Complete Analysis of a Random Forest Model

Jason M. Klusowski
Department of Statistics and Biostatistics
Rutgers University – New Brunswick
Piscataway, NJ, USA, 08019
jason.klusowski@rutgers.edu

September 24, 2018

Abstract

Random forests have become an important tool for improving accuracy in regression problems since their popularization by [Breiman, 2001] and others. In this paper, we revisit a random forest model originally proposed by [Breiman, 2004] and later studied by [Biau, 2012], where a feature is selected at random and the split occurs at the midpoint of the box containing the chosen feature. If the Lipschitz regression function is sparse and only depends on a small, unknown subset of \( S \) out of \( d \) features, we show that, given access to \( n \) observations, this random forest model outputs a predictor that has a mean-squared prediction error \( O((n(\sqrt{\log n})^{S-1})^{-\frac{S}{S+2\pi}}) \). This positively answers an outstanding question of [Biau, 2012] about whether the rate of convergence therein could be improved.

The second part of this article shows that the aforementioned prediction error cannot generally be improved, which we accomplish by characterizing the variance and by showing that the bias is tight for any linear model with nonzero parameter vector. As a striking consequence of our analysis, we show the variance of this forest is similar in form to the best-case variance lower bound of [Lin and Jeon, 2006] among all random forest models with nonadaptive splitting schemes (i.e., where the split protocol is independent of the training data).

1 Introduction

Random forests are ubiquitous among ensemble averaging algorithms because of their ability to reduce overfitting and their efficient implementation. As a method that grows many base tree predictors and then combines them, they are related to kernel regression [Breiman, 2000, Geurts et al., 2006, Scornet, 2016], adaptive nearest neighbors [Lin and Jeon, 2006], and AdaBoost [Wyner et al., 2017]. These connections may explain the success of random forests in various prediction and classification problems, such as those encountered in bioinformatics and computer vision.

One of the most widely used random forests is Breiman’s CART algorithm [Breiman, 2001], which was inspired by the random subspace method of [Ho, 1995], spacial feature selection of [Amit and Geman, 1997], and random decision method of [Dietterich, 2000]. To this date, researchers have spent a great deal of effort in understanding theoretical properties of various streamlined versions of Breiman’s original algorithm [Genner, 2010, 2012, Arlot and...]
where the data may be bootstrapped or the splits determined by optimizing some empirical objective.

We will assume that the conditional mean response function of its "strong" variables $s = \{x_j : j \in S\}$, where $S = |S| \ll d$. Conversely, the output of $f$ does not depend on "weak" variables that belong to $[d] \setminus S$. Per the success of many modern methods in machine learning, the sparsity assumption corresponds to the fact that a large class of high-dimensional functions admit or are well-approximated by sparse representations of simple model forms (e.g., sparse linear combinations of nonlinear ridge compositions or single-hidden-layer neural networks with sparse inner and outer layer parameters). Of course, the set $S$ is not known a priori and must be learned from the data.

As mentioned earlier, many scholars have proposed and studied idealized versions of Breiman's original algorithm $\text{Breiman (2004)}$, largely with the intent of reducing the complexity of their theoretical analysis. On the other hand, recent works have proved properties like asymptotic normality $\text{Mentch and Hooker (2016)}$ or consistency (for additive models) $\text{Scornet et al. (2015a)}$ of Breiman's original random forest model $\text{Breiman (2001)}$, where the data may be bootstrapped or the splits determined by optimizing some empirical objective $\text{Genuer (2012)}$. However, these results are asymptotic in nature, and it is difficult to determine the quality of convergence as a function of the parameters of the random forest (e.g., sample size, dimension, and depth to which the individual trees are grown).

In this paper, we focus on another historically significant model that was proposed by Breiman in a technical report $\text{Breiman (2004)}$. Here, importantly, the individual trees are grown independently of the training sample $\mathcal{D}_n$ (although subsequent work allows the trees to depend on a second sample $\mathcal{D}_n'$, independent of $\mathcal{D}_n$). Such models are referred to as "purely random forests" $\text{Genuer (2012)}$. Despite its simplicity, this random forest model captures a few of the attractive features of Breiman's original algorithm $\text{Breiman (2004)}$, i.e., variance reduction by randomization, and adaptive variable selection.

Later, in an influential paper, $\text{Biau (2012)}$ considered the same model and rigorously established some informal, heuristic-based claims made by Breiman. Both works of Breiman and Biau will serve as the basis for this article, whose primary purpose is to complete the analysis of this model and offer a full picture of its fundamental limits.
Borrowing the terminology of [Scornet, 2016], we shall refer to this model henceforth as a “centered random forest”. In the forthcoming discussion, log is the natural logarithm.

**New contributions.** [Biau, 2012, Corollary 6] showed that if the regression function is sparse in the sense that it only depends on $S$ strong features, then with the aide of a second random sample $D_n'$, the splits concentrate on the informative features in an adaptive manner, without a priori knowledge of the set $S$. Furthermore, the mean-squared prediction error is

$$O\left(n^{-\frac{1}{S(4/3) \log 2 + 1}}\right).$$

A surprising aspect of this error is that the exponent is independent of the ambient dimension $d$, which might partially explain why random forests perform well in high-dimensional settings. Biau also raised the question [Biau, 2012, Remark 7] as to whether this rate could be improved. We will answer this in the affirmative and show that the error can indeed be improved to

$$O\left((n \sqrt{\log \frac{S}{1-n}})^{-\alpha_S}\right),$$

where

$$\alpha_S = \frac{2 \log (1 - S^{-1/2})}{2 \log (1 - S^{-1/2}) - \log 2} = \frac{1}{S \log 2 + 1} (1 + \Delta_S),$$

and $\Delta_S$ is some positive quantity that decreases to zero as $S$ approaches infinity. In particular,

(a) We improve the rate in the exponent from $\frac{1}{S(4/3) \log 2 + 1}$ to $\frac{1}{S \log 2 + 1}$ and, due to the presence of the logarithmic term in (1), improve the convergence by a factor of $O((\log n)^{-\frac{1}{2 \log 2}})$.

(b) We show that the rate (1) is not generally improvable. To accomplish this, we show that the bias is tight for all linear models with nonzero parameter vector. We also give matching upper and lower bounds on the variance, which are, surprisingly, nearly optimal among all purely random forests with nonadaptive splitting schemes.

(c) We show that if the regression function is square-integrable (e.g., it need not be continuous or even bounded), then the random forest predictor is pointwise consistent almost everywhere.

Additional comparisons between our work and Biau’s is provided in Table 1 and Table 2. The improvements in (a) and (b) stem from a new analysis of the bias of the random forest and of the correlation between trees. We also believe our new techniques can be used to improve existing results for other random forest models, i.e., improve the bias/approximation error of “median forests” [Duroux and Scornet, 2016] and the subpar mean-squared prediction error

$$O\left(n^{-\frac{\log (1-0.75/d)}{\log (1-0.75/d) - \log 2}}\right)$$

[Duroux and Scornet, 2016, Theorem 3.1].

**Related results.** We now mention a few related results. [Scornet, 2016] slightly altered the definition of random forests so that they could be rewritten as kernel methods. For what he called “centered kernel random forests (KeRF)”, where the trees are grown according to the same selection and splitting procedure as centered random forests, [Scornet, 2016] Theorem
1] showed that these estimators have mean-squared prediction error $O(n^{-\frac{1}{2(d+1)}} \log^2 n)$. In addition to the computational advantages of centered random forests when $n$ and $d$ are moderately sized, note that (1) is strictly better, even when $S = d$. The improved rate (1) is obtained by growing the trees to a shallower depth than the suboptimal depth used by Scornet, and this may explain why he found centered KeRF to empirically outperform centered random forests for certain regression models [Scornet, 2016, Model 1, Figure 5].

Other results have been established for function classes with additional smoothness assumptions. For example, a multivariate function on $[0,1]^d$ is of class $C_k([0,1]^d)$ if all its $k^{th}$ order partial derivatives exist and are bounded on $[0,1]^d$. Then, for regression functions in $C_2([0,1]^d)$, [Arlot and Genuer, 2014, p. 21] obtained a similar rate of $O(n^{-\alpha S})$ for $S = d \geq 4$ under the so-called “balanced purely random forest (BPRF)” model, where all nodes are split at each stage (in contrast to single splits with centered random forests). However, in addition to requiring that the regression function is of class $C_2([0,1]^d)$ (instead of just Lipschitz), it is unclear whether these random forest models adapt to sparsity (i.e., where only a subset of the variables have an effect on the output). It would be interesting to see if our new techniques could be used to remove the $C_2([0,1]^d)$ condition so that the same rate also holds for $C_1([0,1]^d)$.

Finally, there are online versions of random forests, albeit defined somewhat differently than centered random forests, which achieve optimal rates of estimation. Recently, [Mourtada et al., 2018] have shown that a type of online forest known as a Mondrian forest achieves the minimax optimal rates when $f$ is of class $C_1([0,1]^d)$ or $C_2([0,1]^d)$, i.e., $\Theta(n^{-\frac{1}{d+2}})$ or $\Theta(n^{-\frac{1}{d+1}})$, respectively. As with the BPRF model, a current open question is how to incorporate a data-driven way of selecting informative variables for which the splits are performed along.

**Notation.** Throughout this document, we let $\|x\| = (\sum_{j=1}^d |x^{(j)}|^2)^{1/2}$ denote the $\ell^2$ norm of a $d$-dimensional vector $x = (x^{(1)}, \ldots, x^{(d)})$, $\langle \cdot, \cdot \rangle$ denote the Euclidean inner product, and $\|x\|_\infty = \sup_{1 \leq j \leq d} |x^{(j)}|$ denote the supremum norm of $x$. For a subset $S \subset \{1, \ldots, d\}$ with cardinality $S$, we write $\|x\|_S$ to denote $\|(x^{(j)} : j \in S)\|$, i.e., the norm of $x$ embedded in $\mathbb{R}^S$. For a Lebesgue integrable function $f$, let $\|f\| = (\int_{[0,1]^d} |f(x)|^2 \lambda(dx))^{1/2}$ denote the $L^2(\lambda)$ ($\lambda$ is Lebesgue measure on $[0,1]^d$) norm of $f$ and $\|f\|_\infty = \sup_{x \in [0,1]^d} |f(x)|$ denote the $L^\infty$ norm of $f$.

For a positive integer $m$, let $[m] = \{1, \ldots, m\}$. For positive sequences $\{a_n\}$ and $\{b_n\}$, we write $a_n = O(b_n)$ if $a_n \leq Cb_n$, $a_n = \Omega(b_n)$ if $a_n \geq cb_n$, and $a_n = \Theta(b_n)$ if both $a_n \leq Cb_n$ and $a_n \geq cb_n$, for some constants $c > 0$ and $C > 0$ that may depend on other parameters, e.g., variance, Lipschitz constant. The least integer greater than or equal to a real number $z$ is denoted by $\lceil z \rceil$. The natural and base-2 logarithms are denoted by $\log$ and $\log_2$, respectively.

