Estimation and Inference with Trees and Forests in High Dimensions*

Vasilis Syrgkanis
Microsoft Research
vasy@microsoft.com

Manolis Zampetakis
MIT
mzampet@mit.edu

Abstract

We analyze the finite sample mean squared error (MSE) performance of regression trees and forests in the high dimensional regime with binary features, under a sparsity constraint. We prove that if only \( r \) of the \( d \) features are relevant for the mean outcome function, then shallow trees built greedily via the CART empirical MSE criterion achieve MSE rates that depend only logarithmically on the ambient dimension \( d \). We prove upper bounds, whose exact dependence on the number relevant variables \( r \) depends on the correlation among the features and on the degree of relevance. For strongly relevant features, we also show that fully grown honest forests achieve fast MSE rates and their predictions are also asymptotically normal, enabling asymptotically valid inference that adapts to the sparsity of the regression function.

1 Introduction

Regression Trees [BFOS84] and their ensemble counterparts, Random Forests [Bre01], are one of the most widely used estimation methods by machine learning practitioners. Despite their widespread use, their theoretical underpinnings are far from being fully understood. Early works established sample complexity bounds of decision trees and other data-adaptive partitioning estimators [Nob96, LN96, MM00]. However, sample complexity bounds do not address the computational aspect of how to choose the best tree in the space. In practice, trees and forests are constructed in a greedy fashion, typically identifying the most empirically informative split at each step; an approach pioneered by [BFOS84, Bre01]. The consistency and estimation rates of such greedily built trees has proven notoriously more difficult to analyze.

Recent breakthrough advances has shown that such greedily built trees are asymptotically consistent [Bia10, DMdF14, SBV15] in the low dimensional regime, where the number of features is a constant independent of the sample size. In another line of work, [MH16, WA18] provide asymptotic normality results for honest versions of Random Forests, where each tree is constructed using a random sub-sample of the original data and further each tree construction algorithm sub-divides the sub-sample into a random half-sample that is used for construction of the tree structure and a separate half-sample used for the leaf estimates. However, these results are typically asymptotic or their finite sample guarantees scale exponentially with the number

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of features. Random Forests are used in practice to address estimation with high-dimensional features. Hence, these works, though of immense theoretical importance in our understanding of adaptively built trees and forests, they do not provide theoretical foundations of the finite sample superiority of these algorithms in practice.

In this work, we analyze the performance of regression trees and forests in the high-dimensional regime, where the number of features can grow exponentially with the number of samples. To focus on the high-dimensionality of the features (as opposed to the ability of forests to sub-divide continuous variable spaces), we constrain our analysis to the case when all features are binary.

We show that trees and forests built greedily based on the original CART criterion, provably adapt to sparsity: when only a subset $R$, of size $r$, of the features are relevant, then the mean squared error of appropriately shallow trees, or fully grown honest forests, scales exponentially only with the number of relevant features and depends only logarithmically on the overall number of features. We analyze two variants of greedy tree algorithms: in the level-split variant, the same variable is chosen at all the nodes of each level of the tree and is greedily chosen so as to maximize the overall variance reduction. In the second variant, which is the most popular in practice, the choice of the next variable to split on is locally decided at each node of the tree.

We identify three regimes, each providing different dependence on the number of relevant features. When the relevant variables are “weakly” relevant (in the sense that there is not strong separation between the relevant and irrelevant variables in terms of their ability to reduce variance), then shallow trees achieve “slow rates” on the mean squared error of the order of $2^r / \sqrt{n}$, when variables are independent, and $1/n^{1/(r+2)}$, when variables are dependent. When the relevant variables are “strongly” relevant, in that there is a separation in their ability to reduce variance as compared to the irrelevant ones, by a constant $\beta_{\text{min}}$, then we show that greedily built shallow trees and fully grown honest forests can achieve fast parametric mean squared error rates of the order of $2^r / (\beta_{\text{min}} n)$.

When variables are strongly relevant, we also show that the predictions of sub-sampled honest forests have an asymptotically normal distribution centered around their true values and whose variance scales at most as $O(2^r \log(n) / (\beta_{\text{min}} n))$. Thus sub-sampled honest forests are provably a data-adaptive method for non-parametric inference, that adapts to the latent sparsity dimension of the data generating distribution, as opposed to classical non-parametric regression approaches, whose variance would deteriorate drastically with the overall number of features. Our results show that, at least for the case of binary features, forest based algorithms can offer immense improvement on the statistical power of non-parametric hypothesis tests in high-dimensional regimes.

The main crux of our analysis is showing bounds on the decay of the bias of decision trees, constructed via the mean-squared-error criterion. In particular, we show that either a relevant variable leads to a large decrease in the mean squared error, in which case we prove that with high probability it is chosen in the first few levels of the tree or if not then it’s impact on the mean squared due to the fact that the algorithm failed to choose it can be controlled. For achieving the fast rates of $1/n$ for shallow trees, we also develop a new localized Rademacher analysis [BBM02, Wai19] for adaptive partitioning estimators [GKKW06] to provide fast rates for the “variance” part of the MSE. Our results on honest forests, utilize recent work on the concentration and asymptotic normality of sub-sampled estimators [MH16, WA18, FLW18] and combine it with our proof of the bias decay, which for the case of strongly relevant features, as we show, is exponential in the number of samples.
Several theoretical aspects of variants of CART trees and forests have been analyzed in the recent years [LJ02, Mei06, AG14, Bre04, Sco16]. The majority of these works deal with the low dimensional regime and with few exceptions, these results deal with trees built with random splitting criteria or make no use of the fact that splits are chosen to minimize the CART mean-squared-error criterion. Arguably, closest to our work is that of [WW15], who consider a high dimensional regime with continuous variables, distributed according to a distribution with continuous density and uniformly upper and lower bounded. The main focus of this work is proving a uniform concentration bound on the mean squared error objective locally at every node of the adaptively constructed tree and for this reason makes several assumptions not present in our work: e.g. minimum leaf size constraints, approximately balanced splits. Crucially, their results on random forest consistency require an analogue of our $\beta_{\min}$ condition, and do not offer results without strong relevance. Moreover, their results on the consistency of forests requires a strong modification of the CART algorithm: split variables are selected based on initial median splits, subject to a lower bound on the decrease in variance, and then only the chosen variables are used in subsequent splits, not based on a CART criterion, but rather simply choosing random median splits; invoking an analysis of such random median trees in low dimensions by [DS16]. Moreover, they provide no results on asymptotic normality.

Apart from the literature related to Random Forests and the CART criterion, there has been a great amount of work on the sparse non-parametric regression problem that we consider in this paper. A lot of heuristic methods have been proposed such as: $C_p$ and AIC for additive models [HTF09], MARS [Fri91], Bayesian methods [GM97], Gaussian Processes [SB01] and more. All these methods are very successful in many practical scenarios but our theoretical understanding of their performance is limited. Our work is closer related to the works of [LW+08, LC09, CD12, YT15] and citations therein, where they propose and theoretically analyze greedy algorithms that exploit the sparsity of the input regression function and hence they provide a way to overcome the curse of dimensionality of high dimensional data in non-parametric regression. The main difference of this line of work with our paper is that we do not propose a new algorithm but instead our goal is to analyze the performance of the heuristically proposed CART trees in the setting of sparse high-dimensional non-parametric regression with binary features.

2 Model and Preliminaries

In this work we consider the non-parametric regression model with binary features. More precisely, we assume that we have access to a training set $D_n = \{(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})\}$, which consists of $n$ i.i.d. samples of the form $(x^{(i)}, y^{(i)})$, sampled independently from a common distribution $D$. Each sample is generated according to the following steps:

1. $x^{(i)}$ is sampled from a distribution $D_x$ with support $\{0, 1\}^d$,
2. $\epsilon^{(i)}$ is sampled from a zero mean error distribution $\mathcal{E}$ with support $[-1/2, 1/2]$, i.e. $\mathbb{E}_{\epsilon \sim \mathcal{E}} [\epsilon] = 0$ and $\epsilon^{(i)} \in [-1/2, 1/2]$,
3. $y^{(i)} = m(x^{(i)}) + \epsilon^{(i)}$, where $m : \{0, 1\}^d \rightarrow [-1/2, 1/2]$.

The goal of the regression task is to estimate the target function $m$. Observe from the definition of the non-parametric regression model we have that $y^{(i)} \in [-1,1]$. Our results apply to any case where both the error distribution and the values of the target function are bounded, i.e. $|\epsilon^{(i)}| \leq H$ and $|m(x)| \leq H$. In this case the sample complexity bounds and the rates should be
multiplied by $H$. For simplicity we present the result for the case $|y^{(i)}| \leq 1$.

For any vector $x \in \{0,1\}^d$ we define the vector $x_S$ as the sub-vector of $x$, where we keep only the coordinates with indices in $S \subseteq [d]$. Additionally, we define $D_{x,S}$ as the marginal distribution of $D_x$ in the coordinates $S$. Also, let $x^{(k)}$ be an arbitrary $x^i$ such that $j \in K$. For any training set $D_n$ we define the set $D_{x,n} = \{x^{(1)}, \ldots, x^{(n)}\}$. For any set $S \subseteq [d]$ and an index $i \in [d]$ we sometimes use the notation $S \cup i$ to refer to $S \cup \{i\}$.

All of the results that we present in this paper are in the “high-dimensional” regime, where the number of features is very big but the number of relevant features is small. When this is true we say that the function $m$ is sparse as we explain in the following definition.

**Definition 2.1 (Sparsity).** We say that the target function $m : \{0,1\}^d \to \mathbb{R}$ is $r$-sparse if and only if there exists a set $R \subseteq [d]$, with $|R| = r$ and a function $h : \{0,1\}^r \to \mathbb{R}$ such that for every $z \in \{0,1\}^d$ it holds that $m(z) = h(z_R)$. The set $R$ is called the set of relevant features.

Some of the results that we have in this paper significantly improve if we make the assumption that the feature vector distribution $D_x$ is a product distribution. For this reason we define the “independence of features” assumption.

**Assumption 2.2 (Independence of Features).** We assume that there exist Bernoulli distributions $B_1, \ldots, B_d$ such that $x^{(i)}$ is distributed independently according to $B_i$.

Now we give some definitions, related to the structure of a binary regression tree, that are important for the presentation of our results.

**Definition 2.3 (Partitions, Cells and Subcells).** A partition $\mathcal{P}$ of $\{0,1\}^d$ is a family of sets $\{A_1, \ldots, A_s\}$ such that $A_j \subseteq \{0,1\}^d$, $A_j \cap A_k = \emptyset$ for all $j,k \in [s]$, and $\bigcup_{j=1}^s A_j = \{0,1\}^d$.

Let $\mathcal{P}$ be a partition of $\{0,1\}^d$. Every element $A$ of $\mathcal{P}$ is called a cell of $\mathcal{P}$ or just cell, if $\mathcal{P}$ is clear from the context. Every cell $A$ has two subcells $A^0_i$, $A^1_i$ with respect to any direction $i$, which are defined as $A^0_i = \{x \in A \mid x_i = 0\}$ and $A^1_i = \{x \in A \mid x_i = 1\}$.

For any $x \in \{0,1\}^d$ and any partition $\mathcal{P}$, we define $\mathcal{P}(x) \in \mathcal{P}$ as the cell of $\mathcal{P}$ that contains $x$.

**Definition 2.4 (Split Operator and Refinement).** For any partition $\mathcal{P}$ of $\{0,1\}^d$, any cell $A \in \mathcal{P}$ and any $i \in [d]$ we define the split operator $S(\mathcal{P},A,i)$ that outputs a partition with the cell $A$ split with respect to direction $i$. More formally $S(\mathcal{P},A,i) = (\mathcal{P} \setminus \{A\}) \cup \{A^0_i, A^1_i\}$. We can also extend the definition of the split operator to splits over sets of dimensions $I \subseteq [d]$, inductively as follows: if $i \in I$ then $S(\mathcal{P}, A, I) = S(S(\mathcal{P}, A, i), A^0_i, I \setminus \{i\}), A^1_i, I \setminus \{i\})$.

A partition $\mathcal{P}'$ is a refinement of a partition $\mathcal{P}$ if every element of $\mathcal{P}'$ is a subset of an element of $\mathcal{P}$. Then we say that $\mathcal{P}'$ is finer than $\mathcal{P}$ and $\mathcal{P}$ is coarser than $\mathcal{P}'$ and we use the notation $\mathcal{P}' \subseteq \mathcal{P}$.

### 3 Consistency of Level-Splits Algorithm for Sparse Functions

In this section we present our analysis for the case when we run a level split greedy algorithm to build a tree or a forest that approximates the target function $m$. We start with the necessary definitions to present the algorithm that we use. We refer to Appendix A.1 for a presentation and analysis of the population version of the algorithm, that is useful (though not necessary) to gain intuition on the finite sample proof.
Given a set of splits $S$, we define the expected mean squared error of $S$ as follows:

$$
\mathbb{E}(S) = \mathbb{E}_{x \sim \mathcal{D}_x} \left[ \left( m(x) - \mathbb{E}_{w \sim \mathcal{D}_x} [m(w) \mid w_S = x_S] \right)^2 \right] 
$$

$$
= \mathbb{E}_{x \sim \mathcal{D}_x} [m^2(x)] - \mathbb{E}_{z \sim \mathcal{D}_{x,z}} \left[ \left( \mathbb{E}_{w \sim \mathcal{D}_z} [m(w) \mid w_S = z_S] \right)^2 \right] 
\triangleq \mathbb{E}_{x \sim \mathcal{D}_x} [m^2(x)] - \mathbb{V}(S). \quad (3.2)
$$

It is easy to see that $\mathbb{E}$ is a monotone decreasing function of $S$ and hence $\mathbb{V}$ is a monotone increasing function of $S$. $\mathbb{V}$ can be viewed as a measure of heterogeneity of the within-leaf mean values of the target function $m$, from the leaves created by split $S$.

We present results based on either one of two main assumption about $\mathbb{V}$: approximate submodularity of $\mathbb{V}$ or strong sparsity. These assumptions play a crucial role in the analysis of the performance of the random forest algorithm, both in the finite sample regime and the population regime (presented in Appendix A.1). It is not difficult to see that without any assumption, no meaningful result about the consistency of greedily grown trees in the high dimensional setting is possible, as we illustrate in Appendix G.

**Assumption 3.1 (Approximate Submodularity).** Let $C \geq 1$, we say that the function $\mathbb{V}$ is $C$-approximate submodular, if and only if for any $T, S \subseteq [d]$, such that $S \subseteq T$, and any $i \in [d]$, it holds that $\mathbb{V}(T \cup \{i\}) - \mathbb{V}(T) \leq C \cdot (\mathbb{V}(S \cup \{i\}) - \mathbb{V}(S))$.

**Assumption 3.2 (Strong Sparsity).** A target function $m : \{0,1\}^d \rightarrow [-1/2,1/2]$ is $(\beta,r)$-strongly sparse if $m$ is $r$-sparse with relevant features $R$ and the function $\mathbb{V}$ satisfies: $\mathbb{V}(T \cup \{j\}) - \mathbb{V}(T) + \beta \leq \mathbb{V}(T \cup \{i\}) - \mathbb{V}(T)$, for all $i \in R$, $j \in [d] \setminus R$ and $T \subset [d] \setminus \{i\}$.

We next need to define the estimator that is produced by a level-split tree with a set of splits $S$. Given a set of splits $S$, a training set $\mathcal{D}_n$ and an input $x$ we can define the estimate $m(x;S,\mathcal{D}_n)$ as follows (for simplicity, we use $m_n(\cdot;\cdot), N_n(\cdot;\cdot)$, and $T_n(\cdot;\cdot)$ instead of $m(\cdot;\cdot,\mathcal{D}_n)$, $N(\cdot;\cdot,\mathcal{D}_n)$ and $T(\cdot;\cdot,\mathcal{D}_n)$):

$$
m_n(x;S) = \frac{1}{N_n(x;T_n(S,x))} \sum_{j \in [n]} 1 \{ x^{(j)}_{T_n(S,x)} = x_{T_n(S,x)} \} \cdot y^{(j)} \quad (3.3)
$$

where $N_n(\cdot;\cdot), T_n(\cdot;\cdot)$ are defined as follows

$$
N_n(x;T) = \sum_{j \in [n]} 1\{ x^{(j)}_T = x_T \}, \quad T_n(S,x) = \arg\max_{T \subseteq S, N_n(x;T) > 0} |T|.
$$

In words, the function $T_n(S,x)$ returns the subset $T$ of the splits $S$ that we used to create the leaf of the tree that contains $x$, until the leaf that corresponds to $T$ contains at least one training point. The function $N_n(x;T)$ is the number of training points in the leaf that contains $x$, when we split across the coordinates $T$.

For the presentation of the algorithm we also need the definition of the empirical mean square
error, given as set of splits $S$, as follows:

$$L_n(S) = \frac{1}{n} \sum_{j \in [n]} \left( y^{(j)} - m_n(x^{(j)}; S) \right)^2 = \frac{1}{n} \sum_{j \in [n]} \left( y^{(j)} \right)^2 - \frac{1}{n} \sum_{j \in [n]} m_n^2(x^{(j)}; S)$$  \hspace{1cm} (3.4)$$

$$\Delta = \frac{1}{n} \sum_{j \in [n]} \left( y^{(j)} \right)^2 - V_n(S).$$  \hspace{1cm} (3.5)$$

It is easy to see that $V_n$ is a monotone increasing function and $L_n$ is a monotone decreasing function. We are now ready to present the level-split algorithm both with and without honesty. For this we use the honesty flag $h$, where $h = 1$ means we use honesty and $h = 0$ means we don’t.

**Algorithm 1: Level Split Algorithm**

**Input:** maximum number of splits $\log(t)$, a training data set $D_n$, honesty flag $h$.

**Output:** tree approximation of $m$.

1. $V \leftarrow D_{n,x}$
2. if $h = 1$ then Split randomly $D_n$ in half, $D_{n/2}, D'_{n/2}$, set $n \leftarrow n/2$, set $V \leftarrow D'_{n,x}$;
3. Set $P_0 = \{ \{0,1\}^d \}$ the partition associated with the root of the tree.
4. For all $1 \leq \ell \leq n$, set $P_{\ell} = \emptyset$.
5. level $\leftarrow -1$, $S \leftarrow \emptyset$.
6. while level $< \log(t)$ do
7. level $\leftarrow$ level + 1, $P_{\text{level}+1} = \emptyset$.
8. Select $i \in [d]$ that maximizes $V_n(S \cup \{i\})$ [see (3.2)].
9. for all $A \in P_{\text{level}}$ do
10. Cut the cell $A$ to cells $A^i_k = \{x \mid x \in A \land x_i = k\}$, $k = 0, 1$.
11. if $|V \cap A^i_0| > 1$ and $|V \cap A^i_1| > 1$ then
12. $P_{\text{level}+1} \leftarrow P_{\text{level}+1} \cup \{A^i_0, A^i_1\}$
13. else
14. $P_{\text{level}+1} \leftarrow P_{\text{level}+1} \cup \{A\}$
15. end
16. end
17. $S \leftarrow S \cup \{i\}$
18. end
19. return $(P_n, m_n) = (P_{\text{level}+1}, x \mapsto m_n(x; S))$ [see (3.3)].

Now we are ready to state our main result for the consistency of shallow trees with level splits as described in Algorithm 1. The proof of this theorem can be found in Appendix D.

**Theorem 3.3.** Let $D_n$ be i.i.d. samples from the non-parametric regression model $y = m(x) + \epsilon$, where $m(x) \in [-1/2, 1/2]$, $\epsilon \sim \mathcal{E}$, $\mathbb{E}_{\epsilon \sim \mathcal{E}}[\epsilon] = 0$ and $\epsilon \in [-1/2, 1/2]$. Let also $S_n$ be the set of splits chosen by Algorithm 1, with input $h = 0$. Then the following statements hold.

1. Under the submodularity Assumption 3.1, assuming that $m$ is $r$-sparse and if we set as input the number of splits to be $\log(t) = \frac{C \cdot \log(n)}{\log(d/\delta)}$, then it holds that

$$\mathbb{P}_{D_n \sim D_n} \left( \mathbb{E}_{x \sim D_n} \left[ (m(x) - m_n(x; S))^2 \right] > \Omega \left( C \cdot r \cdot \log(d/\delta) \right) \right) \leq \delta.$$
2. Under the submodularity Assumption 3.1, the independence of features Assumption 2.2 and assuming that \( m \) is \( r \)-sparse, if \( \log(t) = r \) then it holds that

\[
\mathbb{P}_{D_n \sim D^n} \left( \mathbb{E}_{x \sim D_x} \left[ (m(x) - m_n(x; S_n))^2 \right] > \Omega \left( C \cdot \sqrt{\frac{2r \cdot \log(d/\delta)}{n}} \right) \right) \leq \delta.
\]

3. If \( m \) is \((\beta, r)\)-strongly sparse as per Assumption 3.2, and \( n \geq \tilde{\Omega} \left( \frac{2^r \log(d/\delta)}{\beta^2} \right) \), and we set \( \log(t) = r \), then we have

\[
\mathbb{P}_{D_n \sim D^n} \left( \mathbb{E}_{x \sim D_x} \left[ (m(x) - m_n(x; S_n))^2 \right] > \Omega \left( \frac{2^r \log(d/\delta) \log(n)}{n} \right) \right) \leq \delta.
\]

As we can see the rates, naturally, are better as we make our assumptions stronger. The fastest rate is achievable when the \((\beta, r)\) strong sparsity holds (even without the submodularity or the independence condition), the second fastest rate when the features are independent but only the submodularity holds, and we have the slowest rate when only the submodularity holds and there is arbitrary correlation between the features.

### 3.1 Fully Grown Honest Forests with Level Splits

In this section we consider the case of fully grown honest trees. For this case it is necessary to consider forest estimators instead of trees because a fully grown tree has very high variance. For this reason we use the subsampling technique and honesty. For any subset \( D_s \) of size \( s \) of the set of samples \( D_n \), we build one tree estimator \( m(\cdot; D_{s}) \) according to Algorithm 1 with inputs, \( \log(t) \) large enough so that every leaf has two or three samples (fully grown tree), training set \( D_s \) and \( h = 1 \). Then our final estimator \( m_{n,s} \) can be computed as follows

\[
m_{n,s}(x) = \frac{1}{\binom{n}{s}} \sum_{D_i \subseteq D_n \mid |D_i| = s} \mathbb{E}[m(x; D_i)]. \tag{3.6}
\]

Where \( \omega \) is any internal randomness to the tree building algorithm (e.g. the sample splitting). We note that even though we phrase results for the latter estimator, where all sub-samples are being averaged over and the expectation over the randomness \( \omega \) is computed, our results carry over to the monte-carlo approximation of this estimator, where only \( B \) trees are created, each on a randomly drawn sub-sample and for a random draw of the randomness (see e.g. [WA18, OSW19]), assuming \( B \) is large enough (for our guarantees to hold it suffices to take \( B = \Theta(d^{n^2}) \)).

