Supplementary Material:

$$N(\epsilon, \mathcal{Q}_{K,\xi}, \|\cdot\|_{\infty}) \le n^{\phi_j} \left(1 + \frac{2\phi_j \xi}{\epsilon}\right)^{\phi_j}$$

$$\le n^K \left(1 + \frac{2K\xi}{\epsilon}\right)^K, \tag{D.5}$$

where (D.5) is from $\phi_j \leq K$.

Therefore, using Dudley Theorem (Theorem 1.19 in [51]), we have

$$\mathbf{R}(\mathbf{x}_{1},...,\mathbf{x}_{n}) \leq \inf_{0 \leq \epsilon \leq \xi/2} \left\{ 4\epsilon + \frac{12}{\sqrt{n}} \int_{\epsilon}^{\xi} \sqrt{\log N(w, \mathcal{Q}_{K,\xi}, \|\cdot\|_{2,n})} dw \right\}$$

$$\lesssim \inf_{0 \leq \epsilon \leq \xi/2} \left\{ 4\epsilon + 12(\xi - \epsilon) \sqrt{\frac{K \log n}{n}} \right\}$$

$$\leq 12\xi \sqrt{\frac{K \log n}{n}}.$$

That is, we have

$$\mathbf{R}(\mathcal{Q}_{K,\xi}) \le 12\xi\sqrt{\frac{K\log n}{n}}.$$

Using Lemma D.3 in Section D.3 of Supplementary Material, we have

$$\mathbb{E}_{\mathbf{X}}^{n} \left[\sup_{q \in \mathcal{Q}_{K,\xi}} \triangle_{\mathbf{X}^{(n)}}(q) \right] \leq 2\mathbf{R}(\mathcal{Q}_{K,\xi})$$
$$\leq 24\xi \sqrt{\frac{K \log n}{n}}.$$

Finally, we conclude that

$$\mathbb{P}_{\mathbf{X}}^{n} \left\{ \sup_{f_{S} \in \mathcal{F}_{S,K,\xi}^{E}} \|f_{S} - f_{\mathbb{P}_{S},f_{S}}\|_{\infty} \leq (24\xi + 1)2^{|S|} \sqrt{\frac{K \log n}{n}} \right\} \\
\geq \mathbb{P}_{\mathbf{X}}^{n} \left\{ \max_{W \subseteq S} \max_{j \in W} \max_{\boldsymbol{\ell}_{j^{c}}} \sup_{q \in \mathcal{Q}_{K,\xi}} \Delta_{\mathbf{X}^{(n)}}(q) \leq (24\xi + 1) \sqrt{\frac{K \log n}{n}} \right\} \\
\geq 1 - \sum_{W \subseteq S} \sum_{j \in W} \sum_{\boldsymbol{\ell}_{j^{c}}} \mathbb{P}_{\mathbf{X}}^{n} \left\{ \sup_{q \in \mathcal{Q}_{K,\xi}} \Delta_{\mathbf{X}^{(n)}}(q) > (24\xi + 1) \sqrt{\frac{K \log n}{n}} \right\} \\
\geq 1 - 2^{|S|+1} |S|K^{|S|} \exp\left(-\frac{K \log n}{4\xi^{2}}\right). \tag{D.6}$$

The converse of Theorem D.1 is also true. That is, Theorem D.2 proves that the

approximation error bettween a given populationally identifiable multinary-product tree

and its empirically identifiable version is the same as that of Theorem D.1. The proof

can be done by simply interchanging $\mu_{n,S}$ and \mathbb{P}_S in the proof of Theorem D.1 and so is

omitted.

Theorem D.2. Let $\mathcal{F}_{S,K,\xi}^P$ be the set of all populationally identifiable S-component multinaryproduct trees f_S with $\max_{j\in S} |\mathcal{P}_j| \leq K$ and $||f_S||_{\infty} \leq \xi$. Then, we have

$$\mathbb{P}_{\mathbf{X}}^{n} \left\{ \sup_{f_{S} \in \mathcal{F}_{S,K,\xi}^{P}} \|f_{S} - f_{\mu_{n,S},f_{S}}\|_{\infty} \le (24\xi + 1)2^{|S|} \sqrt{\frac{K \log n}{n}} \right\}$$
$$\ge 1 - 2^{|S|+1} |S| K^{|S|} \exp\left(-\frac{K \log n}{4\xi^{2}}\right).$$

D.3 Rademacher complexity bound

Lemma D.3. For function class $Q_{K,\xi}$, we have

$$\mathbb{E}_{\mathbf{X}}^{n} \left[\sup_{q \in \mathcal{Q}_{K,\xi}} \triangle_{\mathbf{X}^{(n)}}(q) \right] \leq 2\mathbf{R}(\mathcal{Q}_{K,\xi}).$$

Proof. Let $\mathbf{X}'_1,...,\mathbf{X}'_n$ be independent identical sample from the distribution $\mathbb{P}_{\mathbf{X}}$, where $\mathbf{X}'_i = (X'_{i,1},...,X'_{i,p})$. Then, we have

$$\mathbb{E}_{\mathbf{X}}^{n} \left[\sup_{q \in \mathcal{Q}_{K,\xi}} \Delta_{\mathbf{X}^{(n)}}(q) \right] \\
= \mathbb{E}_{\mathbf{X}}^{n} \left[\sup_{q \in \mathcal{Q}_{K,\xi}} \left| \frac{1}{n} \sum_{i=1}^{n} q(X_{i,j}) - \mathbb{E}_{\mathbf{X}'_{1}}[q(X'_{1,j})] \right| \right] \\
= \mathbb{E}_{\mathbf{X}}^{n} \left[\sup_{q \in \mathcal{Q}_{K,\xi}} \left| \mathbb{E}_{\mathbf{X}'}^{n} \left[\frac{1}{n} \sum_{i=1}^{n} \left(q(X_{i,j}) - q(X'_{i,j}) \right) \right] \right| \right] \\
\leq \mathbb{E}_{\mathbf{X},\mathbf{X}'}^{n} \left[\sup_{q \in \mathcal{Q}_{K,\xi}} \left| \frac{1}{n} \sum_{i=1}^{n} \left(q(X_{i,j}) - q(X'_{i,j}) \right) \right| \right] \\$$

Since the distribution of $(q(X_{i,j}) - q(X'_{i,j}))$ is identical to that of $\vartheta_i(q(X_{i,j}) - q(X'_{i,j}))$ for i = 1, ..., n, we have

$$\mathbb{E}_{\mathbf{X},\mathbf{X}'}^{n} \left[\sup_{q \in \mathcal{Q}_{K,\xi}} \left| \frac{1}{n} \sum_{i=1}^{n} \left(q(X_{i,j}) - q(X'_{i,j}) \right) \right| \right]$$

$$= \mathbb{E}_{\mathbf{X},\mathbf{X}',\boldsymbol{\vartheta}}^{n} \left[\sup_{q \in \mathcal{Q}_{K,\xi}} \left| \frac{1}{n} \sum_{i=1}^{n} \vartheta_{i} \left(q(X_{i,j}) - q(X'_{i,j}) \right) \right| \right]$$

$$\leq 2\mathbf{R}(\mathcal{Q}_{K,\xi}).$$

E Proof of Theorem 5.2

The proof of Theorem 5.2 consists of the following four steps.

(STEP 1). We derive the posterior convergence rate with respect to the population l_2 norm. That is, we show that

$$\pi_{\xi} \{ (f, \sigma^2) \in \Theta_{\xi}^n : ||f - f_0||_{2, \mathbb{P}_{\mathbf{X}}} + |\sigma^2 - \sigma_0^2| > B_n \epsilon_n |\mathbf{X}^{(n)}, Y^{(n)} \} \to 0,$$
 (E.1)

for any $B_n \to \infty$ in \mathbb{P}_0^n as $n \to \infty$.

