Sparse learning with CART

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Abstract

Decision trees with binary splits are popularly constructed using Classification and Regression Trees (CART) methodology. For regression models, this approach recursively divides the data into two near-homogenous daughter nodes according to a split point that maximizes the reduction in sum of squares error (the impurity) along a particular variable. This paper aims to study the statistical properties of regression trees constructed with CART. In doing so, we find that the training error is governed by the Pearson correlation between the optimal decision stump and response data in each node, which we bound by constructing a prior distribution on the split points and solving a quadratic program. We leverage this connection between the training error and Pearson correlation to show that CART with cost-complexity pruning achieves an optimal complexity/goodness-of-fit tradeoff when the depth scales with the logarithm of the sample size. Data dependent quantities, which adapt to the dimensionality and latent structure of the regression model, are seen to govern the rates of convergence of the prediction error.

1 Introduction

Decision trees are the building blocks of some of the most important and powerful algorithms in statistical learning. For example, ensembles of decision trees are used for some bootstrap aggregated prediction rules (e.g., bagging [1] and random forests [2]). In addition, each iteration of gradient tree boosting (e.g., TreeBoost [6]) fits the pseudo-residuals with decision trees as base learners. From an applied perspective, decision trees have an appealing interpretability and are accompanied by a rich set of analytic and visual diagnostic tools. These attributes make tree-based learning particularly well-suited for applied sciences and related disciplines—which may rely heavily on understanding and interpreting output from a statistical model and the system that generated the data. Although, as with many aspects of statistical learning, good empirical
performance often comes at the expense of rigor. Tree-structured learning with decision trees is no exception—statistical guarantees for popular variants, i.e., those that are actually used in practice, are hard to find. Indeed, the recursive manner in which decision trees are constructed makes them unamenable to analysis, especially when the split protocol involves both the input and output data. Despite these challenges, we take a step forward in advancing the theory of decision trees and aim to tackle the following fundamental question:

When do decision trees adapt to the sparsity of a predictive model?

To make our work informative to the applied user of decision trees, we strive to make the least departure from practice and therefore focus specifically on Classification and Regression Tree (CART) methodology—by far the most popular for regression and classification problems. With this methodology, the tree construction importantly depends on both the input and output data and is therefore data dependent. This aspect lends itself favorably to the empirical performance of CART, but poses unique mathematical challenges. It is perhaps not surprising then that, despite the widespread use of CART, there have been only a small handful of papers that study its theoretical properties. For example, [13] study the asymptotic properties of CART in a fixed dimensional regime, en route to establishing consistency of Breiman’s random forests for additive regression models. Another notable paper [7] provides oracle-type inequalities for the CART pruning algorithm proposed by [3], though the theory does not imply guarantees for out-of-sample prediction. What the existing literature currently lacks, however, is a more fine-grained analysis that reveals the unique advantages of tree learning with CART over other unstructured regression procedures, like vanilla $k$-NN or other kernel based estimators. Filling this theoretical gap, our main message is that, in certain settings, CART can identify low dimensional, latent structure in the data and adapt accordingly. We illustrate the adaptive properties of CART when the model is sparse, namely, when the output depends only on a small, unknown subset of the input variables—thereby circumventing the curse of dimensionality.

Arguably the most difficult technical aspect of studying decision trees (and for that matter, any adaptive partitioning-based predictor) is understanding their approximation error, or pinning down conditions on the data that enable such an endeavor. Indeed, most existing convergence results [13] for decision trees or ensembles thereof begin with a study of the size (i.e., the diameter) of the terminal nodes and show that they vanish with the depth of the tree, ensuring that the approximation error does so also. While this technique can be useful to prove consistency statements, it is not generally delicate enough to capture the adaptive properties of the tree on the data. It also often requires making strong assumptions about the tree construction. To address this shortcoming, one of our crucial insights is that we can avoid using the node diameters as a proxy for the approximation error and, instead, directly bound the training error in terms of data dependent quantities that are more transparent and interpretable.
1.1 Learning setting

Let us now describe the learning setting and framework that we will operate under for the rest of the paper. For clarity and ease of exposition, we focus specifically on regression trees, where the target outcome is a continuous real value. We assume the training data is \( D_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\} \), where \( (X_i, Y_i), 1 \leq i \leq n \) are i.i.d. with common joint distribution \( \mathbb{P}_{X,Y} \). Here, \( X_i \in [0,1]^d \) is the input and \( Y_i \in \mathbb{R} \) is a continuous response (or output) variable. A generic pair of variables will be denoted as \((X, Y)\). A generic coordinate of \( X \) will be denoted by \( X \), unless there is a need to highlight the dependence on the \( j \)-th coordinate index, denoted by \( X_j \), or additionally on the \( i \)-th data point, denoted \( X_{ij} \). Using squared error loss \( L(Y, Y') = (Y - Y')^2 \) as the performance metric, our goal is to predict \( Y \) at a new point \( X = x \) via a tree structured prediction rule \( \hat{Y}(x) = \hat{Y}(X; D_n) \). The training error and mean squared prediction error are, respectively,

\[
\text{Err}(\hat{Y}) := \frac{1}{n} \sum_{i=1}^{n} (Y_i - \hat{Y}(X_i))^2 \quad \text{and} \quad \text{Err}(\hat{Y}) := \mathbb{E}_{(X', Y')}[(Y' - \hat{Y}(X'))^2],
\]

where \((X', Y')\) denotes an independent copy of \((X, Y)\). For data \( \{(X_1, U_1, V_1), \ldots, (X_n, U_n, V_n)\} \), we let

\[
\hat{\rho}(U, V | X \in A) := \frac{\frac{1}{n} \sum_{X_i \in A} (U_i - \bar{U})(V_i - \bar{V})}{\sqrt{\frac{1}{n} \sum_{X_i \in A} (U_i - \bar{U})^2 \times \frac{1}{n} \sum_{X_i \in A} (V_i - \bar{V})^2}}
\]

\( (A \text{ is a subset, } N = \#\{X_i \in A\}, \bar{U} = \frac{1}{N} \sum_{X_i \in A} U_i, \text{ and } \bar{V} = \frac{1}{N} \sum_{X_i \in A} V_i) \) denote the empirical Pearson product-moment correlation coefficient, given \( X \in A \), and let \( \rho(U, V | X \in A) \) be its infinite sample counterpart. If \( U_i = g(X_{ij}) \) for a univariate function \( g(\cdot) \) of a coordinate \( X_j \), we write \( \hat{\rho}(g(X_j), V | X \in A) \) or \( \rho(g(X_j), V | X \in A) \). For brevity, we let \( \hat{\sigma}^2_j \) denote the sample variance of the response values \( Y_1, Y_2, \ldots, Y_n \) in the training data. The \( r \)-th derivative of a real valued function \( g(\cdot) \) is denoted by \( g^{(r)}(\cdot) \). Proofs of all forthcoming results are given in the supplement.

2 Preliminaries

As mentioned earlier, regression trees are commonly constructed with Classification and Regression Tree (CART) methodology. The primary objective of CART is to find partitions of the input variables that produce minimal variance of the response values (i.e., minimal sum of squares error with respect to the average response values). Because of the computational infeasibility of choosing the best overall partition, CART trees are greedily grown with a procedure in which binary splits recursively partition the tree into near-homogeneous terminal nodes. That is, an effective binary split partitions the data from the
parent tree node into two daughter nodes so that the resultant homogeneity of the daughter nodes, as measured through their impurity, is improved from the homogeneity of the parent node.

The CART algorithm is comprised of two elements—a growing procedure and a pruning procedure. The growing procedure constructs from the data a maximal binary tree \( T_{\text{max}} \) by the recursive partitioning scheme; the pruning procedure selects, among all the subtrees of \( T_{\text{max}} \), a sequence of subtrees that greedily optimize a cost function.

2.1 Growing the tree

Let us now describe the tree construction algorithm with additional detail. Consider splitting a regression tree \( T \) at a node \( t \). Let \( s \) be a candidate split for a generic variable \( X \) that splits \( t \) into left and right daughter nodes \( t_L \) and \( t_R \) according to whether \( X \leq s \) or \( X > s \). These two nodes will be denoted by 

\[
\begin{align*}
\hat{t}_L &= \{ X \in t : X \leq s \} \\
\hat{t}_R &= \{ X \in t : X > s \}
\end{align*}
\]

As mentioned previously, a tree is grown by recursively reducing node impurity. Impurity for regression trees is determined by the within node sample variance

\[
\hat{\Delta}(t) := \frac{1}{N(t)} \sum_{X_i \in t} (Y_i - \bar{Y}_t)^2,
\]

where \( \bar{Y}_t = \frac{1}{N(t)} \sum_{X_i \in t} Y_i \) is the sample mean for \( t \) and \( N(t) = \# \{ X_i \in t \} \) is the number of data points in \( t \). Similarly, the within node sample variance for a daughter node is

\[
\begin{align*}
\hat{\Delta}(t_L) &= \frac{1}{N(t_L)} \sum_{X_i \in t_L} (Y_i - \bar{Y}_{t_L})^2, \\
\hat{\Delta}(t_R) &= \frac{1}{N(t_R)} \sum_{X_i \in t_R} (Y_i - \bar{Y}_{t_R})^2,
\end{align*}
\]

where \( \bar{Y}_{t_L} \) is the sample mean for \( t_L \) and \( N(t_L) \) is the sample size of \( t_L \) (similar definitions apply to \( t_R \)). The parent node \( t \) is split into two daughter nodes using the variable and split point producing the largest decrease in impurity. For a candidate split \( s \) for \( X \), this decrease in impurity equals [3, Definition 8.13]

\[
\hat{\Delta}(s, t) := \hat{\Delta}(t) - \left[ \hat{P}(t_L)\hat{\Delta}(t_L) + \hat{P}(t_R)\hat{\Delta}(t_R) \right],
\]

where \( \hat{P}(t_L) = N(t_L)/N(t) \) and \( \hat{P}(t_R) = N(t_R)/N(t) \) are the proportions of data points in \( t \) that are contained in \( t_L \) and \( t_R \), respectively.

The tree \( T \) is grown recursively by finding the variable \( j \) and split point \( s \) that maximizes \( \hat{\Delta}(s, t) \). Note that for notational brevity, we suppress the dependence on the input coordinate index \( j \). The output \( \hat{Y}(T) \) of the tree at a terminal node \( t \) is the least squares predictor, namely, \( \hat{Y}(T, x) = \bar{Y}_t \) for all \( x \in t \).
2.2 Pruning the tree

The CART growing procedure stops once a maximal binary tree $T_{\text{max}}$ is grown (i.e., when the terminal nodes contain at least a single data point). However, $\hat{Y}(T_{\text{max}})$ is generally not a good predictor, since it will tend to overfit the data and therefore generalize poorly to unseen data. This effect can be mitigated by complexity regularization. Removing portions of the overly complex tree (i.e., via pruning) is one way of reducing its complexity and improving performance. We will now describe such a procedure.