For the estimator \( m_{n,s} \) and under the strong sparsity Assumption 3.2 we have the following consistency and asymptotic normality theorems. The proofs of the theorems are presented in Appendices D.3 and F.

**Theorem 3.4.** Let \( D_n \) be i.i.d. samples from the non-parametric regression model \( y = m(x) + \varepsilon \), where \( m(x) \in [-1/2, 1/2], \varepsilon \sim \mathcal{E}, \mathbb{E}_{\mathcal{E}, \varepsilon}[\varepsilon] = 0 \) and \( \varepsilon \in [-1/2, 1/2] \). Let \( m_{n,s} \) be the forest estimator that is built with sub-sampling of size \( s \) from the training set and where every tree \( m(x; D_{s}) \) is built using Algorithm 1, with inputs: \( \log(t) \) large enough so that every leaf has two or three samples and \( h = 1 \). Under the Assumption 3.2, if \( R \) is the set of relevant features and and for every \( \omega \in \{0, 1\}^t \) it holds for the marginal probability that \( \mathbb{P}_{z \sim D_{s}}(z_R = \omega) \neq (0, \frac{2}{2'}) \) and if \( s = \tilde{\Theta} \left( \frac{2^r \log(1/d)}{\beta^2} + \frac{2^r \log(1/d)}{\zeta} \right) \) then it holds that

\[
\mathbb{P}_{D_n \sim D^n} \left( \mathbb{E}_{x \sim D_x} \left[ (m_{n,s}(x) - m(x))^2 \right] \right) \geq \tilde{\Omega} \left( \frac{2^r \log(1/d)}{n} \left( \frac{\log(d)}{\beta^2} + \frac{1}{\zeta} \right) \right) \leq \delta.
\]
Our next goal is to prove the asymptotic normality of the estimate \( m_{n,s} \). To do so we need that our estimation algorithm treats samples, a-priori symmetrically (i.e. the estimate is invariant to permutations of the sample indices). Since for simplicity, we have presented \( m_{n,s} \) based on a deterministic algorithm, this might be violated. For this reason, for the normality result, before computing the \( m_{n,s} \) we apply a random permutation \( \tau \in S_n \) in the training set \( D_n \). The permutation \( \tau \) is part of the internal randomness \( \omega \) of the algorithm. Given the permutation \( \tau \) we denote estimate that we compute by \( m_{n,s,\tau} \). Ideally we would like to compute the expected value of \( m_{n,s,\tau} \) over a uniform choice of \( \tau \) which we denote by \( \overline{m}_{n,s} \). However this is computationally very expensive since we need to repeat the estimate for all the \( n! \) permutations. Instead we compute a Monte Carlo approximation of \( \overline{m}_{n,s} \) by sampling \( B \) permutations from \( S_n \) and then taking the empirical average of those. We denote this estimator as \( m_{n,s,B} \).

**Theorem 3.5.** Under the same conditions of Theorem 3.4 and with the further assumption that: \( \sigma^2(x) = \text{Var}(y^{(i)} \mid x^{(i)} = x) \geq \sigma^2 > 0 \) and that for a priori fixed \( x \) it holds \( \mathbb{P}_{z \sim D_n}(z_R = x_R) \geq \zeta/2^r \), if we set: 
\[
\hat{\Theta} \left( \frac{2^r (\log(d) + \log(n))}{\sigma^2} + \frac{2^r \log(n)}{\zeta} \right) \leq s \leq o(\sqrt{n}),
\]
then for \( \sigma_n^2(x) = O \left( \frac{\zeta^2}{n} \right) \), it holds that:
\[
\sigma_n^{-1}(x) (m_{n,s,B}(x) - m(x)) \rightarrow_d N(0, 1) \tag{3.7}
\]
where \( B \geq n^2 \log(n) \).

The latter asymptotic normality theorem enables the construction of asymptotically valid normal based intervals, using estimates of the variance of the prediction. These estimates can be constructed either via the bootstrap or via methods particular to random forests such as the infinitesimal jackknife proposed in [WHE14].

### 4 Consistency of Breiman’s Algorithm for Sparse Functions

In this section we present our analysis for the case when the tree construction algorithm, at every iteration, chooses a different direction to split on at every cell of the current partition. We start with the necessary definitions to present the algorithm that we use. We refer to Appendix A.2 for a presentation and analysis of the population version of the algorithm, that contains some relevant definitions and lemmas used in our main proof.

We define the total expected mean squared error that is achieved by a partition \( \mathcal{P} \) of \( \{0,1\}^d \), in the population model, as follows:
\[
\overline{\mathcal{L}}(\mathcal{P}) \triangleq \mathbb{E}_{x \sim D_x} \left[ \left( m(x) - \mathbb{E}_{z \sim D_x} [m(z) \mid z \in \mathcal{P}(x)] \right)^2 \right] \tag{4.1}
\]
\[
= \mathbb{E}_x [m^2(x)] - \mathbb{E}_{x \sim D_x} \left[ \left( \mathbb{E}_{z \sim D_x} [m(z) \mid z \in \mathcal{P}(x)] \right)^2 \right]
\]
\[
\triangleq \mathbb{E}_x [m^2(x)] - \overline{\mathcal{V}}(\mathcal{P}). \tag{4.2}
\]
For simplicity, we use the shorthand notation \( \overline{\mathcal{V}}(\mathcal{P}, A, i) \) and \( \overline{\mathcal{L}}(\mathcal{P}, A, i) \) to denote \( \overline{\mathcal{V}}(S(\mathcal{P}, A, i)) \) and \( \overline{\mathcal{L}}(S(\mathcal{P}, A, i)) \). Observe that the function \( \overline{\mathcal{L}} \) is increasing with respect to \( \mathcal{P} \) is the sense that if \( \mathcal{P}' \subseteq \mathcal{P} \) then \( \overline{\mathcal{L}}(\mathcal{P}') \leq \overline{\mathcal{L}}(\mathcal{P}) \) and hence \( \overline{\mathcal{V}} \) is decreasing with respect to \( \mathcal{P} \).
In order to define the splitting criterion of our algorithm, we will need to define a local version of the mean squared error, locally at a cell $A$, as follows:

$$\mathcal{T}_\ell(A, P) \triangleq \mathbb{E}_{x \sim D_x} \left( \frac{1}{2} (m(x) - \mathbb{E}_{z \sim D_z} [m(z) \mid z \in P(x)])^2 \right) \mid x \in A$$

$$= \mathbb{E}_{x \sim D_x} [m^2(x) \mid x \in A] - \mathbb{E}_{x} \left[ \mathbb{E}_{z \sim D_z} [m(z) \mid z \in P(x)]^2 \right] \mid x \in A$$

$$\triangleq \mathbb{E}_{x} [m^2(x) \mid x \in A] - \mathcal{V}_\ell(A, P).$$

(4.3)

For shorthand notation, for any $P$ that contains $A$, we will use $\mathcal{V}_\ell(A, I) = \mathcal{V}_\ell(A, S(P, A, I))$, for any set of directions $I \subseteq [d]$ (observe that the quantity is independent of the choice of $P$, as long as it contains $A$). Similarly, we will use the shorthand notation $\mathcal{T}_\ell(A, I)$. Finally, we will use the shorthand notation: $\mathcal{T}_\ell(A), \mathcal{V}_\ell(A)$ for $\mathcal{T}_\ell(A, \emptyset)$ and $\mathcal{V}_\ell(A, \emptyset)$ correspondingly.

We now need to define the corresponding property of submodularity and strong sparsity in this more complicated setting. Inspired by the economics literature we call the analogue of submodularity for this setting the *diminishing returns* property. Moreover, we call the analogue of strong sparsity, strong partition sparsity.

**Assumption 4.1 (Approximate Diminishing Returns).** For $C \geq 1$, we say that the function $\mathcal{V}$ has the approximate diminishing returns property if for any cells $A, A'$, any $i \in [d]$ and any $T \subseteq [d]$ such that $A' \subseteq A$ it holds that $\mathcal{V}_\ell(A', T \cup \{i\}) - \mathcal{V}_\ell(A', T) \leq C \cdot (\mathcal{V}_\ell(A, i) - \mathcal{V}_\ell(A))$.

**Assumption 4.2 (Strong Partition Sparsity).** A target function $m : \{0, 1\}^d \rightarrow [-1/2, 1/2]$ is $(\beta, r)$-strongly partition sparse if $m$ is $r$-sparse with relevant features $R$ and the function $\mathcal{V}$ satisfies: $\mathcal{V}_\ell(A, T \cup j) - \mathcal{V}_\ell(A, T) + \beta \leq \mathcal{V}_\ell(A, T \cup i) - \mathcal{V}_\ell(A, T)$, for all possible cells $A$ and for all $i \in R$, $j \in [d] \setminus R$.

For some of the results in this section we need to assume that the density or the marginal density with respect to $x$ is lower bounded by some constant. The reason that we need this assumption is that the greedy decision made by the Algorithm 2 are separate for every leaf of the tree. Therefore we need to make sure that, at least in the first important splits, every leaf has enough samples to choose the correct greedy option. For this reason we define the following assumption on the lower bound of the marginal density.

**Assumption 4.3 (Marginal Density Lower Bound).** We say that the density $D_x$ is $(\zeta, q)$-lower bounded, if for every set $Q \subseteq [d]$ with size $|Q| = q$ then for every $w \in \{0, 1\}^q$ it holds that $P_{x \sim D_x} (x_Q = w) \geq \zeta / 2^q$.

We next need to define the estimator that is defined by a tree that produces a partition $P$ of the space $\{0, 1\}^d$. Given a training set $D_n$ and a cell $A \in P$, we define:

$$g_n(A) = \frac{1}{N_n(A)} \sum_{j \in [n]} y^{(j)} \cdot \mathbb{1}\{x^{(j)} \in A\} = \sum_{j \in [n]} W_n(x^{(j)}; A) \cdot y^{(j)},$$

(4.5)

where in both the aforementioned definition $N_n(\cdot)$ and $W_n(\cdot; \cdot)$ are defined as follows

$$N_n(A) = \sum_{j \in [n]} \mathbb{1}\{x^{(j)} \in A\}, \quad W_n(x; A) = \frac{\mathbb{1}\{x \in A\}}{N_n(A)}$$

(4.6)
In words, the function \( N_n(A) \) is the number of training point in the cell \( A \) and \( W_n(x; A) \) is the coefficient of the training points that lie in the cell \( A \), when computing the local estimate at \( A \). We also define the set \( Z_n(A) \), as the subset of the training set \( Z_n(A) = \{ j \mid x^{(j)} \in A \} \). Based on this we also define the partition \( \mathcal{U}_n(\mathcal{P}) \) of the training set \( D_n \) as \( \mathcal{U}_n(\mathcal{P}) = \{ Z_n(A) \mid A \in \mathcal{P} \} \). Given an input \( x \) we define the estimate \( m(x; \mathcal{P}, D_n) \) as follows (for simplicity, we use \( m_n(\cdot; \cdot), N_n(\cdot) \) and \( W_n(\cdot; \cdot) \) instead of \( m(\cdot; \cdot; D_n), N(\cdot; D_n) \) and \( W(\cdot; \cdot; D_n) \)):

\[
m_n(x; \mathcal{P}) = g_n(\mathcal{P}(x)),
\]

For the presentation of the algorithm we also need the definition of the empirical mean squared error, conditional on a cell \( A \) and a potential split direction \( i \), as follows.

\[
L_n^\ell(A, i) \triangleq \sum_{z \in \{0,1\}} \frac{N_n(A^i_z)}{N_n(A)} \sum_{j \in Z_n(A^i_z)} \frac{1}{N_n(A^i_z)} \left( y^{(j)} - m_n \left( x^{(j)}; \mathcal{P} \left( x^{(j)} \right) \right) \right)^2 \quad (4.8)
\]

\[
= \frac{1}{N_n(A)} \sum_{j \in Z_n(A)} \left( y^{(j)} \right)^2 - \sum_{z \in \{0,1\}} \frac{N_n(A^i_z)}{N_n(A)} \left( g_n(A^i_z) \right)^2 \\
\triangleq \frac{1}{N_n(A)} \sum_{j \in Z_n(A)} \left( y^{(j)} \right)^2 - V_n^\ell(A, i), \quad (4.9)
\]

We are now ready to present the Breiman’s tree construction algorithm both with and without honesty (we use the honesty flag \( h \), where \( h = 1 \) means we use honesty).

---

**Algorithm 2: Breiman’s Tree Construction Algorithm**

**Input:** maximum number of nodes \( t \), a training data set \( D_n \), honesty flag \( h \).

**Output:** tree approximation of \( m \).

1. \( \mathcal{V} \leftarrow D_{n,x} \)
2. if \( h = 1 \) then Split randomly \( D_n \) in half, \( D_{n/2}, D'_{n/2} \), set \( n \leftarrow n/2 \), set \( \mathcal{V} \leftarrow D'_{n,x} \);
3. Set \( \mathcal{P}_0 = \{ \{0,1\}^d \} \) the partition associated with the root of the tree.
4. For all \( 1 \leq \ell \leq t \), set \( \mathcal{P}_\ell = \emptyset \).
5. level \( \leftarrow 0 \), \( n_{\text{nodes}} \leftarrow 1 \), \( \text{queue} \leftarrow \mathcal{P}_0 \).
6. while \( n_{\text{nodes}} < t \) do
   7. if \( \text{queue} = \emptyset \) then
      8. level \( \leftarrow \) level + 1, \( \text{queue} \leftarrow \mathcal{P}_\text{level} \)
      9. Pick \( A \) the first element in \( \text{queue} \)
   10. if \( | \mathcal{V} \cap A | \leq 1 \) then
       11. \( \text{queue} \leftarrow \text{queue} \setminus \{ A \}, \mathcal{P}_{\text{level}+1} \leftarrow \mathcal{P}_{\text{level}+1} \cup \{ A \} \)
   12. else
     13. Select \( i \in [d] \) that maximizes \( V_n^\ell(A, i) \) [see (4.9)]
     14. Cut the cell \( A \) to cells \( A^i_k = \{ x \mid x \in A \land x_i = k \}, k = 0,1 \)
     15. \( \text{queue} \leftarrow \text{queue} \setminus \{ A \}, \mathcal{P}_{\text{level}+1} \leftarrow \mathcal{P}_{\text{level}+1} \cup \{ A_0, A^i_1 \} \)
   16. end
17. \( \mathcal{P}_{\text{level}+1} \leftarrow \mathcal{P}_{\text{level}+1} \cup \text{queue} \)
18. return \((\mathcal{P}_n, m_n) = (\mathcal{P}_{\text{level}+1}, x \mapsto m_n(x; \mathcal{P}_{\text{level}+1})) \) [see (4.7)]
We can now state our main result for the consistency of shallow trees with Breiman’s splits as described in Algorithm 2. The proof of this theorem can be found in the Appendix E. As we can see in Theorem 4.4 the rates are better as we make our assumptions stronger similar to the results for the level-split algorithm. The main difference between the results in this section and the results for the level-split algorithm is that for the analysis of Breiman’s algorithm we need to assume that the probability mass function of the distribution $\mathcal{D}_x$ is lower bounded by $\zeta/2^d$.

**Theorem 4.4.** Let $D_n$ be i.i.d. samples from the non-parametric regression model $y = m(x) + \varepsilon$, where $m(x) \in [-1/2, 1/2]$, $\varepsilon \sim \mathcal{E}$, $\mathbb{E}_{x \sim \mathcal{E}}[\varepsilon] = 0$ and $\varepsilon \in [-1/2, 1/2]$ with $m$ an $r$-sparse function. Let also $\mathcal{P}_n$ be the partition that the Algorithm 2 returns with input $h = 0$. Then the following statements hold.

1. Let $q = \frac{Cr}{C + 3} \left( \log(n) - \log(\log(d/\delta)) \right)$ and assume that the approximate diminishing returns Assumption 4.1 holds. Moreover if we set the number of nodes $t$ such that $\log(t) \geq q$, and if we have number of samples $n \geq \tilde{\Omega} \left( \log(d/\delta) \right)$ then it holds that

$$
\mathbb{P}_{D_n \sim \mathcal{D}^n} \left[ \mathbb{E}_{x \sim \mathcal{D}_x} \left[ (m(x) - m_n(x, \mathcal{P}_n))^2 \right] > \tilde{\Omega} \left( C \cdot r \cdot \frac{C \cdot r}{\log(d/\delta)} \right) \right] \leq \delta.
$$

2. Suppose that the distribution $\mathcal{D}_x$ is a product distribution (see Assumption 2.2) and that the Assumption 4.1 holds. Moreover if $\log(t) \geq r$, then it holds that

$$
\mathbb{P}_{D_n \sim \mathcal{D}^n} \left[ \mathbb{E}_{x \sim \mathcal{D}_x} \left[ (m(x) - m_n(x, \mathcal{P}_n))^2 \right] > \tilde{\Omega} \left( \frac{3}{C} \cdot 2^{r} \cdot \frac{\log(d/\delta)}{\log(n)} \right) \right] \leq \delta.
$$

3. Suppose that the distribution $\mathcal{D}_x$ is a product distribution (see Assumption 2.2), that is also $(\zeta, r)$-lower bounded (see Assumption 4.3) and that the Assumption 4.1 holds. Moreover if $\log(t) \geq r$, then it holds that

$$
\mathbb{P}_{D_n \sim \mathcal{D}^n} \left[ \mathbb{E}_{x \sim \mathcal{D}_x} \left[ (m(x) - m_n(x, \mathcal{P}_n))^2 \right] > \tilde{\Omega} \left( \frac{3}{C} \cdot 2^{r} \cdot \frac{\log(d/\delta)}{\zeta \cdot n} \right) \right] \leq \delta.
$$

4. Suppose that $m$ is $(\beta, r)$-strongly sparse (see Assumption 4.2) and that $\mathcal{D}_x$ is $(\zeta, r)$-lower bounded (see Assumption 4.3). If $n \geq \tilde{\Omega} \left( \frac{2^{r} \log(d/\delta)}{\zeta \beta^{2}} \right)$, and $\log(t) \geq r$, then we have

$$
\mathbb{P}_{D_n \sim \mathcal{D}^n} \left[ \mathbb{E}_{x \sim \mathcal{D}_x} \left[ (m(x) - m_n(x, \mathcal{P}_n))^2 \right] > \tilde{\Omega} \left( \frac{2^{r} \log(d/\delta) \log(n)}{n} \right) \right] \leq \delta.
$$

**4.1 Fully Grown Honest Forests with Breiman’s Algorithm**

In this section we consider the case of fully grown honest trees. As in the case of level splits we are going to use the subsampling technique and honesty. That is, for any subset $D_s$ of size $s$ of the set of samples $D_n$, we build one tree estimator $m(\cdot; D_s)$ according to Algorithm 2 with inputs, $\log(t)$ large enough so that every leaf has two or three samples, training set $D_s$ and $h = 1$. Then our final estimator $m_{n,s}$ can be computed as follows

$$
m_{n,s}(x) = \frac{1}{\binom{n}{s}} \sum_{D_s \subseteq D_n, |D_s| = s} \mathbb{E}[m(x; D_s)]. \quad (4.10)
$$

Where $\omega$ is the internal randomness of the tree building algorithm. For this estimator $m_{n,s}$ and under the strong partition sparsity Assumption 4.2 we have the following consistency and
asymptotic normality theorems. The proof of the following theorems is presented in Appendices E.3 and F.

**Theorem 4.5.** Let $D_n$ be i.i.d. samples from the non-parametric regression model $y = m(x) + \epsilon$, where $m(x) \in [-1/2, 1/2]$, $\epsilon \sim \mathcal{E}$, $\mathbb{E}_{\epsilon \sim \mathcal{E}}[\epsilon] = 0$ and $\epsilon \in [-1/2, 1/2]$. Suppose that $\mathcal{D}_x$ is $(\zeta, r)$-lower bounded (see Assumption 4.3). Let $m_{n,s}$ be the forest estimator that is built with sub-sampling of size $s$ from the training set and where every tree $m(x; D_s)$ is built using the Algorithm 2, with inputs: $\log(t)$ large enough so that every leaf has two or three samples, training set $D_s$ and $h = 1$. Then using $s = \tilde{\Theta}\left(\frac{2^\xi \log(d/\delta)}{\zeta \beta^2}\right)$ and under Assumption 4.2:

$$
\mathbb{P}_{D_n \sim D^n} \left(\mathbb{E}_{x \sim D_s} [(m(x) - m_{n,s}(x))^2] > \Omega \left(\frac{2^\xi \log(d/\delta)}{n \cdot \zeta \cdot \beta^2}\right)\right) \leq \delta.
$$

Our next goal is to prove the asymptotic normality of the estimate $m_{n,s}$. As we have already discussed for the level-splits algorithm, to prove the asymptotic normality we need that our estimation algorithm treats samples, a priori symmetrically (i.e. the estimate is invariant to permutations of the sample indices). Since for simplicity, we have presented $m_{n,s}$ based on a deterministic algorithm, this might be violated. For this reason, for the normality result, before computing the $m_{n,s}$ we apply a random permutation $\tau \in S_n$ in the training set $D_n$. The permutation $\tau$ is part of the internal randomness $\omega$ of the algorithm. Given the permutation $\tau$ we denote estimate that we compute by $m_{n,s,\tau}$. Ideally we would like to compute the expected value of $m_{n,s,\tau}$ over a uniform choice of $\tau$ which we denote by $\overline{m}_{n,s}$. However this is computationally very expensive since we need to repeat the estimate for all the $n!$ permutations. Instead we compute a Monte Carlo approximation of $\overline{m}_{n,s}$ by sampling $B$ permutations from $S_n$ and then taking the empirical average of those. We denote this estimator as $m_{n,s,B}$.

**Theorem 4.6.** Under the same conditions of Theorem 4.5 and with the further assumption that: $\sigma^2(x) = \text{Var}(y^{(i)} | x^{(i)} = x) \geq \sigma^2 > 0$ and that for a priori fixed $x$ it holds $\mathbb{P}_{z \sim D_1} (z_R = x_R) \geq \zeta/2^\xi$, if we set:

$$
\tilde{\Theta}\left(\frac{2^\xi \log(d \cdot n)}{\zeta \beta^2}\right) \leq s \leq o(\sqrt{n}),
$$

then for $\sigma_n^2(x) = \Theta\left(\frac{s^2}{n}\right)$ it hold that

$$
\sigma_n^{-1}(x) (m_{n,s,B}(x) - m(x)) \xrightarrow{d} N(0, 1).
$$

(4.11)

where $B \geq n^2 \log(n)$.

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A  Population Models

In this section we present the population versions of the algorithms that we analyze in the main part of the paper, together with their analysis of convergence. We suggest to the reader to start studying these results first and then read the complete finite sample analysis.

A.1 Population Algorithm using Level-Splits

We start with the presentation of the level-splits algorithm in the population model.