**Organization.** This paper is organized as follows. We formally define centered random forests and a few related quantities in Section 2. In Section 3, we present our main results, which are derived from an analysis of the bias and variance of the forest. Finally, in Section 4, we show that the bias and variance bounds derived in Section 3 cannot be generally improved. Proofs of all supporting lemmas are given in Appendix A.
2 Centered random forests

In general terms, a random forest is an estimator that is built from an ensemble of randomized base regression trees \( \{ f_n(x; \Theta_m, D_n) \}_{1 \leq m \leq M} \). The sequence \( \{ \Theta_m \}_{1 \leq m \leq M} \) consists of i.i.d. realizations of a random variable \( \Theta \), which governs the probabilistic mechanism that builds each tree. These individual random trees are aggregated to form the final output

\[
\bar{f}_n^M(x; \Theta_1, \ldots, \Theta_M) = \frac{1}{M} \sum_{m=1}^{M} f_n(x; \Theta_m, D_n).
\]

When \( M \) is large, the law of large numbers justifies using

\[
\bar{f}_n(x) \triangleq \mathbb{E}_\Theta [f_n(x; \Theta, D_n)],
\]

in lieu of \( \bar{f}_n^M(x; \Theta_1, \ldots, \Theta_M) \), where \( \mathbb{E}_\Theta \) denotes expectation with respect to \( \Theta \), conditionally on \( X \) and \( D_n \). We shall henceforth work with these population level versions (i.e., infinite number of trees) of their empirical counterparts (i.e., finite number of trees).

Let us now formally define how each base tree of a centered random forest is constructed. Every node of the tree has a corresponding box \((d\text{-dimensional hyperrectangle})\) and at each stage of the construction of the tree, the collection of boxes among the leaves of the tree forms a partition of \([0,1]^d\). In fact, we will see that the boxes are dyadic cubes.

(i) Initialize with \([0,1]^d\) as the root.

(ii) At each node, select a coordinate of \(X = (X^{(1)}, \ldots, X^{(d)})\) at random, with the \(j^{th}\) feature having a probability \(p_{nj}\) of being selected, where \(\sum_{j=1}^{d} p_{nj} = 1\).

(iii) Split at the midpoint of the selected variable at the node.

(iv) Repeat steps (ii) and (iii) \(\lceil \log_2 k_n \rceil\) times, where \(k_n \geq 2\) is a tuning parameter.\(^2\)

The ideal selection probabilities should satisfy \(p_{nj} = 1/S\) for \(j \in S\) and \(p_{nj} = 0\) otherwise. We do not know the set \(S\) a priori, but nevertheless, we can adaptively select candidate variables using a second sample \(D'_n = \{ (X'_i, Y'_i) \}_{i=1}^{n}\), independent of \(D_n\) (which can be done, for example, by sample-splitting). Then candidate “strong” coordinates are those that maximizes the weighted conditional variance decrement \(V_n(j, z)\) within a current leaf \(A_j = [a_j, b_j]\),

\[
\frac{1}{n} \sum_{i=1}^{n} (Y_i' - \bar{Y}_{A_j})^2 \mathbb{I} \{ x_i^{(j)} \in A_j \} - \frac{1}{n} \sum_{i=1}^{n} (Y_i' - \bar{Y}_{A_j}^{L})^2 \mathbb{I} \{ x_i^{(j)} \in A_j^{L} \} - \frac{1}{n} \sum_{i=1}^{n} (Y_i' - \bar{Y}_{A_j}^{R})^2 \mathbb{1} \{ x_i^{(j)} \in A_j^{R} \}, \tag{2}
\]

where \(A_j^{L} = [a_j, z]\) and \(A_j^{R} = [z, b_j]\) and, for \(A \subset [0,1]\), \(\bar{Y}_A = \frac{1}{n} \sum_{i=1}^{n} Y_i \mathbb{I} \{ x_i^{(j)} \in A \}\). The idea is to first randomly select a subset \(M_n\) of \(M_n\) of the \(d\) coordinates. Then, for each selected coordinate, calculate the split \(z_j^*\) that maximizes \(2\) and store the corresponding maximum value \(V_n(j, z_j^*)\). Finally, select one variable at random among the largest of \(\{V_n(j, z_j^*)\}_{j \in M_n}\).

\(^2\)Its value will be determined by optimizing the tradeoff between the variance and bias of \(f_n(X)\)
to split along. Define \( p_{nj} \) as the probability that the \( j^{th} \) variable is selected. As is argued in \cite{Biau2012} Section 3, for large \( n \), this empirical maximization procedure (à la CART) will produce \( p_{nj} \) that concentrate approximately around \( 1/S \) for \( j \in S \) and zero otherwise, viz.,

\[
p_{nj} \approx \frac{1}{S} \left[ 1 - \left( 1 - \frac{S}{d} \right)^{M_{n}} \right] (1 + \xi_{nj}) \approx \frac{1}{S}(1 + \xi_{nj}), \quad j \in S,
\]

and \( p_{nj} \approx \xi_{nj} \) otherwise, where \( \xi_{nj} = O(k_{n}/n) \). The reader is encouraged to consult \cite{Biau2012} Section 3] for further details. This argument justifies assuming henceforth that the \( p_{nj} \) admit such a form.

The randomized base regression tree \( f_{n}(X; \Theta, D_{n}) \) is a local weighted average of all \( Y_{i} \) for which the corresponding \( X_{i} \) falls into the same box of the random partition as \( X \). For concreteness, let \( A_{n}(X, \Theta) \) be the box of the random partition containing \( X \) and define the individual tree predictor via

\[
f_{n}(X; \Theta, D_{n}) = \frac{\sum_{i=1}^{n} Y_{i} 1\{X_{i} \in A_{n}(X, \Theta)\}}{\sum_{i=1}^{n} 1\{X_{i} \in A_{n}(X, \Theta)\}} 1\varepsilon_{n}(X, \Theta),
\]

where \( \varepsilon_{n}(X, \Theta) \) is the event that \( \sum_{i=1}^{n} 1\{X_{i} \in A_{n}(X, \Theta)\} \) is nonzero. We then take the expectation of these individual predictors with respect to the randomizing variable \( \Theta \) yielding

\[
\bar{f}_{n}(X) = \sum_{i=1}^{n} \mathbb{E}_{\Theta} [W_{ni}(X, \Theta)] Y_{i},
\]

where

\[
W_{ni}(X, \Theta) = \frac{1\{X_{i} \in A_{n}(X, \Theta)\}}{N_{n}(X, \Theta)} 1\varepsilon_{n}(X, \Theta)
\]

are the weights corresponding to each observed output and

\[
N_{n}(X, \Theta) = \sum_{i=1}^{n} 1\{X_{i} \in A_{n}(X, \Theta)\}
\]

is the total number of observations that fall into the same box of the random partition as \( X \). The box \( A_{n}(X, \Theta) \) can be decomposed into the product of its sides \( \prod_{j=1}^{d} A_{nj}(X, \Theta) \), where \( A_{nj}(X, \Theta) = [a_{nj}(X, \Theta), b_{nj}(X, \Theta)] \) and \( a_{nj}(X, \Theta) \) and \( b_{nj}(X, \Theta) \) are its left and right endpoints, respectively. Since \( X^{(j)} \) is uniformly distributed on \([0, 1]\), it has a binary expansion

\[
X^{(j)} \overset{\mathcal{D}}{=} \sum_{k \geq 1} B_{k}(X)2^{-k},
\]

where \( \{B_{k}(X)\}_{k=1}^{\infty} \) are i.i.d. Bern(1/2). Thus, if \( K_{nj}(X, \Theta) \) is the number of times the box \( A_{n}(X, \Theta) \) is split along the \( j^{th} \) coordinate, it is not hard to see that each endpoint of \( A_{nj}(X, \Theta) \) is a randomly stopped binary expansion of \( X^{(j)} \), viz.,

\[
a_{nj}(X, \Theta) \overset{\mathcal{D}}{=} \sum_{k=1}^{K_{nj}(X, \Theta)} B_{k}(X)2^{-k}, \quad j \in S,
\]

(3)
Theorem 1. Suppose \( f \) is square-integrable, i.e., \( \int_{[0,1]^d} |f(x)|^2 \lambda(dx) < +\infty \), \( p_{nj} \) log \( k_n \to +\infty \) for all \( j = 1, \ldots, d \) and \( k_n/n \to 0 \) as \( n \to +\infty \). Then, for \( \lambda \)-almost all \( x \in [0,1]^d \),

\[
\mathbb{E} \left[ \tilde{f}_n(x) - f(x) \right]^2 \to 0, \quad n \to +\infty.
\]

For the next set of results, we assume that \( f \) is \( L \)-Lipschitz, i.e., \( |f(x) - f(x')| \leq L \|x - x'\| \) for all \( x \) and \( x' \) in \( \mathbb{R}^d \) for some positive constant \( L \).

We begin our analysis with the standard variance/bias decomposition

\[
\mathbb{E} \left[ \tilde{f}_n(X) - f(X) \right]^2 = \mathbb{E} \left[ \tilde{f}_n(X) - \mathbb{E} \left[ \tilde{f}_n(X) \mid X \right] \right]^2 + \mathbb{E} \left[ \mathbb{E} \left[ \tilde{f}_n(X) \mid X \right] - f(X) \right]^2. \tag{5}
\]

Each of these terms will be controlled in Theorem 3 and Theorem 4. The next result is proved by combining the bounds in Theorem 3 and Theorem 4 with the variance/bias decomposition in (5).

In accordance with the discussion in Section 2, we assume throughout that \( p_{nj} = (1/S)(1 + \xi_{nj}) \) for \( j \in \mathcal{S} \) and \( p_{nj} = \xi_{nj} \) otherwise, where \( \{\xi_{nj}\} \) is a sequence that tends to zero as \( n \) tends to infinity. Furthermore, let \( p_n = (1/S)(1 + \xi_n) \), where \( \xi_n = \min_{j \in \mathcal{S}} \xi_{nj} \).