We say that $T$ is a pruned subtree of $T'$, written as $T \preceq T'$, if $T$ can be obtained from $T'$ by collapsing any number of its internal nodes. A pruned subtree of $T_{\text{max}}$ is defined as any binary subtree of $T_{\text{max}}$ having the same root node as $T_{\text{max}}$. The number of terminal nodes in a tree $T$ is denoted $|T|$. Given a subtree $T$ and temperature $\alpha > 0$, we define the penalized cost function

$$R_{\alpha}(\hat{Y}(T)) := \text{err}(\hat{Y}(T)) + \alpha |T|. \quad (3)$$

As shown in [3, Section 10.2], the smallest minimizing subtree for the temperature $\alpha$, $\hat{T} \in \arg \min_{T \preceq T_{\text{max}}} R_{\alpha}(\hat{Y}(T))$, exists and is unique (smallest in the sense that if $T' \in \arg \min_{T \preceq T_{\text{max}}} R_{\alpha}(\hat{Y}(T))$, then $T \preceq T'$). For a fixed $\alpha$, the optimal subtree $\hat{T}$ can be found efficiently by weakest link pruning [3, 8], i.e., by successively collapsing the internal node that increases $\text{err}(\hat{Y}(T))$ the least, until we arrive at the single-node tree consisting of the root node. Good values of $\alpha$ can be selected using cross-validation, for example, though analyzing the effect of such a procedure is outside the scope of the present paper.

Our first result shows that, with high probability, the test error of the pruned tree $\hat{T}$ on new data is bounded by a multiple of $\min_{T \preceq T_{\text{max}}} R_{\alpha}(\hat{Y}(T))$.

**Theorem 1.** Let $\hat{T}$ be the smallest minimizer of (3). Suppose $Y = f(X)$, $B = \sup_x |f(x)| < \infty$, $n > (d + 1)/2$, and $\alpha > \frac{18B^2(d+1)\log(2en/(d+1))}{n}$. Then, with probability at least $1 - \delta$ over the training sample $D_n$,

$$\text{Err}(\hat{Y}(\hat{T})) \leq 2 \min_{T \preceq T_{\text{max}}} R_{\alpha}(\hat{Y}(T)) + \frac{18B^2\log(1/\delta^2)}{n} + 4B^2\delta.$$

Similar bounds hold for binary classification, i.e., $Y \in \{0, 1\}$, since, in this case, the squared error impurity [1] equals one-half of the so-called Gini impurity used for classification trees.

In what follows, we let $T_K \preceq T_{\text{max}}$ denote a fully grown binary tree of depth $K = \Theta(\log_2(n))$, i.e., we grow the tree until each node contains a single data point or a depth of $K$ is reached, whichever occurs sooner. We also let $\hat{T}$ be the smallest minimizer of the cost function (3) with temperature $\alpha = \Theta((d/n)\log(n/d))$. 


3 Bounding the training error

In the previous section, Theorem 1 showed that, with high probability, the test error is bounded by the cost function (3) at its minimum. Since the cost function is defined as the training error plus penalty term, the next step in our course of study is to understand how the training error of CART behaves.

3.1 Splitting criterion and Pearson correlation

Before we begin our analysis of the training error, we first digress back to the tree construction algorithm and give an alternative characterization of the objective. Now, the use of the sum of squares impurity criterion \( \hat{\Delta}(s, t) \) with averages in the terminal nodes permits further simplifications of the formula (2) above. For example, using the sum of squares decomposition, \( \hat{\Delta}(s, t) \) can equivalently be expressed as [3, Section 9.3]

\[
\hat{P}(t_L)\hat{P}(t_R)\left(\overline{Y}_{t_L} - \overline{Y}_{t_R}\right)^2,
\]

which is commonly used for its computational appeal—that is, one can find the best split for a continuous variable with just a single pass over the data, without the need to calculate multiple averages and sums of squared differences for these averages, as required with (2). Yet another way to view \( \hat{\Delta}(s, t) \), which does not appear to have been considered in past literature and will prove to be useful for our purposes, is via its equivalent representation as

\[
\hat{\Delta}(t) \times \hat{\rho}^2(\tilde{Y}, Y | X \in t),
\]

where

\[
\hat{\rho}(\tilde{Y}, Y | X \in t) := \frac{1}{N(t)} \sum_{X_i \in t} (\tilde{Y}_i - \overline{Y}_t)(Y_i - \overline{Y}_t)
\]

\[
\sqrt{\frac{1}{N(t)} \sum_{X_i \in t} (\tilde{Y}_i - \overline{Y}_t)^2 \times \frac{1}{N(t)} \sum_{X_i \in t} (Y_i - \overline{Y}_t)^2}
\]

is the Pearson product-moment correlation coefficient between the decision stump

\[
\tilde{Y} := \overline{Y}_{t_L}1_{\{X \leq s\}} + \overline{Y}_{t_R}1_{\{X > s\}}
\]

and response variable \( Y \) within \( t \) (for the proof, see Lemma 2 in the supplement). Hence, at each node, CART seeks the decision stump most correlated in magnitude with the response variable along a particular variable, i.e.,

\[
\hat{s} \in \arg \max_s \hat{\Delta}(s, t) = \arg \max_s |\hat{\rho}(\tilde{Y}, Y | X \in t)|. \tag{7}
\]

We let \( \tilde{Y} \) denote the decision stump \( \tilde{Y} \) with the optimal direction \( \hat{j} \in \arg \max_{j=1,2,...,d} \hat{\Delta}(\hat{s}, t) \) and corresponding optimal split \( \hat{s} \). It should be stressed that the alternative characterization of the splitting criterion (2) in terms of a correlation is unique to the squared error impurity with (constant) averages in the terminal nodes of the tree.
We now introduce a data dependent quantity that will play a central role in determining the rates of convergence of the prediction error. For a univariate function class $\mathcal{G}$, we let $\hat{\rho}_\mathcal{G}$ be the largest Pearson correlation between the response data $Y$ and a function in $\mathcal{G}$ of a single input coordinate for a worst-case node, i.e.,

$$\hat{\rho}_\mathcal{G} := \min_t \sup_{g(\cdot) \in \mathcal{G}, j=1,2,\ldots,d} |\hat{\rho}(g(X_j), Y | X \in t)|,$$

where the minimum runs over all internal nodes $t$ in $T_K$. We will specifically focus on classes $\mathcal{G}$ that consist of decision stumps, and more generally, monotone functions.

### 3.2 Location of splits and Pearson correlation

Having already revealed the intimate role the correlation between the decision stump and response values (5) plays in the tree construction, it is instructive to explore this relationship with the location of the splits. In order to study this cleanly, let us for the moment work in an asymptotic data setting to determine the coordinates to split and their split points, i.e.,

$$\hat{\Delta}(s, t) \xrightarrow{n \to \infty} \Delta(s, t) := \Delta(t) - [P(t_L)\Delta(t_L) + P(t_R)\Delta(t_R)],$$

where quantities without hats are the population level counterparts of the empirical quantities defined previously in (2). The decision stump (6) with the optimal theoretical direction $j^*$ with corresponding optimal theoretical split $s^*$ is denoted by $\hat{Y}^*$. Now, if the number of data points within $t$ is large and $\Delta(s, t)$ has a unique global maximum, then we can expect $\hat{s} \approx s^*$ (via an empirical process argument) and hence the infinite sample setting is a good approximation to CART with empirical splits, giving us some insights into its dynamics. Indeed, if $s^*$ is unique, [10, Theorem 2] shows that $\hat{s}$ converges in probability to $s^*$.

With additional assumptions, one can go even further and characterize the rate of convergence. For example, [4, Section 3.4.2] provide cube root asymptotics for $\hat{s}$, i.e., $n^{1/3}(\hat{s} - s^*)$ converges in distribution.

Each node $t$ is a Cartesian product of intervals. As such, the interval along variable $X$ in $t$ is denoted by $[a, b]$, where $a < b$. The next theorem characterizes the relationship between the optimal theoretical split $s^*$ and infinite sample correlation $\rho(\hat{Y}^*, Y | X \in t)$:

$$\lim_{n \to \infty} \hat{\rho}(\hat{Y}^*, Y | X \in t) = A$$

for a deterministic node $t$ (the limit exists by the law of large numbers). The proof is based on the first-order optimality condition, namely, $\frac{\partial}{\partial s} \Delta(s, t) |_{s=s^*} = 0.$

**Theorem 2.** Suppose $X$ is uniformly distributed and $\Delta(s^*, t) > 0$. For a deterministic parent node $t$, the optimal theoretical split $s^* \in [a, b]$ along variable $X$ has the form

$$\frac{a + b}{2} \pm \frac{b - a}{2} \sqrt{\frac{v}{v + \rho^2(\hat{Y}^*, Y | X \in t)}}.$$
Expression (10) in Theorem 2 reveals that the optimal theoretical split \( s^* \) is a perturbation of the median \( (a + b)/2 \) of the conditional distribution \( X \mid X \in t \), where the gap is governed by the correlation \( \rho(\hat{Y}^*, Y \mid X \in t) \). These correlations control the local and directional granularity of the partition of the input domain. Splits along input coordinates that contain a strong signal, i.e., \(|\rho(\hat{Y}^*, Y \mid X \in t)| \gg 0\), tend to be further away from the parent node edges, thereby producing side lengths \([a, b]\) that are on average narrower. At the other extreme, the correlation is weakest when there is no signal in the splitting direction or when the response values in the node are not fit well by a decision stump—yielding either \( s^* \approx a \) or \( s^* \approx b \)—and hence the predicted output in one of the daughter nodes does not change by much. For example, if \( Y = g(X) \) is a sinusoidal waveform with large frequency \( w \) (not fit well by a single decision stump) and \( t \) is the root node \([0, 1]^d\), then \( \rho(\hat{Y}^*, Y \mid X \in t) = \Theta(1) \approx a \) or \( s^* \approx b \) (see Lemma 3 in the supplement). This phenomenon, where optimal splits concentrate at the endpoints of the node along noisy directions, has been dubbed ‘end-cut preference’ in the literature and has been known empirically since the inception of CART [10], [3, Section 11.8]. The theory above is also consistent with empirical studies on the adaptive properties of Breiman’s random forests which use CART [11, Section 4].

### 3.3 Training error and Pearson correlation

In addition to determining the location of the splits, the correlation is also directly connected to the training error. Intuitively, the training error should small when CART finds decision stumps that have strong correlation with the response values in each node. More precisely, the following lemma reveals the importance of the correlation (5) in controlling the training error. It shows that each time a node \( t \) is split, yielding the optimal decision stump \( \hat{Y} \), the training error in \( t \) is reduced by a constant factor, namely, \( \exp(-\hat{\rho}^2(\hat{Y}, Y \mid X \in t)) \) or, uniformly, by \( \exp(-\hat{\rho}_H^2) \), where \( H \) is the collection of all decision stumps (i.e., a step function with two constant pieces) and \( \hat{\rho}_H \) is the quantity defined in (8).

Recursing this contraction inequality over nodes at each level of the tree leads to the conclusion that the training error should be exponentially small in the depth \( K \), provided the correlation at each node is large.