**Algorithm 3: Level Split Algorithm – Population Model**

**Input:** maximum number of splits log(t).

**Output:** tree approximation of m.

1. Set $P_0 = \{0, 1\}^d$ the partition associated with the root of the tree.
2. level ← −1, S ← Ø.
3. **while** level < log(t) **do**
   4. level ← level + 1, $P_{\text{level+1}} = \emptyset$.
   5. Select $i \in [d]$ that maximizes $\nabla(S \cup \{i\})$ (see (3.2)).
   6. **for all** $A \in P_{\text{level}}$ **do**
      7. Cut the cell $A$ to cells $A'_i = \{x \mid x \in A \land x_i = k\}$, $k = 0, 1$.
      8. $P_{\text{level+1}} \leftarrow P_{\text{level+1}} \cup \{A'_0, A'_1\}$
   9. **end**
10. $S \leftarrow S \cup \{i\}$
11. **end**
12. return $(P, \overline{m}) = (P_{\text{level}}, x \mapsto E((z, y) \sim \mathcal{D} \mid y \in \overline{P}(x)))$

**Definition A.1 (Relevant Variables).** Given a set $S$, we define the set of remaining relevant features $\mathcal{R}(S) = \{i \in [d] \mid \nabla(S \cup \{i\}) > \nabla(S)\}$.

**Lemma A.2.** For every set $S \subseteq [d]$, under the Assumption 3.1, if $\mathcal{R}(S) = \emptyset$, then for any $x, x' \in \{0, 1\}^d$ such that $x_S = x'_S$ it holds that $m(x) = m(x')$.

**Proof.** We prove this by contradiction. If there exist $x, x' \in \{0, 1\}^d$ such that $x_S = x'_S$ and $m(x) \neq m(x')$ then obviously there exists an $\bar{x} \in A$ such that $m(\bar{x}) \neq E_{x,z}[m((x_S, x_{-S}))]$, where $A$ is the cell of the input space that contains all vectors $z$ with $z_S = x_S$. Therefore it holds that $\mathcal{L}(S) > \mathcal{L}([d]) = 0$ and hence $\nabla([d]) > \nabla(S)$. Now let’s assume an arbitrary enumeration $\{i_1, \ldots, i_k\}$ of the set $S^c = [d] \setminus S$. Because the function $\nabla$ is monotone and $\nabla([d]) > \nabla(S)$, there has to be a number $j \in [k]$ such that $\nabla(S \cup \{i_1, \ldots, i_j\}) > \nabla(S \cup \{i_1, \ldots, i_{j-1}\})$. But because of the approximate submodularity of $\nabla$ it holds that $\nabla(S \cup \{i_1, \ldots, i_j\}) - \nabla(S \cup \{i_1, \ldots, i_{j-1}\}) \leq C \cdot (\nabla(S \cup \{i_j\}) - \nabla(S))$, which implies that $\nabla(S \cup \{i_j\}) > \nabla(S)$ and this contradicts our assumption that $\mathcal{R}(S) = \emptyset$.

**Theorem A.3.** Consider the non-parametric regression model $y = m(x) + \varepsilon$, where $m : \{0, 1\}^d \rightarrow [-\frac{1}{2}, \frac{1}{2}]$ is a r-sparse function and $\varepsilon \sim \mathcal{E}$, with $\varepsilon \in [-\frac{1}{2}, \frac{1}{2}]$ and $E[\varepsilon] = 0$. Let $\overline{m}$ be the function that the
Algorithm 3 returns with input $t \geq (1/\eta)^{C \cdot r}$, then under the Assumption 3.1 it holds that

$$\mathbb{E}_x \left[ (m(x) - \overline{m}(x))^2 \right] \leq \eta.$$ 

Moreover under the Independence of Features Assumption 2.2 if $\log(t) \geq r$ then $\overline{m} = m$.

**Proof.** Let $R \subseteq [d]$ be the set of size $|R| = r$ of the relevant features of the target function $m$. Let $S$ the set of splits that Algorithm 3 chooses. Observe that it holds that $\mathcal{L}(S \cup R) = 0$ and hence $\nabla(S \cup R) \triangleq V^*$ is maximized. Since $m(x) \in [-1/2, 1/2]$, the maximum value of $\nabla$ is 1.

For the first part of the theorem, let $\{i_1, \ldots, i_r\}$ and be an arbitrary enumeration of $R$ and let $R_j = \{i_1, \ldots, i_j\}$ then by adding and subtracting terms of the form $\nabla(S \cup R_j)$ we have the following equality

$$(\nabla(S \cup R) - \nabla(S \cup R_{r-1})) + \cdots + (\nabla(S \cup R_2) - \nabla(S \cup \{i_1\})) + \nabla(S \cup \{i_1\}) = V^*.$$ 

From the approximate submodularity of $\nabla$ we hence have that

$$(\nabla(S \cup \{i_r\}) - \nabla(S)) + \cdots + (\nabla(S \cup \{i_2\}) - \nabla(S)) + (\nabla(S \cup \{i_1\}) - \nabla(S)) \geq \frac{V^* - \nabla(S)}{C}$$

which implies

$$\max_{j \in [r]} (\nabla(S \cup \{i_j\}) - \nabla(S)) \geq \frac{V^* - \nabla(S)}{C \cdot r}.$$ 

Let $i_{\text{level}}$ be the coordinate that the algorithm chose to split at level level. Now from the greedy criterion that Algorithm 3 uses we get that the coordinate $i_{\text{level}}$ that we picked to split was at least as good as the best of the coordinates in $R$, hence it holds that

$$\nabla \left(S \cup \{i_{\text{level}}\}\right) \geq \nabla(S) + \frac{V^* - \nabla(S)}{C \cdot r}$$

which in turn using $L^* \triangleq \mathcal{L}(S \cup R) = 0$ implies that

$$\mathcal{L} \left(S \cup \{i_{\text{level}}\}\right) \leq \mathcal{L}(S) \left(1 - \frac{1}{C \cdot r}\right). \tag{A.1}$$

Again we fix $S_{\text{level}}$ to be the set of splits after the step level of Algorithm 3, it holds that

$$\mathcal{L} \left(S_{\text{level}+1}\right) \leq \mathcal{L} \left(S_{\text{level}}\right) \left(1 - \frac{1}{C \cdot r}\right).$$

Inductively and using the fact that $m(x) \in [-1/2, 1/2]$ implies that

$$\mathcal{L}(S_{\text{level}}) \leq \mathcal{L}(\emptyset) \left(1 - \frac{1}{C \cdot r}\right)^{\text{level}} \leq \left(1 - \frac{1}{C \cdot r}\right)^{\text{level}}. \tag{A.2}$$

Finally from the choice of $t$ we have that for level $= C \cdot r \ln(1/\eta)$ it holds $\mathcal{L}(S_{\text{level}}) \leq \eta$ and since $\mathcal{L}(S)$ is a decreasing function of $S$ the first part of the theorem follows.

For the second part, we observe that for any coordinate $i \in [d] \setminus R$ and for any $S \subseteq [d]$ it holds that $\nabla(S \cup \{i\}) - \nabla(S) = 0$ and hence the Algorithm 3 will pick a coordinate in $[d] \setminus R$ only after it picks all the coordinates in $R$. Hence for $\log(t) \geq r$ we have that $\mathcal{R}(S) = \emptyset$ and from Lemma A.2 the second part of the theorem follows. 

\[\square\]
A.2 Population Algorithm of Breiman’s Algorithm

In this section we present the analysis of Breiman’s algorithm in the population model, defined in Algorithm 4.

**Algorithm 4: Breiman’s Tree Construction Algorithm – Population Model**

| Input:   | maximum number of nodes $t$. |
| Output:  | tree approximation of $m$. |
| 1. Set $P_0 = \{0, 1\}^d$ the partition associated with the root of the tree. |
| 2. $\text{level} \leftarrow 0$, $n_{\text{nodes}} \leftarrow 1$, $\text{queue} \leftarrow P_0$. |
| 3. while $n_{\text{nodes}} < t$ do |
| 4. if $\text{queue} = \emptyset$ then |
| 5. $\text{level} \leftarrow \text{level} + 1$, $\text{queue} \leftarrow P_{\text{level}}$ |
| 6. end |
| 7. Pick $A$ the first element in $\text{queue}$ |
| 8. Select $i \in [d]$ that maximizes $\nabla_\ell(A, i)$ [see (4.4)] |
| 9. Cut the cell $A$ to cells $A^i_k = \{x \mid x \in A \land x_i = k\}$, $k = 0, 1$ |
| 10. $\text{queue} \leftarrow \text{queue} \setminus \{A\}$, $P_{\text{level}+1} \leftarrow P_{\text{level}+1} \cup \{A_0, A^i_1\}$ |
| 11. end |
| 12. $P_{\text{level}+1} \leftarrow P_{\text{level}+1} \cup \text{queue}$. |
| 13. return $(\overline{P}, \overline{m}) = (P_{\text{level}+1}, x \mapsto E_{(z, y) \sim \mathcal{D}}[y \mid z \in P_{\text{level}+1}(x)])$ |

We now prove some important properties of the functions $\nabla, \nabla_\ell, \overline{L}$ and $\overline{L}_\ell$ as presented in Equations (3.1), (3.2), (3.3) and (4.4).

**Lemma A.4.** For any partition $\mathcal{P}$ and any cell $A \in \mathcal{P}$ the following hold

1. $\nabla(\mathcal{P}) = \sum_{A \in \mathcal{P}} \mathbb{P}_x (x \in A) \cdot \nabla(A)$,
2. $\overline{L}(\mathcal{P}) = \sum_{A \in \mathcal{P}} \mathbb{P}_x (x \in A) \cdot \overline{L}(A)$,
3. $\nabla(\mathcal{P}, A, i) - \nabla(\mathcal{P}) = \mathbb{P}_x (x \in A) \cdot (\nabla(A, i) - \nabla(A))$,
4. Under Assumption 4.1 for any two partitions $\mathcal{P}', \mathcal{P}$ and any cells $A, A'$, such that $A' \subseteq A$ and $A' \in \mathcal{P}'$, $A \in \mathcal{P}$, it holds that $\nabla(\mathcal{P}', A', i) - \nabla(\mathcal{P}) \leq C \cdot (\nabla(\mathcal{P}, A, i) - \nabla(\mathcal{P}))$.
5. Under Assumption 4.1 for any two partitions $\mathcal{P}', \mathcal{P}$ and any cells $A, A'$, such that $A' \subseteq A$ and $A' \in \mathcal{P}'$, $A \in \mathcal{P}$ and for any $T \subseteq [d], i \in [d]$ it holds that $\nabla(\mathcal{P}', A', T \cup \{i\}) - \nabla(\mathcal{P}', A', T) \leq C \cdot (\nabla(\mathcal{P}, A, i) - \nabla(\mathcal{P}))$.

**Proof.** The equations (1), (2) follow from the definitions of $\nabla, \nabla_\ell, \overline{L}, \overline{L}_\ell$. For equation 3. we have

$$
\nabla(\mathcal{P}, A, i) - \nabla(\mathcal{P}) = \mathbb{P}_x \left( x \in A_0 \right) \cdot \nabla(A_0) + \mathbb{P}_x \left( x \in A_1 \right) \cdot \nabla(A_1) - \mathbb{P}_x \left( x \in A \right) \cdot \nabla(A)
$$

$$
\nabla(A, i) - \nabla(A) = \mathbb{P}_x \left( x \in A_0 \mid x \in A \right) \cdot \nabla(A_0) + \mathbb{P}_x \left( x \in A_1 \mid x \in A \right) \cdot \nabla(A_1) - \nabla(A)
$$

and therefore we have that

$$
\nabla(\mathcal{P}, A, i) - \nabla(\mathcal{P}) = \mathbb{P}_x \left( x \in A \right) \cdot (\nabla(A, i) - \nabla(A))
$$

and equation (3) follows. Now from Assumption 4.1 we have that

$$
\nabla(A', i) - \nabla(A') \leq C \cdot (\nabla(A, i) - \nabla(A)) \implies
$$
\[ \mathbb{P}(x \in A) \cdot (\nabla_{l}(A',i) - \nabla_{l}(A')) \leq \mathbb{P}(x \in A) \cdot C \cdot (\nabla_{l}(A,i) - \nabla_{l}(A)) \]

but now since \( A' \subseteq A \) this implies \( \mathbb{P}(x \in A') \leq \mathbb{P}(x \in A) \) and hence
\[ \mathbb{P}(x \in A') \cdot (\nabla_{l}(A',i) - \nabla_{l}(A')) \leq \mathbb{P}(x \in A) \cdot C \cdot (\nabla_{l}(A,i) - \nabla_{l}(A)) \]
combining the last inequality with equation 3. we get a proof of equation (4). The statement in (5.) can be proven in an identical manner to (4.).

**Definition A.5.** Given a cell \( A \), we define the set \( R(A) = \{i \in [d] \mid \nabla_{l}(A,i) > \nabla_{l}(A)\} \). We also define the set \( I(A) = \{i \in [d] \mid A_{0}^{i} \subset A\} \) and \( O(A) = [d] \setminus I(A) \).

**Lemma A.6.** For every partition \( P \), under the Assumption 4.1, if for every \( A \in P \) it holds that \( R(A) = \emptyset \), then for every \( B \in P \), with \( \mathbb{P}_{x}(x \in B) > 0 \), and \( x,x' \in B \) it holds that \( m(x) = m(x') \).

*Proof.* We prove this by contradiction. Let \( B \in P \), if there exist \( x,x' \in B \) such that \( m(x) \neq m(x') \) then obviously there exists a \( \bar{x} \in B \) such that \( m(\bar{x}) \neq \mathbb{E}_{x}[m(x)|x \in B] \). Therefore it holds that \( \mathbb{I}(P) > \mathbb{I}(P,B,[d]) \) and hence \( \nabla(P,B,[d]) > \nabla(P) \). Now let’s assume an arbitrary enumeration \( \{i_{1}, \ldots, i_{k}\} \) of the set \( I(B) \). Because the function \( \nabla \) is decreasing with respect to \( P \) and \( \nabla(P,B,[d]) > \nabla(P) \), there has to be a number \( j \in [k] \) such that \( \nabla(P,B,\{i_{1}, \ldots, i_{j}\}) > \nabla(P,B,\{i_{1}, \ldots, i_{j-1}\}) \). But because of Assumption 4.1 of \( \nabla_{l} \) and Lemma A.4 it holds that
\[ 0 < \nabla(P,B,\{i_{1}, \ldots, i_{j}\}) - \nabla(P,B,\{i_{1}, \ldots, i_{j-1}\}) \leq C \cdot (\nabla(P,B,i_{j}) - \nabla(P,B)) \],
by Lemma A.4 we have that \( \nabla_{l}(B,i_{j}) > \nabla_{l}(B) \) and together with \( \mathbb{P}_{x\sim D_{x}}(x \in B) > 0 \) these contradict the assumption \( R(B) = \emptyset \).

**Theorem A.7.** Consider the non-parametric regression model \( y = m(x) + \varepsilon \), where \( m : \{0,1\}^{d} \to [-\frac{1}{2}, \frac{1}{2}] \) is a \( r \)-sparse function and \( \varepsilon \sim \mathcal{E} \), with \( \varepsilon \in [-\frac{1}{2}, \frac{1}{2}] \) and \( \mathbb{E}[\varepsilon] = 0 \). Let \( \mathbb{M} \) be the function that the Algorithm 4 returns with input \( t \geq (1/\eta)^{C \cdot r} \), then under the Assumption 4.1 it holds that
\[ \mathbb{E}_{x}[\frac{(m(x) - \mathbb{M}(x))^{2}}{\eta}] \leq \eta. \]
Also, under the Independence of Features Assumption 2.2 if \( t \geq 2^{r} \) then \( \mathbb{P}_{x\sim D_{x}}(\mathbb{M}(x) = m(x)) = 1 \).

*Proof.* When the value of level changes, then the algorithm considers separately every cell \( A \) in \( \mathcal{P}_{\text{level}} \). For every such cell \( A \) it holds that \( \mathbb{I}_{l}(A,R) = 0 \) and hence \( \mathbb{V}_{l}(A,R) = V^{*}(A) \) is maximized. Since \( m(x) \in [-1,1] \) it holds that the maximum value of \( \mathbb{V}_{l} \) is 1. Now let \( \{i_{1}, \ldots, i_{r}\} \) be an arbitrary enumeration of \( R \) and let \( R_{j} = \{i_{1}, \ldots, i_{j}\} \) then by adding and subtracting terms of the form \( \nabla_{l}(A,R_{j}) \) we have the following equality
\[ \nabla_{l}(A,R) - \nabla_{l}(A,R_{r-1}) + \cdots + \nabla_{l}(A,R_{2}) - \nabla_{l}(A,i_{1}) + \mathbb{V}_{l}(A,i_{1}) = V^{*}(A). \]
From Assumption 4.1 we have that
\[ (\nabla_{l}(A,i_{r}) - \nabla_{l}(A)) + \cdots + (\nabla_{l}(A,i_{2}) - \nabla_{l}(A)) + (\nabla_{l}(A,i_{1}) - \nabla_{l}(A)) \geq \frac{V^{*}(A) - \mathbb{V}_{l}(A)}{C} \]
which implies
\[ \max_{j \in [r]}(\nabla_{l}(A,i_{j}) - \nabla_{l}(A)) \geq \frac{V^{*}(A) - \mathbb{V}_{l}(A)}{C \cdot r}. \]
Let \( i^\text{level}_A \) be the coordinate that the algorithm chose to split cell \( A \) at level \( \text{level} \). Now from the greedy criterion that we use to pick the next coordinate to split in Algorithm 4 we get that for the coordinate \( i^\text{level}_A \) that we picked to split \( A \) was at least as good as the best of the coordinates in \( R \), hence it holds that

\[
\nabla_{\text{level}}(A, i^\text{level}_A) \geq \nabla_{\text{level}}(A) + \frac{V^*(A) - \overline{V}_t(A)}{C \cdot r}
\]

which in turn because \( L^*(A) \triangleq \nabla_{\text{level}}(A, R) = 0 \) implies that

\[
\nabla_{\text{level}}(A, i^\text{level}_A) \leq \nabla_{\text{level}}(A) \left(1 - \frac{1}{C \cdot r}\right).
\]

(A.3)

Again we fix \( Q_{\text{level}} \) to be the partition \( P_{\text{level}} \) when level changed and \( P_{\text{level}} \) is a full partition of \( \{0, 1\}^d \). Then because of A.3 and Lemma A.4 it holds that

\[
\mathcal{T}(Q_{\text{level}}) = \sum_{A \in Q_{\text{level}}} \mathbb{P}(x \in A) \nabla_{\text{level}}(A, i^\text{level}_A) \leq \sum_{A \in Q_{\text{level}}} \nabla_{\text{level}}(A) \left(1 - \frac{1}{C \cdot r}\right)
\]

(A.4)

\[
= \overline{L}(Q_{\text{level}}) \left(1 - \frac{1}{C \cdot r}\right). 
\]

(A.5)

Inductively and using the fact that \( m(x) \in [-1, 1] \) implies that

\[
\overline{L}(Q_{\text{level}}) \leq \overline{L}(P_0) \left(1 - \frac{1}{C \cdot r}\right)^{\text{level}} \leq \left(1 - \frac{1}{C \cdot r}\right)^{\text{level}}.
\]

(A.6)

Finally from the choice of \( t \) we have that \( \text{level} \geq C \cdot r \cdot \ln(1/\eta) \) and hence \( \overline{L}(Q_{\text{level}}) \leq \eta \) and hence the first part of the theorem follows.

For the second part, we observe that for any coordinate \( i \in [d] \setminus R \) and for any cell \( A \) it holds that \( \nabla_{\text{level}}(A, i) - \nabla_{\text{level}}(A) = 0 \) and hence the Algorithm 4 will pick a coordinate in \( [d] \setminus R \) only after it picks all the coordinates in \( R \). Hence for \( t \geq 2^t \) we have that \( \mathcal{R}(A) = \emptyset \) for all the cells \( A \) in the output partition and from Lemma A.6 the second part of the theorem follows. \( \square \)
B Bias-Variance Decomposition of Shallow Trees

In this section, we prove a bias-variance decomposition of estimators defined via partitions of the function space; a special case of which are tree-based estimators. Moreover, we prove a bound on the variance via an adaptation of the localized Rademacher complexity analysis, to account for partition-based estimators (which are not necessarily global minimizers of the empirical risk).

Definition B.1. Given a partition \( \mathcal{P} = \{A_1, \ldots, A_k\} \) of \( \{0, 1\}^d \) we define the set \( \mathcal{F}(\mathcal{P}) \) of piecewise constant functions that have the value for every set in \( \mathcal{P} \), i.e.

\[
\mathcal{F}(\mathcal{P}) = \{ m : \{0, 1\}^d \rightarrow [-1, 1] \mid \forall A \in \mathcal{P}, \forall x, x' \in A, m(x) = m(x') \}.
\]

If \( Z = \{\mathcal{P}_1, \ldots, \mathcal{P}_s\} \) is a family of partitions of \( \{0, 1\}^d \), then we define \( \mathcal{F}(Z) \) to be the union of \( \mathcal{F}(\mathcal{P}) \) for all \( \mathcal{P} \in Z \).

For any function class \( \mathcal{G} \), we define the critical radius as any solution to the inequality:

\[
\mathcal{R}(\delta; \mathcal{G}) \leq \delta^2
\]

where \( \mathcal{R}(\delta; \mathcal{G}) \) is the localized Rademacher complexity, defined as:

\[
\mathcal{R}(\delta; G) = \mathbb{E}_{D_n \sim \mathcal{P}^n, \epsilon \sim \text{Rad}^n} \left( \sup_{\mathcal{G} \in \mathcal{G}: \|g\|_2 \leq \delta} \frac{1}{s} \sum_i \epsilon_i g(x_i, y_i) \right)
\]

where \( \epsilon_i \) are independent Rademacher random variables taking values equi-probably in \( \{-1, 1\} \). Moreover, we define the star-hull of the function class as: \( \text{star}(G) = \{ \kappa g : g \in G, \kappa \in [0, 1]\} \).

Lemma B.2 (Bias-Variance Decomposition). Consider a mapping \( \mathcal{P}(D_n) \) (for simplicity \( \mathcal{P}_n \)), that maps a set of training samples into a partition of the space \( \{0, 1\}^d \). Let \( \overline{\mathcal{P}} \) be the image of this mapping, i.e. the union of \( \mathcal{P}_n \) for all possible \( D_n \). Suppose that an estimator \( \hat{m} \), minimizes the empirical mean squared error among all piece-wise constant functions \( f \in \mathcal{F}(\mathcal{P}_n) \), i.e.:

\[
\hat{m} = \arg\min_{f \in \mathcal{F}(\mathcal{P}_n)} \sum_{i \in [n]} (y^{(i)} - f(x_i))^2.
\]

Let \( \overline{\mathcal{F}} = \mathcal{F}(\overline{\mathcal{P}}) \) and let \( \delta_n^2 \geq \Theta \left( \frac{\log(\log(n))}{n} \right) \) be an upper bound on the critical radius of \( \text{star}(\overline{\mathcal{F}} - m) \).