(STEP 2). From (E.1), for any $S \subseteq [p]$ we establish that

$$\pi_{\xi} \{ (f, \sigma^2) \in \Theta_{\xi}^n : ||f_S - f_{0,S}||_{2, \mathbb{P}_{\mathbf{X}}} + |\sigma^2 - \sigma_0^2| > B_n \epsilon_n |\mathbf{X}^{(n)}, Y^{(n)} \} \to 0,$$
 (E.2)

for any $B_n \to \infty$ in \mathbb{P}_0^n as $n \to \infty$.

(STEP 3). We modify (E.2) for the empirical l_2 norm. That is, we show that

$$\pi_{\xi} \{ (f, \sigma^2) \in \Theta_{\xi}^n : ||f_S - f_{0,S}||_{2,n} + |\sigma^2 - \sigma_0^2| > B_n \epsilon_n |\mathbf{X}^{(n)}, Y^{(n)} \} \to 0,$$
 (E.3)

for any $B_n \to \infty$ in \mathbb{P}_0^n as $n \to \infty$.

(STEP 4). Finally, we establish

$$\pi_{\xi} \left\{ \Theta_{\xi} \backslash \Theta_{\xi}^{n} \middle| \mathbf{X}^{(n)}, Y^{(n)} \right\} \to 0$$
 (E.4)

E.1 Proof of (E.1)

We rely on the following result (See Theorem 19.3 of [15] for its proof).

Lemma E.1 (Theorem 19.3 of [15]). Let $X, X_1, ..., X_n$ be independent and identically distributed random vectors with values in \mathbb{R}^d . Let $K_1, K_2 \geq 1$ be constants and let \mathcal{G} be a class of functions $g : \mathbb{R}^d \to \mathbb{R}$ with

$$|g(\boldsymbol{x})| \le K_1, \quad \mathbb{E}[g(\boldsymbol{X})^2] \le K_2 \mathbb{E}[g(\boldsymbol{X})].$$
 (E.5)

Let $0 < \kappa < 1$ and $\zeta > 0$. Assume that

$$\sqrt{n}\kappa\sqrt{1-\kappa}\sqrt{\zeta} \ge 288\max\left\{2K_1,\sqrt{2K_2}\right\}$$

and that, for all $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$ and for all $t \geq \frac{\zeta}{8}$,

$$\frac{\sqrt{n}\kappa(1-\kappa)t}{96\sqrt{2}\max\{K_1, 2K_2\}} \ge \int_{\frac{\kappa(1-\kappa)t}{16\max\{K_1, 2K_2\}}}^{\sqrt{t}} \sqrt{\log N\left(u, \left\{g \in \mathcal{G} : \frac{1}{n}\sum_{i=1}^{n}g\left(\mathbf{x}_i\right)^2 \le 16t\right\}, ||\cdot||_{1,n}\right)} du. \tag{E.6}$$

Then,

$$\mathbb{P}_{\mathbf{X}}^{n} \left\{ \sup_{g \in \mathcal{G}} \frac{\left| \mathbb{E}[g(\boldsymbol{X})] - \frac{1}{n} \sum_{i=1}^{n} g\left(\boldsymbol{X}_{i}\right) \right|}{\zeta + \mathbb{E}[g(\boldsymbol{X})]} > \kappa \right\} \leq 60 \exp\left(-\frac{n\zeta\kappa^{2}(1-\kappa)}{128 \cdot 2304 \max\left\{K_{1}^{2}, K_{2}\right\}}\right).$$

First, since \mathcal{F}_{ξ}^{n} depends on the data $\mathbf{X}^{(n)}$, we cannot directly apply Lemma E.1. To resolve this problem, as in (D.4), we consider a class of linear combinations of binary product trees not necessarily identifiable, which we denote $\mathcal{F}_{\xi,\text{general}}^{n}$, and show that the

covering number is of the same order as that of \mathcal{F}^n_{ξ} .

For given $S \subseteq [p]$, $\mathbf{s} = (s_j, j \in S)$, and $\boldsymbol{\beta} = (\beta_{\mathbf{v}}, \mathbf{v} \in \{-1, 1\}^{|S|})$, let $\mathbb{T}^G(\mathbf{x}_S : S, \mathbf{s}, \boldsymbol{\beta})$ be a binary-product tree given as

$$\mathbb{T}^G(\mathbf{x}_S: S, \mathbf{s}, \boldsymbol{\beta}) = \sum_{\mathbf{v} \in \{-1,1\}^{|S|}} \beta_{\mathbf{v}} \prod_{j \in S} \mathbb{I}^{(v_j)}(x_j - s_j > 0).$$

Note that we do not impose the identifiability condition on β . Now, we define $\mathcal{F}_{\text{general}}^n$ as

$$\mathcal{F}_{\text{general}}^n = \left\{ f : f(\mathbf{x}) = \sum_{t=1}^T \mathbb{T}^G \left(\mathbf{x}_{S_t} : S_t, \mathbf{s}_t, \boldsymbol{\beta}_t \right), \quad T \in [M_n] \text{ and } \max_t \|\boldsymbol{\beta}_t\|_{\infty} \le n^{p+1} \right\},$$

and $\mathcal{F}_{\xi,\text{general}}^n = \{ f \in \mathcal{F}_{\text{general}}^n, \|f\|_{\infty} \leq \xi \}$. Note that $\mathcal{F}_{\xi}^n \subseteq \mathcal{F}_{\xi,\text{general}}^n$. By a similar approach used in to Section C.4 of Supplementary Material, we can show

$$N(\epsilon, \mathcal{F}_{\xi, \text{general}}^n, \|\cdot\|_{\infty}) \lesssim M_n n^{M_n p} \left(1 + \frac{n^{p+1} M_n 2^{p+1}}{\epsilon}\right)^{M_n 2^p}.$$
 (E.7)

For $K_1 = K_2 = 4\xi^2$, $\kappa := \frac{1}{2}$, $\zeta = \epsilon_n^2$, and $\mathcal{G} = \{g : g = (f_0 - f)^2, f \in \mathcal{F}_{\xi,\text{general}}^n\}$, we first verify Condition (E.5) and Condition (E.6) in Lemma E.1.

Verifying Condition (E.5): Since $||f||_{\infty} \leq \xi$ for $f \in \mathcal{F}_{\xi,general}^n$, we have

$$\sup_{\mathbf{x}} g(\mathbf{x}) = \sup_{\mathbf{x}} (f_0(\mathbf{x}) - f(\mathbf{x}))^2 \le 4\xi^2$$

for all $g \in \mathcal{G}$.

Verifying Condition (E.6): Since

$$\forall f_1, f_2 \in \mathcal{F}_{\xi, \text{general}}^n, \quad \|(f_1 - f_0)^2 - (f_2 - f_0)^2\|_{1,n} \le 4\xi \|f_1 - f_2\|_{1,n},$$

we have

$$N(u, \mathcal{G}, \|\cdot\|_{1,n}) \leq N\left(\frac{u}{4\xi}, \mathcal{F}_{\xi, \text{general}}^{n}, \|\cdot\|_{1,n}\right)$$

$$\lesssim \frac{n\epsilon_{n}^{2}}{\log n} n^{n\epsilon_{n}^{2}p/\log n} \left(1 + \frac{4\xi n^{p+1}\epsilon_{n}^{2}2^{p+1}}{u\log n}\right)^{n\epsilon_{n}^{2}/\log n}$$
(E.8)

for any u > 0, where (E.8) is derived from (E.7). Therefore, for $t \ge \epsilon_n^2/8$, $\frac{t/4}{16 \max(K_1, 2K_2)} \le u \le \sqrt{t}$, we have

$$\log N(u, \mathcal{G}, \|\cdot\|_{1,n}) \lesssim \log \frac{n\epsilon_n^2}{\log n} + \frac{n\epsilon_n^2}{\log n} p \log n + \frac{n\epsilon_n^2}{\log n} \log \left(1 + \frac{4\xi n^{p+1}\epsilon_n^2 2^{p+1}}{u \log n}\right)$$
$$\lesssim n\epsilon_n^2.$$