**Lemma 1.** Almost surely,

\[
\frac{1}{N(t)} \sum_{X_i \in t} (Y_i - \hat{Y}_i)^2 \leq \frac{1}{N(t)} \sum_{X_i \in t} (Y_i - \bar{Y}_t)^2 \times \exp(-\hat{\rho}^2(\hat{Y}, Y \mid X \in t)),
\]

and hence

\[
\text{err}(\hat{Y}(T_K)) \leq \hat{\sigma}_Y^2 \exp(-K \times \hat{\rho}_H^2),
\]

where \( H \) is the collection of all decision stumps.
Lemma 1 also has an analog in the infinite sample setting with a similar conclusion for the mean squared error.

### 3.4 Size of Pearson correlation

Due to the importance of the correlation in controlling the training error, it is natural to ask when it will be large. We accomplish this by studying its size relative to the correlation between the data and another more flexible model. That is, we fit an arbitrary univariate function \( g(X) \) of a generic coordinate \( X \) to the data in the node and ask how large \( |\hat{\rho}(\hat{Y}, Y | X \in t)| \) is relative to \( |\hat{\rho}(g(X), Y | X \in t)| \). Such a relationship will enable us to conclude that if \( Y \) is locally correlated with \( g(X) \) in the node, then so will \( Y \) with the optimal decision stump \( \hat{Y} \). Before we continue, let us mention that studying \( |\hat{\rho}(\hat{Y}, Y | X \in t)| \) directly is hopeless since it almost never admits a closed form expression. Furthermore, it is difficult to rely on concentration of measure when \( t \) contains insufficient data; a likely situation among deep nodes. Nevertheless, by definition of \( \hat{Y} \) via (7), we can construct a prior \( \Pi(j, s) \) on coordinates \( j \) and splits \( s \), and lower bound \( |\hat{\rho}(\hat{Y}, Y | X \in t)| \) by

\[
\int |\hat{\rho}(\hat{Y}, Y | X \in t)| d\Pi(j, s),
\]

which is much less burdensome to analyze. Importantly, the prior can involve unknown quantities from the distribution of \((X, Y)\). For a special choice of prior \( \Pi \), (13) can be further lower bounded by

\[
|\hat{\rho}(\hat{Y}, Y | X \in t)| \geq \text{constant} \times |\hat{\rho}(g(X), Y | X \in t)|.
\]

(14)

The constant in (14) depends on \( g(\cdot) \), though importantly it is invariant to the scale of \( g(\cdot) \). If \( g(\cdot) \) belongs to a univariate model class \( \mathcal{G} \), this constant can either be studied directly for the specific \( g(\cdot) \) or minimized over \( g(\cdot) \in \mathcal{G} \) to yield a more insightful lower bound. The minimization problem turns out to be equivalent to a quadratic program, and for certain model classes \( \mathcal{G} \), the solution can be obtained explicitly and used to prove the next set of results. Our first result shows that, relative to an arbitrary univariate function, the optimal decision stump produces a correlation with the data that is always above the \( 1/\sqrt{N(t)} \) noise level in the node.

**Fact 1.** Almost surely, uniformly over all functions \( g(\cdot) \) of \( X \) that change from (strictly) increasing to decreasing or vice versa at most \( V \) times over their domain in the node, we have

\[
|\hat{\rho}(\hat{Y}, Y | X \in t)| \geq \frac{1}{\sqrt{N(t) \times (V + 1)}} \times |\hat{\rho}(g(X), Y | X \in t)|.
\]

(15)

Additional assumptions on \( g(\cdot) \) are required to obtain a useful lower bound. The next result shows that despite fitting the data with a decision stump with one
degree of freedom (i.e., the location of the split), CART behaves almost as if it fit the data with an arbitrary monotone function with $N(t) - 1$ degrees of freedom, at the expense of a sublogarithmic factor in $N(t)$. For example, the correlation between the response variable and the decision stump is, up to a sub-logarithmic factor, at least as strong as the correlation between the response variable and a linear or isotonic fit.

**Fact 2.** Almost surely, uniformly over all monotone functions $g(\cdot)$ of $X$ in the node, we have

$$|\hat{\rho}(\hat{Y}, Y \mid X \in t)| \geq \frac{1}{\sqrt{1 + \log(2N(t))}} \times |\hat{\rho}(g(X), Y \mid X \in t)|.$$  \tag{16}$$

The previous fact also suggests that CART is quite good at fitting response values that have a local, low-dimensional, monotone relationship with the input variables. Note that because correlation is merely a measure of linear association, $|\hat{\rho}(g(X), Y \mid X \in t)|$ can still be large for some monotone $g(\cdot)$, even if $Y$ is not approximately monotone in one coordinate. That is, $Y$ need only be locally correlated with such a function.

## 4 Main results

In this section, we use the training error bound (12) and the device (13) for obtaining correlation comparison inequalities (à la Fact 1 and Fact 2) to give bounds on the prediction error of CAR T. We first outline the high-level strategy. By Theorem 1, with high probability, the leading behavior of the prediction error $\text{Err}(\hat{Y}(\hat{T}))$ is governed by $\inf_{\hat{T} \leq T_{\text{max}}} R_\alpha(\hat{Y}(\hat{T}))$, which is smaller than the minimum of $R_\alpha(\hat{Y}(T_K)) = \text{err}(\hat{Y}(T_K)) + \alpha |T_K|$ over all fully grown trees $T_K$ of depth $K$ with $|T_K| \leq 2^K$, i.e.,

$$\inf_{K \geq 1} \{\text{err}(\hat{Y}(T_K)) + \alpha 2^K\}.$$  \tag{17}$$

Coupled with an informative bound on $\text{err}(\hat{Y}(T_K))$, (17) can then be further bounded and solved. The proofs reveal that a good balance between the tree size and its goodness of fit occurs when $K$ is logarithmic in the sample size.

### 4.1 Asymptotic consistency rates for sparse additive models

Applying the training error bound (12) to (17) with $K = (\hat{\rho}_H^2 + \log 2)^{-1} \log(\hat{\sigma}_Y^2 / \alpha)$, we have from Theorem 1 that with probability at least $1 - \delta$,

$$\text{Err}(\hat{Y}(\hat{T})) = O\left(\hat{\sigma}_Y^2 \left(\frac{d \log(n/d)}{n \hat{\sigma}_Y^2} \right)^{\hat{\rho}_H^2 + \log(1/\delta)} \frac{\log(1/\delta)}{n} + \delta\right).$$  \tag{18}$$
It turns out that if $X$ is uniformly distributed and $Y$ is a sparse additive model with $d_0$ component functions $g_j(\cdot)$, then $\hat{\rho}_H^2$ is asymptotically lower bounded by a constant multiple of $1/d_0$. Thus, we find from (18) that if $d_0$ is fixed, then $\lim_n \text{Err}(\hat{Y}(\hat{T})) \overset{a.s.}{=} 0$ even when the ambient dimension grows as $d = o(n)$. Note that such a statement is not possible for vanilla $k$-NN or other kernel based regression methods with nonadaptive weights, unless feature selection is performed beforehand. In fact, we show next that the prediction error rate that CART achieves is the same as what would be achieved by a standard kernel predictor if one had a priori knowledge of the locations of the $d_0$ input variables that determine the output. A routine computer experiment on synthetic data easily confirms this theory.

**Theorem 3.** Suppose $X$ is uniformly distributed and $Y = \sum_j g_j(X_j)$ is a sparse additive model with $d_0 \ll d$ smooth component functions $g_j(\cdot)$, where each function is not too ‘flat’ in the sense that

$$\sup_x \inf\{r \geq 1 : g_j^{(r)}(\cdot) \text{ exists, continuous, and nonzero at } x\} < \infty.$$  

Then there exists a constant $C > 0$ that is independent of $d_0$ such that, almost surely, $\lim\inf_n \hat{\rho}_H^2 \geq C/d_0$, and

$$\lim\sup_n \frac{\text{Err}(\hat{Y}(\hat{T}))}{((d/n) \log(n/d))^{1/3}} \overset{a.s.}{=} O(1).$$

Any nonconstant component function $g_j(\cdot)$ that admits a power series representation satisfies the hypothesis of Theorem 3, though, in general, the condition (19) accommodates functions that are not infinitely differentiable. In fact, even differentiability is not necessary—in the supplement (see Theorem 5 after the proof of Theorem 3) we also show that Theorem 3 holds verbatim if the $g_j(\cdot)$ are step functions.

### 4.2 Finite sample consistency rates and general sparse models

Using Fact 2 we now provide results of a similar flavor for more general regression models under a mild assumption on the largest number of data points in a node at level $k$ in $T_K$—denoted by $N_k$. Importantly, our theory only requires that each $N(t)$ is upper bounded at each level of the tree. This condition still allows for nodes that have very few data points, which is typical for trees trained in practice. Contrast this assumption with past work on tree learning algorithms (include tree ensembles like random forests) that requires each $N(t)$ to be lower bounded [3, Section 12.2] [12, 14, 5].

**Assumption 1.** For some constants $a \geq 0$ and $A > 0$, the largest number of data points in a node at level $k$ in $T_K$ satisfies $N_k \leq A nk^a/2^k$, for $k = 1, 2, \ldots, K = \Theta(\log_2(n))$.  

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Recall the quantity $\hat{\rho}_G$ defined in (8), namely, the largest correlation between the response data $Y$ and a function in $G$ for a worst-case node. Our next theorem shows that if $\mathcal{M}$ is the collection of all monotone (i.e., increasing or decreasing) functions, then

$$\hat{\rho}_\mathcal{M} = \min_t \sup_{g(\cdot) \text{ monotone}, \, j=1,2,\ldots,d} |\hat{\rho}(g(X_j), Y \mid X \in t)|$$

governs the rate at which the training error and prediction error decrease. Both errors are small if the local monotone dependence between $X$ and $Y$ is high; that is, if CAR T partitions the input domain into pieces where the response variable is locally monotone in a few of the input coordinates.