Moreover, let \( \hat{m}_n(\cdot) = \mathbb{E}_{z \sim D_x} [m(z) \mid z \in \mathcal{P}_n(\cdot)] \). Then for a universal constant \( C \), w.p. \( 1 - \zeta \):

\[
\mathbb{E}_{x \sim D_x} \left[ (\hat{m}(x) - m(x))^2 \right] \leq C \left( \delta_n + \sqrt{\frac{\log(1/\zeta)}{n}} \right)^2 + \mathbb{E}_{x \sim D_x} \left[ (\hat{m}_n(x) - m(x))^2 \right]
\]

B.1 Proof of Lemma B.2

Notation. To simplify the exposition we introduce here some notation that we need for our local Rademacher complexity analysis. We define \( c(x, y; m) \) to be represent the error of the sample \( (x, y) \) according to the function \( m \). In our setting we have that \( c(x, y; m) = (y - m(x))^2 \) and we may drop the argument \( m \) from \( c \) when \( m \) is clear from the context. We define \( D_x \) to be the marginal with respect to \( x \) of the distribution of \( D \). Also we use the notation \( \|m\|_2 = \)
\[ \sqrt{\mathbb{E}_{x \sim D_x}[m(x)]}. \] In this section we sometimes use \( \hat{m} \) is place for \( m_n \) but they have the same meaning. We next give a formal definition of the set of piece-wise constant functions. Finally, let \( \mathbb{E}_n \) denote the empirical expectation with respect to \( D_n \).

For simplicity of notation, let \( \mathcal{F}(D_n) = \mathcal{F}_n \triangleq \mathcal{F}(\mathcal{P}_n) \) and \( \mathcal{F} \triangleq \mathcal{F}(\mathcal{P}) \). From the definition of \( \hat{m} \) we have that

\[ \sum_{i \in [n]} \left( y^{(i)} - \hat{m}(x^{(i)}) \right)^2 \leq \inf_{f \in \mathcal{F}_n} \sum_{i \in [n]} \left( y^{(i)} - f(x) \right)^2. \] (B.5)

Now for any function \( g : \{0, 1\}^d \to \mathbb{R} \) we have that

\[ \mathbb{E}_{(x,y) \sim D} \left[ (y - g(x))^2 - (y - m(x))^2 \right] = \mathbb{E}_{(x,y) \sim D} \left[ g^2(x) - m^2(x) - 2y(g(x) + m(x)) \right] = \mathbb{E}_{x \sim D_x} \left[ g^2(x) - m^2(x) - 2 \mathbb{E}[y | x] (g(x) + m(x)) \right] = \mathbb{E}_{x \sim D_x} \left[ g^2(x) + m^2(x) - 2m(x)g(x) \right] = \| g - m \|_2^2. \] (B.6)

If we plug in \( g = \hat{m} \) in (B.6) then we get that

\[ \| \hat{m} - m \|_2^2 = \mathbb{E}_{(x,y) \sim D} [c(x, y; \hat{m}) - c(x, y; m)] \] (B.7)

We define also the following function

\[ \hat{m}_n = \arg\min_{f \in \mathcal{F}_n} \mathbb{E}_{x \sim D_x} \left[ (f(x) - m(x))^2 \right]. \] (B.8)

Observe that the solution to this optimization takes the form:

\[ \hat{m}_n = \mathbb{E}_{z \sim D_n} [m(z) | z \in \mathcal{P}_n] \] (B.9)

Conditional on the training set \( D_n \), we have:

\[ \| \hat{m} - m \|_2^2 = \mathbb{E}_{(x,y) \sim D} [c(x, y; \hat{m}) - c(x, y; m)] = \mathbb{E}_{(x,y) \sim D} [c(x, y; \hat{m}) - c(x, y; \hat{m}_n)] + \mathbb{E}_{(x,y) \sim D} [c(x, y; \hat{m}_n) - c(x, y; m)] = \mathbb{E}_{(x,y) \sim D} [c(x, y; \hat{m}) - c(x, y; \hat{m}_n)] + \| \hat{m}_n - m \|_2^2 \] (by (B.6))

Now we can relate the population generalization error with the empirical.

\[ \mathbb{E}_{(x,y) \sim D} [c(x, y; \hat{m}) - c(x, y; \hat{m}_n)] = \mathbb{E}_n [c(x, y; \hat{m}) - c(x, y; \hat{m}_n)] + \mathbb{E}_{(x,y) \sim D} [c(x, y; \hat{m}) - c(x, y; \hat{m}_n)] - \mathbb{E}_n [c(x, y; \hat{m}) - c(x, y; \hat{m}_n)] \]

Since by definition \( \hat{m} \) minimizes the empirical loss over \( \mathcal{F}_n \) and since \( \hat{m}_n \in \mathcal{F}_n \) the first term is non-positive and hence

\[ \mathbb{E}_{(x,y) \sim D} [c(x, y; \hat{m}) - c(x, y; \hat{m}_n)] \leq \mathbb{E}_{(x,y) \sim D} [c(x, y; \hat{m}) - c(x, y; m)] - \mathbb{E}_n [c(x, y; \hat{m}) - c(x, y; \hat{m}_n)] \]

\[ = \mathbb{E}_{(x,y) \sim D} [c(x, y; \hat{m}) - c(x, y; m)] - \mathbb{E}_n [c(x, y; \hat{m}) - c(x, y; m)] + \mathbb{E}_{(x,y) \sim D} [c(x, y; m) - c(x, y; \hat{m}_n)] - \mathbb{E}_n [c(x, y; m) - c(x, y; \hat{m}_n)] \]
Observe that the space of functions $F_n$ is a subset of the space of functions $\overline{F}$, which is independent of $D_n$. Thus it suffices to prove a uniform convergence tail bound for all functions in the latter space.

By Lemma 7 of [FS19], we have that if $\delta_n^2 = \Theta \left( \frac{\log(\log(n))}{n} \right)$ is any solution to the inequality:

$$
\mathcal{R}(\delta; \text{star}(\overline{F} - m)) \leq \delta^2
$$

(B.10)

then for some universal constant $C$, we have that with probability $1 - \delta$ for all $f \in \overline{F}$ it holds that

$$
\left| \mathbb{E}_{(x,y) \sim D} [c(x,y,f) - c(x,y;m)] - \frac{1}{n} \sum_{i=1}^{n} c(x_i,y_i,f) - c(x_i,y_i;m) \right| \leq C (\delta_n + \zeta) \|f - m\|_2 + C (\delta_n + \zeta)^2
$$

for $\zeta = \sqrt{\frac{\log(1/\delta)}{n}}$. Applying the same lemma to loss function $-c$, we get

$$
\left| \mathbb{E}_{(x,y) \sim D} [c(x,y,m) - c(x,y;m)] - \frac{1}{n} \sum_{i=1}^{n} c(x_i,y_i;m) - c(x_i,y_i;m) \right| \leq C (\delta_n + \zeta) \|f - m\|_2 + C (\delta_n + \zeta)^2.
$$

Applying the first inequality for $f = \hat{m}$ and the second for $f = \tilde{m}_n$ and taking a union bound over both events, we have that for $\zeta = \sqrt{\frac{\log(2/\delta)}{n}}$, w.p. $1 - \delta$:

$$
\mathbb{E}_{(x,y) \sim D} [c(x,y,\hat{m}) - c(x,y;m)] - \mathbb{E}_{n} [c(x,y,\hat{m}) - c(x,y;m)] \leq C (\delta_n + \zeta) \|\hat{m} - m\|_2 + C (\delta_n + \zeta)^2
$$

and

$$
\mathbb{E}_{(x,y) \sim D} [c(x,y,m) - c(x,y,\tilde{m}_n)] - \mathbb{E}_{n} [c(x,y,m) - c(x,y,\tilde{m}_n)] \leq C (\delta_n + \zeta) \|\tilde{m}_n - m\|_2 + C (\delta_n + \zeta)^2.
$$

Combining all these we have, w.p. $1 - \delta$ over the training set:

$$
\|\hat{m} - m\|_2^2 \leq C (\delta_n + \zeta)(\|\hat{m} - m\|_2 + \|\tilde{m}_n - m\|_2) + 2C (\delta_n + \zeta)^2 + \|\tilde{m}_n - m\|_2^2
$$

$$
\leq C \left( C (\delta_n + \zeta)^2 + \frac{1}{4C}(\|\hat{m} - m\|_2 + \|\tilde{m}_n - m\|_2)^2 \right) + 2C (\delta_n + \zeta)^2 + \|\tilde{m}_n - m\|_2^2
$$

$$
\leq C (2 + C) (\delta_n + \zeta)^2 + \frac{1}{2} \left( \|\hat{m} - m\|_2 + \|\tilde{m}_n - m\|_2^2 \right) + \|\tilde{m}_n - m\|_2^2
$$

Re-arranging the last inequality, yields:

$$
\|\hat{m} - m\|_2 \leq 2C (1 + C) (\delta_n + \zeta)^2 + 3 \|\tilde{m}_n - m\|_2^2
$$

(B.11)

B.2 Critical Radius of Shallow Trees

**VC dimension of $\overline{F}$** We now show that when the partition $P_n \triangleq P(D_n)$ is defined by a tree with $t$ leaves, then the function class $\overline{F}$ is a VC-subgraph class. Let $\overline{F}(\zeta)$ denote the subgraph of $\overline{F}$ at any level $\zeta$ (i.e. the space of binary functions $\overline{F}(\zeta) \triangleq \{ x \rightarrow 1 \{ f(x) > \zeta \} : f \in \overline{F} \}$). To show that $\overline{F}$ is VC-subgraph with VC dimension $v$, we need to show that $\overline{F}(\zeta)$ has VC dimension at most $v$.

Observe that the number of all possible observationally equivalent functions that the function class $\overline{F}(\zeta)$ can output on $n$ samples is at most $(nd)^t 2^t$. This follows by the following argument: the number of possible functions is equal to the number of possible partitions of the $n$ samples
that can be induced by a tree with $t$ leaves, multiplied by the number of possible binary value assignments at the leaves. The latter is $2^t$. The former is at most $(nd)^t$.

On the other hand, the set of all binary functions on $n$ points is $2^n$. Thus for the function class $\mathcal{F}(\zeta)$ to be able to shatter a set of $n$ points, it must be that $2^n \leq (2nd)^t$. Equivalently:

$$n \leq t \log(2d) + t \log(n) \Rightarrow m \leq 4t \log(t) + 2t \log(2d) = O(t \log(dt)) \quad (B.12)$$

Thus we get that the function class $\mathcal{F}(\zeta)$ has VC dimension at most $v = O(t \log(dt))$. Thus $\mathcal{F}$ is a VC-subgraph class of VC dimension $v = O(t \log(dt))$.

**Bounding the critical radius** We will use the fact that the critical radius of star $(\mathcal{F} - m)$ is $O(\delta_n)$, where $\delta_n$ is any solution to the inequality (see e.g. [Wai19]):

$$\int_{\delta^2/8}^\delta \sqrt{\frac{H_2(\varepsilon, \text{star}(\mathcal{F} - m)_{\delta,n}, z_{1:n})}{n}} \leq \delta^2 \quad (B.13)$$

where $G_{\delta,n} = \{g \in G : \|g\|_n = \sqrt{\frac{1}{n} \sum_i g(z_i)^2} \leq \delta\}$ and $H_2(\varepsilon, G, z_{1:n})$ is the logarithm of the size of the smallest $\varepsilon$-cover of $G$, with respect to the empirical $\ell_2$ norm $\|g\|_n$ on the samples $z_{1:n}$.

First observe that the star hull can only add at most a logarithmic extra factor to the metric entropy, by a simple discretization argument on the parameter $\delta$, i.e.:

$$H_2(\varepsilon, \text{star}(\mathcal{F} - m)_{\delta,n}, z_{1:n}) \leq H_2(\varepsilon/2, (\mathcal{F} - m)_{\delta,n}, z_{1:n}) + \log(2 \sup_{f \in (\mathcal{F} - m)_{\delta,n}} \|f\|_{2,n}/\varepsilon)$$

$$\leq H_2(\varepsilon, (\mathcal{F} - m)_{\delta,n}, z_{1:n}) + \log(2\delta/\varepsilon)$$

Moreover, observe that the metric entropy of $(\mathcal{F} - m)_{\delta,n}$ is at most the metric entropy of $\mathcal{F} - m$, which is at most the metric entropy of $\mathcal{F}$ (since $m$ is a fixed function). Thus it suffices to bound the metric entropy of $\mathcal{F}$.

Theorem 2.6.7 of [VW96] shows that for any VC-subgraph class $G$ of VC dimension $v$ and bounded in $[-1, 1]$ we have:

$$H_2(\varepsilon, G, z_{1:n}) = O(v(1 + \log(1/\varepsilon))) \quad (B.14)$$

This implies that the critical radius of star $(\mathcal{F} - m)$ is of the order of any solution to the inequality:

$$\int_{\delta^2/8}^\delta \sqrt{\frac{v(1 + \log(2\delta/\varepsilon)) + \log(2\delta/\varepsilon)}{n}} \leq \delta^2$$

The left hand side is of order $\delta \sqrt{\frac{v(1 + \log(1/\delta))}{n}}$. Thus the critical radius needs to satisfy for some constant $D$, that:

$$\delta \geq D \sqrt{\frac{v(1 + \log(1/\delta))}{n}} \quad (B.15)$$

---

This can be shown by induction; Let $S_{s,t}$ be the number of possible partitions induced by a tree with $t$ leaves. Then $S_{s,1} = 1$ and in order to create a tree with $t$ leaves, we need to take a tree with $t - 1$ leaves and expand the leaf that one of the $s$ samples belongs to along the dimension of one of the $d$ features. Thus we have $ds$ total choices, leading to $S_{s,t} = S_{s,t-1} ds = (ds)^t$
This is satisfied for:

\[ \delta = \Theta \left( \sqrt{\frac{\nu(1+\log(n))}{n}} \right) \]  

(B.16)

Thus the critical radius of \( \star(\mathcal{F} - m) \) is \( \Theta \left( \sqrt{\frac{t \log(d/t)(1+\log(n))}{n}} \right) \).

**Corollary B.3** (Critical Radius of Shallow Trees). Let \( \mathcal{P}(D_n) \), be a function that maps any set of training samples \( D_n \) into a partition of \( \{0,1\}^d \), defined in the form of a binary tree with \( t \) leaves. Then the critical radius of \( \star(\mathcal{F} - m) \), as defined in Lemma B.2 is \( \Theta \left( \sqrt{\frac{t \log(d/t)(1+\log(n))}{n}} \right) \).
C Bias-Variance Decomposition of Deep Honest Forests

We next need the notion of diameter of a cell $A$ with respect to the value of $m(x)$.

**Definition C.1 (Value-Diameter of a Cell).** Given set $B \subseteq \{0,1\}^d$ we define the subset $\overline{B} \subseteq B$ such that $x \in \overline{B}$ if and only if $\Pr_{z \sim D_x}(z \in B) > 0$. The value-diameter $\Delta(B)$ of $B$ to be equal to $\Delta_B = \max_{x,y \in \overline{B}} (m(x) - m(y))^2$. For any partition $\mathcal{P}$ of $\{0,1\}^d$ we define the value-diameter of the partition $\mathcal{P}$ to be $\Delta_B(\mathcal{P}) = \max_{A \in \mathcal{P}} \Pr_{x \sim D_x}(x \in A) \cdot \Delta_B(A)$.

**Lemma C.2.** Consider any forest with $B$ trees, where each tree is built with honesty and on a random sub-sample of size $s$. Let $\epsilon(s) = \mathbb{E}_{x \sim D_x, D_{z,s} \sim D^n} \left[ \Delta_B(\mathcal{P}_{s/2}(x)) \right]$. Then

$$
\Pr_{D_{n} \sim D^n} \left( \mathbb{E}_{x \sim D_x} \left[ (m_{n,s}(x) - m(x))^2 \right] \leq O \left( \frac{s \log(n/\delta)}{n} + \frac{d \log(1/\delta)}{B} \right) + \epsilon(s) \right) \geq 1 - \delta.
$$

**Proof.** We start with defining the following function

$$
\overline{m}_s(x) = \mathbb{E}_{D_{n} \sim D^n} \left[ m_{n,s}(x) \right] = \mathbb{E}_{D_{x} \sim D_x} \left[ m_s(x) \right].
$$

(C.1)

For mean squared error of $m_{n,s}$ we have:

$$
\frac{\mathbb{E}_{x \sim D_x, D_{n} \sim D^n} \left[ (m_{n,s}(x) - m(x))^2 \right]}{\mathbb{E}_{x \sim D_x, D_{n} \sim D^n} \left[ (m_{n,s}(x) - \overline{m}_s(x))^2 \right] + \mathbb{E}_{x \sim D_x} \left[ (\overline{m}_s(x) - m(x))^2 \right]}
$$

The first part we know that it is bounded for every $x$ and with exponential tails due to concentration of U-statistics [Hoe94, PAR10], i.e. for any fixes $x$ with probability $1 - \delta$ it holds that

$$
(m_{n,s}(x) - \overline{m}_s(x))^2 \leq O \left( \frac{s \log(1/\delta)}{n} \right)
$$

(C.2)

Thus integrating over $x \sim D_x$, we have:

$$
\Pr_{x \sim D_x, D_{n} \sim D^n} \left( (m_{n,s}(x) - \overline{m}_s(x))^2 \geq O \left( \frac{s \log(1/\delta)}{n} \right) \right) \leq \delta.
$$

(C.3)

Let $T(x) = (m_{n,s}(x) - \overline{m}_s(x))^2$ and $\epsilon = \Theta \left( \frac{s \log(1/\delta)}{n} \right)$. Suppose that with probability more than $n \delta$ over the training set $D_n \sim D^n$, we had that $\Pr_{x \sim D_x}(T(x) \geq \epsilon \mid D_n) \geq 1/n$. Then we have that $\Pr_{x \sim D_x, D_{n} \sim D^n}(T(x) \geq \epsilon) \geq \delta$, which contradict C.3. Thus we know that with probability $1 - n \delta$ over $D_n \sim D^n$ it holds that $\Pr_{x \sim D_x}(T(x) \geq \epsilon \mid D_n) \leq 1/n$. Hence with probability $1 - n \delta$ over the training set $D_n \sim D^n$ it holds that

$$
\mathbb{E}_{x \sim D_x} \left[ (m_{n,s}(x) - \overline{m}_s(x))^2 \right] \leq \epsilon + \Pr_{x \sim D_x}(T(x) \geq \epsilon) \leq \epsilon + \frac{1}{n} = O \left( \frac{s \log(1/\delta)}{n} \right) + \frac{1}{n}
$$

Setting $\delta' = n \delta$, we have the following

$$
\Pr_{D_{n} \sim D^n} \left( \mathbb{E}_{x \sim D_x} \left[ (m_{n,s}(x) - \overline{m}_s(x))^2 \right] \leq O \left( \frac{s \log(n/\delta')}{n} \right) \right) \geq 1 - \delta'.
$$

(C.4)
For the bias term we define for simplicity \( w^{(j)}(x) = \frac{1}{N_n(P_n(x^{(j)}))} \) and hence \( m_n(x) = \sum_{i=1}^s w^{(i)}(x)y^{(i)} \) and we have:

\[
\mathbb{E}_{x \sim D_x} [(m_n(x) - m(x))^2] = \mathbb{E}_{x \sim D_x} \left[ \left( \mathbb{E}_{D_{n-s} \sim D_{n-s}} [m_{n,s}(x)] - m(x) \right)^2 \right]
\]

\[
= \mathbb{E}_{x \sim D_x} \left[ \left( \mathbb{E}_{D_{n-s} \sim D_{n-s}} \left[ \sum_{j=1}^s w^{(j)}(x) (y^{(j)} - m(x^{(j)})) \right] \right) + \mathbb{E}_{D_{n-s} \sim D_{n-s}} \left[ \sum_{j=1}^s w^{(j)}(x) (m(x^{(j)}) - m(x)) \right] \right]^2
\]

Due to honesty \( w^{(j)}(x) \) is independent of \( y^{(j)} \) and we have that the first term is equal to 0 by a tower law. Thus we have:

\[
\mathbb{E}_{x \sim D_x} [(m_n(x) - m(x))^2] = \mathbb{E}_{x \sim D_x} \left[ \mathbb{E}_{D_{n-s} \sim D_{n-s}} \left[ \sum_{j=1}^s w^{(j)}(x) (m(x^{(j)}) - m(x)) \right] \right]^2
\]

\[
\leq \mathbb{E}_{x \sim D_x, D_{n-s} \sim D_{n-s}} \left[ \left( \sum_{j=1}^s w^{(j)}(x) (m(x^{(j)}) - m(x)) \right)^2 \right]
\]

\[
\leq \mathbb{E}_{x \sim D_x, D_{n-s} \sim D_{n-s}} \left[ \Delta_m(D_{n-s}/2(x)) \right]
\]

□
D Proofs for Level Splits Algorithms

In this section we present the proofs of Theorem 3.3 and Theorem 3.4. We start with a proof about the bias of the trees that are produced by Algorithm 1 and then we show how we can bound the variance term. First, we define the set $\mathcal{K}_n(S; D_n)$, or for simplicity $\mathcal{K}_n(S)$, as the partition of the samples induced by the set of splits $S$, i.e. $\mathcal{K}_n(S) = \{ \mathcal{K}_n(S, z) \mid z \in \{0, 1\}^d \}$ where we define $\mathcal{K}_n(S, z)$ as the following set $\mathcal{K}_n(S, z) = \{ j \mid x^{(j)}_{\mathcal{T}_n(z, S)} = z_{\mathcal{T}_n(z, S)}, j \in [n] \}$. Observe that $\mathcal{K}_n$ is the same as the partition of the samples implied by the partition $\mathcal{P}_n$ of the space $\{0, 1\}^d$, returned by Algorithm 1.

D.1 Bounding The Bias

We first prove a technical lemma for the concentration of the function $V_n$ around the function $\nabla$.

**Lemma D.1.** Assuming that $d > 1$, $q \in [d]$ and $k > 1$, we have that

$$\mathbb{P}_{D_n \sim D^n} \left( \sup_{S \subseteq [d], |S| \leq q} \left| V_n(S) - \nabla(S) \right| \geq 10 \sqrt{\frac{2^{q} \cdot (q \log(d \cdot q) + t)}{n}} \right) \leq \exp(-t).$$

**Proof.** For the purpose of the proof we will define the following function that interpolates between then sample based function $V_n$ and the population based function $\nabla$.

$$J_n(S) \triangleq \sum_{K \in \mathcal{K}_n(S)} \frac{|K|}{n} \left( \mathbb{E}_{(x,y) \sim D} \left[ y \mid x_S = x_S^{(K)} \right] \right)^2 \quad (D.1)$$

First we bound the difference $|V_n(S) - J_n(S)|$ in the following claim.