Hence, for all $t \ge \epsilon_n^2/8$, the following inequality holds:

$$\int_{\frac{t/4}{16\max(K_1, 2K_2)}}^{\sqrt{t}} \sqrt{\log N(u, \mathcal{G}, \|\cdot\|_{1,n})} \lesssim \sqrt{t} \sqrt{n} \epsilon_n$$

$$= o\left(\frac{\sqrt{n}t/4}{96\sqrt{2}\max\{K_1, 2K_2\}}\right).$$

Proof of Condition (E.1): From Lemma E.1, we obtain the following bound:

$$\mathbb{P}_{\mathbf{X}}^{n} \left\{ \sup_{f \in \mathcal{F}_{\xi}^{n}} \frac{\left| ||f - f_{0}||_{2,\mathbb{P}_{\mathbf{X}}}^{2} - ||f - f_{0}||_{2,n}^{2} \right|}{\varepsilon_{n}^{2} + ||f - f_{0}||_{2,\mathbb{P}_{\mathbf{X}}}^{2}} > \frac{1}{2} \right\} \\
\leq \mathbb{P}_{\mathbf{X}}^{n} \left\{ \sup_{f \in \mathcal{F}_{\xi, \text{general}}^{n}} \frac{\left| ||f - f_{0}||_{2,\mathbb{P}_{\mathbf{X}}}^{2} - ||f - f_{0}||_{2,n}^{2} \right|}{\varepsilon_{n}^{2} + ||f - f_{0}||_{2,\mathbb{P}_{\mathbf{X}}}^{2}} > \frac{1}{2} \right\} \\
\leq 60 \exp\left(-\frac{n\varepsilon_{n}^{2}/8}{128 \cdot 2304 \cdot 16\xi^{4}} \right).$$

It implies that

$$\forall f \in \mathcal{F}_{\xi}^{n}, \quad 2\|f - f_0\|_{2,n}^2 \ge \|f - f_0\|_{2,\mathbb{P}_{\mathbf{X}}}^2 - \epsilon_n^2$$

with probability at least $1-60\exp\left(-\frac{n\varepsilon_n^2/8}{128\cdot 2304\cdot 16\xi^4}\right)$ under the probability distribution $\mathbb{P}_{\mathbf{X}}^n$. We refer to this event as Ω_n^* .

On the event Ω_n^* , we have

$$\pi_{\xi} \Big\{ (f, \sigma^{2}) \in \Theta_{\xi}^{n} : \|f - f_{0}\|_{2, \mathbb{P}_{\mathbf{X}}} + |\sigma^{2} - \sigma_{0}^{2}| > B_{n} \epsilon_{n} \Big| \mathbf{X}^{(n)}, Y^{(n)} \Big\}$$

$$\leq \pi_{\xi} \Big\{ (f, \sigma^{2}) \in \Theta_{\xi}^{n} : \|f - f_{0}\|_{2, n} + |\sigma^{2} - \sigma_{0}^{2}| > B_{n} \epsilon_{n} \Big| \mathbf{X}^{(n)}, Y^{(n)} \Big\}$$

$$\to 0$$

for any $B_n \to \infty$ in \mathbb{P}_0^n as $n \to \infty$ by Theorem 5.1. Since $\mathbb{P}_0^n(\Omega_n^*) \to 1$ as $n \to \infty$, we have

$$\pi_{\xi} \Big\{ (f, \sigma^2) \in \Theta_{\xi}^n : \|f - f_0\|_{2, \mathbb{P}_{\mathbf{X}}} + |\sigma^2 - \sigma_0^2| > B_n \epsilon_n \Big| \mathbf{X}^{(n)}, Y^{(n)} \Big\} \to 0$$

for any $B_n \to \infty$ in \mathbb{P}_0^n as $n \to \infty$, which completes the proof of (E.1).

E.2 Proof of (E.2)

Let C_L and C_U be positive constants such that

$$C_L \le \inf_{\mathbf{x} \in \mathcal{X}} \frac{p_{\mathbf{X}}(\mathbf{x})}{p_{\mathbf{X}}^{\text{ind}}(\mathbf{x})} \le \sup_{\mathbf{x} \in \mathcal{X}} \frac{p_{\mathbf{X}}(\mathbf{x})}{p_{\mathbf{X}}^{\text{ind}}(\mathbf{x})} \le C_U.$$

Any $f \in \mathcal{F}_{\xi}^n$ can be decomposed into the sum of identifiable multinary-product trees f_S s, i.e.,

$$f(\mathbf{x}) = \sum_{S \subset [p]} f_S(\mathbf{x}_S),$$

where f_S is the ensemble of T_S many identifiable binary-product trees. Let $K_S = \prod_{j \in S} |\mathcal{P}_j|$, where $\mathcal{P}_j s$ are partitions in f_S . Since $T_S \leq \sum_{S \subseteq [p]} T_S \leq M_n$, it follows that

$$K_S \le (T_S^{\frac{1}{|S|}} + 1)^{|S|} \le C_1 n\epsilon_n^2 / \log n.$$

Therefore by Theorem D.1, we have

$$\mathbb{P}_{\mathbf{X}}^{n} \left\{ \sup_{f_{S}: f \in \mathcal{F}_{\xi}^{n}} \|f_{S} - f_{\mathbb{P}_{S}, f_{S}}\|_{\infty} \lesssim \epsilon_{n} \right\} \geq 1 - 2^{|S|+1} |S| (C_{1} n \epsilon_{n}^{2} / \log n)^{|S|} \exp\left(-\frac{C_{1} n \epsilon_{n}^{2}}{4 \xi^{2}}\right).$$

For notational simplicity, we denote $f_{\mathbb{P}_S,f_S}$ by f_S^P . Let $f^P = \sum_{S \subseteq [p]} f_S^P$.

For f^P , we have

$$\|f^{P} - f_{0}\|_{2,\mathbb{P}_{\mathbf{X}}}^{2} = \int_{\mathcal{X}} \left\{ \sum_{S \subseteq [p]} (f_{S}^{P}(\mathbf{x}_{S}) - f_{0,S}(\mathbf{x}_{S})) \right\}^{2} \mathbb{P}_{\mathbf{X}}(d\mathbf{x})$$

$$\geq \frac{1}{C_{L}} \int_{\mathcal{X}} \left\{ \sum_{S \subseteq [p]} (f_{S}^{P}(\mathbf{x}_{S}) - f_{0,S}(\mathbf{x}_{S})) \right\}^{2} \prod_{j=1}^{p} \mathbb{P}_{j}(dx_{j})$$

$$= \frac{1}{C_{L}} \sum_{S \subseteq [p]} \int_{\mathcal{X}} (f_{S}^{P}(\mathbf{x}_{S}) - f_{0,S}(\mathbf{x}_{S}))^{2} \prod_{j=1}^{p} \mathbb{P}_{j}(dx_{j})$$

$$\geq \frac{C_{U}}{C_{L}} \sum_{S \subseteq [p]} \|f_{S}^{P} - f_{0,S}\|_{2,\mathbb{P}_{\mathbf{X}}}^{2}$$

$$\geq \|f_{S}^{P} - f_{0,S}\|_{2,\mathbb{P}_{\mathbf{X}}}^{2},$$

$$(E.9)$$

for all $S \subseteq [p]$, where the equality (E.9) holds since f_S^P s satisfy the populational identifiability condition. Thus, we obtain the following lower bound for $||f - f_0||_{2,\mathbb{P}_{\mathbf{X}}}$:

$$||f - f_0||_{2,\mathbb{P}_{\mathbf{X}}} \ge ||f^P - f_0||_{2,\mathbb{P}_{\mathbf{X}}} - ||f - f^P||_{2,\mathbb{P}_{\mathbf{X}}}$$

$$\gtrsim ||f^P - f_0||_{2,\mathbb{P}_{\mathbf{X}}} - \epsilon_n$$

$$\gtrsim ||f_S^P - f_{0,S}||_{2,\mathbb{P}_{\mathbf{X}}} - \epsilon_n$$

$$\gtrsim ||f_S - f_{0,S}||_{2,\mathbb{P}_{\mathbf{X}}} - 2\epsilon_n$$

To sum up, we conclude that

$$\pi_{\xi} \Big\{ (f, \sigma^2) \in \Theta_{\xi}^n : \|f_S - f_{0,S}\|_{2, \mathbb{P}_{\mathbf{X}}} + |\sigma^2 - \sigma_0^2| > B_n \epsilon_n \Big| \mathbf{X}^{(n)}, Y^{(n)} \Big\} \to 0,$$

for any $B_n \to \infty$ in \mathbb{P}_0^n as $n \to \infty$.