**Theorem 4.** Let $Y = f(X)$, where $f(\cdot)$ is a bounded function. Under Assumption 1, almost surely,

$$\text{Err}(\hat{Y}(T_K)) \leq \sigma_Y^2 \left(1 - \frac{K}{\log_2(4K^aAn)}\right)^{\hat{\rho}_\mathcal{M}^2}. \tag{21}$$

Furthermore, with probability at least $1 - \delta$,

$$\text{Err}(\hat{Y}(\hat{T})) = O\left(\sigma_Y^2 \left(\frac{\log((d/\sigma_Y^2) \log^{2+a}(n))}{\log(n)}\right)^{\hat{\rho}_\mathcal{M}^2} + \frac{\log(1/\delta)}{n} + \delta \right). \tag{22}$$

We will now argue that $\hat{\rho}_\mathcal{M}$ is an empirical measure of the local dimensionality of $Y$. More specifically, we argue that if CAR T effectively partitions the input domain so that, in each node, $Y$ is locally correlated with sparse additive models $Y_0 = \sum_j g_j(X_j)$ with $d_0 \ll d$ monotone component functions, then $\hat{\rho}_\mathcal{M}^2 = \Omega(1/d_0)$. To see why this assertion is true, suppose $g_1(X_1), g_2(X_2), \ldots, g_d(X_d)$ is an arbitrary collection of $d$ univariate functions (if they belong to $\mathcal{M}$, then they are monotone and so, for example, $Y_0$ could be a linear model). However, in reality, suppose that only a subset of $d_0$ of the input variables locally affect $Y$ in the node. Then, by constructing a special prior $\pi(j)$ on the $j$th direction, it can be shown (see Lemma 4 in the supplement) that there is a sparse additive model $Y_0$ with $d_0$ component functions of the form $\pm g_j(X_j)$, corresponding to the $d_0$ input variables that locally affect $Y$, such that, almost surely,

$$\max_{j=1,2,\ldots,d} \hat{\rho}^2(g_j(X_j), Y \mid X \in t) \geq \frac{\hat{\rho}^2(Y_0, Y \mid X \in t)}{d_0} = \Omega(1/d_0). \tag{23}$$

The above statement is reminiscent of Theorem 3 in which $\hat{\rho}_H = \Omega(1/d_0)$ controls the convergence rate of the prediction error when the underlying regression model is additive. Though, in contrast, note that (23) holds regardless of the dependence structure between the $d_0$ input coordinates that matter and the $d-d_0$ input coordinates that do not. Thus, (23) and Theorem 4 together suggest that it is possible to achieve rates of the form $(\log(d)/\log(n))^{\Omega(1/d_0)}$—which vanish even with growing ambient dimension, i.e., $d = e^{o(\log(n))}$, despite the (likely) presence of confounding input variables.
5 Conclusion and discussion

A key strength of CART decision trees is that they can exploit local, low dimensionality of the model—via a built-in, automatic dimension reduction mechanism. This is particularly useful since many real-world input/output systems are locally approximated by simple model forms with only a few variables. Adaptivity with CART is made possible by the recursive partitioning of the input space, in which optimal splits are increasingly affected by local qualities of the data as the tree is grown. To illustrate this ability, we identified settings where CART adapts to the unknown sparsity of the model. To the best of our knowledge, the consistency rates given here are the first of their kind for CART decision trees.

Let us conclude by making a few comments on ensembles of decision trees. One of the key insights for our analysis of CART was the ability to connect the training error to the objective function of the growing procedure, as in Lemma[1]. This connection enabled us to reveal how certain data dependent quantities adapt to the true dimensionality of the model and control the rates of convergence. Establishing similar relationships is not as easy with tree ensembles like bagging or random forests, due to the subsampling step and form of predicted output as an average of trees. Nevertheless, by convexity [2, Section 11] or [1, Section 4.1] show that the prediction error of a random forest or bagged regression trees is at most the weighted correlation between the residuals of the trees times the average prediction error of the individual trees. In that sense, tree ensembles should, on average, perform at least as well as individual trees, and so our theory for CART can be regarded as a benchmark of sorts.

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Supplementary material

In Appendix A, we provide proofs of Theorem 1, Theorem 2, Lemma 1, Fact 1, Fact 2, Theorem 3, Theorem 4 from the main body of the paper. We also state and prove any supporting lemmas in Appendix B.

As a general rule, if the coordinate index \( j \) is omitted on any quantity that should otherwise depend on \( j \), it should be understood that we are considering a generic variable \( X \). Similar conventions apply to the optimal empirical and theoretical split coordinate index, \( j^* \) and \( \hat{j}^* \), respectively.

A Proofs of in-text statements, lemmas, and theorems

Lemma 2 (Equivalence between the decrease in impurity and Pearson correlation from Section 3.1).

\[
\hat{\rho}(\hat{Y}, Y | X \in t) = \sqrt{\Delta(s, t)/\hat{\Delta}(t)}.
\]

Proof. By expanding the sum of squares in (2), it can easily be shown that \( \hat{\Delta}(s, t) \) equals

\[
\hat{P}(t_L)(\hat{Y}_{t_L})^2 + \hat{P}(t_R)(\hat{Y}_{t_R})^2 - (\hat{Y}_{t})^2,
\]

which is further equal to both \( \frac{1}{N(t)} \sum_{X_i \in t}(\hat{Y}_i - \hat{Y}_t)^2 \) and \( \frac{1}{N(t)} \sum_{X_i \in t}(\hat{Y}_i - \hat{Y}_t)(Y_i - Y_t) \).

Thus,

\[
\hat{\rho}(\hat{Y}, Y | X \in t) = \frac{\frac{1}{N(t)} \sum_{X_i \in t}(\hat{Y}_i - \hat{Y}_t)(Y_i - Y_t)}{\sqrt{\frac{1}{N(t)} \sum_{X_i \in t}(\hat{Y}_i - \hat{Y}_t)^2 \times \frac{1}{N(t)} \sum_{X_i \in t}(Y_i - Y_t)^2}}
\]

\[
= \frac{\hat{P}(t_L)(\hat{Y}_{t_L})^2 + \hat{P}(t_R)(\hat{Y}_{t_R})^2 - (\hat{Y}_{t})^2}{\sqrt{(\hat{P}(t_L)(\hat{Y}_{t_L})^2 + \hat{P}(t_R)(\hat{Y}_{t_R})^2 - (\hat{Y}_{t})^2)(\hat{\Delta}(t))}}
\]

\[
= \sqrt{\Delta(s, t)/\hat{\Delta}(t)}.
\]

Note that the mean of the decision stump \( \hat{Y} \) in \( t \) is in fact \( \bar{Y}_t \), which is why it appears in the formula (21) for the Pearson correlation. \( \square \)

Lemma 3 (Example from Section 3.2). Let \( Y = \sin(2\pi w X) \) for some positive integer \( w \) and \( t = [0, 1]^d \). Then,

\[
|\rho(\hat{Y}^*, Y | X \in t)| = \Theta(1/\sqrt{w}), \ s^* = \Theta(1/w), \ and \ s^* = 1 - \Theta(1/w).
\]

Proof. Elementary calculations reveal that \( \Delta(s, t) = \frac{(1 - \cos(2\pi w))}{4\pi^2w^2(1-s)} \). It can be seen from this expression that the maximizers satisfy \( s^* = \Theta(1/w) \) and \( s^* = 1 - \Theta(1/w) \) and thus \( \Delta(s^*, t) = \Theta(1/w) \).
Since $\Delta(t) = 1/2$, we have from the infinite sample analog of Lemma 2 that $|\rho(\hat{Y}, Y | X \in t)| = \sqrt{\Delta(x^*, t)/\Delta(t)} = \Theta(1/\sqrt{w})$.

Lemma 4 (Inequality (23) from Section 4.2). Let $g_1(X_1), g_2(X_2), \ldots, g_d(X_d)$ be univariate functions and let $Y_0 = \sum_j w_j g_j(X_j)$ consist of a subset of $d_0$ component functions $g_j(\cdot)$, where $w_j \in \{-1, +1\}$, and $w = (w_j)_j$. Then,

$$\max_{j=1,2,\ldots,d} \hat{\rho}^2(g_j(X_j), Y | X \in t) \geq \frac{\min_w \hat{\rho}^2(Y_0, Y | X \in t)}{d_0}.$$  \hfill (25)

Furthermore, if each $g_j(\cdot)$ has nonnegative Pearson correlation with the others in the node, then

$$\max_{j=1,2,\ldots,d} \hat{\rho}^2(g_j(X_j), Y | X \in t) \geq \frac{\hat{\rho}^2(Y_0, Y | X \in t)}{d_0},$$  \hfill (26)

where $Y_0 = \sum_j g_j(X_j)$.

Proof. Before we proceed with proving the lemma, we first establish some shorthand notation. Let $\hat{\sigma}_h^2(t)$ denote the empirical variance of a function $h(X)$ in $t$, i.e., $\hat{\sigma}_h^2(t) = \overline{\text{VAR}(h(X)) | X \in t}$. Define the discrete prior $\pi(j, w)$ on the component function index $j$ and sign vector $w$ of $Y_0$ by

$$\pi(j, w) = \frac{\hat{\sigma}_{w_j g_j(t)}(t)}{2^{d_0} \sum_{j', \sigma_{w_{j'}} g_{j'}(t)}(t)} = \frac{\hat{\sigma}_{g_j(t)}(t)}{2^{d_0} \sum_{j', \sigma_{g_{j'}(t)}}(t)}. $$

We are now in a position to prove (25). Since a maximum is greater than or equal to an average (with respect to the coordinate index $j$ and sign vector $w$), we have

$$\max_{j=1,2,\ldots,d} \hat{\rho}^2(g_j(X_j), Y | X \in t) = \max_{j=1,2,\ldots,d} \hat{\rho}^2(w_j g_j(X_j), Y | X \in t) \geq \sum_{(j, w)} \pi(j, w) \hat{\rho}^2(w_j g_j(X_j), Y | X \in t).$$

Jensen’s inequality for the square function yields

$$\sum_{(j, w)} \pi(j, w) \hat{\rho}^2(w_j g_j(X_j), Y | X \in t) \geq \sum_{w} \pi(w) | \sum_{j} \pi(j | w) \hat{\rho}(w_j g_j(X_j), Y | X \in t) |^2$$

$$= \sum_{w} \pi(w) \frac{\hat{\sigma}_{\omega_j}^2(t)}{(\sum_{j'} \sigma_{g_{j'}}(t))^2} \hat{\rho}^2(Y_0, Y | X \in t)$$

$$\geq \sum_{w} \pi(w) \hat{\sigma}_{\omega_j}^2(t) \frac{\hat{\rho}^2(Y_0, Y | X \in t)}{(\sum_{j'} \sigma_{g_{j'}}(t))^2} \cdot \min_w \hat{\rho}^2(Y_0, Y | X \in t) \quad (27)$$

Next, note that $\sum_{w} \pi(w) \hat{\sigma}_{\omega_j}^2(t) = \sum_{j} \hat{\sigma}_{\omega_j}^2(t)$, since the covariance terms of $\hat{\sigma}_{\omega_j}^2(t)$ have mean zero with respect to $\pi(w) = 2^{-d_0}$; that is,

$$\sum_{w} \pi(w) \hat{\sigma}_{\omega_j}^2(t) = \sum_{w} \sum_{j} \pi(w) \hat{\sigma}_{w_j g_j(t)} + \sum_{w} \sum_{j} \pi(w) \overline{\text{COV}(w_j g_j(X_j), w_{j'} g_{j'}(X_{j'})) | X \in t}$$

$$= \sum_{j} \hat{\sigma}_{\omega_j}^2(t) \sum_{w} \pi(w) + \sum_{j, j'} \overline{\text{COV}(g_j(X_j), g_{j'}(X_{j'})) | X \in t} \sum_{w} \pi(w) w_j w_{j'}$$

$$= \sum_{j} \hat{\sigma}_{\omega_j}^2(t).$$
Combining this with (27) shows that \( \max_{j=1,\ldots,d} \tilde{\rho}^2(g_j(X_j), Y | X \in t) \) is at least

\[
\frac{\sum_{j} \rho^2_{\tilde{\sigma}_{\tilde{g}_j}(t)}}{(\sum_{j} \rho^2_{\tilde{\sigma}_{\tilde{g}_j}(t)})^2} \min_w \tilde{\rho}^2(Y_0, Y | X \in t) \geq \frac{\min_w \tilde{\rho}^2(Y_0, Y | X \in t)}{d_0},
\]

where the last inequality follows from the Cauchy-Schwarz inequality. If each \( g_j(\cdot) \) has nonnegative Pearson correlation with the others in the node, then \( \tilde{\rho}^2_{\tilde{\sigma}_{\tilde{g}_j}(t)} \geq \sum_{j} \tilde{\rho}^2_{\tilde{g}_j}(t) \) and thus the same argument as above can be repeated with \( Y_0 = \sum_{j} g_j(X_j) \) to prove (26).