**Claim D.2.** Assuming that $d > 1$, $r \in [d]$ and $t > 1$, we have that

$$\mathbb{P}_{D_n \sim D^n} \left( \sup_{S \subseteq [d], |S| \leq r} \left| V_n(S) - J_n(S) \right| \geq 5 \sqrt{\frac{2^{r} \cdot (r \log(d \cdot r) + t)}{n}} \right) \leq \exp(-t).$$

**Proof.** For the first part of the proof, we fix a particular set of splits $S$. Using the fact that both $y^{(j)}, m(\cdot)$ take values in $[0, 1]$ we get that

$$|V_n(S) - J_n(S)| = \left| \sum_{K \in \mathcal{K}_n(S)} \frac{|K|}{n} \left( \left( \sum_{j \in K} \frac{1}{|K|} y^{(j)} \right)^2 - \mathbb{E}_{(x,y) \sim D} \left[ y \mid x_S = x_S^{(K)} \right]^2 \right) \right| \leq 2 \sum_{K \in \mathcal{K}_n(S)} \frac{|K|}{n} \left| \left( \sum_{j \in K} \frac{1}{|K|} y^{(j)} \right)^2 - \mathbb{E}_{(x,y) \sim D} \left[ y \mid x_S = x_S^{(K)} \right]^2 \right| .$$

Now let $\mathcal{Y}_S(x_S)$ be the distribution of the random variable $y$ conditional that the random variable $x$ takes value $x_S$ at the subset $S$ of the coordinates. Observe that conditional on $x_S^{(j)}$, the variables $y^{(j)}$ for $j \in K \in \mathcal{K}_n(S)$ are i.i.d. samples from the distribution $\mathcal{Y}_S(x_S^{(K)})$. Hence, using the Hoeffding’s inequality we have that for any $K \in \mathcal{K}_n(S)$ it holds that

$$\mathbb{P}_{y^{(j)} \sim \mathcal{Y}_S(x_S^{(K)})} \left( \left| \sum_{j \in K} \frac{1}{|K|} y^{(j)} - \mathbb{E}_{(x,y) \sim D} \left[ y \mid x_S = x_S^{(K)} \right] \right| \geq \sqrt{\frac{2t}{|K|}} \right) \leq \exp(-t).$$
which, by a union bound over $\mathcal{K}_n(S)$, implies that
\[
\mathbb{P}_{y^{(j)} \sim y_S(x_S^{(j)})} \left( \frac{1}{|K|} \sum_{j \in K} |y^{(j)}_{x_S} - \mathbb{E}_{(x,y)}[y | x_S = x_S^{(K)}]| \geq \sqrt{\frac{2(|S| + t)}{|K|}} \right) \leq \exp(-t),
\]
where we have used the fact that after splitting on $|S|$ coordinates we can create at most $2^{|S|}$ leaf nodes, i.e. $|\mathcal{K}_n(S)| \leq 2^{|S|}$. Hence we have that
\[
\mathbb{P}_{y^{(j)} \sim y_S(x_S^{(j)})} \left( |V_n(S) - J_n(S)| \geq \sqrt{\frac{8(|S| + t) \sum_{K \in \mathcal{K}_n(S)} \sqrt{|K|}}{n}} \right) \leq \exp(-t). \tag{D.2}
\]
But we know that $\sum_{K \in \mathcal{K}_n(S)} |K| = n$, and also we have that the for any vector $w \in \mathbb{R}^k$ it holds that $\|w\|_1 \leq \sqrt{k} \|w\|_2$. Therefore if we define the vector $w = (\sqrt{|K|})_{K \in \mathcal{K}_n(S)}$ we have that
\[
\frac{\sum_{K \in \mathcal{K}_n(S)} \sqrt{|K|}}{n} = \frac{\|w\|_1}{\|w\|_2} \leq \frac{\sqrt{|\mathcal{K}_n(S)|}}{\|w\|_2} \leq \sqrt{\frac{2^{|S|}}{n}}.
\]
Now using this in the inequality (D.2) and taking the expectation over $x_S^{(j)}$ for all $j$ we get the following inequality for any $S \subseteq [d]$:
\[
\mathbb{P}_{D_n \sim \mathcal{D}^n} \left( |V_n(S) - J_n(S)| \geq \sqrt{\frac{8(|S| + t)2^{|S|}}{n}} \right) \leq \exp(-t). \tag{D.3}
\]
To finalize the proof, using a union bound over all $S \subseteq [d]$ with $|S| \leq r$ we get that
\[
\mathbb{P}_{D_n \sim \mathcal{D}^n} \left( \sup_{S \subseteq [d], |S| \leq r} |V_n(S) - J_n(S)| \geq \sqrt{\frac{8(r + t)2^r}{n}} \right) \leq \left( \sum_{i=0}^r \begin{pmatrix} d \cr i \end{pmatrix} \right) \exp(-t). \tag{D.4}
\]
Finally using the fact that $\log \left( \sum_{i=0}^r \begin{pmatrix} d \cr i \end{pmatrix} \right) \leq (r + 1) \log(d \cdot r)$ and assuming that $d > 1$, we have that $r + (r + 1) \log(d \cdot r) \leq 3r \log(dr)$ and the claim follows.

Next we bound the difference $|J_n(S) - \nabla(S)|$.

**Claim D.3.** *If we assume that $d > 1$, $r \in [d]$, $t > 1$ then we have that
\[
\mathbb{P}_{D_n \sim \mathcal{D}^n} \left( \sup_{S \subseteq [d], |S| \leq r} |J_n(S) - \nabla(S)| \geq \sqrt{\frac{2r \cdot \log(d \cdot r) + t}{n}} \right) \leq \exp(-t). \]
*Proof.* For the first part of the proof, we fix a particular set of splits $S$. We then have that
\[
\left( \mathbb{E}_{(x,y) \sim \mathcal{D}}[y | x_S = z_S] \right)^2 = \left( \mathbb{E}_{x \sim \mathcal{D}_x}[m(x) | x_S = z_S] \right)^2 \triangleq M_S(z_S),
\]
and hence
\[
J_n(S) - \nabla(S) = \sum_{K \in \mathcal{K}_n(S)} \frac{|K|}{n} \left( \mathbb{E}_{x \sim \mathcal{D}_x}[m(x) | x_S = x_S^{(K)}] \right)^2 - \mathbb{E}_{x_S} \left[ \left( \mathbb{E}_{x}[m(x) | x_S] \right)^2 \right] = \frac{1}{n} \sum_{j \in [n]} M_S(x_S^{(j)}) - \mathbb{E}_{x_S}[M_S(x_S)].
\]

Now since $m(\cdot) \in \left[ -\frac{1}{2}, \frac{1}{2} \right]$, we have that for any $x \in \{0, 1\}^d$ it holds that $|M_S(x_S)| \leq 1$ and hence from Hoeffding’s inequality we get that

$$P_{D_n \sim D^n} \left( \left| \frac{1}{n} \sum_{j \in [n]} M_S(x_S^{(j)}) - \mathbb{E}_{x_S} [M_S(x_S)] \right| \geq \sqrt{\frac{t}{2n}} \right) \leq \exp(-t).$$

Finally if we apply the union bound over all sets $S \subseteq [d]$, with $|S| = r$, the claim follows. \[Q.E.D.\]

If we combine Claim D.2 and D.3, the Lemma D.1 follows. \[Q.E.D.\]

Towards bounding the bias term we provide a relaxed version of the Definition A.1.

**Definition D.4.** Given a set $S$, a positive number $\eta$ and a training set $D_n$, we define the sets $\mathcal{R}^\eta_n(S) = \{ i \in [d] \mid V_n(S \cup \{i\}) - V_n(S) > \eta \}$ and $\mathcal{R}^\eta(S) = \{ i \in [d] \mid V(S \cup \{i\}) - V(S) > \eta \}$. For simplicity for $\eta = 0$ we use the simpler notation $\mathcal{R}(S)$ and $\mathcal{R}_n(S)$.

Since $V_n$ is a monotone increasing function we have that $V_n(S \cup i) \geq V_n(S)$. Hence given $S$ the Algorithm 1 chooses the direction $i$ that maximizes the positive quantity $V_n(S \cup i) - V_n(S)$. So the bad event is that for all $j \in [d]$, $V_n(S \cup i) - V_n(S) > V_n(S \cup j) - V_n(S)$ but $V(S \cup i) - V(S) = 0$ and there exists a $k \in [d]$ such that $V(S \cup k) - V(S) > 0$. A relaxed version of this bad event can be described using the Definition D.4. In this language the bad event is that the index $i \in [d]$ that the Algorithm 1 chooses to split does not belong to $\mathcal{R}^\eta(S)$ although $\mathcal{R}^\eta_n(S) \neq \emptyset$. We bound the probability of this event in the next lemma.

**Lemma D.5.** Let $\eta = 10 \sqrt{\frac{2^t (r \log(d - r) + t)}{n}}$ and assume that $d > 1$, $r \in [d]$ and $t > 1$, then it holds that

$$P_{D_n \sim D^n} \left( \bigvee_{S \subseteq [d], |S| \leq r} \left( \left( \arg\max_{i \in [d]} V_n(S \cup i) \right) \notin \mathcal{R}(S) \mid \mathcal{R}_n(S) \neq \emptyset \right) \right) \leq 2 \exp(-t)$$

**Proof.** Directly applying Lemma D.1 to Definition D.4 we have that

$$P_{D_n \sim D^n} \left( \bigvee_{i, S} (i \in \mathcal{R}_n(S) \mid i \notin \mathcal{R}(S)) \right) \leq \exp(-t), \quad \text{(D.5)}$$

where $\eta = 10 \sqrt{\frac{2^t (r \log(d - r) + t)}{n}}$. Similarly we have that

$$P_{D_n \sim D^n} \left( \bigvee_{i, S} (i \notin \mathcal{R}_n(S) \mid i \in \mathcal{R}_n(S)) \right) \leq \exp(-t). \quad \text{(D.6)}$$

If we combine the above inequalities we get that there is a very small probability that there exists an index $i \in \mathcal{R}_n(S)$ but an index $j \notin \mathcal{R}(S)$ is chosen instead. This is summarized in the following inequality

$$P_{D_n \sim D^n} \left( \bigvee_{S} \left( \left( \arg\max_{i \in [d]} V_n(S \cup i) \notin \mathcal{R}(S) \mid \mathcal{R}_n(S) \neq \emptyset \right) \right) \right) \leq 2 \exp(-t) \quad \text{(D.7)}$$

and the lemma follows. \[Q.E.D.\]
Lemma D.6. For every set \( S \subseteq [d] \), under Assumption 3.1, if \( \mathcal{R}^\eta(S) = \emptyset \), then

\[
\mathbb{E}_{(x,y) \sim \mathcal{D}} \left[ \left( m(x) - \mathbb{E}_{(x,y) \sim \mathcal{D}} [m(x) | x_S] \right)^2 \right] \leq C \cdot \eta \cdot |\mathcal{R}(S)|.
\]

Proof. We know that \( \overline{\ell}([d]) = 0 \) and under the Assumption 3.1, the function \( \overline{\ell}(\cdot) \) is approximate supermodular. We first prove that \( \overline{\ell}(S \cup \mathcal{R}(S)) = 0 \). If this is not the case then there exists an \( i \notin \mathcal{R}(S) \) such that \( \overline{\ell}(S \cup \mathcal{R}(S) \cup i) - \overline{\ell}(S \cup \mathcal{R}(S)) < 0 \). But because of the approximate supermodularity of \( \overline{\ell} \) we have that

\[
\overline{\ell}(S \cup i) - \overline{\ell}(S) < C \cdot (\overline{\ell}(S \cup \mathcal{R}(S) \cup i) - \overline{\ell}(S \cup \mathcal{R}(S))) < 0
\]

which contradicts with the assumption that \( i \notin \mathcal{R}(S) \).

Now assume that \( \mathcal{R}^\eta(S) = \emptyset \) and for the sake of contradiction also assume that \( \overline{\ell}(S) > C \cdot \eta \cdot |\mathcal{R}(S)| \). Let \( \{r_1, \ldots, r_i\} \) be an arbitrary enumeration of the set \( \mathcal{R}(S) \). From the argument before we have that \( \overline{\ell}(S \cup \mathcal{R}(S)) = 0 \) hence there exists an element \( r_j \in \mathcal{R}(S) \) such that

\[
\overline{\ell}(S \cup \{r_1, \ldots, r_{j-1}\}) - \overline{\ell}(S \cup \{r_1, \ldots, r_j\}) > C \cdot \eta,
\]

otherwise we would immediately have \( \overline{\ell}(S) \leq C \cdot \eta \cdot |\mathcal{R}(S)| \). But because of the approximate supermodularity of \( \overline{\ell}(\cdot) \) we have that

\[
C \cdot (\overline{\ell}(S) - \overline{\ell}(S \cup r_j)) \geq \overline{\ell}(S \cup \{r_1, \ldots, r_j\}) - \overline{\ell}(S \cup \{r_1, \ldots, r_j\}) > C \cdot \eta,
\]

but this last inequality implies \( r_j \in \mathcal{R}^\eta(S) \) which contradicts with our assumption that \( \mathcal{R}^\eta(S) = \emptyset \). Hence \( \overline{\ell}(S) \leq C \cdot \eta \cdot |\mathcal{R}(S)| \) and the lemma follows.

Finally we need one more Lemma to handle the case where Assumption 3.2 holds.

Lemma D.7. Let \( m \) be a target function that is \((\beta, r)\)-strongly sparse, with set of relevant features \( R \), and suppose \( n \geq 256 \cdot \frac{2^{(r \log(d,r)+t)}}{\beta^2} \), then it holds that

\[
\mathbb{P}_{D_n \sim D^n} \left( \bigvee_{S \subseteq [d], |S| \leq r} \left( \argmax_{i \in [d]} V_n(S \cup i) \notin R \mid (R \setminus S) \neq \emptyset \right) \right) \leq 2 \exp(-t)
\]

Proof. Directly applying Lemma D.1 to Definition D.4 we have that

\[
\mathbb{P}_{D_n \sim D^n} \left( \bigvee_{i, S} \left( i \in \mathcal{R}^\eta_n(S) \mid i \notin \mathcal{R}(S) \right) \right) \leq \exp(-t), \quad (D.8)
\]

where \( \eta = 10 \sqrt{2^{r \log(d,r)+t}} \). Similarly we have that

\[
\mathbb{P}_{D_n \sim D^n} \left( \bigvee_{i, S} \left( i \notin \mathcal{R}^\eta_n(S) \mid i \in \mathcal{R}^{2\eta}(S) \right) \right) \leq \exp(-t). \quad (D.9)
\]

If we combine the above inequalities with the Assumption 3.2 the lemma follows.

We are now ready to upper bound the bias of the Algorithm 1 under the Assumption 3.1.
Theorem D.8. Let $D_n$ be i.i.d. samples from the non-parametric regression model $y = m(x) + \epsilon$, where $m(x) \in [-1/2, 1/2]$, $\epsilon \sim \mathcal{E}$, $E_{\epsilon \sim \mathcal{E}}[\epsilon] = 0$ and $\epsilon \in [-1/2, 1/2]$. Let also $\mathcal{P}_n$ be the partition that Algorithm 1 returns. Then under the submodularity Assumption 3.1 the following statements hold.

1. If $m$ is $r$-sparse and we set $\log(t) \geq \frac{C_r}{\sqrt{r+2}} \left( \log(n) - \log(\log(d/\delta)) \right)$, then it holds that

$$
\mathbb{P}_{D_n \sim \mathbb{D}^n} \left( \mathbb{E}_{x \sim D_n} \left[ \left( m(x) - \mathbb{E}_{z \sim D_n} [m(z) \mid z \in \mathcal{P}_n(x)] \right)^2 \right] \right) \geq \Omega \left( C \cdot r \cdot \sqrt{\frac{\log(d/\delta)}{n}} \right) \leq \delta.
$$

2. Under the independence of features Assumption 2.2 and assuming that $m$ is $r$-sparse and if $\log(t) \geq r$, then it holds that

$$
\mathbb{P}_{D_n \sim \mathbb{D}^n} \left( \mathbb{E}_{x \sim D_n} \left[ \left( m(x) - \mathbb{E}_{z \sim D_n} [m(z) \mid z \in \mathcal{P}_n(x)] \right)^2 \right] \right) \geq \Omega \left( C \cdot \sqrt{\frac{2r \cdot \log(d/\delta)}{n}} \right) \leq \delta.
$$

Proof. We fix $S$ to be the set of splits that Algorithm 1 chooses. Our goal in this lemma is to show that with high probability the following quantity is small

$$
\overline{L}(\mathcal{P}_n) = \mathbb{E}_{x \sim D_n} \left[ \left( m(x) - \mathbb{E}_{z \sim D_n} [m(z) \mid z \in \mathcal{P}_n(x)] \right)^2 \right].
$$

(D.10)

We prove this in two steps. First we show that after the completion of the level level of the algorithm the quantity $\overline{L}(S_{\text{level}})$ is small. Then we bound the difference $|\overline{L}(\mathcal{P}_{\text{level}}) - \overline{L}(S_{\text{level}})|$ in Claim D.9. Finally we use the monotonicity of $\overline{L}$ to argue about the upper bound on $\mathcal{P}_n$.

Let $R \subseteq [d]$ be the set of size $|R| = r$ of the relevant features of the target function $m$. Observe that it holds that $\overline{L}(S \cup R) = 0$ and hence $\nabla(S \cup R) \triangleq V^*$ is maximized. Since $m(x) \in [-1/2, 1/2]$, the maximum value of $\nabla$ is 1.

For the first part of the theorem, let $\{i_1, \ldots, i_r\}$ and be an arbitrary enumeration of $R$ and let $R_j = \{i_1, \ldots, i_j\}$ then by adding and subtracting terms of the form $\nabla(S \cup R_j)$ we have the following equality

$$
(\nabla(S \cup R) - \nabla(S \cup R_{r-1})) + \cdots + (\nabla(S \cup R_2) - \nabla(S \cup \{i_1\})) + \nabla(S \cup \{i_1\}) = V^*.
$$

From the approximate submodularity of $\nabla$ we hence have that

$$
(\nabla(S \cup \{i_r\}) - \nabla(S)) + \cdots + (\nabla(S \cup \{i_2\}) - \nabla(S)) + (\nabla(S \cup \{i_1\}) - \nabla(S)) \geq \frac{V^* - \overline{L}(S)}{C}
$$

which implies

$$
\max_{j \in [r]} (\nabla(S \cup \{i_j\}) - \nabla(S)) \geq \frac{V^* - \overline{L}(S)}{C \cdot r}.
$$

Let $i_{\text{level}}$ be the coordinate that the algorithm chose to split at level level. Now from the greedy criterion of Algorithm 1 we get that the coordinate $i_{\text{level}}$ that we picked to split was at least as good as the best of the coordinates in $R$, hence using Lemma D.1 and if we define $\eta = \frac{\sqrt{2r \cdot (q \log(d-q) + \log(1/\delta))}}{n}$, where $q$ is the maximum depth of the tree for which we are applying Lemma D.1, we have that with probability at least $1 - \delta$ it holds that

$$
\nabla \left( S \cup \{i_{\text{level}}\} \right) \geq \nabla(S) + \frac{V^* - \overline{L}(S)}{C \cdot r} - 2\eta
$$
which in turn because \( L^* \triangleq \bar{L}(S \cup R) = 0 \) implies that
\[
\bar{L} \left( S \cup \{i^{\text{level}}\} \right) \leq \bar{L}(S) \left( 1 - \frac{1}{C \cdot r} \right) + 2\eta. \tag{D.11}
\]
Let \( S_{\text{level}} \) to be the set of splits after the step level of Algorithm 1. Then it holds that
\[
\bar{L}(S_{\text{level}+1}) \leq \bar{L}(S_{\text{level}}) \left( 1 - \frac{1}{C \cdot r} \right) + 2\eta.
\]
Inductively and using the fact that \( m(x) \in [-1/2, 1/2] \), the latter implies that
\[
\bar{L}(S_{\text{level}}) \leq \bar{L}(\emptyset) \left( 1 - \frac{1}{C \cdot r} \right)_{\text{level}} ^{level} + 2\text{level} \cdot \eta \leq \left( 1 - \frac{1}{C \cdot r} \right)_{\text{level}} ^{level} + 2\text{level} \cdot \eta. \tag{D.12}
\]
From the choice of \( t \) we have that for \( \text{level} = C \cdot r \ln(1/\eta) \) it holds \( \bar{L}(S_{\text{level}}) \leq 3 \cdot C \cdot r \ln(1/\eta) \eta \). For this analysis to be consistent we have to make sure that the maximum depth \( q \) for which we are applying Lemma D.1 is at least the value required for level. Thus we need to find values for \( q, \eta \) such that \( q \geq C \cdot r \ln(1/\eta) \) at the same time when \( \eta \geq 8 \sqrt{\frac{2n \cdot (q \log(d \cdot q) + \log(1/\delta))}{r}} \). It is easy to see that the smallest possible value for \( \eta \) is hence achieved for \( q = \frac{C \cdot r}{c \cdot r + 2} \left( \log(n) - \log(\log(d / \delta)) \right) \) and \( \eta = \Theta \left( \sqrt{\frac{\log(d / \delta)}{n}} \right) \). Hence the inequality \( \bar{L}(S_{\text{level}}) \leq 3 \cdot C \cdot r \ln(1/\eta) \eta \) which implies
\[
\bar{L}(S_{\text{level}}) \leq \tilde{O} \left( C \cdot r \cdot \frac{c \cdot r + 2}{n} \sqrt{\frac{\log(d / \delta)}{n}} \right). \tag{D.13}
\]
For the second part of the theorem we use Lemma D.5 and we have that at every step either the algorithm chooses to split with respect to a direction \( i \in R(S) \) or \( R^x(S) = \emptyset \). Because of our assumption that \( m \) is \( r \)-sparse and because we assume that the features are distributed independently we have that at any step \( |R(S)| \leq r \). Hence, when \( \text{level} = r \) it has to be that the set \( S_{\text{level}} \) during the execution of the Algorithm 1 satisfies \( R^x(S) = \emptyset \). Then using Lemma D.6 we have that \( \bar{L}(S_{\text{level}}) \leq C \cdot \eta \cdot r \) from which we get that
\[
\bar{L}(S_{\text{level}}) \leq O \left( C \cdot \sqrt{\frac{2r \cdot \log(d / \delta)}{n}} \right). \tag{D.14}
\]
Next we need to compare \( \bar{L}(S_{\text{level}}) \) with \( \bar{L}(P_{\text{level}}) \).