Theorem 2. Suppose \( f \) is \( L \)-Lipschitz and has \( L^\infty \) norm at most \( B \). Then,

\[
\mathbb{E} \left[ \tilde{f}_n(X) - f(X) \right]^2 \leq \frac{SL^2k_n^2\log_2(1-p_{n}/2)+1}{n+1} + SL^2k_n^2\log_2(1-p_{n}/2) + B\left(\frac{12\sigma^2k_n}{n}\right) \left(\frac{(8S)^{S-1}}{(1+\xi_n)^{S-1}\sqrt{\log_2^{S-1}k_n}}\right).
\]
The leading terms in the risk bound from Theorem 2 are $S^2 L^2 k_n^{2\log_2(1-p_n/2)}$ and $\frac{12\sigma^2 k_n}{n^{(1+\xi_n)S^{-1}}\sqrt{\log_2 S^{-1} k_n}}$. Optimizing their sum over $k_n$ leads to the following corollary.

**Corollary 1.** Assume the same setup as Theorem 2. Let $\alpha_S = \frac{2\log(1-p_n/2)}{2\log(1-p_n/2)-\log 2}$ and $k_n = \left(\frac{S^{-S+3}(L/\sigma)^2n\sqrt{\log_2 S^{-1} n}}{\log_2 S^{-1} n}\right)^{1-\alpha_S}$, and assume the same setup as Theorem 2. There exists a constant $C > 0$, depending only on $B$, $S$, $L$, and $\sigma$, such that

$$E[\hat{f}_n(X) - f(X)]^2 \leq C \left(\frac{n\sqrt{\log_2 S^{-1} n}}{\sqrt{\log_2 S^{-1} n}}\right)^{-\alpha_S}.$$ 

A conclusion of these results is that this random forest model produces a computationally feasible, adaptive predictor for learning sparse regression functions, which beats the minimax optimal rate $\Theta(n^{-2/3})$ [Yang and Barron, 1999, Example 6.5] (for Lipschitz function classes in $d$ dimensions) when $\alpha_S \geq \frac{2}{\sqrt{d+2}}$, or roughly when $S \leq \lceil 0.72d \rceil$.

As with [Biau, 2012, Remark 10], the assumption of uniform design is not crucial to our analysis. If instead $X$ has density $f$ which satisfies $1/c \leq f(x) \leq c$ for some universal constant $c > 0$ and for all $x \in [0, 1]^d$, the conclusions of Theorem 1, Theorem 2, and Corollary 1 remain true, with only minor adjustments to the constants.

**Remark 1.** Compare our choice of the optimal number of leaf nodes $k_n = \Theta(n^{1-\alpha_S}) \approx \Theta(n^{S\log_2 S^{-1}})$ (ignoring logarithmic factors) with that of [Biau, 2012, Corollary 6], $k'_n = \Theta(n^{S(4/3)\log_2 S^{-1}})$. Thus, better performance is achieved if the trees are grown less aggressively.

**Remark 2.** When $S = d = 1$, Corollary 2 gives the optimal minimax rate $\Theta(n^{-2/3})$ for Lipschitz regression functions in one dimension [Yang and Barron, 1999, Example 6.5].

![Figure 1: A plot of the new rate $\alpha_S \approx \frac{1}{S\log_2 S^{-1} + 1}$ for $S = d$ from Corollary 1 versus the rate $\frac{1}{d(1/3)\log_2 S^{-1} + 1}$ from Biau, 2012, Corollary 6]
In Table 1, we catalogue our improvements to [Biau, 2012] in terms of the bias, variance, and mean-squared prediction error of an optimally chosen $k_n$. Table 2 shows that centered random forests almost surely convergence to the true regression function, even under quite weak conditions. For ease of exposition, we replaced $\log(1 - p_n/2)$ by an approximation $-1/(2S)$, valid for for large $n$ and $S$. In this case, for example, $\alpha_S$ becomes $\frac{1}{S \log 2 + 1}$.

| Bias | Variance | $k_n$ | Rate |
|------|----------|------|------|
| $k_n$ | $\frac{1}{n \log 2}$ | $\frac{k_n}{n} (\log_2 k_n) - \frac{S}{2}$ | $n^{-\frac{S(4/3) \log 2}{n S \log 2 + 1}}$ |
| Improvement | $n^{-\frac{S(4/3) \log 2}{n S \log 2 + 1}}$ | $(n \sqrt{\log S^{-1} n})^{-\frac{1}{S \log 2 + 1}}$ |

Table 1: Comparison of convergence rates to [Biau, 2012].

| Convergence | $\mathbb{E}[ Y \mid X = x]$ |
|-------------|--------------------------|
| Improvement | Mean squared-error | Almost sure |
| Improvement | Lipschitz continuous | Square-integrable |

Table 2: Comparison of convergence strength to [Biau, 2012].

**Variance term.** In this subsection, we bound the variance of the random forest. Suppose for the moment that $\text{Var}[ Y \mid X ] \equiv \sigma^2$. Note that in [Lin and Jeon, 2006, Theorem 1, Lemma 1, and Theorem 3], it was shown that if $w_{\max}$ is the maximum number of observations per leaf node for any nonadaptive random forest (with uniform input $X$), then there exists a universal constant $C > 0$ such that the variance is at least

$$C \sigma^2 w_{\max}^{-1} (d - 1)! (2 \log n)^{-(d-1)}. \quad (6)$$

By Stirling’s formula, (6) can be further lower bounded by

$$\frac{C' \sigma^2 w_{\max}^{-1} (d - 1)! (2 \log n)^{-(d-1)}}{\log^{d-1} n}, \quad (7)$$

where $C' = C \sqrt{2 \pi (d-1)/(2e)^{d-1}}$. The number of observations per leaf node of a centered random forest is on average about $w_{\text{avg}} = n/k_n$ and hence the next theorem shows that centered random forests nearly achieve (7) when $S = d$ and $k_n = n/w_{\text{avg}}$, mainly,

$$\sigma^2 w_{\text{avg}}^{-1} (d - 1)^{d-1} \left(\log^{d-1}(n/w_{\text{avg}})\right)^{-1}. \quad (8)$$

**Theorem 3.** For any regression function $f(x) = \mathbb{E}[ Y \mid X = x]$ with $\sup_{x \in [0,1]^d} \text{Var}[ Y \mid X = x] \leq \sigma^2$,

$$\mathbb{E} \left[ \hat{f}_n(X) - \mathbb{E} \left[ \hat{f}_n(X) \mid X \right] \right]^2 \leq \frac{12 \sigma^2 k_n}{n} \frac{(8S)^{S-1}}{(1 + \xi_n)^{S-1} \sqrt{\log_2^{S-1} k_n}}. \quad (9)$$

Actually, the lower bound in [Lin and Jeon, 2006, Theorem 3] is for the mean-squared prediction error, but the proof gives it for the variance.
We do not know of any other random forest model that achieves (6) or improves upon (8). Taken together, (7) and (8) imply that centered random forests have nearly optimal variance among all purely random forests with nonadaptive splitting schemes.

Remark 3. Compare our result with [Biau, 2012, Proposition 2], which shows that the variance of \( f_n \) is \( O((k_n/n)(\sqrt{\log_2 k_n})^{-S/d}) \). In particular, we improve the exponent in the logarithmic factor from \( S/d \) to \( S - 1 \) (which is a strict improvement whenever \( S > 2 \)). In the fully grown case when \( k_n = n \) (i.e., when there is on average one observation per leaf node), the variance still decays at a reasonably fast rate \( O((\sqrt{\log_2 n})^{-(S-1)}) \). In addition to the term \( k_n/n \), which is due to the aggregation of the individual tree predictors, the extra logarithmic factor arises from the correlation between trees.

Proof of Theorem 3: It is shown in [Biau, 2012, Section 5.2, p. 1085] that

\[
\mathbb{E} \left[ (\bar{f}_n(X) - \mathbb{E}[\bar{f}_n(X) | X])^2 \right] \leq \frac{12\sigma^2 k_n^2}{n} \mathbb{E} \left[ \lambda(A_n(X, \Theta) \cap A_n(X, \Theta')) \right].
\]

where \( \Theta' \) is an independent copy of \( \Theta \). We can use the representations (3) and (4) to show that for any \( \Theta \) and \( \Theta' \), the sides of the box are nested according to \( A_{nj}(X, \Theta) \subseteq A_{nj}(X, \Theta') \) if and only if \( K_{nj}(X, \Theta) \geq K_{nj}(X, \Theta') \) and hence

\[
\lambda(A_{nj}(X, \Theta) \cap A_{nj}(X, \Theta')) = 2^{-\max\{K_{nj}(X, \Theta), K_{nj}(X, \Theta')\}}.
\]

Using this, we have

\[
\lambda(A_n(X, \Theta) \cap A_n(X, \Theta')) = \prod_{j \in [d]} \lambda(A_{nj}(X, \Theta) \cap A_{nj}(X, \Theta'))
\]

\[
= 2^{-\sum_{j \in [d]} \max\{K_{nj}(X, \Theta), K_{nj}(X, \Theta')\}} = 2^{-[\log_2 k_n] - \frac{1}{2} \sum_{j \in [d]} |K_{nj}(X, \Theta) - K_{nj}(X, \Theta')|},
\]

where the equality in (12) follows from the identity

\[
\sum_{j \in [d]} \max\{K_{nj}(X, \Theta), K_{nj}(X, \Theta')\} = \frac{1}{2} \sum_{j \in [d]} K_{nj}(X, \Theta) + \frac{1}{2} \sum_{j \in [d]} K_{nj}(X, \Theta')
\]

\[
+ \frac{1}{2} \sum_{j \in [d]} |K_{nj}(X, \Theta) - K_{nj}(X, \Theta')|
\]

\[
= [\log_2 k_n] + \frac{1}{2} \sum_{j \in [d]} |K_{nj}(X, \Theta) - K_{nj}(X, \Theta')|.
\]

Here we depart from the strategy of [Biau, 2012], which we now briefly outline. His approach consists of applying Hölder’s inequality to the expectation of (12) and resultant expected product

\[
\mathbb{E} \left[ 2^{-\sum_{j \in [d]} \max\{K_{nj}(X, \Theta), K_{nj}(X, \Theta')\}} \right] \leq k_n^{-1} \prod_{j \in [d]} \mathbb{E} \left[ 2^{-\frac{1}{2} |K_{nj}(X, \Theta) - K_{nj}(X, \Theta')|} \right]^{1/d}.
\]
He uses this together the fact that, for \( d \geq 2 \),
\[
\mathbb{E}
\left[
2^{-\frac{d}{2}|K_{nj}(X,\Theta) - K_{nj}(X,\Theta')}|ight]
\leq \mathbb{P}
\left[
M_1 = M'_1
\right]
+ \mathbb{E}
\left[
2^{-|M_1 - M'_1|} \1_{\{M_1 > M'_1\}}
\right]
= \mathbb{P}
\left[
M_1 = M'_1
\right]
+ 2\mathbb{E}
\left[
2^{-|M_1 - M'_1|} \1_{\{M_1 > M'_1\}}
\right]
\leq 2\mathbb{E}
\left[
2^{-|K_{nj}(X,\Theta) - K_{nj}(X,\Theta')}| \1_{\{K_{nj}(X,\Theta) \geq K_{nj}(X,\Theta')\}}
\right]
\leq \frac{12}{\sqrt{\pi p_{nj}(1 - p_{nj}) \log_2 k_n}},
\]
where the last inequality follows from [Biau 2012, Proposition 13], to conclude that the bias is of order \( O((k_n/n) (\log_2 k_n)^{-S/(2d)}) \).