**Proof of Theorem 7.** Let \( \text{Err}(\tilde{Y}) = \frac{1}{n} \sum_{i=1}^{n} (Y'_i - \tilde{Y}(T_i, X'_i))^2 \) denote the test error of \( \tilde{Y}(T) \) on a test sample \( D'_n = \{(X'_i, Y'_i)\}_{i=1}^{n} \) of size \( n \). Let \( \mathcal{T} \) denote the collection of tree-structured partitions constructed on the grid \( \{X_i\}_{i=1}^{n} \cup \{X'_i\}_{i=1}^{m} \) with 2n points. Note that the VC-dimension of the collection of axis-parallel splits is at most the VC-dimension of the collection of all half-spaces, or, \( d+1 \). Lemma B.2 in [7] shows that the number of trees in \( \mathcal{T} \) with exactly \( |T| \) nodes is at most \( (2ne/(d+1))^{|T|(d+1)} \). Using this, we have

\[
\sum_{T \in \mathcal{T}} e^{-L(T)} \leq \sum_{k:|T|=k \geq 1} \exp \left( -L(T) + |T|(d+1) \log(2ne/(d+1)) \right) \leq 1,
\]

if \( L(T) \geq 2|T|(d+1) \log(2en/(d+1)) \geq |T| \log(1/\delta) \log(2ne/(d+1))) \). Thus, a penalty equal to \( L(T) := 2|T|(d+1) \log(2en/(d+1)) \geq |T| \log(2+\log(2ne/(d+1))) \) satisfies Kraft’s inequality, i.e., \( \sum_{T \in \mathcal{T}} e^{-L(T)} \leq 1 \). Observe also that \( \mathcal{T} \) is invariant with respect to permutations of the data points on the grid \( \{X_i\}_{i=1}^{n} \cup \{X'_i\}_{i=1}^{m} \). By Lemma 2.1 in [8], for all \( u \geq 0 \),

\[
P \left( \max_{T \in \mathcal{T}} \frac{\text{Err}(\tilde{Y}(T)) - \text{Err}(\tilde{Y}(T))}{u + \frac{L(T)}{n} + \frac{1}{n} \sum_{i=1}^{n} (Y'_i - \tilde{Y}(X'_i))^2} < 1 \right) \geq 1 - \exp \left( -\frac{n}{\gamma} \right), \tag{28}
\]

where \( S^2(\tilde{Y}(T)) = \frac{1}{n} \sum_{i=1}^{n} (Y'_i - \tilde{Y}(X'_i))^2 - (Y_i - \tilde{Y}(X_i))^2 \). Using the fact that \( S^2(\tilde{Y}(T)) \leq 8B^2(\text{Err}(\tilde{Y}(T)) + \text{Opt}(\tilde{Y}(T))) \) and choosing \( u = \frac{\gamma \log(1/\delta^2)}{\gamma - 4B^2} \), we find that the event whose probability is lower bounded in (28) is contained in the event

\[
\text{Err}(\tilde{Y}(\tilde{T})) < \frac{\gamma + 4B^2}{\gamma - 4B^2} R_\alpha(\tilde{Y}(\tilde{T})) + \frac{\gamma^2}{\gamma - 4B^2} \log(1/\delta^2) \frac{n}{\gamma - 4B^2}.
\]

which occurs with probability at least \( 1 - \delta^2 \). Next, we use a truncation argument to obtain high probability bounds in terms of \( \text{Err}(\tilde{Y}(\tilde{T})) \). To this end, we have

\[
\text{Err}(\tilde{Y}(\tilde{T})) = \mathbb{E}_{D'_{n}}[\text{Err}(\tilde{Y}(\tilde{T}))] \\
\leq \frac{\gamma + 4B^2}{\gamma - 4B^2} R_\alpha(\tilde{Y}(\tilde{T})) + \frac{\gamma^2}{\gamma - 4B^2} \log(1/\delta^2) \frac{n}{\gamma - 4B^2} + 4B^2 \mathbb{P}_{D'_{n}} \left( \text{Err}(\tilde{Y}(\tilde{T})) > \frac{\gamma + 4B^2}{\gamma - 4B^2} R_\alpha(\tilde{Y}(\tilde{T})) + \frac{\gamma^2}{\gamma - 4B^2} \log(1/\delta^2) \frac{n}{\gamma - 4B^2} \right),
\]

where we used the fact that \( \text{Opt}(\tilde{Y}(\tilde{T})) \leq 4B^2 \). By Markov’s inequality and (28), the random variable \( \mathbb{P}_{D'_{n}} \left( \text{Err}(\tilde{Y}(\tilde{T})) > \frac{\gamma + 4B^2}{\gamma - 4B^2} R_\alpha(\tilde{Y}(\tilde{T})) + \frac{\gamma^2}{\gamma - 4B^2} \log(1/\delta^2) \frac{n}{\gamma - 4B^2} \right) \) is at least \( \delta \) with probability less than \( \delta \).
Hence, with probability at least $1 - \delta$,

$$\text{Err}(\hat{Y}(\hat{T})) \leq \frac{\gamma + 4B^2}{\gamma - 4B^2} R_\alpha(\hat{Y}(\hat{T})) + \frac{\gamma^2}{\gamma - 4B^2} \frac{\log(1/\delta^2)}{n} + 4B^2 \delta.$$  

The conclusion of the theorem follows from the definition of $\hat{T}$ as a minimizer of $R_\alpha(\hat{Y}(\hat{T}))$ and choosing $\gamma = 12B^2$. \hfill \Box

**Proof of Theorem**. The identity (10) is shown by first noting that, in the special case of uniform $X$, the probability $\mathbb{P}(X \leq s^* \mid X \in t)$ from Lemma 5 in Appendix A is equal to $(s^* - a)/(b - a)$. Rearranging the resulting expression yields the desired identity. \hfill \Box

**Proof of Lemma**. We first prove (11) for a general decision stump $\hat{Y}$. The training error in $t$ after splitting is

$$\frac{1}{N(t)} \sum_{X_i \in t} (Y_i - \hat{Y}_i)^2 = \frac{1}{N(t)} \sum_{X_i \in L} (Y_i - \hat{Y}_L)^2 + \frac{1}{N(t)} \sum_{X_i \in R} (Y_i - \hat{Y}_R)^2$$

$$= \hat{\Delta}(t) \left(1 - \frac{\hat{\Delta}(s, t)}{\Delta(t)}\right)$$

$$= \frac{1}{N(t)} \sum_{X_i \in t} (Y_i - \hat{Y}_i)^2 \times (1 - \hat{\rho}^2(\hat{Y}, Y \mid X \in t)),$$

where the last equality follows from Lemma 2. Finally, $1 - \hat{\rho}^2(\hat{Y}, Y \mid X \in t) \leq \exp(-\hat{\rho}^2(\hat{Y}, Y \mid X \in t))$ follows from $1 - z \leq e^{-z}$ for $z \geq 0$. To show (12), we use (11) with $\hat{Y} = \hat{Y}$ recursively together with the identity

$$\text{err}(\hat{Y}(T_K)) = \sum_t \hat{P}(t)\hat{\Delta}(t),$$

where the sum extends over all terminal nodes $t$ of $T_K$. We stop once we reach the root node, at which point the training error is simply $\hat{\sigma}^2$. \hfill \Box

**Proof of Fact**. Let $g(\cdot)$ be any function of a generic coordinate $X$ and assume that the data points in the node are labeled for simplicity as $\{X_i : X \in t\} = \{X_1, X_2, \ldots, X_{N(t)}\}$. Let $\tau$ be a permutation of the data in the node such that $X_{\tau(1)} \leq X_{\tau(2)} \leq \cdots \leq X_{\tau(N(t))}$. Without loss of generality, we can assume that $g(\cdot)$ linearly interpolates between the values $g(X_{\tau(1)}), g(X_{\tau(2)}), \ldots, g(X_{\tau(N(t))})$. We look at the (empirical Bayesian) prior $\Pi$ on splits $s \in [0, 1]$ with density

$$\frac{d\Pi(s)}{ds} = \frac{|g'(s)|\sqrt{\hat{P}(t_L)\hat{P}(t_R)}}{\int_0^1 |g'(s')|\sqrt{\hat{P}(t_L)\hat{P}(t_R)}ds'},$$

where we remind the reader that $\hat{P}(t_L) = 1 - \hat{P}(t_R) = \frac{1}{N(t)} \sum_{X_i \in t} 1\{X_i \leq s\}$. Here, $g'(s)$ equals the divided difference $\frac{g(X_{\tau(s+1)}) - g(X_{\tau(s)})}{X_{\tau(s+1)} - X_{\tau(s)}}$ when $X_{\tau(s)} \leq s < X_{\tau(s+1)}$. Accordingly, observe that $\Pi$ has a piecewise constant density with knots at the data points.
Since, by definition, \( \hat{\rho} \) maximizes \( s \mapsto \hat{\rho}^2(Y, Y | X \in t) \) and a maximum is larger than an average, we have
\[
\hat{\rho}^2(Y, Y | X \in t) = \max_s \hat{\rho}^2(Y, Y | X \in t) \\
\geq \int_0^1 \hat{\rho}^2(Y, Y | X \in t) d\Pi(s) = \int_0^1 \frac{\Delta(s, t)}{\Delta(t)} d\Pi(s), \tag{29}
\]
where the last equality follows from Lemma \( \ref{lemma:1} \). Next, working from the representation \( \Delta(s, t) = \sqrt{P(t_L)P(t_R)} \), note that the reduction in impurity admits the form
\[
\Delta(s, t) = \left( \frac{1}{\sqrt{P(t_L)P(t_R)}} \left( \frac{1}{N(t)} \sum_{X_i \in t} \left( 1_{s < X_i} - \hat{P}(t_R)(Y_i - \overline{Y}_t) \right) \right) \right)^2, \tag{30}
\]
and, hence, integrating inside the square in \( \ref{eq:30} \) against \( g'(s) \sqrt{P(t_L)P(t_R)} \), we have
\[
\int_0^1 g'(s) \left( \frac{1}{N(t)} \sum_{X_i \in t} \left( 1_{s < X_i} - \hat{P}(t_R)(Y_i - \overline{Y}_t) \right) \right) ds \\
= \frac{1}{N(t)} \sum_{X_i \in t} \left( g(X_i) - \frac{1}{N(t)} \sum_{X_i' \in t} g(X_i') \right)(Y_i - \overline{Y}_t) \\
= \widehat{\text{COV}}(g(X), Y | X \in t). \tag{31}
\]
Using the inequality \( \ref{inequality:31} \) together with the identities \( \ref{eq:30} \) and \( \ref{eq:31} \) and Jensen’s inequality for the square function, we have
\[
\hat{\rho}^2(Y, Y | X \in t) \geq \int_0^1 \frac{\Delta(s, t)}{\Delta(t)} d\Pi(s) \\
\geq \frac{\text{VAR}(g(X) | X \in t)}{\left( \int_0^1 |g'(s)| \sqrt{P(t_L)P(t_R)} ds \right)^2} \hat{\rho}^2(g(X), Y | X \in t). \tag{32}
\]
Therefore, from \( \ref{eq:32} \), we are led to determine how small the ratio
\[
\frac{\text{VAR}(g(X) | X \in t)}{\left( \int_0^1 |g'(s)| \sqrt{P(t_L)P(t_R)} ds \right)^2. \tag{33}
\]
can be, ideally in terms of some simple structural characteristics of \( g(\cdot) \). Our next task is to simplify \( \ref{eq:33} \) so that its numerator and denominator can be more easily compared. To this end, observe that
\[
\int_0^1 |g'(s)| \sqrt{P(t_L)P(t_R)} ds \\
= \sum_{i=0}^{N(t)} \int_{N(t)\hat{P}(t_L)=i} |g'(s)| \sqrt{\frac{i}{N(t)} \left( 1 - \frac{i}{N(t)} \right)} ds \\
= \sum_{i=1}^{N(t)-1} \int_{X_{\tau(i)}}^{X_{\tau(i+1)}} |g'(s)| ds \sqrt{\frac{i}{N(t)} \left( 1 - \frac{i}{N(t)} \right)} \\
= \frac{1}{N(t)} \sum_{i=1}^{N(t)-1} \left| g(X_{\tau(i+1)}) - g(X_{\tau(i)}) \right| \sqrt{i(N(t) - i)}, \tag{34}
\]
where the penultimate equality follows from the fact that \( \hat{P}(t_k) = i/N(t) \) if and only if \( X_{\tau(i)} \leq s < X_{\tau(i+1)} \). Next, we further simplify the above expression (34) using summation by parts, that is,