**Claim D.9 (Dealing with Empty Cells).** It holds that with probability \( 1 - \delta \)
\[
|\bar{L}(P_{\text{level}}) - \bar{L}(S_{\text{level}})| \leq 8 \cdot \frac{2^{\text{level}} \ln(2d \text{ level}) + \ln(1/\delta)}{n}.
\]

**Proof.** Fix any possible cell \( A \) after doing a full partition on the first \( q \triangleq \text{level} \) level splits of the algorithm. For simplicity of the exposition of this proof we define for every subset \( B \) of \( \{0, 1\}^n \) the probability \( P_B \triangleq P_{x \sim D_x} \{ x \in B \} \) and the empirical probability \( \hat{P}_B \triangleq \frac{1}{n} \sum_{i=1}^n 1 \{ x(i) \in B \} \). Using the Chernoff-Hoeffding bound we get that
\[
\Pr_{D_n \sim D^n} \left( \hat{P}_A \geq P_A - \sqrt{\frac{2 \ln(1 / \delta) P_A}{n}} \right) \geq 1 - \delta.
\]

33
If the empirical probability $\hat{P}_A$ is zero then we get the following

$$\mathbb{P}_{D_n \sim D^n} \left( P_A \leq \frac{2 \ln(1/\delta)}{n} + 1 \{ \hat{P}_A \neq 0 \} \right) \geq 1 - \delta. $$

The number of possible cells from a tree of depth $q$ is at most $2^d d^q q^d$. Therefore, by union bound over all the possible cells $A$, we have that

$$\mathbb{P}_{D_n \sim D^n} \left( \bigvee_A \left( P_A \leq \frac{2q \ln(2dq) + 2 \ln(1/\delta)}{n} + 1 \{ \hat{P}_A \neq 0 \} \right) \right) \geq 1 - \delta. \quad (D.15)$$

Next, we consider the difference $\mathcal{I}(\mathcal{P}_{\text{level}}) - \mathcal{I}(\mathcal{S}_{\text{level}})$. Let $\mathcal{P}_{\text{level}}^S$ be the partition of space if we split along all the coordinates in $\mathcal{S}_{\text{level}}$. It is easy to see that $\mathcal{P}_{\text{level}}^S$ is a refinement of the partition $\mathcal{P}_{\text{level}}$. Hence in the difference $\mathcal{I}(\mathcal{P}_{\text{level}}) - \mathcal{I}(\mathcal{S}_{\text{level}})$ we only have terms of the form

$$\mathbb{P}_{x \sim D_x} (x \in B) \mathbb{E}_{z \sim D_z} \left[ \left( m(x) - \mathbb{E}_{z \sim D_z} [m(z) \mid z \in B] \right)^2 \mid x \in B \right] - $$

$$- \sum_{j=1}^\ell \mathbb{P}_{x \sim D_x} (x \in A_j) \mathbb{E}_{z \sim D_z} \left[ \left( m(x) - \mathbb{E}_{z \sim D_z} [m(z) \mid z \in A_j] \right)^2 \mid x \in A_j \right].$$

Where $B \in \mathcal{P}_{\text{level}}$, $A_j \in \mathcal{P}_{\text{level}}^S$ and $B$ is the union of the cells $A_1, \ldots, A_\ell$. In order for $B$ to remain unsplit in $\mathcal{P}_{\text{level}}$ it has to be that for all but one of $A_j$’s it holds that $\hat{P}_{A_j} = 0$. We denote with $\mathcal{E}(B)$ the above difference and we observe that it is equal to the following

$$\sum_{j=1}^\ell P_{A_j} \mathbb{E}_{x \sim D_x} \left[ \left( m(x) - \mathbb{E}_{z \sim D_z} [m(z) \mid z \in B] \right)^2 - \left( m(x) - \mathbb{E}_{z \sim D_z} [m(z) \mid z \in A_j] \right)^2 \mid x \in A_j \right].$$

Without loss of generality we will assume that $A_1$ is the only subcell of $B$ that is not empty. We define $Q(A_1)$ the following quantity

$$P_{A_1} \mathbb{E}_{x \sim D_x} \left[ \left( m(x) - \mathbb{E}_{z \sim D_z} [m(z) \mid z \in B] \right)^2 - \left( m(x) - \mathbb{E}_{z \sim D_z} [m(z) \mid z \in A_1] \right)^2 \mid x \in A_1 \right].$$

Since $m(x) \in [-1/2, 1/2]$, we get that

$$\mathcal{E}(B) \leq Q(A_1) + 2 \sum_{j=2}^\ell P_{A_j}. \quad (D.16)$$

Next we also bound $Q(A_1)$ by the measure of cells in $B \setminus A_1$. The intuition why $Q(A_1)$ is small is that, since the cells $B \setminus A_1$ have small measure, then the conditional expectation of $m(z)$ conditional on $z \in B$ is very close to the conditional expectation of $m(z)$ conditional on $z \in A_1$.

More formally, since $x^2$ is 2-Lipschitz for $x \in [-1, 1]$, $m(z) \in [-1/2, 1/2]$ and $A_1 \subseteq B$:

$$Q(A_1) \leq 2P_{A_1} \left| \mathbb{E}_{z \sim D_z} [m(z) \mid z \in B \setminus A_1] - \mathbb{E}_{z \sim D_z} [m(z) \mid z \in A_1] \right|$$

$$= 2P_{A_1} \left| \mathbb{E}_{z \sim D_z} [m(z) \mid z \in B \setminus A_1] - \mathbb{E}_{z \sim D_z} [m(z) \mid z \in A_1] \right| \mathbb{P}(z \in B \setminus A_1 \mid z \in B)$$

$$\leq 2 \frac{P_{A_1}}{P_B} \cdot (P_B - P_{A_1}) \leq 2 (P_B - P_{A_1}) = 2 \left( \sum_{j=2}^\ell P_{A_j} \right)$$
Since all the cells \( A_j \), with \( j \geq 2 \), have \( \hat{P}_{A_j} = 0 \), this means that \( P_{A_j} \leq \frac{2q \ln(2dq) + 2 \ln(1/\delta)}{n} \) due to (D.15). Putting this together with (D.16) we get that

\[
\mathcal{E}(B) \leq 4 \sum_{j=2}^{\ell} P_{A_j} \leq 8(\ell - 1) \frac{q \ln(2dq) + \ln(1/\delta)}{n}.
\]

Let \( \ell_B \) the number of subcells of \( B \in \mathcal{P}_{\text{level}} \) that are inside \( \mathcal{P}_{\text{level}}^S \). If we sum over all \( B \in \mathcal{P}_{\text{level}} \) we get that

\[
| \mathcal{E}(\mathcal{P}_{\text{level}}) - \mathcal{E}(S_{\text{level}}) | \leq 8 \left( \sum_{B \in \mathcal{P}_{\text{level}}} \ell_B \right) \frac{q \ln(2dq) + \ln(1/\delta)}{n}
\]

but the sum \( \sum_{B \in \mathcal{P}_{\text{level}}} \ell_B \) is less than the size of \( \mathcal{P}_{\text{level}}^S \) which is \( 2^q \) and hence we get that

\[
| \mathcal{E}(\mathcal{P}_{\text{level}}) - \mathcal{E}(S_{\text{level}}) | \leq 8 \cdot 2^q \frac{q \ln(2dq) + \ln(1/\delta)}{n}.
\]

\( \square \)

Using Claim D.9 and equations (D.13) and (D.14) we get the first two parts of the theorem by observing that the error term in Claim D.9 is less than the error terms in (D.13) and (D.14). \( \square \)

Recall the definition of the value-diameter of a cell C.1. We are now ready to upper bound the bias under the strong sparsity Assumption 3.2.

**Theorem D.10.** Let \( D_n \) be i.i.d. samples from the non-parametric regression model \( y = m(x) + \epsilon \), where \( m(x) \in [-1/2, 1/2] \), \( \epsilon \sim \mathcal{E} \), \( \mathbb{E}_{\epsilon \sim \mathcal{E}}[\epsilon] = 0 \) and \( \epsilon \in [-1/2, 1/2] \). Let also \( \mathcal{P}_n \) be the partition that Algorithm 1 returns. If \( m \) is \((\beta, r)\)-strongly sparse as per Assumption 3.2 then the following statements hold for the bias of the output of Algorithm 1.

1. If \( n \geq \Omega \left( \frac{2^l(\log(d/\delta))}{\beta^2} \right) \) and we set \( \log(t) \geq r \), then it holds that

\[
\mathbb{P}_{D_n \sim D^n} \left( \mathbb{E}_{x \sim \mathcal{D}_n} \left[ m(x) - \mathbb{E}_{z \sim \mathcal{D}_n} [m(z) | z \in \mathcal{P}_n(x)] \right]^2 \right) \geq \Omega \left( \frac{2^l \cdot \log(d/\delta)}{n} \right) \leq \delta.
\]

2. If \( R \) is the set of relevant features and and for every \( w \in \{0, 1\}^r \) it holds for the marginal probability that \( \mathbb{P}_{z \sim \mathcal{D}_n} (z_R = w) \neq 0, \zeta/2' \) and if \( n \geq \Omega \left( \frac{2^l(\log(d/\delta)) + 2^l(\log(1/\delta))}{\zeta} \right) \) and we set \( \log(t) \geq r \), then it holds that

\[
\mathbb{P}_{D_n \sim D^n} (\Delta_m(\mathcal{P}_n) = 0) \geq 1 - \delta.
\]

3. Let \( R \) be the set of relevant features, \( x \in \{0, 1\}^d \) such that \( \mathbb{P}_{z \sim \mathcal{D}_n} (z_R = x_R) \geq \zeta/2' \), and assume that we run Algorithm 1 with input \( h = 1 \) and \( \log(t) \geq r \). If \( n \geq \Omega \left( \frac{2^l(\log(d/\delta)) + 2^l(\log(1/\delta))}{\zeta} \right) \), then it holds that

\[
\mathbb{E}_{D_n \sim D^n} (m_R(x) - m(x))^2 \leq \delta.
\]
Proof. For the first part of the theorem we observe that Lemma D.7 implies that \( \overline{L}(S_{\text{level}}) = 0 \). Then using Claim D.9 the first part of the theorem follows.

For the second part of the theorem we fix any possible cell \( A \) after doing a full partition on the first \( r \) splits of the Algorithm 1. For simplicity of the exposition of this proof we define for every subset \( B \) of \( \{0,1\}^n \) the probability \( P_B \triangleq \mathbb{P}_{x \sim D_n}[x \in B] \) and the empirical probability \( \hat{P}_B \triangleq \frac{1}{n} \sum_{i=1}^n \mathbb{1}\{x^{(i)} \in B\} \). Using the multiplicative form of the Chernoff bound we get that

\[
\mathbb{P}_{D_n \sim D^n} \left( n\hat{P}_A \geq \left( 1 - \sqrt{\frac{2\log(1/\delta)}{nP_A}} \right) nP_A \right) \geq 1 - \delta.
\]

Hence for \( n \geq \frac{8\log(1/\delta)}{P_A} \) we have that

\[
\mathbb{P}_{D_n \sim D^n} \left( \sum_{i=1}^n \mathbb{1}\{x^{(i)} \in A\} \geq 1 \right) \geq 1 - \delta.
\]

Next we can apply a union bound over all possible cell \( A \) that split according to the \( R \) coordinates and using our assumption that \( P_A \geq \frac{\varepsilon}{2} \) we get that for \( n \geq \frac{242}{\varepsilon} (r + \log(1/\delta)) \) it holds that

\[
\mathbb{P}_{D_n \sim D^n} \left( \bigvee_A \left( \sum_{i=1}^n \mathbb{1}\{x^{(i)} \in A\} \geq 1 \right) \right) \geq 1 - \delta. \tag{D.17}
\]

Now let \( S \) be the set of splits after \( r \) iterations of the Algorithm 1. Then the Lemma D.7 implies that \( S = R \) and \( \overline{L}(S) = 0 \). Finally from (D.17) we also have that the partition \( P_r \) after \( r \) iterations of Algorithm 1 is the partition the full partition to all the cells of \( R \) and hence

\[
\mathbb{E}_{x \sim D_x} \left[ \left( m(x) - \mathbb{E}_{z \sim D_z}[m(z) \mid z \in P_n(x)] \right)^2 \right] \leq \mathbb{E}_{x \sim D_x} \left[ \left( m(x) - \mathbb{E}_{z \sim D_z}[m(z) \mid z_S = x_S] \right)^2 \right]
\]

where the latter is 0 with high probability because of Lemma D.7. This means that with probability at least \( 1 - \delta \) it holds that

\[
\sum_{A \in P_n} \mathbb{P}_{x \sim D_x} (x \in A) \cdot \mathbb{E}_{x \sim D_x} \left[ \left( m(x) - \mathbb{E}_{z \sim D_z}[m(z) \mid z \in A] \right)^2 \mid x \in A \right] = 0.
\]

Since all the summands in the above expression are positive, it has to be that for every cell \( A \in P_n \) it holds that either

\[
\mathbb{P}_{x \sim D_x} (x \in A) = 0 \quad \text{or} \quad \mathbb{E}_{x \sim D_x} \left[ \left( m(x) - \mathbb{E}_{z \sim D_z}[m(z) \mid z \in A] \right)^2 \mid x \in A \right] = 0.
\]

which from the definition of value-diameter implies that

\[
\mathbb{P}_{x \sim D_x} (x \in A) = 0 \quad \text{or} \quad \Delta_m(A) = 0
\]

and in turn this implies \( \Delta_m(P_n) = 0 \) with probability at least \( 1 - \delta \).

For the third part of the theorem we define for simplicity \( w^{(j)}(x) = \frac{\mathbb{1}\{x^{(j)} = x_T^n(S, x)\}}{N_n(x; T^n(S, x))} \) and hence

36
\[ m_n(x) = \sum_{i=1}^n w^{(i)}(x)y^{(i)} \] and we have:
\[
\left( \mathbb{E}_{D_n \sim D^n} [m_n(x) - m(x)] \right)^2 = \\
= \left( \mathbb{E}_{D_n \sim D^n} \left[ \sum_{j=1}^n w^{(j)}(x)(y^{(j)} - m^{(j)}) \right] + \mathbb{E}_{D_n \sim D^n} \left[ \sum_{j=1}^n w^{(j)}(x)(m^{(j)} - m(x)) \right] \right)^2
\]

Due to honesty \( w^{(j)}(x) \) is independent of \( y^{(j)} \) and we have that the first term is equal to 0 by a tower law. Thus we have:
\[
\left( \mathbb{E}_{D_n \sim D^n} [m_n(x) - m(x)] \right)^2 = \left( \mathbb{E}_{D_n \sim D^n} \left[ \sum_{j=1}^n w^{(j)}(x)(m^{(j)} - m(x)) \right] \right)^2 \\
\leq \mathbb{E}_{D_n \sim D^n} \left[ \left( \sum_{j=1}^n w^{(j)}(x)(m^{(j)} - m(x)) \right)^2 \right]
\]

Let also \( A = \{ z \mid z_R = x_R \} \), then using the multiplicative form of the Chernoff Bound from the proof of the second part of the theorem above we get \( \mathbb{P}_{D_n \sim D^n} \left( \sum_{i=1}^n 1 \{ x^{(i)} \in A \} \geq 1 \right) \geq 1 - \delta \). Therefore with probability \( 1 - \delta \) the path of the tree that leads to \( x \) has split all the relevant coordinates \( R \) and hence for all \( j \) such that \( w^{(j)}(x) > 0 \) it holds that \( x^{(j)}_R = x_R \) which in turn implies that \( m^{(j)} = m(x) \). With the rest \( \delta \) probability the square inside the expectation is at most 1 since \( m(\cdot) \in [-\frac{1}{2}, \frac{1}{2}] \), hence we get
\[
\left( \mathbb{E}_{D_n \sim D^n} [m_n(x) - m(x)] \right)^2 \leq \delta.
\]

\[ \square \]

### D.2 Proof of Theorem 3.3

Observe that the output estimate \( m_n(\cdot; S) \) and partition \( \mathcal{P}_n \) of Algorithm 1, satisfies the conditions of Lemma B.2. Moreover, by Corollary B.3, we have that the critical radius quantity \( \delta_n \) is of order \( \Theta \left( \frac{\log(d) + \log(n)}{n} \right) \), if we grow the tree at depth \( \log(f) \). Thus applying the bound presented in (B.4) with the bound on \( \delta_n \) we have the following cases:

1. from case 1 of Theorem D.8 we get case 1 of Theorem 3.3,
2. from case 2 of Theorem D.8 we get case 2 of Theorem 3.3 and
3. from case 1 of Theorem D.10 we get case 3 of Theorem 3.3.

### D.3 Proof of Theorem 3.4

From case 2. of Theorem D.10 and since the maximum possible value diameter is 1, we have that if \( s \geq \tilde{\Omega} \left( \frac{2'(\log(d)/\delta')}{\beta^2} + \frac{2' \log(1/\delta')}{\xi} \right) \) then \( \mathbb{E}_{D_n \sim D^n} [\Delta_m(P_s)] \leq \delta \) which implies \( \mathbb{E}_{x \sim D_s} [m_s(x) - m(x)] \) \( \leq \delta \). Putting this together with the Lemma C.2 we get that if \( s = \tilde{\Omega} \left( \frac{2'(\log(d)/\delta')}{\beta^2} + \frac{2' \log(1/\delta')}{\xi} \right) \) then
\[
\mathbb{P}_{D_n \sim D^n} \left( \mathbb{E}_{x \sim D_s} [(m_{n,x}(x) - m(x))^2] \geq \tilde{\Omega} \left( \frac{2'(\log(d) \cdot \delta')}{n \cdot \beta^2} + \frac{2' \log(1/(\delta \cdot \delta'))}{n \cdot \xi} \right) + \delta \right) \leq \delta'.
\]
From the above we get Theorem 3.4 by setting \(\delta = \tilde{\Omega}\left(\frac{2'(\log(d/d'))}{n^{p\epsilon}} + \frac{2'(1/d')}{n^{\epsilon}}\right)\).

## E Proofs for Breiman’s Algorithm

In this Section we present the proof of the Theorem 4.4 and the Theorem 4.5. We start with a proof about the bias of the trees that are produced by the Algorithm 2 and then we show how we can combine this with a bias-variance decomposition and bounds on the variance part.

### E.1 Bounding The Bias

We start with definitions of the empirical mean squared error for a given partition \(\mathcal{P}\) and the empirical mean squared error of a leaf for a particular leaf \(A\). For the derivations below, we remind the following definitions from Section 4: for a cell \(Z\), we define the set \(Z_n(A)\), as the subset of the training set \(Z_n(A) = \{j \mid x^{(j)} \in A\}\) and we define the partition \(U_n(\mathcal{P})\) of the training set \(D_n\) as \(U_n(\mathcal{P}) = \{Z_n(A) \mid A \in \mathcal{P}\}\).

#### E.1.1 Bounding the Bias

We first prove a technical lemma for the concentration of the function \(V_n^{\ell}\) around the function \(\nabla_{\ell}\). Observe that \(\nabla_{\ell}\) is not the expected value of \(V_n^{\ell}\) and hence this concentration bound is not a trivial one.
**Definition E.1** (Large Cells). Let \( \mathcal{A}(q, \zeta) \) be the set of \((q, \zeta)\)-large cells such that \( A \in \mathcal{A}(q, \zeta) \) if and only if \(|A| \geq 2^{d-q} \) and \( \mathbb{P}_{x \sim \mathcal{D}_n}(x \in A) \geq \frac{\zeta}{2^q} \).

**Lemma E.2.** If \( d > 1, r \in [d], t > 1 \) and \( n \geq \frac{2^{1+q}}{\zeta}(q \log(d) + t) \) then we have that

\[
\mathbb{P}_{D_n \sim \mathcal{D}^n} \left( \sup_{A \in \mathcal{A}(q, \zeta)} \left| \mathbb{V}_n(A, i) - \mathbb{V}_t(A, i) \right| \geq \sqrt{\frac{2^{18+q}(q \log(d) + t)}{\zeta \cdot n}} \right) \leq \exp(-t).
\]

**Proof.** For the purpose of the proof we will define the following function that interpolates between the sample based function \( \mathbb{V}_n(A, i) \) and the population based function \( \mathbb{V}_t \).

\[
J_n(A, i) \triangleq \sum_{z \in \{0, 1\}} \frac{N_n(A^j_z)}{N_n(A)} \left( \mathbb{E}_{(x, y) \sim \mathcal{D}} \left[ y \mid x \in A^j_z \right] \right)^2
\]

(E.5)

First we bound the difference \( |\mathbb{V}_n(A, i) - J_n(A, i)| \) in the following claim.