E.3 Proof of (E.3)

In the same manner as in (E.1), using Lemma E.1 with $\mathcal{G} = \{g : g = (f_{0,S} - f_S)^2, f \in \mathcal{F}_{\xi,\text{general}}^n\}$, we can obtain the following:

$$\pi_{\xi} \Big\{ (f, \sigma^2) \in \Theta_{\xi}^n : \|f_S - f_{0,S}\|_{2,n} + |\sigma^2 - \sigma_0^2| > B_n \epsilon_n \Big| \mathbf{X}^{(n)}, Y^{(n)} \Big\} \to 0$$

for any $B_n \to \infty$ in \mathbb{P}_0^n as $n \to \infty$.

E.4 Proof of (E.4)

For given $\mathbf{x}^{(n)} \in A_n$, where A_n is defined in Section C.3 of Supplementary Material, we have

$$\frac{\pi_{\xi}\{\Theta_{\xi}\backslash\Theta_{\xi}^{n}\}}{\pi_{\xi}\{\mathbb{B}_{n}\}} \leq \exp\left(-2n\epsilon_{n}^{2}\right)$$

since Condition (C.17) and Condition (C.18) hold. Thus, Lemma 1 of [11] implies that for any $\mathbf{x}^{(n)} \in A_n$ and an arbitrary $\delta > 0$,

$$\lim_{n\to\infty} \mathbb{P}_{Y^{(n)}} \left\{ \pi_{\xi} \{ \Theta_{\xi} \backslash \Theta_{\xi}^{n} | \mathbf{X}^{(n)}, Y^{(n)} \} > \delta \middle| \mathbf{X}^{(n)} = \mathbf{x}^{(n)} \right\} = 0.$$

Since $\mathbb{P}^n_{\mathbf{X}}(A_n) \to 1$, we have

$$\lim_{n \to \infty} \mathbb{P}_0^n \left\{ \pi_{\xi} \{ \Theta_{\xi} \backslash \Theta_{\xi}^n | \mathbf{X}^{(n)}, Y^{(n)} \} > \delta \right\} = 0,$$

for any $\delta > 0$, which completes the proof of (E.4).

F Proof of Theorem C.1

The proof consists of three steps. In the first step, we approximate $f_{0,S}$ by a specially designed multinary-product tree called the equal probability-product tree, which is populationally identifiable. The second step is to approximate the equal probability-product tree by an identifiable multinary-product tree using Theorem D.2. The third step is to transfer the identifiable multinary-product tree obtained in the second step into a sum of identifiable binary-product trees whose heights are bounded.

F.1 Approximation of $f_{0,S}$ by the equal probability-product tree

We first approximate $f_{0,S}$ by a specially designed populationally identifiable multinary-product tree so called the EP-product (equal probability-product) tree. For a positive integer r, let $q_{j,\ell}, \ell = 1, \ldots, r$ be the $\ell \cdot 100/r\%$ quantiles of \mathbb{P}_j , the distribution of X_j . Let $\mathcal{P}_{r,j}^{\mathrm{EP}}$ be the partition of \mathcal{X}_j consisting of $(q_{j,(\ell-1)}, q_{j,\ell}], \ell = 1, \ldots, r$ with $q_{j,0} = 0$, which we call the equal-probability partition of size r. Then, the EP-product tree with the parameters $S, \mathcal{P}_r^{\mathrm{EP}} = \prod_{j \in S} \mathcal{P}_{r,j}^{\mathrm{EP}}$ and $\gamma = \{\gamma_{\ell} \in \mathbb{R}, \ell \in \{1, \ldots, r\}^{|S|}\}$ is defined as

$$f_{S,\mathcal{P}_r^{\mathrm{EP}},\gamma}(\mathbf{x}_S) = \sum_{\boldsymbol{\ell}} \gamma_{\boldsymbol{\ell}} \mathbb{I}(\mathbf{x}_S \in I_{\boldsymbol{\ell}}).$$

That is, the EP-product tree is a multinary-product tree defined on the product partition $\mathcal{P}_r^{\text{EP}}$. The next lemma is about the approximation of a smooth function by an EP-product tree.

Lemma F.1. Define

$$\gamma_{\boldsymbol{\ell}} = \frac{1}{\mathbb{P}_S^{ind}(I_{\boldsymbol{\ell}})} \int_{I_{\boldsymbol{\ell}}} f_{0,S}(\mathbf{x}_S) \mathbb{P}_S^{ind}(d\mathbf{x}_S)$$

for all $\ell \in [r]^{|S|}$. Then, $f_{S,\mathcal{P}_r^{EP},\gamma}$ is populationally identifiable and it satisfies the following

error bound:

$$\sup_{\mathbf{x}_S \in \mathcal{X}_S} |f_{0,S}(\mathbf{x}_S) - f_{S,\mathcal{P}_r^{EP},\gamma}(\mathbf{x}_S)| \le ||f_{0,S}||_{\mathcal{H}^{\alpha}} \left(\frac{\sqrt{|S|}}{rp_L}\right)^{\alpha},$$

where $p_L = \inf_{\mathbf{x} \in \mathcal{X}} p_{\mathbf{X}}(\mathbf{x})$.

Proof. For $\mathbf{x}_S \in I_{\ell}$,

$$\begin{aligned} &|f_{0,S}(\mathbf{x}_S) - f_{S,\mathcal{P}_r^{EP},\gamma}(\mathbf{x}_S)| \\ &= \left| f_{0,S}(\mathbf{x}_S) - \frac{1}{\mathbb{P}_S^{\operatorname{ind}}(I_{\boldsymbol{\ell}})} \int_{I_{\boldsymbol{\ell}}} f_{0,S}(\mathbf{x}_S') \mathbb{P}_S^{\operatorname{ind}}(d\mathbf{x}_S') \right| \\ &\leq \frac{1}{\mathbb{P}_S^{\operatorname{ind}}(I_{\boldsymbol{\ell}})} \int_{I_{\boldsymbol{\ell}}} |f_{0,S}(\mathbf{x}_S) - f_{0,S}(\mathbf{x}_S')| \mathbb{P}_S^{\operatorname{ind}}(d\mathbf{x}_S') \\ &\leq \frac{1}{\mathbb{P}_S^{\operatorname{ind}}(I_{\boldsymbol{\ell}})} ||f_{0,S}||_{\mathcal{H}^{\alpha}} \int_{I_{\boldsymbol{\ell}}} ||\mathbf{x}_S - \mathbf{x}_S'||_2^{\alpha} \mathbb{P}_S^{\operatorname{ind}}(d\mathbf{x}_S') \\ &\leq ||f_{0,S}||_{\mathcal{H}^{\alpha}} \sup_{\mathbf{x}_S' \in I_{\boldsymbol{\ell}}} ||\mathbf{x}_S - \mathbf{x}_S'||_2^{\alpha}, \end{aligned}$$

where $\|\cdot\|_2$ is the Euclidean norm for a vector, i.e., for a given vector $\mathbf{e} = (e_1, ..., e_n)$, $\|\mathbf{e}\|_2 = \sqrt{\sum_{i=1}^n e_i^2}$. Since I_{ℓ} is a |S|-dimensional hyper-cube whose side lengths are less than $1/(rp_L)$, we have $\|\mathbf{x}_S - \mathbf{x}_S'\|_2 \leq \sqrt{|S|}/(rp_L)$, which completes the proof of the approximation error bound.