Our approach is different. Instead of reducing the calculations so that the expectations involve only the marginals \( K_{nj}(X,\Theta) \) and \( K_{nj}(X,\Theta') \), we will work with their joint distribution. To this end, note that conditionally on \( X \), \((K_{n1}(X,\Theta), \ldots, K_{nd}(X,\Theta))\) has a multinomial distribution with \( \log_2 k_n \) trials and event probabilities \( \{p_{n1}, \ldots, p_{nd}\} \). We take the expected value of (12) and use the bound
\[
\mathbb{E}
\left[
2^{-\frac{1}{2} \sum_{j \in S} |K_{nj}(X,\Theta) - K_{nj}(X,\Theta')|}
\right]
\leq \mathbb{E}
\left[
2^{-\frac{1}{2} \sum_{j \in S} |K_{nj}(X,\Theta) - K_{nj}(X,\Theta')|}
\right],
\]
Next, let \( \{j_1, j_2, \ldots, j_S\} \) be an enumeration of \( S \). By (A.23) (whose proof is given in Lemma A.5), we have
\[
\mathbb{E}
\left[
2^{-\frac{1}{2} \sum_{j \in S} |K_{nj}(X,\Theta) - K_{nj}(X,\Theta')|} \mid X
\right]
\leq \frac{8^{S-1}}{(\log_2 k_n)^{S-1} \prod_{k=1}^{S-1} p_{njk}} \prod_{k=1}^{S-1} p_{njk}
\leq \frac{(8S)^{S-1}}{(1 + \xi_n)^{S-1} \log_2 k_n}.
\]
Combining (14) and (10) proves (9). \hfill \Box

Remark 4. [Breiman 2004, Equation 3] seems to make the claim that (15) is \( O((\sqrt{\log_2 k_n})^{-S}) \), although in view of the multivariate normal approximation to the multinomial distribution, we see that this cannot be the case since \( \sum_{j \in S} |K_{nj}(X,\Theta) - K_{nj}(X,\Theta')| \) has only \( S - 1 \) degrees of freedom.

Bias term. Here we provide a bound on the bias of the random forest, which will be seen to be \( O(k_n^{2\log_2(1-p_n/2)}) \approx O(k_n^{-\frac{1}{\log_2}}) \). Our bias bound is the same (up to a constant factor) as [Arlot and Genuer 2014, Corollary 9] when \( S = d \geq 4 \), but for the BPRF model and under a stronger assumption that \( f \) is of class \( C_2([0, 1]^d) \).

It will be shown in Section 4 that our bound cannot be improved, even under additional smoothness assumptions.

\(^4\)In an earlier draft of this paper, we experimented with a random number of leaf nodes \( \xi_n \sim \text{Poisson}(\lambda) \), so that \( \{K_{nj}(X,\Theta)\}_{j \in S} \) are independent \( \text{Poisson}(\lambda p_{nj}) \). Then the expected value of the product (12) is simply the product of the expectations, which involves only the marginals \( K_{nj}(X,\Theta) \). Despite the advantages of independence, it can be shown that this random forest has worse mean-squared predictive error, even when the bias and variance are optimized over \( \lambda \).
Theorem 4. Suppose \( f \) is \( L \)-Lipschitz and has \( \ell_\infty \) norm at most \( B \). Then,

\[
\mathbb{E} \left[ \mathbb{E} \left[ \hat{f}_n(X) \mid X \right] - f(X) \right]^2 \leq \frac{S L^2 k_n^2 \log_2 (1 - p_n/2) + 1}{n + 1} + S^2 L^2 k_n^2 \log_2 (1 - p_n/2) + B e^{-n/(2k_n)}. \tag{15}\]

Proof. We first decompose the bias term \( \mathbb{E} \left[ \mathbb{E} \left[ \hat{f}_n(X) \mid X \right] - f(X) \right]^2 \) as follows:

\[
\mathbb{E} \left[ \mathbb{E} \left[ \hat{f}_n(X) \mid X \right] - f(X) \right]^2 = \mathbb{E} \left[ \sum_{i=1}^n \mathbb{E}_\Theta \left[ W_{ni}(X, \Theta) \right] \left( f(X_i) - f(X) \right) + \mathbb{1} \mathcal{E}_n(X, \Theta) f(X) \right]^2
\]

\[
= \mathbb{E} \left[ \sum_{i=1}^n \mathbb{E}_\Theta \left[ W_{ni}(X, \Theta) \right] \left( f(X_i) - f(X) \right) \right]^2 + \mathbb{E} \left[ \mathbb{1} \mathcal{E}_n(X, \Theta) f(X) \right]^2 \tag{16}\]

\[
\leq \mathbb{E} \left[ \sum_{i=1}^n \mathbb{E}_\Theta \left[ W_{ni}(X, \Theta) \right] \left( f(X_i) - f(X) \right) \right]^2 + \|f\|_{\ell_\infty}^2 \mathbb{P} \left[ \mathcal{E}_n^c(X, \Theta) \right]. \tag{17}\]

In \cite{Biau2012}, Section 5.3, p. 1089, it is shown that

\[
\mathbb{E} \left[ \mathbb{1} \mathcal{E}_n(X, \Theta) f(X) \right]^2 \leq \|f\|_{\ell_\infty}^2 \mathbb{P} \left[ \mathcal{E}_n^c(X, \Theta) \right] \leq B e^{-n/(2k_n)}. \]

The remainder of the proof is devoted to bounding the first term in \( (17) \) by

\[
\frac{S L^2 k_n^2 \log_2 (1 - p_n/2) + 1}{n + 1} + S^2 L^2 k_n^2 \log_2 (1 - p_n/2), \tag{18}\]

which is an improvement over the bound of \( 2S L^2 k_n^2 \left( \frac{p_n}{(1/4) \log_2} \right) \) in \cite{Biau2012}, Section 5.3, p. 1089, albeit with an additional factor of \( S \). Let us pause for a moment and discuss how this improvement arises. As is standard with the analysis of purely random forests, \cite{Biau2012}, Section 5.4, pp. 1086-1087] applies Jensen’s inequality to arrive at the bound

\[
\mathbb{E} \left[ \sum_{i=1}^n \mathbb{E}_\Theta \left[ W_{ni}(X, \Theta) \right] \left( f(X_i) - f(X) \right) \right]^2 \leq \sum_{i=1}^n \mathbb{E} \left[ W_{ni}(X, \Theta) \left( f(X_i) - f(X) \right) \right]^2 \leq n \mathbb{E} \left[ W_{n1}(X, \Theta) \left( f(X_1) - f(X) \right) \right]^2. \tag{19}\]

He then proceeds to show that \( (19) \) is at most \( 2S L^2 k_n^2 \left( \frac{p_n}{(1/4) \log_2} \right) \). Instead, we expand the square in \( \mathbb{E} \left[ \sum_{i=1}^n \mathbb{E}_\Theta \left[ W_{ni}(X, \Theta) \right] \left( f(X_i) - f(X) \right) \right]^2 \), and collect diagonal and off-diagonal terms separately, to arrive at

\[
\mathbb{E} \left[ \sum_{i=1}^n \mathbb{E}_\Theta \left[ W_{ni}(X, \Theta) \right] \right]^2 \left( f(X_i) - f(X) \right)^2 \]

\[
\mathbb{E} \left[ \sum_{i \neq i'} \mathbb{E}_\Theta \left[ W_{ni}(X, \Theta) \right] \left( f(X_i) - f(X) \right) \mathbb{E}_\Theta \left[ W_{n'i'}(X, \Theta) \right] \left( f(X_{i'}) - f(X) \right) \right]
\]

\[
= n \mathbb{E} \left[ \mathbb{E}_\Theta \left[ W_{n1}(X, \Theta) \right] \right]^2 \left( f(X_1) - f(X) \right)^2 \tag{20}\]

\[
n(n-1) \mathbb{E} \left[ \mathbb{E}_\Theta \left[ W_{n1}(X, \Theta) \right] \left( f(X_1) - f(X) \right) \mathbb{E}_\Theta \left[ W_{n2}(X, \Theta) \right] \left( f(X_2) - f(X) \right) \right]. \tag{21}\]
exists a universal constant \( \Theta \).

Theorem 5. Which turns out to be significantly smaller than (19).

To see this, consider the linear model \( Y = \langle \beta, X \rangle + \epsilon \), where \( \beta = (\beta^{(1)}, \ldots, \beta^{(d)}) \) is a \( d \)-dimensional, \( S \)-sparse vector. Then we have the following lower bound on the bias of the random forest, whose proof we defer to Appendix A.

\[
\begin{align*}
\mathbb{E} \left[ \sigma^2 k_n^2 / n \right] \bigr| A_n(X, \Theta) \cap A_n(X, \Theta') \bigr|, \\
\end{align*}
\]

where \( \Theta' \) is an independent copy of \( \Theta \). The key observation is that \( A_n(X, \Theta) \) and \( A_n(X, \Theta') \) are nested according to the maximum of \( K_{nj}(X, \Theta) \) and \( K_{nj}(X, \Theta') \), and hence the equality in (12). Thus by (22) and (12), we are done if we can show that \( \mathbb{E} \left[ 2^{-1} \sum_{j \in \mathcal{S}} \left| K_{nj}(X, \Theta) - K_{nj}(X, \Theta') \right| \right] \) has a lower bound similar in form to the upper bound in (14). In fact, by Lemma A.4, (22),

\[
\mathbb{E} \left[ 2^{-1} \sum_{j \in \mathcal{S}} \left| K_{nj}(X, \Theta) - K_{nj}(X, \Theta') \right| \right] = \mathbb{E} \left[ 2^{-1} \sum_{j \in \mathcal{S}} \left| K_{nj}(X, \Theta) - K_{nj}(X, \Theta') \right| \right] \\
\geq \frac{C^{S-1} S^{S/2}}{\log_2^{S-1} k_n},
\]

for some universal constant \( C > 0 \). This proves the following lower bound on the variance of centered random forests and shows that the variance bound in Theorem 3 is tight.