**Claim E.3.** If \( d > 1, q \in [d], t > 1, \) and \( n \geq \frac{2^q}{\zeta}(4q \log d + t) \) then we have that

\[
\mathbb{P}_{D_n \sim \mathcal{D}^n} \left( \sup_{A \in \mathcal{A}(q, \zeta)} \left| \mathbb{V}_n(A, i) - J_n(A, i) \right| \geq \sqrt{\frac{2^{28+q}(q \log(d) + t)}{\zeta \cdot n}} \right) \leq \exp(-t).
\]

**Proof.** We start by fixing a specific cell \( A \in \mathcal{A}(q, \zeta) \). This cell \( A \) is fixed before we observe the training samples \( D_n \). We have that

\[
\left| \mathbb{V}_n(A, i) - J_n(A, i) \right| = \left| \sum_{z \in \{0, 1\}} \frac{N_n(A^j_z)}{N_n(A)} \left( \left( \sum_{j \in \mathcal{Z}_n(A^j_z)} \frac{1}{N_n(A^j_z)} y^{(j)} \right)^2 - \mathbb{E}_{(x, y) \sim \mathcal{D}} \left[ y \mid x \in A^j_z \right] \right) \right|
\]

Since \( m(x) \in \left[ -\frac{1}{2}, \frac{1}{2} \right] \) and \( \epsilon \in \left[ -\frac{1}{2}, \frac{1}{2} \right] \), we have that \( y \in [-1, 1] \) and hence

\[
\leq 4 \sum_{z \in \{0, 1\}} \frac{N_n(A^j_z)}{N_n(A)} \left| \left( \sum_{j \in \mathcal{Z}_n(A^j_z)} \frac{1}{N_n(A^j_z)} y^{(j)} - \mathbb{E}_{(x, y) \sim \mathcal{D}} \left[ y \mid x \in A^j_z \right] \right) \right|.
\]

Now let \( \mathcal{Y}(A) \) be the distribution of the random variable \( y \) conditional on the fact that the random variable \( x \) lies in the cell \( A \). Observe that since \( A \) is cell fixed before observing the training set \( D_n \), the samples \( y^{(j)} \) for \( j \in \mathcal{Z}_n(A) \) are i.i.d. samples from the distribution \( \mathcal{Y}(A) \) conditional on the event that \( x^{(j)} \) is in \( A \). We define \( Q(A, K) \) to be the event that \( \mathcal{Z}_n(A) = K \) where \( K \subseteq [d] \) and we have the following using Hoeffding’s inequality.

\[
\mathbb{P}_{D_n \sim \mathcal{D}^n} \left( \left| \sum_{j \in \mathcal{Z}_n(A)} \frac{1}{N_n(A^j_z)} y^{(j)} - \mathbb{E}_{(x, y) \sim \mathcal{D}} \left[ y \mid x \in A^j_z \right] \right| \geq \sqrt{\frac{t + \ln(2)}{2N_n(A^j_z)}} | Q(A^j_z, K^j) \right) \leq e^{-t},
\]

Where \( z \in \{0, 1\} \) and \( K^0, K^1 \) are two disjoint subsets of \([d]\). Observe that conditional on \( Q(A, K^i) \) the number \( N_n(A^i_z) \) is equal to \(|K^i|\) and hence is not a random variable any more. Then from union bound we have that if we condition on \( Q(A^j_z, K^j) \) then we have that

\[
\mathbb{P}_{D_n \sim \mathcal{D}^n} \left( \left| \sum_{z \in \{0, 1\}} \frac{1}{N_n(A^j_z)} y^{(j)} - \mathbb{E}_{(x, y) \sim \mathcal{D}} \left[ y \mid x \in A^j_z \right] \right| \geq \sqrt{\frac{(2 \ln(2) + t)}{2N_n(A^j_z)}} \right) \leq e^{-t},
\]

Therefore...
where we dropped the condition on \( Q(A^i_0, K^0) \cap Q(A^i_1, K^1) \) from the above notation for simplicity of exposition. Hence we have the following which holds again if we condition on the event \( Q(A^i_0, K^0) \cap Q(A^i_1, K^1) \).

\[
\mathbb{P}_{D_n \sim D^n} \left( \left| V_n^i(A, i) - J_n(A, i) \right| \geq \sqrt{2(2 \ln(2) + t) \sum_{x \in \{0, 1\}} \sqrt{N_n(A^i_x)}} \right) \leq \exp(-t). \quad (E.6)
\]

But we know that \( \sum_{x \in \{0, 1\}} \sqrt{N_n(A^i_x)} = N_n(A) \), and also we have that the for any vector \( w \in \mathbb{R}^k \) it holds that \( \|w\|_1 \leq \sqrt{k} \|w\|_2 \). Therefore we have that

\[
\sum_{x \in \{0, 1\}} \sqrt{N_n(A^i_x)} \leq \sqrt{\frac{2}{N_n(A)}}.
\]

Now using this in inequality (E.6) and taking the expectation over \( D^n \) conditional on the event \( R(A, k) \) that is equal to the event that \( N_n(A) = k \) and by the law of total expectation we get the following inequality for any possible cell \( A \).

\[
\mathbb{P}_{D_n \sim D^n} \left( \left| V_n^i(A, i) - J_n(A, i) \right| \geq \sqrt{\frac{4(2 \ln(2) + t)}{k}} | R(A, k) \right) \leq \exp(-t). \quad (E.7)
\]

Since \( A \) is a cell of size at least \( 2^{d-q} \) we have that there exists a set \( Q_A \subseteq [d] \) with \( q_A = |Q_A| \leq q \) and a vector \( w_A \in \{0, 1\}^{q_A} \) such that \( x \in A \iff x_{Q_A} = w_A \). Therefore by the assumption that \( A \in \mathcal{A}(q, \zeta) \) we have that \( \mathbb{P}_x(x \in A) \geq \frac{\zeta}{2^q} \). Hence from classical Chernoff bound for binary random variables we have that

\[
\mathbb{P}_{D_n \sim D^n} \left( N_n(A) \leq \frac{n \cdot \zeta}{8 \cdot 2^q} \right) \leq \exp \left( -\frac{n \cdot \zeta}{2^q} \right) \quad (E.8)
\]

Then by combining (E.7) and (E.8) in the Bayes rule we get that

\[
\mathbb{P}_{D_n \sim D^n} \left( \left| V_n^i(A, i) - J_n(A, i) \right| \geq \sqrt{\frac{32(2 \ln(2) + t) \cdot 2^q}{\zeta \cdot n}} \right) \leq \exp(-t) + \exp \left( -\frac{n \cdot \zeta}{2^q} \right). \quad (E.9)
\]

It is also easy to see that the number of possible cells \( A \) with size at least \( 2^{d-q} \) is at most \( 2^d \cdot \left( \sum_{i=0}^{d} \binom{d}{i} \right) \) and hence \( |\mathcal{A}(q, \zeta)| \leq \left( \sum_{i=0}^{d} \binom{d}{i} \right) \). Now using a union bound of (E.9) over all possible cells \( A \in \mathcal{A}(q, \zeta) \) we get

\[
\mathbb{P}_{D_n \sim D^n} \left( \sup_{A \in \mathcal{A}(q, \zeta)} |V_n^i(A, i) - J_n(A, i)| \geq \sqrt{\frac{32(2 \ln(2) + t) \cdot 2^q}{\zeta \cdot n}} \right) \leq \left( \sum_{i=0}^{d} \binom{d}{i} \right) \left( \exp(-t) + \exp \left( -\frac{n \cdot \zeta}{2^q} \right) \right). \quad (E.10)
\]

Finally using \( \log \left( \sum_{i=0}^{d} \binom{d}{i} \right) \leq (q + 1) \log(d \cdot q) \) and since \( d > 1 \), the claim follows. \( \square \)

Next we bound the difference \( |J_n(A, i) - \nabla \ell(A, i)| \).

40
Claim E.4. If \( d > 1, r \in [d], t > 1, \) and \( n \geq \frac{2q}{\epsilon} (4q \log d + t) \) then we have that

\[
\mathbb{P}_{D_n \sim D^n} \left( \sup_{A \in \mathcal{A}(q, \zeta)} |J_n(A, i) - \nabla_b(A, i)| \geq \sqrt{\frac{2^{10+q} \cdot (q \log(d) + t)}{n \cdot \zeta}} \right) \leq \exp(-t).
\]

Proof. Since the error distribution has zero mean, i.e. \( \mathbb{E}[\varepsilon] = 0 \), we have that

\[
\left( \mathbb{E}_{(x, y) \sim D} [y \mid x \in A] \right)^2 = \left( \mathbb{E}_{x} [m(x) \mid x \in A] \right)^2 \triangleq M(A)
\]

and hence

\[
|J_n(A, i) - \nabla_b(A, i)| \leq \sum_{z \in \{0, 1\}} \left| \frac{N_n(A^i_z)}{N_n(A)} - P_x(x \in A^i_z \mid x \in A) \right| \left( \mathbb{E}_{(x, y) \sim D} [y \mid x \in A^i_z] \right)^2
\]

\[
\leq 4 \sum_{z \in \{0, 1\}} \left| \frac{N_n(A^i_z)}{N_n(A)} - P_x(x \in A^i_z \mid x \in A) \right|.
\]

Now from Hoeffding bound we have that

\[
\mathbb{P}_{D_n \sim D^n} \left( \left| \frac{N_n(A^i_z)}{k} - P_x(x \in A^i_z \mid x \in A) \right| \geq t \mid N_n(A) = k \right) \leq \exp(-2 \cdot k \cdot t^2)
\]

excluding the case \( N_n(A) \leq \frac{n \cdot \zeta}{16 \cdot 2^q} \) and taking expectation of both sides we get that

\[
\mathbb{P}_{D_n \sim D^n} \left( \left| \frac{N_n(A^i_z)}{N_n(A)} - P_x(x \in A^i_z \mid x \in A) \right| \geq t \right) \leq \mathbb{E}_{D_n \sim D^n} \left[ \exp(-2t^2 \cdot N_n(A)) \mid N_n(A) > \frac{n \cdot \zeta}{16 \cdot 2^q} \right] + \mathbb{P}_{D_n \sim D^n} \left( N_n(A) \leq \frac{n \cdot \zeta}{16 \cdot 2^q} \right)
\]

now we can use (E.8) to get that

\[
\mathbb{P}_{D_n \sim D^n} \left( \left| \frac{N_n(A^i_z)}{N_n(A)} - P_x(x \in A^i_z \mid x \in A) \right| \geq \sqrt{\frac{8 \cdot 2^q \cdot t}{n \cdot \zeta}} \right) \leq \exp(-t) + \exp\left( -\frac{n \cdot \zeta}{2^q} \right)
\]

Finally if we apply the union bound over all possible cells \( A \in \mathcal{A}(q, \zeta) \) together with the assumption that \( n \geq \frac{2q}{\epsilon} (4q \log d + t) \), the claim follows. \( \square \)

If we combine Claim E.3 and E.4, the lemma follows. \( \square \)

We are now ready to prove that the bias of every tree that is constructed by Algorithm 2 is small under the Assumption 4.1. We start by proving the finite sample analogues of Lemma A.6. First we provide a relaxed version of the Definition A.5 and a version with finite samples.

**Definition E.5.** Given a partition \( \mathcal{P} \) and a cell \( A \) of \( \mathcal{P} \), a positive number \( \eta \) and a training set \( D_n \), we define the sets \( \mathcal{L}^b(A) = \{ i \in [d] \mid \nabla_b(A, i) - \nabla_b(A) > \eta \} \) and \( \mathcal{L}^o(A) = \{ i \in [d] \mid \nabla^\ell(A, i) - \nabla^\ell(A) > \eta \} \). Similarly, when \( \eta = 0 \) we use the simpler notation \( \mathcal{L}(A) \) and \( \mathcal{L}(A) \).
Since \( V_n \) is monotone decreasing with respect to \( \mathcal{P} \), we have that \( V_n(\mathcal{P}, A, i) \geq V_n(\mathcal{P}) \). Hence given \( \mathcal{P}, A \) the Algorithm 2 chooses the direction \( i \) that maximizes the positive quantity \( V_n(\mathcal{P}, A, i) - V_n(\mathcal{P}) \). So the bad event is that for all \( j \in [d] \), \( V_n(\mathcal{P}, A, i) - V_n(\mathcal{P}) \geq V_n(\mathcal{P}, A, j) - V_n(\mathcal{P}) \) but \( V(\mathcal{P}, A, i) - V(\mathcal{P}) = 0 \) and there exists a \( k \in [d] \) such that \( V(\mathcal{P}, A, k) - V(\mathcal{P}) > 0 \). A relaxed version of this bad event can be described using the Definition E.5. In this language the bad event is that the index \( i \in [d] \) that the Algorithm 2 chooses to split does not belong to \( \mathcal{L}(\mathcal{P}, A) \) although \( \mathcal{L}(\mathcal{P}, A) \neq \emptyset \). We bound the probability of this event in the next lemma.

**Lemma E.6.** If \( d > 1, r \in [d] \), \( t > 1 \), and \( n \geq \frac{2^{d+q}}{\xi} (q \log(d) + t) \) and let \( \eta = \sqrt{\frac{2^{18+q}(q \log(d) + t)}{\xi n}} \) then we have that

\[
\mathbb{P}_{D_n \sim D^n} \left( \bigvee_{i \in [d]} \left( \arg\max_{A \in \mathcal{A}(q, \xi)} \left( i \in \mathcal{L}_n(A) \right) \right) \notin \mathcal{L}(A) \mid \mathcal{L}^{2\eta}(A) \neq \emptyset \right) \leq 2 \exp(-t)
\]

**Proof.** Directly applying Lemma E.2 to Definition E.5 we have that

\[
\mathbb{P}_{D_n \sim D^n} \left( \bigvee_{i \in [d]} \left( i \notin \mathcal{L}_n(A) \mid i \notin \mathcal{L}(A) \right) \right) \leq \exp(-t), \tag{E.11}
\]

where \( \eta = \sqrt{\frac{2^{18+q}(q \log(d) + t)}{\xi n}} \) and \( n \geq \frac{q^{3+q}}{\xi} (q \log(d) + t) \). Similarly we have that

\[
\mathbb{P}_{D_n \sim D^n} \left( \bigvee_{i \in [d]} \left( i \notin \mathcal{L}_n(A) \mid i \in \mathcal{L}^{2\eta}(A) \right) \right) \leq \exp(-t). \tag{E.12}
\]

If we combine the above inequalities we get that there is a very small probability that there exists an index \( i \in \mathcal{L}^{2\eta}(A) \) but an index \( j \notin \mathcal{L}(A) \) is chosen instead. This is summarized in the following inequality

\[
\mathbb{P}_{D_n \sim D^n} \left( \bigvee_{A \in \mathcal{A}(q, \xi)} \left( \arg\max_{i \in [d]} V_n(A, i) \notin \mathcal{L}(A) \mid \mathcal{L}^{2\eta}(A) \neq \emptyset \right) \right) \leq 2 \exp(-t) \tag{E.13}
\]

and the lemma follows. \( \square \)

**Lemma E.7.** For every partition \( \mathcal{P} \), under the Assumption 4.1, if for every \( A \in \mathcal{P} \) it holds that \( \mathcal{L}(A) = \emptyset \), then

\[
\mathbb{E}_{x \sim D_x^n} \left[ \left( m(x) - \mathbb{E}_{z \sim D_x} [m(z) \mid z \in \mathcal{P}(x)] \right)^2 \right] \leq C \cdot n \cdot \mathbb{E}_{x \sim D_x} [||\mathcal{L}(\mathcal{P}(x))||].
\]

**Proof.** We define \( \overline{\mathcal{P}} \) to be the partition where all the cells contain only one element of the space, that is \( \overline{\mathcal{P}} = \{ \{ x \} \mid x \in \{0,1\}^d \} \). We then know that \( \overline{\mathcal{L}}(\overline{\mathcal{P}}) = 0 \). Let \( \mathcal{P}' \) be the refinement of \( \mathcal{P} \) where every cell \( A \) of \( \mathcal{P} \) has been split with respect to all the coordinates \( \mathcal{R}(A; \mathcal{P}) \). We first prove that \( \overline{\mathcal{L}}(\mathcal{P}') = 0 \). If this is not the case then there exists a cell \( A \) and a direction \( i \notin \mathcal{R}(A; \mathcal{P}) \) such that \( \overline{\mathcal{L}}(\mathcal{P}', A, i) - \overline{\mathcal{L}}(\mathcal{P}) < 0 \). But because of the Assumption 4.1 and item (4) of Lemma A.4 we have that

\[
C \cdot (\overline{\mathcal{L}}(\mathcal{P}, A, i) - \overline{\mathcal{L}}(\mathcal{P})) \leq \overline{\mathcal{L}}(\mathcal{P}', A, i) - \overline{\mathcal{L}}(\mathcal{P}') < 0
\]

42
which contradicts the assumption that \( i \not\in \mathcal{R}(A; \mathcal{P}) \).

Now assume that \( \mathcal{L}^\eta(A) = \emptyset \) and for the sake of contradiction also assume that \( \mathcal{T}_\ell(A) > C \cdot \eta \cdot |\mathcal{L}(A)| \). Let \( \{r_1, \ldots, r_k\} \) be an arbitrary enumeration of the set \( \mathcal{L}(A) \). From the argument before we have that \( \mathcal{T}_\ell(A, \mathcal{L}(A)) = 0 \) hence there exists an element \( r_j \) of \( \mathcal{L}(A) \) such that

\[
\mathcal{T}_\ell(A, \{r_1, \ldots, r_{j-1}\}) - \mathcal{T}_\ell(A, \{r_1, \ldots, r_j\}) > C \cdot \eta,
\]

otherwise we would immediately have \( \mathcal{T}_\ell(A) \leq C \cdot \eta \cdot |\mathcal{L}(A)| \). But because of the diminishing returns property of \( \mathcal{T}(\cdot) \) we have that

\[
C \cdot (\mathcal{T}_\ell(A) - \mathcal{T}_\ell(A, r_j)) \geq \mathcal{T}_\ell(A, \{r_1, \ldots, r_{j-1}\}) - \mathcal{T}_\ell(A, \{r_1, \ldots, r_j\}) > C \cdot \eta,
\]

but this last inequality implies \( r_j \in \mathcal{L}^\eta(A) \) which contradicts with our assumption that \( \mathcal{L}^\eta(A) = \emptyset \). Hence \( \mathcal{T}_\ell(A) \leq C \cdot \eta \cdot |\mathcal{L}(A)| \) and if we take expectation over \( x \), the lemma follows.

Finally we need one more Lemma to handle the case where Assumption 4.2 holds.

**Lemma E.8.** If \( d > 1 \), \( r \in [d] \), \( t > 1 \), assume that \( m \) is \((\ell, r)\)-strongly partition sparse with relevant features \( R \) as per Assumption 4.2 and let \( n \geq \frac{2^3 \cdot q}{\ell} (q \log(d) + t) \) and \( n \geq \frac{2^{3+4} \cdot (q \log(d) + t)}{\ell \cdot \beta^2} \) then we have that

\[
\mathbb{P}_{D_n \sim \mathcal{D}^n} \left( \bigvee_{i, A \in \mathcal{A}(q, \ell)} \left( \argmax_{i \in [d]} \mathcal{V}_n^0(A, i) \not\in R | R \setminus \mathcal{I}(A) \neq \emptyset \right) \right) \leq 2 \exp(-t)
\]

**Proof.** Directly applying Lemma E.2 to Definition E.5 we have that

\[
\mathbb{P}_{D_n \sim \mathcal{D}^n} \left( \bigvee_{i, A \in \mathcal{A}(q, \ell)} \left( i \in \mathcal{L}^\eta_n(A) | i \not\in \mathcal{L}(A) \right) \right) \leq \exp(-t), \tag{E.14}
\]

where \( \eta = \sqrt{\frac{2^{3+4} \cdot (q \log(d) + t)}{\ell \cdot \beta^2}} \) and \( n \geq \frac{2^3 \cdot q}{\ell} (q \log(d) + t) \). Similarly we have that

\[
\mathbb{P}_{D_n \sim \mathcal{D}^n} \left( \bigvee_{i, A \in \mathcal{A}(q, \ell)} \left( i \not\in \mathcal{L}^\eta_n(A) | i \in \mathcal{L}^2(A) \right) \right) \leq \exp(-t). \tag{E.15}
\]

If we combine the above inequalities with Assumption 4.2 the lemma follows.

**Theorem E.9.** Let \( D_n \) be i.i.d. samples from the non-parametric regression model \( y = m(x) + \varepsilon \), where \( m(x) \in [-1/2, 1/2] \), \( \varepsilon \sim \mathcal{E} \), \( \mathbb{E}_{\varepsilon \sim \mathcal{E}}[\varepsilon] = 0 \) and \( \varepsilon \in [-1/2, 1/2] \) with \( m \) an \( r \)-sparse function. Let also \( \mathcal{P}_n \) be the partition that Algorithm 2 returns. Then the following statements hold:

1. Let \( q = \frac{C \cdot r}{r+3} (\log(n) - \log(\log(d/\delta))) \) and assume that the approximate diminishing returns Assumption 4.1 holds. Moreover if we set the number of nodes \( t \) such that \( \log(t) \geq q \), and if we have number of samples \( n \geq \Omega \left( \log(d/\delta) \right) \) then it holds that

\[
\mathbb{P}_{D_n \sim \mathcal{D}^n} \left( \mathbb{E}_{x \sim D_n} \left[ \left( m(x) - \mathbb{E}_{z \sim D_n} [m(z) | z \in \mathcal{P}_n(x)] \right)^2 \right] > \Omega \left( C \cdot r \cdot \frac{\log(d/\delta)}{\sqrt{n}} \right) \right) \leq \delta.
\]
2. Suppose that the distribution \( D_x \) is a product distribution (see Assumption 2.2) and that the Assumption 4.1 holds. Moreover if \( \log(t) \geq r \), then it holds that

\[
\mathbb{P}_{D_x \sim D^n} \left( \mathbb{E}_{x \sim D_x} \left[ \left( m(x) - \mathbb{E}_{z \sim D_x} [m(z) \mid z \in \mathcal{P}_n(x)] \right)^2 \right] > \Omega \left( \sqrt{\frac{C^2 \cdot 2^r \cdot \log(d/\delta)}{n}} \right) \right) \leq \delta.
\]

3. Suppose that the distribution \( D_x \) is a product distribution (see Assumption 2.2), that is also \((\zeta, r)\)-lower bounded (see Assumption 4.3) and that the Assumption 4.1 holds. Moreover if \( \log(t) \geq r \), then it holds that

\[
\mathbb{P}_{D_x \sim D^n} \left( \mathbb{E}_{x \sim D_x} \left[ \left( m(x) - \mathbb{E}_{z \sim D_x} [m(z) \mid z \in \mathcal{P}_n(x)] \right)^2 \right] > \Omega \left( C \cdot \sqrt{\frac{2^r \cdot \log(d/\delta)}{\zeta \cdot n}} \right) \right) \leq \delta.
\]

4. Suppose that \( m \) is \((\beta, r)\)-strongly partition sparse (see Assumption 4.2) and that \( D_x \) is \((\zeta, r)\)-lower bounded (see Assumption 4.3). If \( n \geq \Omega \left( \frac{2^{(\log(d/\delta))}}{\zeta \cdot \beta^2} \right) \), and \( \log(t) \geq r \), then we have

\[
\mathbb{P}_{D_x \sim D^n} \left( \mathbb{E}_{x \sim D_x} \left[ \left. \left( m(x) - \mathbb{E}_{z \sim D_x} [m(z) \mid z \in \mathcal{P}_n(x)] \right)^2 \right| x \in \mathcal{P}_n(A) \right] > 0 \right) \leq \delta.
\]

Proof. When the value of level changes, then the algorithm considers separately every cell \( A \) in \( \mathcal{P}_{level} \). For every such cell \( A \) it holds that \( \mathcal{L}_{t}(A, R) = 0 \) and hence \( \nabla_t(A, R) \triangleq \nabla^*(A) \) is maximized. Since \( m(x) \in [-1, 1] \) it holds that the maximum value of \( \nabla_t \) is 1. Now let \( \{i_1, \ldots, i_r\} \) be an arbitrary enumeration of \( R \) and let \( R_j = \{i_1, \ldots, i_j\} \). Then by adding and subtracting terms of the form \( \nabla_t(A, R_j) \) we have the following equality

\[
(\nabla_t(A, R) - \nabla_t(A, R_{r-1})) + \cdots + (\nabla_t(A, R_2) - \nabla_t(A, i_1)) + \nabla_t(A, i_1) = \nabla^*(A).
\]

From Assumption 4.1 we have that

\[
(\nabla_t(A, i_r) - \nabla_t(A)) + \cdots + (\nabla_t(A, i_2) - \nabla_t(A)) + (\nabla_t(A, i_1) - \nabla_t(A)) \geq \frac{\nabla^*(A) - \nabla_t(A)}{C}
\]

which implies

\[
\max_{j \in [r]} (\nabla_t(A, i_j) - \nabla_t(A)) \geq \frac{\nabla^*(A) - \nabla_t(A)}{C \cdot r}.
\]