For the populational identifiability condition, let $\mathbf{x}_{-j} = (x_{\ell}, \ell \in S, \ell \neq j)$ for a given \mathbf{x}_{S} and let $\boldsymbol{\ell}_{-j}$ be the index in $\{1, \dots, r\}^{|S|-1}$ such that $\mathbf{x}_{-j} \in I_{\boldsymbol{\ell}_{-j}}$. We will show

$$\int_{\mathcal{X}_j} f_{S, \mathcal{P}_r^{EP}, \gamma}(\mathbf{x}_S) \mathbb{P}_j(dx_j) = 0$$

for all $\mathbf{x}_{-j} \in \mathcal{X}_{-j}$ and $j \in S$. For a given $k \in \{1, \dots, r\}$, let $\ell(k) \in \{1, \dots, r\}^{|S|}$ be an index

defined as $\ell(k)_{-j} = \ell_{-j}$ and $\ell(k)_j = k$. Then,

$$\begin{split} &\int_{\mathcal{X}_{j}} f_{S,\mathcal{P}_{r}^{EP},\gamma}(\mathbf{x}_{S}) \mathbb{P}_{j}(dx_{j}) \\ &= \sum_{k=1}^{r} \frac{1}{\mathbb{P}_{S}^{\operatorname{ind}}(I_{\boldsymbol{\ell}(k)})} \int_{I_{\boldsymbol{\ell}(k)}} f_{0,S}(\mathbf{x}_{S}') \mathbb{P}_{S}^{\operatorname{ind}}(d\mathbf{x}_{S}') \mathbb{P}_{j}(I_{j,k}) \\ &= \frac{1}{\mathbb{P}_{S\backslash\{j\}}^{\operatorname{ind}}(I_{\boldsymbol{\ell}-j})} \sum_{k=1}^{r} \int_{I_{\boldsymbol{\ell}(k)}} f_{0,S}(\mathbf{x}_{S}') \mathbb{P}_{S}^{\operatorname{ind}}(d\mathbf{x}_{S}') \\ &= \frac{1}{\mathbb{P}_{S\backslash\{j\}}^{\operatorname{ind}}(I_{\boldsymbol{\ell}-j})} \int_{I_{\boldsymbol{\ell}-j}} \int_{\mathcal{X}_{j}} f_{0,S}(\mathbf{x}_{S}') \mathbb{P}_{j}(dx_{j}') \mathbb{P}_{S\backslash\{j\}}^{\operatorname{ind}}(d\mathbf{x}_{-j}') \\ &= 0, \end{split}$$

since $\int_{\mathcal{X}_j} f_{0,S}(\mathbf{x}_S') \mathbb{P}_j(dx_j') = 0$ for all \mathbf{x}_{-j}' by the populational identifiability of $f_{0,S}$.

F.2 Approximation of the EP-product tree by an identifiable multinary-product tree

Since the EP-product tree $f_{S,\mathcal{P}_r^{EP},\gamma}$ in Section F.1 is a populationally identifiable multinary-product tree, we can apply Theorem D.2 to obtain an identifiable multinary-product tree $f_{S,\mathcal{P}_r^{EP},\hat{\gamma}}$ such that

$$\sup_{\mathbf{x}_{S}} |f_{S,\mathcal{P}_{r}^{EP},\gamma}(\mathbf{x}_{S}) - f_{S,\mathcal{P}_{r}^{EP},\hat{\gamma}}(\mathbf{x}_{S})| \le (24F + 1)2^{|S|} \sqrt{\frac{r^{|S|} \log n}{n}}$$

with probability at least $1 - 2^{|S|+1} |S| r^{|S|} \exp\left(-\frac{r^{|S|} \log n}{4F^2}\right)$ under $\mathbb{P}^n_{\mathbf{X}}$.

To sum up, we have shown that the modified EP tree $f_{S,\mathcal{P}_r^{EP},\hat{\gamma}}$ approximates $f_{0,S}$ well

in the sense that

$$\sup_{\mathbf{x}} |f_{0,S}(\mathbf{x}) - f_{S,\mathcal{P}_r^{EP},\hat{\gamma}}(\mathbf{x})| \leq \sup_{\mathbf{x}} |f_{0,S}(\mathbf{x}) - f_{S,\mathcal{P}_r^{EP},\gamma}(\mathbf{x})| + \sup_{\mathbf{x}} |f_{S,\mathcal{P}_r^{EP},\gamma}(\mathbf{x}) - f_{S,\mathcal{P}_r^{EP},\hat{\gamma}}(\mathbf{x})| \\
\leq ||f_{0,S}||_{\mathcal{H}^{\alpha}} \left(\frac{m}{r}\right)^{\alpha} + (24F + 1)2^{|S|} \sqrt{\frac{r^{|S|} \log n}{n}}.$$

with probability at least $1 - 2^{|S|+1}|S|r^{|S|^2} \exp\left(-\frac{r^{|S|}\log n}{4F^2}\right)$ with resepect to $\mathbb{P}^n_{\mathbf{X}}$, where $m = \sqrt{|S|/p_L}$.

F.3 Decomposition of the modified EP-product tree by a sum of identifiable binary-product trees with bounded heights

The final step is to decompose the modified EP-product tree which satisfies the identifiability condition into the sum of identifiable binary-product trees with bounded heights.

F.3.1 Notations

Let \mathcal{P}_j be an interval partition of \mathcal{X}_j with $|\mathcal{P}_j| = \phi_j$. That is, $\mathcal{P}_j = \{I_{j,k}, k = 1, \ldots, \phi_j\}$, where $I_{j,k}$ s are disjoint intervals of \mathcal{X}_j with $\bigcup_k I_{j,k} = \mathcal{X}_j$. Without loss of generality, we assume that the intervals are ordered such that $I_{j,k} < I_{j,k'}$ whenever k < k'. Here $I_{j,k} < I_{j,k'}$ means that for any $z \in I_{j,k}$ and $z' \in I_{j,k'}$, we have z < z'. That is, the indices of the intervals in each interval partition are sorted from left to right.

For $S \subseteq [p]$, let f be an identifiable multinary-product tree defined on the partitions $\mathcal{P}_j, j \in S$ given as

$$f(\mathbf{x}_S) = \sum_{\ell} \gamma_{\ell} \prod_{j \in S} \mathbb{I}(x_j \in I_{j,\ell_j}),$$

where γ_{ℓ} is the height vector for $\ell \in \prod_{j \in S} [\phi_j]$. We introduce several notations related to f.

• $part(f)_j = \mathcal{P}_j$: interval partition of \mathcal{X}_j .

- order $(f)_j = |\operatorname{part}(f)_j| (= \phi_j)$, order $(f) = (\phi_j, j \in S)$.
- index $(f) = \prod_{j \in S} [\phi_j]$: the set of indices for the product partition $\prod_{j \in S} \mathcal{P}_j$.
- $\gamma = (\gamma_{\ell}, \ell \in index(f)).$
- For given $\ell \in \operatorname{index}(f)$ and $\ell \in [\phi_j]$, let $\ell_{+(j,\ell)}$ be the element in $\operatorname{index}(f)$ obtained by replacing ℓ in the jth position of ℓ . That is $\ell_{+(j,\ell)} = (\ell_1, \dots, \ell_{j-1}, \ell, \ell_{j+1}, \dots, \ell_{|S|})$.

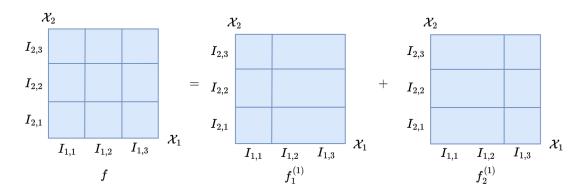


Figure F.4: Example of decomposing the partition of f into the partitions of $f_1^{(1)}$ and $f_2^{(1)}$.