\textbf{Theorem 5.} Suppose \( \mathbb{V} \mathbb{A}r[Y \mid X] \sim \sigma^2 \) and \( p_{nj} = 1 / S \) for \( j \in \mathcal{S} \) and \( p_{nj} = 0 \) otherwise. There exists a universal constant \( C > 0 \) such that

\[
\mathbb{E} \left[ \frac{\sigma^2 k_n^2}{n} \right] \bigr| A_n(X, \Theta) \cap A_n(X, \Theta') \bigr|, \\
\end{align*}
\]

Moreover, the bias bound we have derived in Theorem 4 also cannot be improved in general. To see this, consider the linear model \( Y = \langle \beta, X \rangle + \epsilon \), where \( \beta = (\beta^{(1)}, \ldots, \beta^{(d)}) \) is a \( d \)-dimensional, \( S \)-sparse vector. Then we have the following lower bound on the bias of the random forest, whose proof we defer to Appendix A.
Theorem 6. Suppose \( p_{nj} = 1/S \) for \( j \in S \) and \( p_{nj} = 0 \) otherwise and \( Y = \langle \beta, X \rangle + \varepsilon \), where \( \beta = (\beta^{(1)}, \ldots, \beta^{(d)}) \) is a \( d \)-dimensional, \( S \)-sparse vector. There exist universal constants \( c > 0 \) and \( C > 0 \) such that if \( k_n/n \leq c/S \), then
\[
\mathbb{E} \left[ \mathbb{E} \left[ \hat{f}_n(X) | X \right] - f(X) \right]^2 \geq C \| \beta \|^2 S k_n^{2 \log_2 (1 - S^{-1/2})}.
\]

This lower bound decays with \( k_n \) at the same rate as the upper bound in Theorem 1, which shows that it is tight for all linear models. When combined with the tightness of the variance, this means that the rate \([1]\) is optimal for centered random forests—but slower than the \( S \)-dimensional minimax optimal rate \( \Theta(n^{-1/2}) \) for Lipschitz regression functions on \([0, 1]^S\). In conclusion, while centered random forests enjoy near optimal variance performance (among nonadaptive splitting schemes), their \( O(k_n^{2 \log_2 (1 - p_n/2)}) \approx O(k_n^{-1 \log_2}) \) bias is far from the optimal \( \Theta(k_n^{-2}) \) required to achieve the minimax rate.

5 Conclusion

Although we characterized the fundamental limits of the centered random forest model, there is still much to be done in terms of analyzing Breiman’s original algorithm. As with all data-dependent recursive and/or iterative algorithms, theoretical analysis is challenging (e.g., EM algorithm or gradient descent). A new set of tools will need to be developed to handle the additional complexities that arise from data-entangled splits.

Practically learning the informative variables relies on information gleaned from the decrement in the empirical conditional variance \([2]\), or variance reduction, within an interval defined by a current split [Scornet et al. 2015a, Equation 2], [Breiman et al. 1984, Section 11.2]. If the input distribution is uniform on \([0, 1]^d\) and the one-dimensional partial integrals of the regression function over a subinterval of \([0, 1]\) are constant (i.e., when all but one variable is integrated out, \( \int_{A_{-j}} f(x) \lambda(dx) = C_j \) for \( A_{-j} \subset [0, 1]^{d-1} \) and all \( x^{(j)} \in A_j \subset [0, 1] \)), then any split along any variable results in a zero decrease in the population conditional variance [Scornet et al. 2015b, Technical Lemma 1], despite the fact that the regression function may be nonconstant on its domain [3]. Such a situation may lead us to erroneously classify certain features as “weak” when they may not be so. For example, take \( A_{-j} = [0, 1]^{d-1} \) and the function \( f \) to be a Lipschitz probability density function, i.e., \( f(x) = \partial_x F(x) \), with distribution function
\[
F(x_1, x_2, \ldots, x_d) = \frac{x_1 x_2 \cdots x_d}{1 + (1 - x_1)(1 - x_2) \cdots (1 - x_d)}, \quad (x_1, x_2, \ldots, x_d) \in [0, 1]^d,
\]
and \( F = 0 \) otherwise. Every \( S \)-dimensional \((S < d)\) marginal distribution is uniform on \([0, 1]^S\) and hence any further splitting via the CART protocol will result in zero population conditional variance reduction. Thus, one may be tempted to assume the function is constant on the subbox when in fact \( f \) “strongly” depends on the full set of \( d \) variables. In fact, even if \( S \) \((S < d)\) variables are split along simultaneously, the \( S \)-dimensional partial integrals are still constant on any subbox of \([0, 1]^S\).

This is why theoretical analysis of random forests has tended to focus on special function classes with additional structure, i.e., additive models [Biau 2012, p. 1073], [Scornet et al.]

---

3In fact, the density function of any non-uniform copula has this property.
Proposition 1], for which the aforementioned difficulties are not present. Whether or not one can extend the theory to more general function classes remains to be seen

Acknowledgments

This work was completed while the author was a visiting graduate student at The Wharton School Department of Statistics. He is grateful to Matthew Olson for suggesting relevant literature to review and Edgar Dobriban for helpful discussions.

References

Yali Amit and Donald Geman. Shape quantization and recognition with randomized trees. *Neural Computation*, 9(7):1545–1588, 1997.

Sylvain Arlot and Robin Genner. Analysis of purely random forests bias. *arXiv preprint arXiv:1407.3939*, 2014.

Gérard Biau. Analysis of a random forests model. *Journal of Machine Learning Research*, 13 (Apr):1063–1095, 2012.

Gérard Biau and Erwan Scornet. A random forest guided tour. *Test*, 25(2):197–227, 2016.

Gérard Biau, Luc Devroye, and Gábor Lugosi. Consistency of random forests and other averaging classifiers. *Journal of Machine Learning Research*, 9(Sep):2015–2033, 2008.

Leo Breiman. Some infinity theory for predictor ensembles. *Technical Report 579, UC Berkeley*, 2000.

Leo Breiman. Random forests. *Machine Learning*, 45(1):5–32, 2001.

Leo Breiman. Consistency for a simple model of random forests. *Technical Report 670, UC Berkeley*, 2004.

Leo Breiman, Jerome Friedman, RA Olshen, and Charles J Stone. *Classification and regression trees*. Chapman and Hall/CRC, 1984.

Misha Denil, David Matheson, and Nando De Freitas. Narrowing the gap: Random forests in theory and in practice. In *International Conference on Machine Learning (ICML)*, 2014.

Thomas G. Dietterich. An experimental comparison of three methods for constructing ensembles of decision trees: Bagging, boosting, and randomization. *Machine Learning*, 40(2):139–157, 2000.

Roxane Duroux and Erwan Scornet. Impact of subsampling and pruning on random forests. *arXiv preprint arXiv:1603.04261*, 2016.

Robin Genner. Risk bounds for purely uniformly random forests. *arXiv preprint arXiv:1006.2980*, 2010.

Robin Genner. Variance reduction in purely random forests. *Journal of Nonparametric Statistics*, 24(3):543–562, 2012.
Pierre Geurts, Damien Ernst, and Louis Wehenkel. Extremely randomized trees. *Machine Learning*, 63(1):3–42, 2006.

Tin Kam Ho. Random decision forests. In *Proceedings of the Third International Conference on Document Analysis and Recognition (Volume 1)-Volume 1*, page 278. IEEE Computer Society, 1995.

Børge Jessen, Jan Marcinkiewicz, and Antoni Zygmund. Note on the differentiability of multiple integrals. *Fundamenta Mathematicae*, 25(1):217–234, 1935.

Yi Lin and Yongho Jeon. Random forests and adaptive nearest neighbors. *Journal of the American Statistical Association*, 101(474):578–590, 2006.

Lucas Mentch and Giles Hooker. Quantifying uncertainty in random forests via confidence intervals and hypothesis tests. *Journal of Machine Learning Research*, 17(1):841–881, 2016.

Jaouad Mourtada, Stéphane Gaïffas, and Erwan Scornet. Minimax optimal rates for Mondrian trees and forests. *arXiv preprint arXiv:1803.05784*, 2018.

Volker Scheidemann. *Introduction to Complex Analysis in Several Variables*. Springer, 2005.

Erwan Scornet. Random forests and kernel methods. *IEEE Transactions on Information Theory*, 62(3):1485–1500, 2016.

Erwan Scornet, Gérard Biau, and Jean-Philippe Vert. Consistency of random forests. *Annals of Statistics*, 43(4):1716–1741, 2015a.

Erwan Scornet, Gérard Biau, and Jean-Philippe Vert. Supplement to “Consistency of random forests”. *Annals of Statistics*, 43(4), 2015b. doi: 10.1214/15-AOS1321SUPP.

Stefan Wager. Asymptotic theory for random forests. *arXiv preprint arXiv:1405.0352*, 2014.

Stefan Wager and Susan Athey. Estimation and inference of heterogeneous treatment effects using random forests. *Journal of the American Statistical Association*, 0(ja):0–0, 2017. doi: 10.1080/01621459.2017.1319839. URL https://doi.org/10.1080/01621459.2017.1319839.

Stefan Wager and Guenther Walther. Adaptive concentration of regression trees, with application to random forests. *arXiv preprint arXiv:1503.06388*, 2015.

Abraham J. Wyner, Matthew Olson, Justin Bleich, and David Mease. Explaining the success of AdaBoost and random forests as interpolating classifiers. *Journal of Machine Learning Research*, 18(48):1–33, 2017.

Yuhong Yang and Andrew Barron. Information-theoretic determination of minimax rates of convergence. *Annals of Statistics*, pages 1564–1599, 1999.
A Supplementary lemmas and their proofs

In this supplement, we provide proofs of Theorem 1, Theorem 6, Lemma A.3, Lemma A.4, and Lemma A.5.

We first mention two useful facts that we will exploit many times:

1. Since by construction, \( \sum_{j=1}^{d} K_{nj}(X, \Theta) = \lceil \log_2 k_n \rceil \), we have that, conditionally on \( X \), \( (K_{n1}(X, \Theta), \ldots, K_{nd}(X, \Theta)) \) follows a multinomial distribution with \( \lceil \log_2 k_n \rceil \) trials and event probabilities \( (p_{n1}, \ldots, p_{nd}) \). Note that \cite{Biau2012} only needs that the marginals \( K_{nj}(X, \Theta) \) are binomially distributed Bin\( (p_{nj}, \lceil \log_2 k_n \rceil) \), but we will need to work with their joint distribution.

2. Since by construction, \( N_n(X, \Theta) = \sum_{i=1}^{n} 1 \{ X_i \in A_n(X, \Theta) \} \) and \( \lambda(A_n(X, \Theta)) = 2^{-\lceil \log_2 k_n \rceil} \), we have that conditionally on \( X \) and \( \Theta \), \( N_n(X, \Theta) \) is binomial with \( n \) trials and success probability \( 2^{-\lceil \log_2 k_n \rceil} \).