Let \( l_{A}^{\text{level}} \) be the coordinate that the algorithm chose to split at cell \( A \) at level level. Now from the greedy criterion that Algorithm 2 uses to pick the next coordinate to split on, we have that \( l_{A}^{\text{level}} \) was at least as good as the best of the coordinates in \( R \) with respect to \( V_t^n \). If we set

\[
\zeta = \tilde{O} \left( \frac{C r + 3 \log(d/\delta)}{n} \right), \quad q = \frac{C r}{C r + 3} \left( \log(n) - \log(\log(d/\delta)) \right) \quad \text{and} \quad \tilde{\zeta} = \tilde{O} \left( \frac{C r + 3}{\sqrt{\log(d/\delta)}} \right)
\]

and use Lemma E.2 we get that if \( n \geq \Omega \left( \log(d/\delta) \right) \) and if \( \mathbb{P}_{x \sim D_x} (x \in A) \geq \zeta/2^q \) then it holds with probability at least \( 1 - \delta \) that

\[
\nabla_t \left( A, l_{A}^{\text{level}} \right) \geq \nabla_t(A) + \frac{V^*(A) - \nabla_t(A)}{C \cdot r} - 3\zeta
\]

This condition is necessary to guarantee that we have enough number of samples \( n \) to make the splits that are necessary for the \( q \) splits of every path of the tree.
which in turn because \( L^*(A) \triangleq \bar{\ell}_\ell(A, R) = 0 \) implies that

\[
\bar{\ell}_\ell \left( A, \eta_{A}^{\text{level}} \right) \leq \bar{\ell}_\ell(A) \left( 1 - \frac{1}{C \cdot r} \right) + 3\xi. \tag{E.16}
\]

We fix \( Q_{\text{level}} \) to be the partition \( \mathcal{P}_{\text{level}} \) of \( \{0, 1\}^d \) when level changed. Also we define \( \mathcal{U} \) to be the set of cells \( A \) in \( Q_{\text{level}} \) such that \( \mathbb{I}_{x \sim D_x}(x \in A) \geq \frac{\zeta}{2^q} \) and \( \mathcal{V} \) the rest of the cells \( A \) in \( Q_{\text{level}} \). Then because of E.16 and Lemma A.4 it holds that

\[
\bar{\mathcal{L}}(Q_{\text{level}+1}) = \sum_{A \in Q_{\text{level}}} \mathbb{P}_{x \sim D_x} (x \in A) \bar{\ell}_\ell \left( A, \eta_{A}^{\text{level}} \right) + 3\xi
\]

\[
= \sum_{A \in \mathcal{U}} \mathbb{P}_{x \sim D_x} (x \in A) \bar{\ell}_\ell(A) \left( 1 - \frac{1}{C \cdot r} \right) + \sum_{A \in \mathcal{V}} \mathbb{P}_{x \sim D_x} (x \in A) \bar{\ell}_\ell \left( A, \eta_{A}^{\text{level}} \right) + 3\xi
\]

\[
\leq \bar{\mathcal{L}}(Q_{\text{level}}) \left( 1 - \frac{1}{C \cdot r} \right) + \frac{\zeta}{2^q} \sum_{A \in \mathcal{V}} \bar{\ell}_\ell \left( A, \eta_{A}^{\text{level}} \right) + 3\xi
\]

\[
\leq \bar{\mathcal{L}}(Q_{\text{level}}) \left( 1 - \frac{1}{C \cdot r} \right) + 3\xi + \zeta.
\]

Inductively and using the fact that \( m(x) \in [-1, 1] \), we get that

\[
\bar{\mathcal{L}}(Q_{\text{level}}) \leq \bar{\mathcal{L}}(\mathcal{P}_0) \left( 1 - \frac{1}{C \cdot r} \right)^{\text{level}} + (\xi + \zeta) \cdot \text{level} \leq \left( 1 - \frac{1}{C \cdot r} \right)^{\text{level}} + (\xi + \zeta) \cdot \text{level}. \tag{E.17}
\]

Finally if we set \( \eta = \xi + \zeta = \Theta(\xi) \) from the choice of \( t \) we have that level \( \geq C \cdot r \ln(1/\eta) \) and hence when level is exactly equal to \( C \cdot r \ln(1/\eta) \), it holds that \( \bar{\mathcal{L}}(Q_{\text{level}}) \leq 3 \cdot C \cdot r \ln(1/\eta) \). Now from the monotonicity of the \( \bar{\mathcal{L}} \) function with respect to \( Q_{\text{level}} \) we have that for any level \( \geq C \cdot r \ln(1/\eta) \) it holds that \( \bar{\mathcal{L}}(Q_{\text{level}}) \leq 3 \cdot C \cdot r \ln(1/\eta) \eta \) and the first part of the theorem follows.

For the second part of the theorem we use Lemma E.6 and we have that at every step either the algorithm, if \( A \in \mathcal{A}(r, \zeta) \) then we chose to split with respect to a direction \( i \in \mathcal{L}(A) \) or \( \mathcal{L}^\eta(A) = \emptyset \) for \( \eta = \sqrt{\frac{2^{18+r}(r \log(d)+l)}{\zeta \cdot n}} \). Because of our assumption that \( m \) is \( r \)-sparse and because we assume that the features are distributed independently we have that at any step \( |\mathcal{L}(A)| \leq r \). Hence at \( r \) levels it has to be that for every cell \( A \in \mathcal{A}(r, \zeta) \cap \mathcal{P}_n \), it holds that \( \mathcal{L}^\eta(A) = \emptyset \). Let now \( \mathcal{U} \) be the cells \( A \in \mathcal{P}_n \) such that \( A \in \mathcal{A}(r, \zeta) \), and let \( \mathcal{V} \) be the rest of the cells in \( \mathcal{P}_n \). Then using Lemma E.7 we have that

\[
\bar{\mathcal{L}}(\mathcal{P}_n) = \sum_{A \in \mathcal{U}} \mathbb{P}_{x \sim D_x} (x \in A) \cdot \bar{\ell}_\ell(A) + \sum_{A \in \mathcal{V}} \mathbb{P}_{x \sim D_x} (x \in A) \cdot \bar{\ell}_\ell(A)
\]

\[
\leq C \cdot \eta \cdot r + \zeta
\]

now setting \( \zeta = (C \cdot r)^{2/3} \sqrt{\frac{2^{18+r}(r \log(d)+l)}{\zeta \cdot n}} \) we get

\[
\bar{\mathcal{L}}(\mathcal{P}_n) \leq 2\zeta
\]

and since \( \bar{\mathcal{L}}(\mathcal{P}) \) is a monotone function, the second part of the theorem follows.

For the third part of the theorem we use Lemma E.6 and we have that at every step either the algorithm chose to split with respect to a direction \( i \in \mathcal{L}(A) \) or \( \mathcal{L}^\eta(A) = \emptyset \) for

\[
\eta = \sqrt{\frac{2^{18+r}(r \log(d)+l)}{\zeta \cdot n}}.
\]

Because of our assumption that \( m \) is \( r \)-sparse and because we assume
that the features are distributed independently we have that at any step \(|\mathcal{L}(A)| \leq r\). Hence at \(r\) levels it has to be that for every cell \(A\), it holds that \(\mathcal{L}^r(A) = \emptyset\). Then using Lemma E.7 we have that \(\mathcal{T}(\mathcal{P}_n) \leq C \cdot \eta \cdot r\) and since \(\mathcal{T}(\mathcal{P})\) is a monotone function, the third part of the theorem follows.

The last part of the theorem follows easily from Lemma E.8.

Recall the definition of the value-diameter from Definition C.1. We can prove the following.

**Theorem E.10.** Let \(D_n\) be i.i.d. samples from the non-parametric regression model \(y = m(x) + \varepsilon\), where \(m(x) \in [-1/2, 1/2], \varepsilon \sim \mathcal{E}, \mathbb{E}_{\varepsilon \sim \mathcal{E}}[\varepsilon] = 0\) and \(\varepsilon \in [-1/2, 1/2]\). If \(m\) is \((\beta, r)\)-strongly partition sparse (see Assumption 4.2) and \(D\) is \((\zeta, r)\)-lower bounded (see Assumption 4.3) then the following statements hold for the bias of the output of Algorithm 1.

1. If \(n \geq \Omega \left( \frac{2^r (\log(d/\delta))}{\zeta \delta} \right)\), and \(\log(t) \geq r\), then it holds that
   \[
   \mathbb{P}_{D_n \sim D^n} (\Delta_m(\mathcal{P}_n) = 0) \geq 1 - \delta.
   \]

2. Let \(R\) be the set of relevant features, \(x \in \{0,1\}^d\) and assume that we run Algorithm 2 with input \(h = 1\) and \(\log(t) \geq r\). If \(n \geq \Omega \left( \frac{2 (\log(d/\delta))}{\zeta \delta} \right)\) then it holds that
   \[
   \left( \mathbb{E}_{D_n \sim D^n} \left[ m_n(x; \mathcal{P}_n) - m(x) \right] \right)^2 \leq \delta.
   \]

**Proof.** For the first part of the theorem we fix any possible cell \(A\) after the first \(r\) iterations of the Algorithm 2. For simplicity of the exposition of this proof we define for every subset \(B\) of \(\{0,1\}^n\) the probability \(P_B \triangleq \mathbb{P}_{x \sim D_n} [x \in B]\) and the empirical probability \(\hat{P}_B \triangleq \frac{1}{n} \sum_{i=1}^n \mathbb{I} \{x(i) \in B\}\). Using the multiplicative form of the Chernoff bound we get that
   \[
   \mathbb{P}_{D_n \sim D^n} \left( n\hat{P}_A \geq \left( 1 - \sqrt{\frac{2 \log(1/\delta)}{nP_A}} \right) nP_A \right) \geq 1 - \delta.
   \]

Hence for \(n \geq \frac{8 \log(1/\delta)}{P_A} \) we have that
   \[
   \mathbb{P}_{D_n \sim D^n} \left( \sum_{i=1}^n \mathbb{I} \{x(i) \in A\} \geq 1 \right) \geq 1 - \delta.
   \]

Next we can apply a union bound over all possible cell \(A\) that split according to the \(R\) coordinates and using our assumption that \(P_A \geq \frac{\zeta}{2}\) we get that for \(n \geq \frac{242 (r + \log(1/\delta))}{\zeta}\) it holds that
   \[
   \mathbb{P}_{D_n \sim D^n} \left( \bigvee_A \left( \sum_{i=1}^n \mathbb{I} \{x(i) \in A\} \geq 1 \right) \right) \geq 1 - \delta. \tag{E.18}
   \]

Now let \(Q_r\) be the set of splits after \(r\) iterations of the Algorithm 2. Then the Lemma E.8 implies that \(\mathcal{T}(Q_r) = 0\). Finally from (E.18) we also have that the partition \(Q_r\) is the partition the full partition to all the cells of \(R\) and hence
   \[
   \mathbb{E}_{x \sim D_n} \left[ \left( m(x) - \mathbb{E}_{z \sim D_n} [m(z) \mid z \in \mathcal{P}_n(x)] \right)^2 \right] \leq \mathbb{E}_{x \sim D_n} \left[ \left( m(x) - \mathbb{E}_{z \sim D_n} [m(z) \mid z_R = x_R] \right)^2 \right] \]

46
where the later is 0 with high probability because of Lemma E.8. This means that with probability at least $1 - \delta$ it holds that

$$\sum_{A \in \mathcal{P}_n} \Pr_{x \sim \mathcal{D}_z}(x \in A) \cdot \mathbb{E}_{x \sim \mathcal{D}_z} \left[ \left( m(x) - \mathbb{E}_{z \sim \mathcal{D}_z}[m(z) \mid z \in A] \right)^2 \mid x \in A \right] = 0.$$  

Since all the summands in the above expression are positive, and because we assumed that $\mathcal{D}_z$ is $(\zeta, r)$-lower bounded it has to be that for every cell $A \in \mathcal{P}_n$ it holds that

$$\mathbb{E}_{x \sim \mathcal{D}_z} \left[ \left( m(x) - \mathbb{E}_{z \sim \mathcal{D}_z}[m(z) \mid z \in A] \right)^2 \mid x \in A \right] = 0$$

which from the definition of value-diameter implies that $\Delta_m(A) = 0$ and in turn this implies $\Delta_m(\mathcal{P}_n) = 0$ with probability at least $1 - \delta$.

For the second part of the theorem we define for simplicity $w^{(j)}(x) = \frac{\mathbb{1}_{\{x \in \mathcal{P}_n(x^{(j)})\}}}{N_n(\mathcal{P}_n(x^{(j)}))}$ and hence $m_n(x) = \sum_{j=1}^n w^{(j)}(x) y^{(j)}$ and we have:

$$\left( \mathbb{E}_{\mathcal{D}_n \sim \mathcal{D}^n}[m_n(x)] - m(x) \right)^2 = \left( \mathbb{E}_{\mathcal{D}_n \sim \mathcal{D}^n} \left[ \sum_{j=1}^n w^{(j)}(x) (y^{(j)} - m(x^{(j)})) \right] + \mathbb{E}_{\mathcal{D}_n \sim \mathcal{D}^n} \left[ \sum_{j=1}^n w^{(j)}(x) (m(x^{(j)}) - m(x)) \right] \right)^2$$

Due to honesty, which is implied by $h = 1$ in the input of Algorithm 2, $w^{(j)}(x)$ is independent of $y^{(j)}$ and we have that the first term is equal to 0 by a tower law. Thus we have:

$$\left( \mathbb{E}_{\mathcal{D}_n \sim \mathcal{D}^n}[m_n(x)] - m(x) \right)^2 = \left( \mathbb{E}_{\mathcal{D}_n \sim \mathcal{D}^n} \left[ \sum_{j=1}^n w^{(j)}(x) (m(x^{(j)}) - m(x)) \right] \right)^2 \leq \mathbb{E}_{\mathcal{D}_n \sim \mathcal{D}^n} \left[ \left( \sum_{j=1}^n w^{(j)}(x) (m(x^{(j)}) - m(x)) \right)^2 \right]$$

Let also $A = \{z \mid z_R = x_R\}$, then using the multiplicative form of the Chernoff Bound from the proof of the first part of the theorem we get $\Pr_{\mathcal{D}_n \sim \mathcal{D}^n} \left( \sum_{i=1}^n \mathbb{1}_{\{x^{(i)} \in A\}} \geq 1 \right) \geq 1 - \delta$. Therefore with probability $1 - \delta$ the path of the tree that leads to $x$ has split all the relevant coordinates $R$ and hence for all $j$ such that $w^{(j)}(x) > 0$ it holds that $x_R^{(j)} = x_R$ which in turn implies that $m(x^{(j)}) = m(x)$. With the rest $\delta$ probability the square inside the expectation is at most 1 since $m(\cdot) \in [-\frac{1}{2}, \frac{1}{2}]$, hence we get

$$\left( \mathbb{E}_{\mathcal{D}_n \sim \mathcal{D}^n}[m_n(x)] - m(x) \right)^2 \leq \delta.$$  

\[\square\]

### E.2 Proof of Theorem 4.4

Observe that the output estimate $m_n(\cdot; \mathcal{P}_n)$ and partition $\mathcal{P}_n$ of Algorithm 2, satisfies the conditions of Lemma B.2. Moreover, since the number of vertices in a binary tree upper bounds the
number of leafs we can apply Corollary B.3 and we have that the critical radius quantity $\delta_n$ is of order $\Theta \left( \frac{\sqrt{\log(d)\log(n)}}{n} \right)$, if the total number of nodes is at most $t$. Thus applying the bound presented in (B.4) with the bound on $\delta_n$ we have the following cases each of the cases of Theorem 4.4 by using the corresponding case of Theorem E.9.

E.3 Proof of Theorem 4.5

From case 1. of Theorem E.10 and since the maximum possible value diameter is 1, we have that if $s \geq \tilde{\Omega} \left( \frac{2^{\prime}(\log(d/\delta))}{\zeta \cdot \beta^2} \right)$ then $\mathbb{E}_{D_n \sim D^n} [\Delta_m(\mathcal{P}_n)] \leq \delta$ which implies $\mathbb{E}_{x \sim D_n} [(\overline{m}_s(x) - m(x))^2] \leq \delta$. Putting this together with Lemma C.2 we get that if $s = \tilde{\Omega} \left( \frac{2^{\prime}(\log(d/\delta))}{\zeta \cdot \beta^2} \right)$ then

$$\mathbb{P}_{D_n \sim D^n} \left( \mathbb{E}_{x \sim D_n} [(m_{n,s}(x) - m(x))^2] \geq \Omega \left( \frac{2^{\prime}(\log(d/\delta'))}{n \cdot \zeta \cdot \beta^2} \right) + \delta \right) \leq \delta'.$$

From the above we get Theorem 4.5 by setting $\delta = \tilde{\Omega} \left( \frac{2^{\prime}(\log(d/\delta'))}{n \cdot \zeta \cdot \beta^2} \right)$.

F Proofs of Asymptotic Normality

F.1 Proof of Theorem 3.5

We define $m_{s,\pi}$ to be the output of the Algorithm 1 when the samples have been permuted by the permutation $\pi \in S_s$. We denote by $S_n$ the uniform distribution over the symmetric group $S_n$. We also define

$$\overline{m}_s(x) = \mathbb{E}_{D_n \sim D^n, \pi \sim S_n} [m_{n,s,t}(x)] = \mathbb{E}_{D_n \sim D^n, \pi \sim S_n} [m_{s,\pi}(x)].$$  \hspace{1cm} (F.1)

where the last inequality follows due to symmetry of the distribution $D^n$ and the definition of $m_{n,s,t}$. We also remind that $m_{n,s}$ is equal to $\mathbb{E}_{\pi \sim S_n} [m_{n,s,\pi}]$ and that $m_{n,s,B}$ is the Monte Carlo approximation of $\overline{m}_s$ with $B$ terms. We now have the following.

$$\sigma^{-1}_n(x) (m_{n,s,t}(x) - m(x)) = \sigma^{-1}_n(x) (m_{n,s,B}(x) - \overline{m}_s(x)) + \sigma^{-1}_n(x)(\overline{m}_s(x) - m(x)) + \sigma^{-1}_n(x) (\overline{m}_s(x) - m(x)).$$  \hspace{1cm} (F.2)

We define for simplicity $w^{(j)}(x) = \frac{1}{N_n(x, \pi_n(S, x))}$. By Theorem 2 of [FLW18] we have that:

$$\sigma^{-1}_n(x)(\overline{m}_s(x) - m_s(x)) \rightarrow N(0,1)$$  \hspace{1cm} (F.3)
where:

\[
\sigma_n^2(x) = \frac{s^2}{n} \text{Var} \left( \sum_{j=1}^{s} w^{(j)}(x) y^{(j)} | x^{(1)}, y^{(1)} \right)
\]

\[
\geq \frac{s^2}{n} \mathbb{E} \left( \sum_{j=1}^{s} \mathbb{E} \left[ w^{(1)}(x) | x^{(1)} \right]^2 \sigma^2(x^{(1)}) \right)
\]

\[
\geq \frac{s^2}{n} \mathbb{E} \left( \sum_{j=1}^{s} \left[ w^{(1)}(x) | x^{(1)} \right]^2 \right)
\]

\[
\geq \frac{s^2}{n} \mathbb{E} \left( \sum_{j=1}^{s} w^{(1)}(x) \right)^2
\]

\[
= \frac{s^2 \sigma^2}{n} = \frac{\sigma^2}{4n}
\]

Where the last inequality follows by our assumption that \( \sigma^2(x) \geq \sigma^2 \), uniformly for all \( x \) and the fact that due to the expectation over the random permutation \( \tau \) in the beginning of the algorithm we have symmetry between the samples and hence: \( \mathbb{E}_{D_n \sim D^s \tau \sim S_n}[w^{(1)}(x)] = 1/(2s) \). Also, since \( s \geq \Omega \left( \frac{2(\log(d/\delta))}{\mu^2} + \frac{2\log(n)}{\varepsilon} \right) \), from part 3 of Theorem D.10 with \( \delta = 1/n^2 \) we have that:

\[
\sigma_n^{-1}(x) (\overline{m}_s(x) - m(x)) = o_p(1)
\]  \hspace{1cm} (F.4)

where we have used the fact that the part 3 of Theorem D.10 holds pointwise for every permutation \( \tau \in S_n \). The last step is to bound the error from the Monte Carlo approximation \( m_{n,s,B} \) of \( \overline{m}_n \). Since we have fixed the \( x \in \{0,1\} \) before the execution of the algorithm and since \( m_{n,s,\tau}(x) \in [-1/2,1/2] \), we can use the Hoeffding bound with \( B = n^2 \log(n) \) and get the following

\[
\mathbb{P} \left( |m_{n,s,B}(x) - \overline{m}_n(x)| \geq \frac{1}{n} \right) \leq \frac{2}{n^2}
\]

where the probability is over the randomness that is used to sample the \( B \) permutations uniformly from \( S_n \) to compute the empirical expectation \( m_{n,s,B} \). Hence we have that

\[
\sigma_n^{-1}(x) (m_{n,s,B}(x) - \overline{m}_n(x)) = o_p(1). \]  \hspace{1cm} (F.5)

Finally, putting together (F.2), (F.3), (F.4), (F.5) and invoking Slutsky’s theorem we get that:

\[
\sigma_n^{-1}(x)(m_{n,s,B}(x) - m(x)) \rightarrow_d N(0,1).
\]

F.2 Proof of Theorem 4.6

The proof is almost identical to the proof of Theorem 3.5 presented in the previous section. The only difference is the derivation of (F.4). For this instead of using part 3 of Theorem D.10 we use part 2 of Theorem E.10 again with \( \delta = 1/n \). The rest of the proof remains the same and Theorem 4.6 follows.
G  Necessity of Submodularity

Let \( m : \{0,1\}^d \rightarrow [-1,1] \) be a 2-sparse function such that \( m(x) = x_1 + x_2 - 2x_1x_2 \) where and assume that the feature vector \( x \) is sampled uniformly at random from \( \{0,1\}^d \) and there is no noise, i.e. \( \epsilon_i = 0 \) for all \( i \in [n] \). Then it is easy to see the approximate submodularity does not holds for any constant \( C \). This is due to the fact that \( \nabla(\{1\}) - \nabla(\emptyset) = 0 \) but on the other hand \( \nabla(\{1,2\}) - \nabla(\{2\}) > 0 \). So our theorem do not apply in this case. Nevertheless, we next argue that this is not a limitation of our analysis but a limitation of the greedy algorithms that we are analyzing in this paper.

More precisely, Then it is easy to see that even with infinite number of samples, in the level-split model for any \( S \subseteq [d] \) such that \( S \cap \{1,2\} = \emptyset \) it holds that

\[
\nabla(S \cup \{1\}) = \nabla(S \cup \{2\}) = \nabla(S \cup \{j\}) = \nabla(S).
\]

This implies that until the greedy algorithm picks the coordinates 1 or 2 these relevant coordinates have the same mean square error reduction as any other coordinate. Hence the greedy algorithm picks at every step a coordinate at random with probability \( 1/(d - |S|) \). This means that we need depth at least \( \Omega(d) \) to get small mean square error for this function \( m \). This implies that we need at least \( 2^{\Omega(d)} \) number of samples although the function is 2-sparse, the features are independent and uniform and there is no noise. It is easy to see that the same counter example holds for the Breiman’s algorithm and not only for the level-splits algorithm.

The above lower bound shows the necessity of some assumption to guarantee that the greedy algorithm will be consistent in the high-dimensional regime.