F.3.2 Proof of the decomposition

The strategy of the decomposition is to decompose a given identifiable multinary-product tree into the sum of two sibling identifiable multinary-product trees whose orders are smaller than their parent identifiable multinary-product tree. Figure F.4 presents an example of decomposing the partition of an identifiable multinary-product tree f for $S = \{1, 2\}$ and $\phi_1 = \phi_2 = 3$ into two partitions of child identifiable multinary-product trees $f_1^{(1)}$ and $f_2^{(1)}$, where $\operatorname{order}(f_1)_1 = 2$, $\operatorname{order}(f_1)_2 = 3$, $\operatorname{order}(f_2)_1 = 2$, and $\operatorname{order}(f_2)_2 = 3$. We repeat this decomposition until the orders of all identifiable multinary-product trees become 2. Figure F.5 presents an example of decomposing the partition of a identifiable multinary-product tree f into four partitions of identifiable binary-product trees $f_{1,1}^{(1,2)}$, $f_{1,2}^{(1,2)}$, $f_{2,1}^{(1,2)}$, and $f_{2,2}^{(1,2)}$,

where $\operatorname{order}(f_{i,j}^{(1,2)})_k = 2$ for i = 1, 2, k = 1, 2 and j = 1, 2. The following lemma is the key tool whose proof is given in Section F.3.3 and F.3.4.

Lemma F.2. Let f be an identifiable multinary-product tree of \mathbf{x}_S . Suppose that there exists $h \in S$ such that $order(f)_h > 2$. Then, there exist $order(f)_h - 1$ many identifiable multinary-product trees $f_j, j = 1, \ldots, \phi_h - 1$ such that

$$f(\cdot) = f_1(\cdot) + \dots + f_{\phi_h - 1}(\cdot),$$

where $\operatorname{order}(f_j)_k = \operatorname{order}(f)_k$ for all $j \in [\phi_h - 1]$ when $k \neq h$ and $\operatorname{order}(f_j)_h = 2$ for all $j \in [\phi_h - 1]$. Moreover, $\sup_j \|f_j\|_{\infty} \leq 2\|f\|_{\infty}$.

We will prove the decomposition by use of Lemma F.2. Let f be a given EP-product tree of the component S with $\operatorname{order}(f)_j = r$ for all $j \in S$, which we are going to decompose. Without loss of generality, we let $S = \{1, 2, \dots, |S|\}$. At first, we apply Lemma F.2 to decompose $f(\cdot) = \sum_{k_1=1}^{r-1} f_{k_1}^{(1)}(\cdot)$, where $f_{k_1}^{(1)}$ s are identifiable multinary-product trees such that $\operatorname{order}(f_{k_1}^{(1)})_1 = 2$ and $\operatorname{order}(f_{k_1}^{(1)})_\ell = r, \ell \geq 2$ for all $k_1 = 1, \dots, r-1$ and $\sup_{k_1} \|f_{k_1}^{(1)}\|_{\infty} \leq 2\|f\|_{\infty}$.

In turn, we can decompose each $f_{k_1}^{(1)}$ by a sum of identifiable multinary-product trees such that $f_{k_1}^{(1)}(\cdot) = \sum_{k_2=1}^{m-1} f_{k_1,k_2}^{(1,2)}(\cdot)$, where $\operatorname{order}(f_{k_1,k_2}^{(1,2)})_{\ell} = 2, \ell = 1, 2$ and $\operatorname{order}(f_{k_1,k_2}^{(1,2)})_{\ell} = r, l \geq 3$ and $\sup_{k_1,k_2} \|f_{k_1,k_2}^{(1,2)}\|_{\infty} \leq 2^2 \|f\|_{\infty}$. We repeat this decomposition to have $f_{k_1,\dots,k_{|S|}}^{(1,\dots,|S|)}(\cdot)$ such that

$$f(\cdot) = \sum_{k_1}^{r-1} \cdots \sum_{k_{|S|}=1}^{r-1} f_{k_1,\dots,k_{|S|}}^{(1,\dots,|S|)}(\cdot) \quad \text{with} \quad \operatorname{order}(f_{k_1,\dots,k_{|S|}}^{(1,\dots,|S|)})_{\ell} = 2$$

 $\text{for all } \ell \in S \text{ and } \sup_{k_1, \dots, k_{|S|}} \|f_{k_1, \dots, k_{|S|}}^{(1, \dots, |S|)}\|_{\infty} \leq 2^{|S|} \|f\|_{\infty}, \text{ which completes the proof.}$

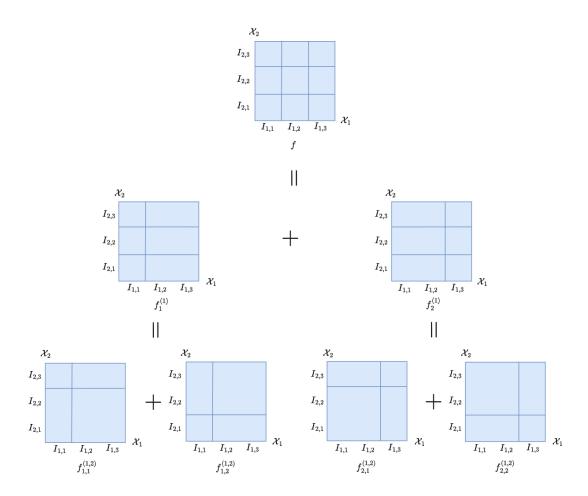


Figure F.5: Example of decomposing partition of f into the partitions of identifiable binary-product trees $f_{1,1}^{(1,2)}$, $f_{1,2}^{(1,2)}$, $f_{2,1}^{(1,2)}$, and $f_{2,2}^{(1,2)}$.

F.3.3 Proof of Lemma F.2 for |S| = 1

For $j \in [r]$, let $\mathbf{1}_j$ be the r-dimensional vector such that the first j many entries are 1 and the others are 0. That is, $\mathbf{1}_j = (\underbrace{1,1,\ldots,1}_{j \text{ times}},\underbrace{0,0,\ldots,0}_{r-j \text{ times}})^{\top}$. Let $\mathbf{1}_j^c = \mathbf{1}_r - \mathbf{1}_j$, that is, $\mathbf{1}_j^c = (\underbrace{0,0,\ldots,0}_{j \text{ times}},\underbrace{1,1,\ldots,1}_{r-j \text{ times}})^{\top}$. Let $\mathcal{S}^r = \{\mathbf{w} \in \mathbb{R}^r : w_j \geq 0, \forall j \in [r], \sum_{j=1}^r w_j = 1\}$. For a given $\mathbf{w} \in \mathcal{S}^r$, let $\mathbb{R}_{\mathbf{w}}^r = \{\mathbf{u} \in \mathbb{R}^r : \mathbf{w}^T \mathbf{u} = 0\}$. In addition, let $\mathbf{w}_{s:t} = \sum_{j=s}^t w_j$.

Claim: Fix $\mathbf{w} \in \mathcal{S}^r$. For any $\mathbf{u} \in \mathbb{R}^r_{\mathbf{w}}$, there exist pairs of real numbers $(a_j, b_j), j =$

 $1, \ldots, r-1$ such that

$$\mathbf{u} = \sum_{j=1}^{r-1} (a_j \mathbf{1}_j + b_j \mathbf{1}_j^c), \tag{F.1}$$

$$\mathbf{w}^{\top}(a_j \mathbf{1}_j + b_j \mathbf{1}_j^c) = 0 \tag{F.2}$$

for all $j \in [r-1]$ and

$$\max\{|a_j|, |b_j| : j \in [r-1]\} \le 2\|\mathbf{u}\|_{\infty}.$$

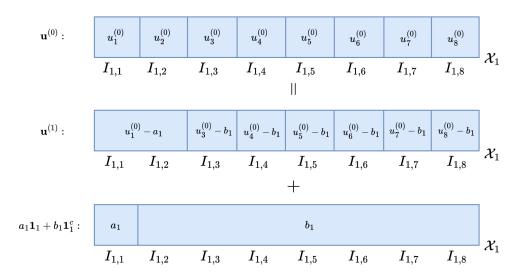


Figure F.6: Decomposition of $\mathbf{u}^{(0)}$ into $\mathbf{u}^{(1)}$ and $(a_1\mathbf{1}_1+b_1\mathbf{1}_1^c)$ in the case of r=8.