To alleviate some notational clutter and promote brevity, we will sometimes omit dependence of certain quantities on \( X \), \( \Theta \), and \( \Theta' \), where \( \Theta' \) is an independent copy of \( \Theta \). Quantities that depend on \( \Theta' \) will be written with a superscript prime in its place. For example, we write \( A_n = A_n(X, \Theta) \) (resp. \( A'_n = A_n(X, \Theta') \)), \( A_{nj} = A_{nj}(X, \Theta) \) (resp. \( A'_{nj} = A_{nj}(X, \Theta') \)), \( N_n = N_n(X, \Theta) \) (resp. \( N'_n = N_n(X, \Theta') \)), \( K_{nj} = K_{nj}(X, \Theta) \) (resp. \( K'_{nj} = K_{nj}(X, \Theta') \)), \( \mathcal{E}_n = \mathcal{E}_n(X, \Theta) \) (resp. \( \mathcal{E}'_n = \mathcal{E}_n(X, \Theta') \)), \( B_{nj} = B_{nj}(X) \), \( a_{nj} = a_{nj}(X, \Theta) \), and \( b_{nj} = b_{nj}(X, \Theta) \). We also define \( \Delta_i = f(X_i) - f(X) \), for \( i = 1, 2, \ldots, n \).

**Lemma A.1.** If \( Z_m \) is binomially distributed Bin\( (M_m, p_m) \) and \( \mathbb{E}[Z_m] = M_m p_m \to +\infty \) as \( m \to +\infty \), then \( Z_m \to +\infty \) a.s.

**Proof.** The desired event is equivalent to, for each positive integer \( M \), the existence of another positive integer \( m' \) such that \( Z_m > M \) for all \( m > m' \). We must show that the complement event \( \bigcup_{m=1}^{\infty} \bigcap_{m=1}^{\infty} \{ Z_m \leq M \} \) has probability content zero. By continuity of probability, its probability is equal to the limit \( \lim_{M \to +\infty} \mathbb{P}[\bigcap_{m=1}^{\infty} \{ Z_m \leq M \}] \), which by monotonicity of probability, is bounded by \( \lim_{M \to +\infty} \liminf_{m \to +\infty} \mathbb{P}[Z_m \leq M] \). Finally, note that for fixed \( M \) and \( 0 \leq z \leq N \), \( \mathbb{P}[Z_m = z] = (M_m)^z p_m^z (1 - p_m)^{M_m - z} \leq (M_m p_m)^z e^{-p_m M_m - z} \to 0 \) as \( M_m p_m \to +\infty \).

**Proof of Theorem 7.** By the standard variance/bias decomposition, we have \[
\mathbb{E}[f_n(x) - f(x)]^2 = \mathbb{E}[f_n(x) - \mathbb{E}[f_n(x)]]^2 + \mathbb{E}[\mathbb{E}[f_n(x)] - f(x)]^2.
\]

By \cite{Biau2012} Section 5.2, p. 1085, the variance term \( \mathbb{E}[f_n(x) - \mathbb{E}[f_n(x)]]^2 \) is at most \( 12\sigma^2(k_n/n) \) and hence, converges to zero provided \( k_n/n \to 0 \) as \( n \to +\infty \). For the bias term, we have from \cite{Biau2012} Section 5.4, pp. 1086-1087 and \cite{Biau2012} Section 5.3, p. 1089.
that

\[
\mathbb{E} \left[ \mathbb{E} \left[ f_n(x) - f(x) \right]^2 \right] \leq \sum_{i=1}^{n} \mathbb{E} \left[ W_{ni}(x, \Theta)(f(X_i) - f(x))^2 \right] + \mathbb{E} \left[ \mathbb{1}_{\mathcal{E}^c(x, \Theta)} f(x) \right]^2
\]

\[
= n\mathbb{E} \left[ \frac{\mathbb{1}_{\{x_i \in A_n(x, \Theta)\}} |f(X_i) - f(x)|^2}{1 + \sum_{i=2}^{n} \mathbb{1}_{\{x_i \in A_n(x, \Theta)\}}} \right] + \mathbb{E} \left[ \mathbb{1}_{\mathcal{E}^c(x, \Theta)} f(x) \right]^2
\]

\[
\leq \mathbb{E}_\Theta \left[ \mathbb{E} \left[ \frac{\mathbb{1}_{\{x_i \in A_n(x, \Theta)\}} |f(X_i) - f(x)|^2}{\mathbb{P}[X_1 \in A_n(x, \Theta) \mid \Theta]} \right] \right] + |f(x)|^2 e^{-n/(2kn)},
\]

where the last inequality uses 2 and \( \mathbb{E} \left[ \frac{1}{1 + \sum_{i=2}^{n} \mathbb{1}_{\{x_i \in A_n(x, \Theta)\}}} \mid \Theta \right] \leq \frac{1}{n^2 - |\log 2 kn|} = \frac{1}{n\mathbb{P}[X_1 \in A_n(x, \Theta) \mid \Theta]}.

By Lemma [A.1] and the representations (3) and (4), the condition that \( p_{nj} \log k_n \to +\infty \) for each \( j = 1, \ldots, d \) as \( n \to +\infty \) enables us to conclude that jointly \( F_{n,j}(x, \Theta) \to +\infty \) for all \( j = 1, \ldots, d \) as \( n \to +\infty \) \( \Theta \)-a.s. and hence \( \text{diam}(A_n(x, \Theta)) \to 0 \) as \( n \to +\infty \) \( \Theta \)-a.s. By the Lebesgue differentiation theorem (for hyperrectangles) [Jessen et al., 1935, Theorem 6], \( \lambda \)-almost every point in \([0, 1]^d\) is a Lebesgue point and hence by the assumption that \( f \) is square-integrable, we have for \( \lambda \)-almost every \( x \in [0, 1]^d \),

\[
F_n(x, \Theta) \triangleq \mathbb{E} \left[ \frac{\mathbb{1}_{\{x_i \in A_n(x, \Theta)\}} |f(X_i) - f(x)|^2}{\mathbb{P}[X_1 \in A_n(x, \Theta) \mid \Theta]} \right] \to 0, \quad n \to +\infty, \quad \Theta \text{-a.s.}
\]

Furthermore, \( F_n(x, \Theta) \) is bounded above by the Hardy-Littlewood maximal function (for hyperrectangles), which is independent of \( n \) and \( \Theta \) and finite \( \lambda \)-almost everywhere. Thus, we can use the Lebesgue bounded convergence theorem to conclude that for \( \lambda \)-almost every \( x \in [0, 1]^d \), \( \mathbb{E}_\Theta [F_n(x, \Theta)] \to 0 \) as \( n \to +\infty \).

**Lemma A.2.** There exist universal constants \( C_1 > 0 \) and \( C_2 > 0 \) such that if

\[
\frac{k_n}{n} \leq C_1 \frac{\mathbb{E} \left[ \mathbb{E} \left[ \mathbb{1}_{\{x_i \in A_n\}} (f(X_1) - f(X)) \mid X \right] \right]^2}{\mathbb{E} \left[ \mathbb{E} \left[ \mathbb{1}_{\{x_i \in A_n\}} |f(X_1) - f(X)| \mid X \right] \right]^2},
\]

then

\[
\mathbb{E} \left[ \mathbb{E} \left[ f_n(X) \mid X \right] - f(X) \right]^2 \geq C_2 k_n^2 \mathbb{E} \left[ \mathbb{E} \left[ \mathbb{1}_{\{x_i \in A_n\}} (f(X_1) - f(X)) \mid X \right] \right]^2.
\]

**Proof.** Combining (16) and (20) from Theorem 4 we obtain the following lower bound on the bias:

\[
\mathbb{E} \left[ \mathbb{E} \left[ f_n(X) \mid X \right] - f(X) \right]^2 \geq \mathbb{E} \left[ \sum_{i=1}^{n} \mathbb{E}_\Theta [W_{ni}] \Delta_i \right]^2 \geq n(n-1) \mathbb{E} \left[ W_{n,1} \Delta_1 W_{n,2}' \Delta_2 \right],
\]

\(^6\) If each component of a joint random vector converges a.s., then the joint random vector also converges a.s. to the limit vector defined by its individual component limits.
where $\Theta'$ is an independent copy of $\Theta$. The remaining strategy of the proof is to lower bound $E[W_{n1}\Delta_1 W_{n2}'\Delta_2]$.

Recall the form of the weights,

$$E_{n1} = \frac{\mathbb{1}\{x_1 \in A_n\}}{\sum_{i=1}^n \mathbb{1}\{x_i \in A_n\}} - \frac{\mathbb{1}\{x_1 \in A_n\}}{1 + \mathbb{1}\{x_2 \in A_n\} + \sum_{i \geq 3} \mathbb{1}\{x_i \in A_n\}},$$

and

$$E_{n2}' = \frac{\mathbb{1}\{x_2 \in A_n'\}}{\sum_{i=1}^n \mathbb{1}\{x_i \in A_n'\}} - \frac{\mathbb{1}\{x_2 \in A_n'\}}{1 + \mathbb{1}\{x_1 \in A_n'\} + \sum_{i \geq 3} \mathbb{1}\{x_i \in A_n'\}}.$$

Define $T = \sum_{i \geq 3} \mathbb{1}\{x_i \in A_n\}$ and $T' = \sum_{i \geq 3} \mathbb{1}\{x_i \in A_n'\}$. Then, we can also write $W_{n1}$ and $W_{n2}'$ as follows:

$$W_{n1} = \frac{\mathbb{1}\{x_1 \in A_n\}}{1 + T} - \frac{\mathbb{1}\{x_1 \in A_n\}\mathbb{1}\{x_2 \in A_n\}}{(1 + T)(2 + T)},$$

and

$$W_{n2}' = \frac{\mathbb{1}\{x_2 \in A_n'\}}{1 + T'} - \frac{\mathbb{1}\{x_2 \in A_n'\}\mathbb{1}\{x_1 \in A_n'\}}{(1 + T')(2 + T')}.$$  \hspace{1cm} (A.1)

Multiplying $W_{n1}$ and $W_{n2}'$ together and expanding the products according to the representations (A.1) and (A.2), we have

$$W_{n1}W_{n2}' = \frac{\mathbb{1}\{x_1 \in A_n\}\mathbb{1}\{x_2 \in A_n'\}}{(1 + T)(2 + T)} - \frac{\mathbb{1}\{x_1 \in A_n \cap A_n'\}\mathbb{1}\{x_2 \in A_n'\}}{(1 + T)(2 + T)(1 + T')} - \frac{\mathbb{1}\{x_2 \in A_n' \cap A_n\}\mathbb{1}\{x_2 \in A_n'\}}{(1 + T)(2 + T)(1 + T')} + \frac{\mathbb{1}\{x_1 \in A_n \cap A_n'\}\mathbb{1}\{x_2 \in A_n \cap A_n'\}}{(1 + T)(2 + T)(1 + T')(2 + T')}.$$ \hspace{1cm} (A.3)