\[
\frac{1}{N(t)} \sum_{i=1}^{N(t)-1} |g(X_{\tau(i+1)}) - g(X_{\tau(i)})| \sqrt{i/N(t) - i} = \frac{1}{N(t)} \sum_{i=1}^{N(t)} g(X_{\tau(i)})(b_i - b_{i-1}), \tag{35}
\]

where \( b_i = \text{sgn}(g(X_{\tau(i+1)}) - g(X_{\tau(i)})) \times \sqrt{i/N(t) - i} \) with \( b_0 = b_{N(t)} = 0 \). Next, since \( \sum_i (b_i - b_{i-1}) = 0 \), (35) can be written as

\[
\frac{1}{N(t)} \sum_{i=1}^{N(t)} g(X_{\tau(i)}) - \frac{1}{N(t)} \sum_{X' \in \mathbb{N}} g(X_{\tau'}) (b_i - b_{i-1}). \tag{36}
\]

Moreover, we can express the variance \( \overline{\text{VAR}}(g(X) \mid X \in t) \) in a similar form, viz.,

\[
\overline{\text{VAR}}(g(X) \mid X \in t) = \frac{1}{N(t)} \sum_{i=1}^{N(t)} (g(X_{\tau(i)}) - \frac{1}{N(t)} \sum_{X' \in \mathbb{N}} g(X_{\tau'}))^2. \tag{37}
\]

To obtain the best lower bound on the ratio (33), we attempt to solve the program

\[
\min_{g(\cdot) \in \mathcal{G}} \overline{\text{VAR}}(g(X) \mid X \in t) \left( \int_0^1 |g'(s)| \sqrt{\hat{P}(t_k) - \hat{P}(t_k)} ds \right)^2, \tag{38}
\]

where \( \mathcal{G} \) is a collection of functions. In light of the expressions (35) and (37), the program (38) is equivalent to the following program:

\[
\min_{a \in A} \sum_{t=1}^{N(t)} |a_t|^2 \quad \text{s.t.} \quad \frac{1}{N(t)} \sum_{i=1}^{N(t)} a_i (b_i - b_{i-1}) = 1, \tag{39}
\]

where \( b_i = \text{sgn}(a_{i+1} - a_i) \sqrt{i/N(t) - i} \) and \( A \) is a collection of vectors in \( \mathbb{R}^{N(t)} \). In order to incorporate structural and/or regularity properties of \( g(\cdot) \), we will need to impose conditions on \( \mathcal{G} \), or since we associate \( a_t \) with \( g(X_{\tau(i)}) - \frac{1}{N(t)} \sum_{X' \in \mathbb{N}} g(X_{\tau'}) \), equivalently, on \( A \). However, not all specifications make the program tractable to solve, or even convex. As a compromise, we fix the signs of the \( b_i \) in advance. That is, we specify two sets where \( b_i = 0 \), \( b_i > 0 \), and \( b_i < 0 \)—corresponding to locations where \( g(\cdot) \) is constant, increasing, and decreasing, respectively—and solve the resulting (quadratic) program. More formally, let \( M \) denote the number of constant pieces of \( g(\cdot) \) and let \( S = \{i_k\}_{0 \leq k \leq M-1} \) and \( S' \subset S \) be two subsets of \( \{1, 2, \ldots, N(t)\} \) with \( i_0 = 0 \) and \( i_M = N(t) \). Let \( A = \{a \in \mathbb{R}^{N(t)} : b_i = 0 \text{ for } i \notin S, b_i > 0 \text{ for } i \in S', b_i < 0 \text{ for } i \notin S'\} \), and \( D_k = i_k - i_{k-1} \). With these specifications fixed, the program (39) becomes

\[
\min_{a \in A} \sum_{k=1}^{M} |a_{ik}|^2 D_k \quad \text{s.t.} \quad \frac{1}{\sqrt{N(t)}} \sum_{k=1}^{M} a_{ik} (b_{ik} - b_{ik-1}) = 1. \tag{40}
\]

Using the method of Lagrange multipliers, it is easy to see that the solution to (40) is

\[
a_{ik}^* = \frac{\sqrt{N(t)}(b_{ik} - b_{ik-1})/D_k}{\sum_{k=1}^{M} (b_{ik} - b_{ik-1})^2/D_k}, \quad k = 1, 2, \ldots, M, \tag{41}
\]
and the value of the program is
\[ N(t) = \sum_{k=1}^{M} \left( b_k - b_{k-1} \right)^2 / D_k. \] (42)

Next, let \( V \) denote the number of times \( g(\cdot) \) changes from increasing to decreasing or vice versa and let \( D \) be the smallest number of data points contained in each constant piece of \( g(\cdot) \) with at least one data point. Lemma 7 in Appendix B shows that (42) is at least
\[ \frac{1}{\sqrt{D-1} V N(t) + (M - V - 1) \land (1 + \log(2N(t)))}, \]
where \( D = \min_{2 \leq k \leq M-1} D_k \), and hence by (32),
\[ |\hat{\rho}(\hat{Y}, Y \mid X \in t)| \geq \frac{1}{\sqrt{D-1} V N(t) + (M - V - 1) \land (1 + \log(2N(t)))} \times \hat{\rho}(g(X), Y \mid X \in t)|. \] (43)

Fact 2 follows immediately from (43) by noting that, in this case, \( V = 0 \). Fact 1 follows similarly since, \( D \geq 1 \) and \( M \leq N(t) \).

**Proof of Theorem 3.** We first employ a technique similar to (42) in the proofs of Fact 1 and Fact 2 to lower bound each \( \rho^2(\hat{Y}, Y \mid X \in t) \)—that is, for each function \( g(\cdot) \) of \( X \) and node \( t \),
\[ \rho^2(\hat{Y}, Y \mid X \in t) \geq \Lambda \times \rho^2(g(X), Y \mid X \in t), \] (44)
where
\[ \Lambda := \frac{\text{VAR}(g(X) \mid X \in [a, b])}{\left( \int_{a}^{b} |g'(s)| \sqrt{\frac{s-a}{b-a}} ds \right)^2}. \]

In contrast with the proofs of Fact 1 and Fact 2, here we do not attempt to minimize \( \Lambda \) over all \( g(\cdot) \) in some function class. Rather, we attempt to lower bound it for a fixed \( g(\cdot) \). Now, (44) is valid for all \( g_j(X_j) \) and so we can instead consider the maximum correlation over all \( g_j(X_j) \), i.e., \( \max_j \rho^2(g_j(X_j), Y \mid X \in t) \), where now \( \Lambda \) is the minimum over all \( g_j(X_j) \). By the infinite sample analog of (20) in Lemma 4, we have
\[ \max_j \rho^2(g_j(X_j), Y \mid X \in t) \geq \rho^2(Y, Y \mid X \in t) = 1/d_0, \]
and hence
\[ \rho^2(\hat{Y}, Y \mid X \in t) \geq \Lambda / d_0. \] (45)

Next, we show that \( \Lambda \) can be further lower bounded by a positive constant that is independent of \( t \). To this end, note that \( \Lambda \) is continuous in \((a, b)\) and strictly positive for all \( a < b \) and, furthermore by Lemma 7 in Appendix B
\[ \inf_{c} \lim_{(a, b) \to (c, c)} \Lambda = \Omega(1/R), \]
where \( R = \sup_{c \in [0, 1]} \inf \{ r \geq 1 : g^{(r)}(\cdot) \text{ exists and is continuous and nonzero at } c \} \)—which means that \( \inf_{(a, b)} \Lambda > 0 \). Note that, in particular, \( R \) is finite if \( g(\cdot) \) admits a power series representation. Taking the minimum of \( \inf_{(a, b)} \Lambda \) over all \( g_j(\cdot) \)—each of which has finite \( R \)—results in a positive quantity that depends only on each \( g_j(\cdot) \) individually. This shows that \( \inf_{t} \rho^2(\hat{Y}, Y \mid X \in t) \geq C/d_0 \) for some positive constant \( C \) that depends only on each \( g_j(\cdot) \) individually and not on \( d_0 \). Next, we will show that, almost surely,
\[ \lim_{n} \inf_{t} \rho^2_H = \lim_{n} \inf_{t} \hat{\rho}^2(\hat{Y}, Y \mid X \in t) \geq \inf_{t} \rho^2(\hat{Y}, Y \mid X \in t), \]
that is independent of \( d \) vanishes, and \( X \) never vanishes. We first show that with probability at least \( \delta \),

\[
\lim \inf_n \inf_t \rho^2(\hat{Y}, Y \mid X \in t) \geq \lim \inf_n \inf_t \hat{\rho}^2(\hat{Y}, Y \mid X \in t).
\]

Next, note that \( \hat{\rho}(\hat{Y}^*, Y \mid X \in t) \) is invariant to scale. Working instead with \( \frac{\hat{N}(\hat{Y}^*)}{n} \) and \( N(Y) \), we find that the correlation involves terms (empirical processes) of the form \( \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{\{X_i \in t\}} + \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{\{X_i \in t\}} Y_i \), and \( t' \) is either the parent node \( t \) or one of the daughter nodes, \( t'_L := \{ X \in t : X \leq s^* \} \) and \( t'_R := \{ X \in t : X > s^* \} \) at the optimal theoretical split \( s^* \). The collection of hyperrectangles in \( \mathbb{R}^d \) is a finite VC-class with VC-dimension \( 2d \), and hence these terms converge almost surely, uniformly over all nodes \( t' \), to their respective population level counterparts when \( d = o(n) \). Thus, \( \lim \inf_n \inf_t \rho^2(\hat{Y}^*, Y \mid X \in t) \Rightarrow \inf_t \lim \inf_n \rho^2(\hat{Y}^*, Y \mid X \in t) \Rightarrow a.s., \)

\[
\text{as } \inf_t \rho^2(\hat{Y}^*, Y \mid X \in t).
\]

The almost sure limit (20) in Theorem 3 follows from (18) with \( \delta = 1/n^2 \) and \( \lim \inf_n \hat{\rho}_n^2 \geq C/d_0 \) almost surely. 