Proof. Let $\mathbf{u}^{(0)} = \mathbf{u}$ and we define $\mathbf{u}^{(1)}$ as

$$\mathbf{u}^{(1)} = \mathbf{u}^{(0)} - (a_1 \mathbf{1}_1 + b_1 \mathbf{1}_1^c),$$

where $a_1 = (1 - w_1)(u_1^{(0)} - u_2^{(0)})$ and $b_1 = w_1(u_2^{(0)} - u_1^{(0)})$. It is easy to see that $\mathbf{w}^{\top}(a_1\mathbf{1}_1 + b_1\mathbf{1}_1^c) = 0$ and thus $\mathbf{w}^{\top}\mathbf{u}^{(1)} = 0$. Moreover, we have $u_j^{(1)} = u_j^{(0)} - b_1$ for j = 3, ..., r and $u_1^{(1)} = u_1^{(0)} - a_1$. In addition, it can be shown that $u_1^{(1)} = u_2^{(1)}$. Figure F.6 presents an

example of this decomposition in the case of r = 8.

For $k \in \{2, ..., r-2\}$, we define $\mathbf{u}^{(k)}$ recursively as

$$\mathbf{u}^{(k)} := \mathbf{u}^{(k-1)} - (a_k \mathbf{1}_k + b_k \mathbf{1}_k^c), \tag{F.3}$$

where $a_k = (1 - \mathbf{w}_{1:k})(u_k^{(k-1)} - u_{k+1}^{(k-1)})$ and $b_k = \mathbf{w}_{1:k}(u_{k+1}^{(k-1)} - u_k^{(k-1)})$. It is not difficult to see that $\mathbf{w}^{\top}(a_k \mathbf{1}_k + b_k \mathbf{1}_k^c) = 0$ (and thus $\mathbf{w}^{\top}\mathbf{u}^{(k)} = 0$) because $\mathbf{w}^{\top}\mathbf{u}^{(k-1)} = 0$. In addition, we have $u_1^{(k-1)} = \cdots = u_k^{(k-1)}$ for $k \in [r-2]$.

To complete the proof, we will show that $\mathbf{u}^{(r-2)}$ can be expressed as

$$\mathbf{u}^{(r-2)} = a_{r-1} \mathbf{1}_{r-1} + b_{r-1} \mathbf{1}_{r-1}^c$$

where $a_{r-1} = w_r(u_{r-1}^{(r-3)} - u_r^{(r-3)})$ and $b_{r-1} = (1 - w_r)(u_r^{(r-3)} - u_{r-1}^{(r-3)})$. Note that, since $u_1^{(r-3)} = \cdots = u_{r-2}^{(r-3)}$ and $\mathbf{w}^{\top} \mathbf{u}^{(r-3)} = 0$, it holds that

$$\mathbf{w}_{1:r-2}u_s^{(r-3)} + w_{r-1}u_{r-1}^{(r-3)} + w_ru_r^{(r-3)} = 0$$
(F.4)

for $s \in [r-2]$. For $s \in [r-2]$, we have

$$u_s^{(r-2)} = u_s^{(r-3)} - a_{r-2}$$

$$= u_s^{(r-3)} - (w_{r-1} + w_r)(u_{r-2}^{(r-3)} - u_{r-1}^{(r-3)})$$

$$= w_r(u_{r-1}^{(r-3)} - u_r^{(r-3)}).$$
(F.5)

In turn, it follows that

$$u_{r-1}^{(r-2)} = u_{r-1}^{(r-3)} - b_{r-2}$$

$$= u_{r-1}^{(r-3)} - \mathbf{w}_{1:r-2} (u_{r-1}^{(r-3)} - u_{r-2}^{(r-3)})$$

$$= u_{r-1}^{(r-3)} - \mathbf{w}_{1:r-2} u_{r-1}^{(r-3)} - w_{r-1} u_{r-1}^{(r-3)} - w_r u_r^{(r-3)}$$

$$= w_r (u_{r-1}^{(r-3)} - u_r^{(r-3)}).$$
(F.6)

and

$$u_r^{(r-2)} = u_r^{(r-3)} - b_{r-2}$$

$$= u_r^{(r-3)} - \mathbf{w}_{1:r-2} (u_{r-1}^{(r-3)} - u_{r-2}^{(r-3)})$$

$$= u_r^{(r-3)} - \mathbf{w}_{1:r-2} u_{r-1}^{(r-3)} - w_{r-1} u_{r-1}^{(r-3)} - w_r u_r^{(r-3)}$$

$$= (1 - w_r) (u_r^{(r-3)} - u_{r-1}^{(r-3)}).$$
(F.7)

Here, (F.5), (F.6), and (F.7) are due to $u_1^{(r-3)} = \cdots = u_{r-2}^{(r-3)}$ and (F.4). Thus, (F.3) holds with $\mathbf{u}^{(r-1)} = \mathbf{0}$. Hence, we complete the proof of the existence of the real numbers $(a_j, b_j), j = 1, ..., r-1$, satisfies (F.1).

Now, we will prove the upper bound of $\max\{|a_j|, |b_j| : j \in [r-1]\}$. For $k \in [r-2]$, we have $u_{k+1}^{(k-1)} - u_k^{(k-1)} = u_{k+1}^{(0)} - u_k^{(0)}$ and thus $|a_k| \le 2 \|\mathbf{u}\|_{\infty}$ and $|b_k| \le 2 \|\mathbf{u}\|_{\infty}$ which completes the proof of **Claim**.

Let f be an identifiable multinary-product tree f for $S = \{h\}$, i.e, $f(x_h) = \sum_{j=1}^r \gamma_j \mathbb{I}(x_h \in I_{h,j})$, where $I_{h,j}$ s are an interval partition of \mathcal{X}_h . We let $\mathbf{u} = (\gamma_j, j \in [r])$ and $\mathbf{w} = (\mu_{n,h}\{I_{h,j}\}, j \in [r])$ and apply **Claim** to have $f(x_h) = \sum_{j=1}^{r-1} f_j^{(h)}(x_h)$, where each $f_j^{(h)}$ is an identifiable binary-product tree with the binary partition $\{\bigcup_{\ell=1}^{j+1} I_{h,\ell}, \bigcup_{\ell=j+1}^r I_{h,\ell}\}$ and

the height vector (a_j, b_j) .

F.3.4 Proof of Lemma F.2 for general S

Fix $\ell \in \operatorname{index}(f)$ and $h \in S$. Let $\mathbf{u}_{\ell,h} = (\gamma_{\ell_{+(h,j)}}, j \in [r])$. Applying **Claim** in Section F.3.3 of Supplementary Material to $\mathbf{u}_{\ell,h}$ with $\mathbf{w} = (\mu_{n,h}\{I_{h,j}\}, j \in [r])$, we have

$$\mathbf{u}_{\ell,h} = \sum_{j=1}^{r-1} (a_j^{(\ell,h)} \mathbf{1}_j + b_j^{(\ell,h)} \mathbf{1}_j^c).$$

Now, for $j \in [r-1]$, we define $f_j^{(h)}$ as the multinary-product tree with the interval partitions $\mathcal{P}_k^{(j)}, k \in S$ and the height vector $\boldsymbol{\gamma}^{(j)}$ such that $\mathcal{P}_k^{(j)} = \mathcal{P}_k$ for $k \neq h$, $\mathcal{P}_h^{(j)} = \{\bigcup_{m=1}^{j} I_{h,m}, \bigcup_{m=j+1}^{r} I_{h,m}\}, \ \boldsymbol{\gamma}_{\boldsymbol{\ell}+(h,1)}^{(j)} = a_j^{(\boldsymbol{\ell},h)}, \ \text{and} \ \boldsymbol{\gamma}_{\boldsymbol{\ell}+(h,2)}^{(j)} = b_j^{(\boldsymbol{\ell},h)} \ \text{for} \ \boldsymbol{\ell} \in \text{index}(f).$ Since $|a_j^{(\boldsymbol{\ell},h)}| \vee |b_j^{(\boldsymbol{\ell},h)}| \leq 2\|\mathbf{u}_{\boldsymbol{\ell},h}\|_{\infty} \leq 2\|f\|_{\infty}$, we have $\|f_j^{(h)}\|_{\infty} \leq 2\|f\|_{\infty}$ for j = [r-1].