We will multiply each of the four terms in (A.3) by $\Delta_1$ and $\Delta_2$ and analyze their expectations. For the purposes of providing a lower bound on $E[W_{n1}\Delta_1 W_{n2}'\Delta_2]$, the term

$$E\left[\frac{\mathbb{1}\{x_1 \in A_n \cap A_n'\}\mathbb{1}\{x_2 \in A_n \cap A_n'\}}{(1 + T)(2 + T)(1 + T')(2 + T')}\Delta_1 \Delta_2\right]$$

can be ignored, since it is seen to equal the positive quantity

$$E\left[\mathbb{E}_{X_1} \left[\mathbb{1}\{x_1 \in A_n \cap A_n'\}\Delta_1\right]^2 \right].$$

Thus, $E[W_{n1}\Delta_1 W_{n2}'\Delta_2]$ is at least

$$E\left[\frac{\mathbb{1}\{x_1 \in A_n\}\mathbb{1}\{x_2 \in A_n'\}}{(1 + T)(1 + T')}\Delta_1 \Delta_2\right] - \frac{\mathbb{1}\{x_1 \in A_n \cap A_n'\}\mathbb{1}\{x_2 \in A_n'\}}{(1 + T)(2 + T')(1 + T')},$$

$$\frac{\mathbb{1}\{x_1 \in A_n \cap A_n'\}\mathbb{1}\{x_2 \in A_n \cap A_n'\}}{(1 + T)(2 + T')(1 + T')} - \frac{\mathbb{1}\{x_1 \in A_n \cap A_n'\}\mathbb{1}\{x_2 \in A_n \cap A_n'\}}{(1 + T)(2 + T')(1 + T')}.$$ \hspace{1cm} (A.4)

Evaluating the first expectation in (A.4) leads to

$$E\left[\frac{\mathbb{1}\{x_1 \in A_n\}\mathbb{1}\{x_2 \in A_n'\}}{(1 + T)(1 + T')}\Delta_1 \Delta_2\right] = E\left[\mathbb{E}_{X_1, \Theta} \left[\mathbb{1}\{x_1 \in A_n\}\Delta_1\right]^2 \right].$$ \hspace{1cm} (A.5)
By Jensen’s inequality, (A.5) is lower bounded by
\[
E \left[ \left( \frac{1}{1+T} \sum_{i=1}^{n} X_i \right)^2 \right] \geq E \left[ \left( \frac{1}{1+T} \sum_{i=1}^{n} X_i \right)^2 \right] \geq E \left[ \left( \frac{1}{1+T} \sum_{i=1}^{n} X_i \right)^2 \right],
\]
where the last line follows because \( E_{x_1, \ldots, x_n} \left[ \frac{1}{1+T} \right] \) is independent of \( \Theta \), a consequence of the fact that \( T \) is conditionally distributed \( \text{Bin}(n - 2, 2^{-\lfloor \log_2 k_n \rfloor}) \) given \( \Theta \). Finally, we can use Jensen’s inequality again to lower bound
\[
E_{x_1, \ldots, x_n} \left[ \frac{1}{1+T} \right] \geq \frac{1}{1 + E_{x_1, \ldots, x_n} [T | \Theta]} = \frac{1}{1 + (n - 2)2^{-\lfloor \log_2 k_n \rfloor}}.
\]
Hence, we obtain that \( E \left[ \left( \frac{1}{1+T} \sum_{i=1}^{n} X_i \right)^2 \right] \) is at least
\[
\frac{E \left[ \left( \frac{1}{1+T} \sum_{i=1}^{n} X_i \right)^2 \right]}{(1 + (n - 2)2^{-\lfloor \log_2 k_n \rfloor})^2} \geq C'' \left( \frac{k_n}{n} \right)^2 \frac{1}{E \left[ \left( \frac{1}{1+T} \sum_{i=1}^{n} X_i \right)^2 \right]},
\]
for some universal constant \( C'' > 0 \).

By symmetry, the expectations of the two final terms in (A.4) are both equal to
\[
E \left[ E_{x_1, \ldots, x_n} \left[ \frac{1}{1+T} \sum_{i=1}^{n} X_i \right] \right],
\]
and bounded by
\[
E \left[ \frac{1}{1+T} \sum_{i=1}^{n} X_i, \Theta, \Theta' \right] E_{x_1, \ldots, x_n} \left[ \frac{1}{1+T} \sum_{i=1}^{n} X_i \right] E_{x_2, \ldots, x_n} \left[ \frac{1}{1+T} \sum_{i=1}^{n} X_i \right].
\]
Now, by the Cauchy-Schwarz inequality,
\[
E \left[ \frac{1}{1+T} \sum_{i=1}^{n} X_i, \Theta, \Theta' \right] \leq E \left[ \frac{1}{1+T} \sum_{i=1}^{n} X_i, \Theta \right] E \left[ \frac{1}{1+T} \sum_{i=1}^{n} X_i, \Theta' \right] \leq \sqrt{E \left[ \frac{1}{1+T} \right]^2} \sqrt{E \left[ \frac{1}{1+T} \right]^2} \leq C(k_n/n)^2C''(k_n/n)^3.
\]
The last inequality is established using \( C' \) which implies that \( T \) and \( T' \) are conditionally distributed \( \text{Bin}(n - 2, 2^{-\lfloor \log_2 k_n \rfloor}) \) given \( X, \Theta, \) and \( \Theta' \) and the fact that for \( Z \sim \text{Bin}(m, p) \),
\[
E \left[ \frac{1}{(1+T)^{\Delta}} \right] \leq C_k \frac{m^{\Delta p}}{m^{\Delta + \Delta p}},
\]
for some positive constant \( C_k \). Thus, we have shown that \( E \left[ W_{n1} \Delta_1 W_{n2} \Delta_2 \right] \) is at least
\[
E \left[ \left( \frac{1}{1+T} \sum_{i=1}^{n} X_i \right)^2 \right] - 2E \left[ \frac{1}{1+T} \sum_{i=1}^{n} X_i \right] E_{x_2, \ldots, x_n} \left[ \frac{1}{1+T} \sum_{i=1}^{n} X_i \right] \geq C''(k_n/n)^2E \left[ \left( \frac{1}{1+T} \sum_{i=1}^{n} X_i \right)^2 \right] - 2CC'(k_n/n)^3E \left[ \left( \frac{1}{1+T} \sum_{i=1}^{n} X_i \right)^2 \right].
\]
Choosing \( C_1 = \frac{C''}{4CC'} \) and \( C_2 = C''/2 \) completes the proof.
\[ \square \]
Proof of Theorem A.6. By Lemma A.2, there exist universal constants $C_1 > 0$ and $C_2 > 0$ such that if
\[
k_n/n \leq C_1 \frac{\mathbb{E} \left[ \frac{\mathbb{E} \left[ 1_{\{X_1 \in A_n\}} \langle \beta, X_1 - X \rangle \mid X \right]^2}{\mathbb{E} \left[ 1_{\{X_1 \in A_n\}} \langle \beta, X_1 - X \rangle \mid X \right]^2} \right]}{C_2 k_n^2 \mathbb{E} \left[ 1_{\{X_1 \in A_n\}} \langle \beta, X_1 - X \rangle \mid X \right]^2},
\] (A.6)
then
\[
\mathbb{E} \left[ \mathbb{E} \left[ \tilde{f}_n(X) \mid X \right] - f(X) \right]^2 \geq C_2 k_n^2 \mathbb{E} \left[ \mathbb{E} \left[ 1_{\{X_1 \in A_n\}} \langle \beta, X_1 - X \rangle \mid X \right]^2 \right].
\]
Let us now find lower and upper bounds for the expressions in the numerator and denominator of the ratio in (A.6), respectively. For the expression in the denominator,
\[
\mathbb{E} \left[ 1_{\{X_1 \in A_n\}} \langle \beta, X_1 - X \rangle \mid X, \Theta \right]
\leq \mathbb{E} \left[ 1_{\{X_1 \in A_n\}} \sum_{j \in S} |\beta(j)||X_1^{(j)} - X^{(j)}| \mid X, \Theta \right]
= \sum_{j \in S} |\beta(j)| \mathbb{E} \left[ 1_{\{X_1 \in A_n\}} \|X_1^{(j)} - X^{(j)}\| \mid X, \Theta \right]
= \sum_{j \in S} |\beta(j)| \prod_{k \neq j} \lambda(A_{nk}) \mathbb{E} \left[ X_1^{(j)} \mid 1_{\{X_1^{(j)} \in A_{nj}\}} \right] \mathbb{E} \left[ X_1^{(j)} - X^{(j)} \mid X, \Theta \right]
\leq \frac{1}{2} \sum_{j \in S} |\beta(j)| \prod_{k \neq j} \lambda(A_{nk}) \lambda^2(A_{nj}) = \frac{2^{-\lfloor \log_2 k_n \rfloor}}{2} \sum_{j \in S} |\beta(j)| \lambda(A_{nj})
\leq \frac{2^{-\lfloor \log_2 k_n \rfloor}}{2} \|\beta\|_S \lambda(A_{nj}).
\]
Finally, note that by $1_{\{X_1 \in A_n\}} \|\lambda(A_{nj}) \mid X \right] = \mathbb{E} \left[ 2^{-K_{nj}} \mid X \right] = (1 - p_{nj}/2)^{\lfloor \log_2 k_n \rfloor} = (1 - S^{-1/2})^{\lfloor \log_2 k_n \rfloor}$. Hence the denominator of the ratio in (A.6) is bounded above by
\[
\frac{2^{-2\lfloor \log_2 k_n \rfloor} \|\beta\|^2_2 (1 - S^{-1/2})^{\lfloor \log_2 k_n \rfloor}}{4}.
\] (A.7)
Next, in giving a lower bound on the numerator of the ratio in (A.6), we will show that
\[
\mathbb{E} \left[ 1_{\{X_1 \in A_n\}} \langle \beta, X_1 - X \rangle \mid X \right]
\] (A.8)
can be written as a weighted sum of $S$ independent Uniform(0, 1) variables minus their mean, 1/2. Consequently, the squared expectation of (A.8) with respect to $X$ is the sum of the respective variances. Using this, we will show that
\[
\mathbb{E} \left[ \mathbb{E} \left[ 1_{\{X_1 \in A_n\}} \langle \beta, X_1 - X \rangle \mid X \right]^2 \right] = \frac{2^{-2\lfloor \log_2 k_n \rfloor} \|\beta\|^2_2 (1 - S^{-1/2})^2}{12} \|\beta\|^2_2 (1 - S^{-1/2})^{\lfloor \log_2 k_n \rfloor}.
\] (A.9)
Combining (A.7) and (A.9), we find that
\[
\frac{\mathbb{E} \left[ \mathbb{E} \left[ 1_{\{X_1 \in A_n\}} \langle \beta, X_1 - X \rangle \mid X \right]^2 \right]}{\mathbb{E} \left[ \mathbb{E} \left[ 1_{\{X_1 \in A_n\}} \langle \beta, X_1 - X \rangle \mid X \right]^2 \right]} \geq \frac{1}{3S}.
\]
To prove (A.9), observe that
\[
E \left[ \mathbb{1}_{\{X_1 \in A_n\}} \langle \beta, X_1 - X \rangle \mid X, \Theta \right] \\
= \sum_{j \in S} E \left[ \mathbb{1}_{\{X_1 \in A_n\}} \langle \beta^{(j)}(X_1^{(j)} - X^{(j)}) \rangle \mid X, \Theta \right] \\
= \sum_{j \in S} \beta^{(j)} \prod_{k \neq j} \lambda(A_{nk})E_{X_1^{(j)}} \left[ \mathbb{1}_{\{X_1^{(j)} \in A_{nj}\}} \langle X_1^{(j)} - X^{(j)} \rangle \mid X, \Theta \right]. \tag{A.10}
\]