As indicated in the main text, we can also prove an analogous statement to Theorem 3 when the \( g_i(\cdot) \) are step functions.

**Theorem 5.** Suppose \( X \) has independent coordinates and their joint density never vanishes, and \( Y = \sum_j g_j(X_j) \) is a sparse additive model with \( d_0 \ll d \) component functions \( g_j(\cdot) \), where each \( g_j(\cdot) \) is a step function. Then there exists a constant \( C > 0 \) that is independent of \( d_0 \) such that, almost surely, \( \lim \inf_n \hat{\rho}_n^2 \geq C/d_0 \), and

\[
\lim \sup_n \frac{\text{Err}(\hat{Y}(\hat{T}))}{\left( \frac{d}{n} \right)^2 \log(n/d)^{2(1/d)}} \Rightarrow a.s. \bigO(1). \tag{46}
\]

**Proof.** Let \( I_{1j}, I_{2j}, \ldots, I_{M_j} \) be the (non-degenerate) intervals along \( X_j \) for which \( g_j(\cdot) \) is constant and define \( q \) to be the smallest marginal probability content of all these intervals, i.e.,

\[
q := \min_j \min_{1 \leq k \leq M_j} \mathbb{P}(X_j \in I_{kj}).
\]

Also, let \( M = \max_j M_j \). Note that \( q > 0 \) since, by assumption, the joint density of \( X \) never vanishes. We first show that with probability at least \( 1 - d_0 M e^{-qn/8} \), each interval \( I_{kj} \) on which \( g_j(\cdot) \) is constant contains at least \( qn/2 \) data points. This event may equivalently be written as

\[
\bigcap_{j} \bigcap_{1 \leq k \leq M_j} \left\{ \sum_{i=1}^{n} \mathbb{1}_{\{X_{ij} \in I_{kj}\}} \geq qn/2 \right\}. \tag{47}
\]

By a union bound, we can bound the probability of the complement event of (47) by \( d_0 M \min_{1 \leq k \leq M_j} \mathbb{P}(\sum_{i=1}^{n} \mathbb{1}_{\{X_{ij} \in I_{kj}\}} \leq qn/2) \). Next, the multiplicative version of Chernoff’s inequality yields

\[
\mathbb{P}(\sum_{i=1}^{n} \mathbb{1}_{\{X_{ij} \in I_{kj}\}} \leq qn/2) \leq \mathbb{P}(\sum_{i=1}^{n} \mathbb{1}_{\{X_{ij} \in I_{kj}\}} \leq \mathbb{P}(X_j \in I_{kj})n/2) \\
\leq e^{-\mathbb{E}(X_j \in I_{kj})n/8} \\
\leq e^{-qn/8}.
\]
On the event \(\mathcal{E}_j\), in the notation of (43), \(D \geq 2n/2 \geq qN(t)/2\) and \(V + 2 \leq M \leq 2/q\), where each \(g_j(\cdot)\) changes from increasing to decreasing or vice versa at most \(V\) times. Therefore, by (43), with probability at least \(1 - d_0M e^{-qn/M}\), in each node \(t\) of \(T_K\),

\[
|\hat{\rho}(\hat{Y}, Y | X \in t)| \geq \sqrt{\frac{1}{D^{-1} \log N(t) + M - V - 1}} \times \max_j |\hat{\rho}(g_j(X), Y | X \in t)|
\]

\[
\geq \sqrt{\frac{1}{(2/q - 1)(V + 1)}} \times \max \hat{\rho}(g_j(X), Y | X \in t)|
\]

\[
\geq \sqrt{\frac{q}{2(V + 1)}} \times \max \hat{\rho}(g_j(X), Y | X \in t)|.
\]

Next, note that \(\hat{\rho}(g_j(X), Y | X \in t)\) is invariant to scale. Working instead with \(\frac{N(t)}{n} g_j(X)\) and \(\frac{N(t)}{n} Y\), the correlation can be written in terms of empirical processes of the form \(\frac{1}{n} \sum_{i=1}^n 1_{X_i \in t} + \frac{1}{n} \sum_{i=1}^n 1_{Y_i \in t} + \frac{1}{n} \sum_{i=1}^n 1_{X_i \in t} g_j(X_i) + \frac{1}{n} \sum_{i=1}^n 1_{X_i \in t} Y_i\), \(\frac{1}{n} \sum_{i=1}^n 1_{X_i \in t} g_j(X_i)\). The collection of hyperrectangles in \(\mathbb{R}^d\) is a finite VC-class with VC-dimension \(2d\), and hence these terms converge almost surely, uniformly over all nodes \(t\), to their respective population level counterparts when \(d = o(n)\). Thus, \(\lim inf_t \lim inf_n \hat{\rho}^2(g_j(X), Y | X \in t) \equiv \lim inf_t \lim inf_n \hat{\rho}^2(g_j(X), Y | X \in t) \equiv \lim inf_t \hat{\rho}^2(g_j(X), Y | X \in t)\). Finally, by the infinite sample analog of (26) in Lemma 4 we have \(\max_j \hat{\rho}^2(g_j(X), Y | X \in t) \geq \rho^2(\hat{Y}, Y | X \in t) = 1/d_0\). Thus, almost surely,

\[
\lim inf_t \rho^2_H = \lim inf_n \lim inf_t \hat{\rho}^2(\hat{Y}, Y | X \in t) \geq \frac{q}{2d_0(V + 1)} = C/d_0,
\]

where \(C = q/(2(V + 1))\). The almost sure limit (40) follows from (13) with \(\delta = 1/n^2\) and \(\lim inf_n \rho^2_H \geq C/d_0\) (almost surely) together with the Borel-Cantelli lemma.

Proof of Theorem 4. We first show that

\[
\text{err}(\hat{Y}(T_K)) \leq \sigma_t^2 \exp \left(-\hat{\rho}^2_M \sum_{k=1}^K (\log_2(4N_k))^{-1}\right).
\]

By (11) in Lemma 1 the training error in the node is decreased by a factor of \(\exp(-\hat{\rho}^2(\hat{Y}, Y | X \in t))\) each time the node is split. By Fact 2, almost surely, \(\hat{\rho}^2(\hat{Y}, Y | X \in t) \geq \frac{1}{D^{-1} \log N(t)} \times \hat{\rho}^2_M \geq \frac{1}{\log_2(4N(t))} \times \hat{\rho}^2_M \geq \frac{1}{\log_2(4N(t))} \times \hat{\rho}^2_M\), if \(t\) is a node at level \(k\). Thus, the training error at level \(k + 1\) is at most \(\exp(-\hat{\rho}^2_M (\log_2(4N_k))^{-1})\) times the training error at level \(k\) in other words, the training error is geometrically decreasing. The proof of (45) can then be completed using an induction argument, noting that the training error at the root node is simply \(\sigma_t^2\).

For the training error bound (21), we use the inequality \(\sum_{k=1}^K \frac{1}{\log_2(4N_k+2^k)} \geq \log \left(\frac{\log_2(4K^2 A_n)}{\log_2(4K^2 A_n) - K}\right)\) for integers \(K \geq 1\). By (48), if \(T_K\) is a fully grown tree of
depth $K$, then under Assumption 1, i.e., $N_k \leq Ank^a/2^{k}$, we have

$$\hat{\mathbb{err}}(\hat{Y}(T_K)) \leq \hat{\sigma}_Y^2 \exp \left( - \hat{\rho}_M^2 \sum_{k=1}^{K} \frac{1}{\log_2(4Ank^a/2^{k})} \right)$$

$$\leq \hat{\sigma}_Y^2 \exp \left( - \hat{\rho}_M^2 \sum_{k=1}^{K} \frac{1}{\log_2(4Ank^a/2^{k})} \right)$$

$$\leq \hat{\sigma}_Y^2 \left( 1 - \frac{K}{\log_2(4AnK^a)} \right)^{\hat{\rho}_M^2}$$

(49)

Next, we show (22), i.e., the bound on the prediction error. By Theorem 1, with high probability, the leading behavior of the test error $\text{Err}(\hat{Y}(\hat{T}))$ is governed by

$$\inf_{T \preceq \hat{T}_{\text{max}}} R_\alpha(\hat{Y}(\hat{T})),$$

(50)

where the temperature $\alpha$ is $\Theta((d/n) \log(n/d))$. Note that (50) is smaller than the minimum of $R_\alpha(\hat{Y}(\hat{T}_K)) = \hat{\mathbb{err}}(\hat{Y}(\hat{T}_K)) + \alpha|\hat{T}_K|$ over all fully grown trees $\hat{T}_K$ of depth $K$ with $|\hat{T}_K| \leq 2^K$, i.e.,

$$\inf_{K \geq 1} \{ \hat{\mathbb{err}}(\hat{Y}(\hat{T}_K)) + \alpha 2^K \}.$$

(51)

Combining the training error bound (49) with (51), we are led to optimize

$$\hat{\sigma}_Y^2 \left( 1 - \frac{K}{\log_2(4AnK^a)} \right)^{\hat{\rho}_M^2} + \alpha 2^K$$

(52)

over $K \geq 1$, although suboptimal choices of $K$ will suffice for our purposes. Choosing $K$ to satisfy $K = \log_2 \left( \log_2(4AnK^a) / \hat{\sigma}_Y^2 \right) < \log_2(\hat{\sigma}_Y^2 / \alpha)$, we find that (52) is equal to

$$\hat{\sigma}_Y^2 \left( \frac{\log_2(4AnK^a) \log_2(4AnK^a) \hat{\rho}_M^2 / \hat{\sigma}_Y^2}{\log_2(4AnK^a)} \right)^{\hat{\rho}_M^2} + \hat{\sigma}_Y^2 \left( \frac{1}{\log_2(4AnK^a)} \right)^{\hat{\rho}_M^2}$$

$$= O \left( \frac{\log_2((d/\hat{\sigma}_Y^2) \log_2(n) \hat{\rho}_M^2 / \log(n)}{\log(n)} \right)^{\hat{\rho}_M^2}.$$

Combining this bound with Theorem 1 proves (22).