The final mission is to show that $f_j^{(h)}$ s satisfy the identifiability condition, i.e.,

$$\int_{\mathcal{X}_k} f_j^{(h)}(\mathbf{x}_S) \mu_{n,k}(dx_k) = 0$$

for $k \in S$. First, $\int_{\mathcal{X}_k} f_j^{(h)}(\mathbf{x}_S) \mu_{n,k}(dx_k) = 0$ for k = h by (F.2). For $k \neq h$, the proof of **Claim** reveals that there exists r-dimensional vectors $\mathbf{v}_1^{(j)}$ and $\mathbf{v}_2^{(j)}$ such that $\gamma_{\boldsymbol{\ell}_+(h,m)}^{(j)} = \mathbf{v}_m^{(j)\top} \gamma_{\boldsymbol{\ell}_+(h,\cdot)}$, for m = 1, 2, where $\gamma_{\boldsymbol{\ell}_+(h,\cdot)} = (\gamma_{\boldsymbol{\ell}_+(h,j)}, j \in [r])$. Thus, for m = 1, 2, we have

$$\mathbb{E}_{\mu_n,k}(\gamma_{\boldsymbol{\ell}_{+(h,m)}}^{(j)}) = \mathbf{v}_m^{(j)\top} \mathbb{E}_{\mu_n,k}(\gamma_{\boldsymbol{\ell}_{+(h,\cdot)}}) = 0$$
 (F.8)

since γ satisfies the identifiability condition, where

$$\mathbb{E}_{\mu_n,k}(\gamma_{\boldsymbol{\ell}_{+(h,\cdot)}}) = \left(\mathbb{E}_{\mu_n,k}(\gamma_{\boldsymbol{\ell}_{+(h,1)}}),...,\mathbb{E}_{\mu_n,k}(\gamma_{\boldsymbol{\ell}_{+(h,r)}})\right)^{\top}$$

and $\mathbb{E}_{\mu_n,k}(\cdot)$ is defined in (D.1).

In conclusion, the function f can be decomposed as

$$f(\cdot) = \sum_{j=1}^{r-1} f_j^{(h)}(\cdot),$$

where $f_j^{(h)}$ satisfies the identifiability condition and $||f_j^{(h)}||_{\infty} \le 2||f||_{\infty}$ for j = [r-1]. By applying **Claim** sequentially to $f_j^{(h)}$ s for other variables $S \setminus \{h\}$, the proof is done.

G Discussion about the posterior concentration rate for the X-fixed Design

A key issue of ANOVA-BART for the X-fixed design is how to define $f_{0,S}$. For a given f_0 , Theorem 2.1 yields a unique ANOVA decomposition with respect to μ_n , whose interactions are identifiable. Recall that the proof of the posterior convergence rate for the X-random design consists of the two main parts: (1) for $\mathbf{x}^{(n)} \in A_n$, where A_n is defined in (C.8), the posterior convergence rate is ϵ_n and (2) the probability of A_n converges to 1. Thus, for the X-fixed design, the mission is to figure out sufficient conditions for $\mathbf{x}^{(n)} \in A_n$ with $f_{0,S}$ defined in Theorem 2.1 with respect to μ_n .

In order that $\mathbf{x}^{(n)} \in A_n$, there exists a sum of identifiable binary-product trees that approximates $f_{0,S}$ closely for each $S \subseteq [p]$. In Section F.1, we show that the EP-tree, which satisfies the populational identifiability condition, approximates $f_{0,S}$ closely for the X-random design. We can modify this proof to show that the empirical EP-tree, which satisfies the identifiability condition, approximates $f_{0,S}$ closely for the X-fixed design when there exists a positive constant C_2 such that, for all $r \in [n]$,

$$\max_{A \in \mathcal{P}_r^{nEP}} \operatorname{Diam}(A) \le C_2/r,$$

where $\operatorname{Diam}(A) := \max_{\mathbf{v}, \mathbf{w} \in A} \|\mathbf{v} - \mathbf{w}\|_2$ and \mathcal{P}_r^{nEP} denotes the equal-probability partition induced by the quantiles of the empirical distribution. Then, by letting the modified EP-tree defined in Section F.2 to be equal to the empirical EP-tree, all the results in Section F.2 to Section F.3 are satisfied. Thus, we conclude that the posterior convergence rate is ϵ_n as long as $\max_{A \in \mathcal{P}_r^{nEP}} \operatorname{Diam}(A) \leq C_2/r$ for all $r \in [n]$.

H Details of the experiments

In this section, we provide details of the experiments including hyperparameter selections.

H.1 Data standardization

The minimax scaling is applied to NAM, while the mean-variance standardization is used for ANOVA-BART, BART, SSANOVA and MARS. In addition, the one-hot encoding is applied to categorical covariates.

H.2 Hyperparameter selection

H.2.1 Experiments for prediction performance

For each method, we select the hyperparameters among the candidates based on 5-fold cross-validation. The candidate hyperparameters for each method are given as follows.

• ANOVA-BART

 $-\alpha_{\rm split}$ and $\gamma_{\rm split}$ in (9) are set to 0.95 and 2, respectively, following [4].

$$-v = \{1, 3, 5, 7, 9\}$$

– For λ , we reparameterize it to q_{λ} , where $q_{\lambda} = \pi(\sigma^2 \leq \hat{\sigma}^2)$ and $\hat{\sigma}^2$ is the variance of the residuals from a linear regression model estimated by the least square method. For the candidates of q_{λ} , we set $q_{\lambda} = \{0.90, 0.95, 0.99\}$. This approach is used in [4].

$$- T_{\text{max}} = \{100, 200, 300\}$$

$$-C_* = \{1e-6, 1e-4, 1e-2, 1\}$$

$$- \sigma_{\beta}^{2} = \{1e - 2, 1e - 1, 1\}$$

• BART ([4])

– $\alpha_{\rm split}, \gamma_{\rm split}, v, \lambda$: set to the same values as for ANOVA-BART

$$-T = \{50, 100, 200\}$$

$$- \sigma_{\beta}^2 = 1/T$$

• SSANOVA

- The smoothing parameter $\phi = \{1e-4, 1e-2, 1, 1e2, 1e4\}$
- The number of knots = $\{10, 30, 50\}$
- The maximum order of interaction = $\{1, 2\}$
- Further details on the hyperparameters of SSANOVA can be found in [13].

• MARS

- Maximum number of terms in the pruned model = $\{10, 30, 50, 100\}$
- The maximum order of interaction = $\{1, 2, 3\}$
- The smoothing parameter = $\{1, 2, 3, 4\}$
- Further details on the hyperparameters of MARS can be found in [38].

• NAM

- The number of hidden layers = 3 and the numbers of hidden nodes = (64, 32, 16)(the architecture used in [1, 44])
- Adam optimizer with learning rate 1e-4 and weight decay 7.483e-9

- Batch size = 256
- Epoch = $\{500, 1000\}$
- The maximum order of interaction = $\{1, 2\}$.

H.2.2 Experiments for component Selection

For the experiment of component selection on synthetic data, the hyperparameters for ANOVA-BART are set to $T_{\text{max}} = 300, v = 3, q_{\lambda} = 0.95, \text{ and } C_* = 1e - 2.$

H.2.3 Experiments for uncertainty quantification

The candidates of the hyperparameters of ANOVA-BART and BART are the same as those used in the prediction performance experiments.

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