B Supplementary lemmas

Lemma 5. Suppose the density of $X$ never vanishes and $\Delta(s^*, t) > 0$. Then the conditional probability of the left daughter node along the splitting variable, i.e., $P(X \leq s^* \mid X \in t)$, has the form

$$\frac{1}{2} \pm \frac{1}{2} \sqrt{v}$$

(53)

where $v = \frac{\mathbb{E}[Y \mid X \leq s^*] - \mathbb{E}[Y \mid X \leq t]}{\mathbb{V}aR(Y \mid X \in t)}^2.$

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Proof. Recall from (40) (albeit, the infinite sample version) that one can write
\[ \Delta(s, t) = P(t_L)P(t_R)[E[Y \mid X \leq s] - E[Y \mid X > s]^2]. \] (54)

Next, define
\[ \Xi(s) = P(t_L)P(t_R)[E[Y \mid X \leq s] - E[Y \mid X > s)], \]
so that
\[ \Delta(s, t) = \Xi(s)^2/(P(t_L)P(t_R)). \] (55)

An easy calculation shows that
\[ \frac{\partial}{\partial s} \Xi(s) = p(t_L)[E[Y \mid X = s] - E[Y \mid X = t)] = p(t_L)G(s), \] (56)
where \( p(t_L) = \frac{\partial}{\partial s} P(X \leq s \mid X \in t) \) and \( G(s) = E[Y \mid X \leq s] - E[Y \mid X > s] \).

Taking the derivative of \( \Delta(s, t) \) with respect to \( s \), we find that
\[ \frac{\partial}{\partial s} \Xi(s, t) = \frac{\Xi(s)p(t_L)(2P(t_L)P(t_R)G(s) - \Xi(s)(1 - 2P(t_L)))}{(P(t_L)P(t_R))^2}. \] (57)

Suppose \( s^* \) is a global maximizer of (55) (in general, it need not be unique). Then a necessary condition (first-order optimality condition) is that the derivative of \( \Delta(s, t) \) is zero at \( s^* \). That is, from (57), \( s^* \) satisfies
\[ \Xi(s^*)p(t_L^*)G(s^*) - \Xi(s^*)(1 - 2P(t_L^*)) = 0, \] (58)
where we denote the daughter nodes with the optimal theoretical split \( s^* \) by \( t_L^* \) and \( t_R^* \), i.e., \( t_L^* = \{X \in t : X \leq s^*\} \) and \( t_R^* = \{X \in t : X > s^*\} \). By assumption, \( p(t_L^*) > 0 \) (since the density of \( X \) never vanishes) and \( \Delta(s^*, t) > 0 \). It follows from rearranging (58) and using the identity (55) that
\[ P(t_L^*) = \frac{1}{2} - \frac{\text{sgn}(\Xi(s^*)) \times G(s^*)}{\sqrt{\Delta(s^*, t)}} \\sqrt{P(t_L^*)P(t_R^*)}. \] (59)

The solution to (59) is obtained by solving a simple quadratic equation of the form \( p = 1/2 \pm c \sqrt{p(1 - p)} \), \( 0 \leq p \leq 1 \), and noting from Lemma 3 that \( \Delta(s^*, t) = \Delta(t) \times \rho^2(Y^* \mid X \in t) \), which proves the identity (53). □

Lemma 6. Suppose \( X \) is uniformly distributed on the unit interval and \( R = \inf \{r \geq 1 : g^{(r)}(\cdot) \text{ exists and is continuous and nonzero at } c \} < \infty \). Then
\[ \liminf_{(a, b) \to (c, c)} \left\{ \frac{\text{VAR}(g(X) \mid X \in [a, b])}{\left( \int_a^b |g'(x)| \sqrt{1/\frac{b-a}{(b-a)^2}} \, dx \right)^2} \right\} = \Omega(1/R). \] (60)

Proof. Since the distribution of \( (X - a)/(b - a) \) given \( X \in [a, b] \) is uniform on the unit interval, the ratio in the limit infimum (60) is
\[ \frac{\text{VAR}(g(X(b - a) + a))}{((b - a) \int_0^1 |g'(x(b - a) + a)| \sqrt{1 - x} \, dx)^2}. \]
Let $\delta = (c-a)/(b-a)$. By a Taylor expansion of $g'(\cdot)$ and the definition of $R$, for fixed $\delta$,

$$
\lim_{(a,b)\to(c,c)} (b-a)^{-R} \int_0^1 |g'(x(b-a)+a)| \sqrt{x(1-x)} dx = \frac{|g^{(R)}(c)|}{(R-1)!} \int_0^1 |x-\delta|^{R-1} \sqrt{x(1-x)} dx.
$$

(61)

For the variance, first note that

$$
\text{VAR}(g(X(b-a) + a)) = \int_0^1 (g(x(b-a) + a) - \int_0^1 g(x'(b-a) + a) dx')^2 dx.
$$

Let $D(x)$ denote the divided difference $\frac{g(a(b-a)+a)-g(c)}{(a-b)+a-c)R}$. Then, we can rewrite $(b-a)^{-R} (g(x(b-a) + a) - \int_0^1 g(x'(b-a) + a) dx')$ as

$$
D(x)(x-\delta)^R - \int_0^1 D(x')(x'-\delta)^R dx'.
$$

(62)

Next, use a Taylor expansion of $g(\cdot)$ about the point $c$ and continuity of $g^{(R)}(\cdot)$ at $c$ to argue that

$$
\lim_{(a,b)\to(c,c)} D(x) = \frac{g^{(R)}(c)}{R!},
$$

where the convergence is uniform and the limit is nonzero by definition of $R$. Therefore, for fixed $\delta$,

$$
\lim_{(a,b)\to(c,c)} (b-a)^{-2R} \text{VAR}(g(X(b-a) + a)) = \left(\frac{g^{(R)}(c)}{R!}\right)^2 \int_0^1 (x-\delta)^R - \int_0^1 (x'-\delta)^R dx' dx
$$

$$
= \left(\frac{g^{(R)}(c)}{R!}\right)^2 \text{VAR}((X-\delta)^R).
$$

(63)

Combining (61) and (63), we have that the limit infimum (60) is at least

$$
\inf_{\delta} \left( \frac{\text{VAR}((X-\delta)^R)}{R! \int_0^1 (x-\delta)^{R-1} \sqrt{x(1-x)} dx} \right).
$$

(64)

Tجادic calculations show that the infimum is achieved at $\delta = 1/2$ and hence (64) is $\Omega(1/R)$.

**Lemma 7.** Consider the expression (64). Then,

$$
\frac{N(t)}{\sum_{k=1}^M (b_k - b_{k-1})^2 / D_k} \geq \frac{1}{D^{-1} V N(t) + (M - V - 1) \wedge (1 + \log(2N(t)))}.
$$

(65)

**Proof.** For brevity, we omit dependent on t and write $N$ instead of $N(t)$.

Suppose that $b_i$ changes sign at index $i_k$ (one of the $V$ many indices such that $b_{i_k-1} b_i < 0$). Then, since $b_i = \text{sgn}(a_{i_k} - a_{i_k-1}) \sqrt{i_k(N-I_k)}$, we have

$$
\sum_{k: b_k < 0} \frac{(b_k - b_{k-1})^2}{ND_k} = \sum_{k: b_k < 0} \frac{|b_k| + |b_{k-1}|)^2}{ND_k} \leq \sum_{k: b_k < 0} \frac{|b_k| + |b_{k-1}|)^2}{ND} \leq D^{-1} V N,
$$

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where the last line is from $(|b_{i_k}| + |b_{i_{k-1}}|)^2 = (\sqrt{i_i(N - i_k)} + \sqrt{i_{k-1}(N - i_{k-1})})^2 \leq N^2$.

Next, for the remaining $M - V$ indices such that $b_{i_{k-1}}b_{i_k} > 0$ we have,

$$\sum_{k: b_{i_{k-1}}b_{i_k} > 0} \frac{(|b_{i_k}| - |b_{i_{k-1}}|)^2}{ND_k} \leq \sum_{k: b_{i_{k-1}}b_{i_k} > 0} \frac{|N - i_k - i_{k-1}|}{N} \leq M - V - 1,$$

where the last line follows from the fact there is always one index such that $|N - i_k - i_{k-1}| + |N - i_{k+1} - i_k| = |i_{k+1} - i_{k-1}|$. Thus, it follows that $rac{\sum_{k=1}^M (b_{i_k} - b_{i_{k-1}})^2}{D_k}$ is at least

$$\frac{1}{D^{-1}VN + (M - V - 1) \land \sum_{k=1}^M \frac{(|b_{i_k}| - |b_{i_{k-1}}|)^2}{ND_k}}.$$

We now obtain an upper bound for

$$\sum_{k=1}^M \frac{(|b_{i_k}| - |b_{i_{k-1}}|)^2}{ND_k} = \sum_{k=1}^M \frac{D_k(N - i_k - i_{k-1})^2}{N(\sqrt{i_i(N - i_k)} + \sqrt{i_{k-1}(N - i_{k-1})})^2}. \tag{67}$$

Let $k^* = \min\{k : i_k + i_{k-1} \geq N\}$. Then, $(\sqrt{i_i(N - i_k)} + \sqrt{i_{k-1}(N - i_{k-1})})^2 \geq (2N - i_k - i_{k-1})(i_k + i_{k-1} - N)$ for all $k \geq k^*$. Thus, the sum

$$\sum_{k \geq k^*} \frac{D_k}{N(\sqrt{i_i(N - i_k)} + \sqrt{i_{k-1}(N - i_{k-1})})^2}$$

is at most

$$\sum_{k > k^*} \frac{D_k}{2N - i_k - i_{k-1}} \left( \frac{i_{k-1} + i_k}{N} - 1 \right) \leq \sum_{k > k^*} \frac{i_k - i_{k-1}}{2N - i_k - i_{k-1}}. \tag{68}$$

where we used the fact that $D_k = i_k - i_{k-1}$. Next, $(\sqrt{i_i(N - i_k)} + \sqrt{i_{k-1}(N - i_{k-1})})^2 \geq (i_k + i_{k-1})(N - i_k - i_{k-1})$ for all $k < k^*$ and hence the sum

$$\sum_{k < k^*} \frac{D_k}{N(\sqrt{i_i(N - i_k)} + \sqrt{i_{k-1}(N - i_{k-1})})^2}$$

is at most

$$\sum_{k < k^*} \frac{D_k}{i_k + i_{k-1}} (1 - \frac{i_{k-1} + i_k}{N}) \leq \sum_{k < k^*} \frac{i_k - i_{k-1}}{i_k + i_{k-1}}. \tag{69}$$

Combining (68) and (69), we have shown that (64) is at most

$$\sum_{k < k^*} \frac{i_k - i_{k-1}}{i_k + i_{k-1}} + \sum_{k \geq k^*} \frac{i_k - i_{k-1}}{2N - i_k - i_{k-1}}. \tag{70}$$

The sum (70) is largest when $M = N$, yielding

$$\sum_{i=1}^{(N-1)/2} \frac{1}{2i - 1} + \sum_{i=1}^{(N+1)/2} \frac{1}{2i - 1} \leq 1 + \log(2N). \tag{71}$$

Combining (70) and (71) with (65) proves (63).