Next, note that because \( X^{(j)} \sim \text{Uniform}(0, 1) \), we have
\[
E_{X_1^{(j)}} \left[ \mathbb{1}_{\{X_1^{(j)} \in A_{nj}\}} \langle X_1^{(j)} - X^{(j)} \rangle \mid X, \Theta \right] \\
= (b_{nj} - a_{nj}) \left( \frac{a_{nj} + b_{nj}}{2} - X^{(j)} \right),
\]
where \( a_{nj} \) and \( b_{nj} \) are the left and right endpoints of \( A_{nj} \). Since \( b_{nj} - a_{nj} = 2^{-K_{nj}} \), we have
\[
E_{X_1^{(j)}} \left[ \mathbb{1}_{\{X_1^{(j)} \in A_{nj}\}} \langle X_1^{(j)} - X^{(j)} \rangle \mid X, \Theta \right] \\
= 2^{-K_{nj}} \left( \frac{a_{nj} + b_{nj}}{2} - X^{(j)} \right).
\]

Combining this with (A.10) and \( \prod_{k \in [d]} 2^{-K_{nk}(X, \Theta)} = 2^{-[\log_2 k_n]} \) yields
\[
E \left[ \mathbb{1}_{\{X_1 \in A_n\}} \langle \beta, X_1 - X \rangle \mid X, \Theta \right] \\
= 2^{-[\log_2 k_n]} \sum_{j \in S} \beta^{(j)} \left( \frac{a_{nj} + b_{nj}}{2} - X^{(j)} \right).
\]

Now, by expressions (3) and (4), which express the endpoints of the interval along the \( j \)th variable as randomly stopped binary expansions of \( X^{(j)} \), we have
\[
\frac{a_{nj} + b_{nj}}{2} - X^{(j)} \overset{D}{=} 2^{-K_{nj} - 1} - \sum_{k \geq K_{nj} + 1} B_{kj} 2^{-k} \\
= 2^{-K_{nj}} \left( \frac{1}{2} - \sum_{k \geq 1} B_{(k+K_{nj})j} 2^{-k} \right) \\
\overset{D}{=} 2^{-K_{nj}} (\bar{X}, \Theta)(1/2 - \bar{X}^{(j)}),
\]
where \( \bar{X} \) is uniformly distributed on \([0, 1]^d\). Taking expectations with respect to \( \Theta \), we have that
\[
E_{X_1^{(j)}} \left[ \mathbb{1}_{\{X_1^{(j)} \in A_{nj}\}} \langle X_1^{(j)} - X^{(j)} \rangle \mid X_1 \right] \\
\overset{D}{=} 2^{-[\log_2 k_n]} \sum_{j \in S} \beta^{(j)} \left( 1 - p_{nj}/2 \right)^{[\log_2 k_n]} \left( 1/2 - \bar{X}^{(j)} \right). \tag{A.11}
\]
Observe that (A.11) is a sum of mean zero independent random variables, and hence, its squared expectation is equal to the sum of the individual variances, viz.,

\[
\mathbb{E} \left[ \left( \mathbb{E} \left[ \mathbb{I}_{\{X_i \in A_n\}} (\beta, X_1 - X) \mid X \right] \right)^2 \right] = 2^{-2\log_2 k_n} \sum_{j \in S} \|\beta(j)\|^2 (1 - p_{nj}/2)^2 \log_2 k_n \text{Var}(\bar{X}(j))
\]

\[
= \frac{2^{-2\log_2 k_n}}{12} \sum_{j \in S} \|\beta(j)\|^2 (1 - S^{-1}/2)^2 \log_2 k_n
\]

\[
= \frac{2^{-2\log_2 k_n} \|\beta\|^2 _S (1 - S^{-1}/2)^2 \log_2 k_n}{12}.
\]

Thus, we have shown that if \( k_n/n \leq C_1/(3S) \), then

\[
\mathbb{E} \left[ \mathbb{E} \left[ \bar{f}_n(X) \mid X \right] - f(X) \right]^2 \geq C_2 k_n^2 2^{-2\log_2 k_n} \|\beta\|^2 _S (1 - S^{-1}/2)^2 \log_2 k_n
\]

\[
\geq \frac{C_2 (1 - S^{-1}/2)}{24} \|\beta\|^2 _S k_n^{2 \log_2 (1-S^{-1}/2)}.
\]

Thus, the conclusion follows with \( c = C_1/3 \) and \( C = C_2(1-S^{-1}/2) \).

**Lemma A.3.**

\[
\mathbb{E} \left[ \mathbb{E}_{\Theta} \left[ W_{n1}(X, \Theta) \right] (f(X_1) - f(X)) \mathbb{E}_{\Theta} \left[ W_{n2}(X, \Theta) \right] (f(X_2) - f(X)) \right] \leq \frac{S^2 L^2 k_n^{2 \log_2 (1 - p_n/2)}}{4n(n - 1)}.
\]  \hspace{1cm} (A.12)

and

\[
\mathbb{E} \left[ \left( \mathbb{E}_{\Theta} \left[ W_{n1}(X, \Theta) \right] \right)^2 (f(X_1) - f(X))^2 \right] \leq \frac{2SL k_n^{2 \log_2 (1 - p_n/2) + 1}}{3n(n + 1)}.
\]  \hspace{1cm} (A.13)

**Proof.** We will first prove (A.12), followed by (A.13). By the Lipschitz condition and sparsity assumption on \( f \), we have

\[
\mathbb{E} \left[ \mathbb{E}_{\Theta} \left[ W_{n1} \right] \mathbb{E}_{\Theta} \left[ W_{n2} \right] \Delta_1 \mathbb{E}_{\Theta} \left[ W_{n2} \right] \Delta_2 \right]
\]

\[
= \mathbb{E} \left[ \mathbb{E}_{\Theta} \left[ W_{n1} \right] (f^*(X_1 S) - f^*(X_S)) \mathbb{E}_{\Theta} \left[ W_{n2} \right] (f^*(X_2 S) - f^*(X_S)) \right]
\]

\[
\leq L^2 \mathbb{E} \left[ W_{n1} W_{n2}' \|X_1 - X\|_S \|X_2 - X\|_S \right], \hspace{1cm} (A.14)
\]

where \( \Theta' \) is an independent copy of \( \Theta \). Define \( T = \sum_{i \geq 3} \mathbb{I}_{\{X_i \in A_n\}} \) and \( T' = \sum_{i \geq 3} \mathbb{I}_{\{X_i \in A'_n\}} \).

Next, note that

\[
W_{n1} W_{n2}' = \mathbb{I}_{\{X_1 \in A_n\}} \mathbb{I}_{\{X_2 \in A'_n\}} \frac{1}{N_n N'_n} \xi_n
\]

\[
\leq \frac{\mathbb{I}_{\{X_1 \in A_n\}} \mathbb{I}_{\{X_2 \in A'_n\}}}{(1 + T)(1 + T')}.
\]
By the Cauchy-Schwarz inequality,

$$
\mathbb{E} \left[ \frac{1}{(1 + T)(1 + T')} X, \Theta, \Theta' \right] \leq \sqrt{\mathbb{E} \left[ \left( \frac{1}{1 + T} \right)^2 | X, \Theta, \Theta' \right]} \sqrt{\mathbb{E} \left[ \left( \frac{1}{1 + T'} \right)^2 | X, \Theta, \Theta' \right]}
$$

$$
\leq \frac{2 \log k_n}{\sqrt{n(n-1)}} \frac{2 \log k_n}{\sqrt{n(n-1)}} = \frac{4 \log k_n}{n(n-1)}. \tag{A.15}
$$

The final inequality (A.15) above follows from the fact that \( \mathbb{E} \left[ \frac{1}{1+Z} \right]^2 \leq \frac{1}{(m+1)(m+2)p^2} \) if \( Z \sim \text{Bin}(m, p) \). Thus, we have

$$
\mathbb{E} \left[ W_{n1} W_{n2}' \| X_1 - X \|_S \| X_2 - X \|_S \right]
$$

$$
\leq \mathbb{E} \left[ \mathbb{E} \left[ \frac{1}{(1 + T)(1 + T')} X, \Theta, \Theta' \right] \mathbb{E}_{X_1, X_2} \left[ \mathbb{I}_{\{X_1 \in A_n\}} \mathbb{I}_{\{X_2 \in A_n'\}} \| X_1 - X \|_S \| X_2 - X \|_S \right] \right.
$$

$$
\leq \frac{4 \log k_n}{n(n-1)} \mathbb{E} \left[ \mathbb{I}_{\{X_1 \in A_n\}} \mathbb{I}_{\{X_2 \in A_n'\}} \| X_1 - X \|_S \| X_2 - X \|_S \right] \tag{A.16}
$$

$$
= \frac{4 \log k_n}{n(n-1)} \mathbb{E} \left[ \left( \mathbb{E} \left[ \mathbb{I}_{\{X_1 \in A_n\}} \| X_1 - X \|_S | X \right] \right)^2 \right]. \tag{A.17}
$$

The last step in our argument will be to show that

$$
\mathbb{E} \left[ \mathbb{I}_{\{X_1 \in A_n\}} \| X_1 - X \|_S | X \right] \leq S 2^{-\log k_n - 1} 2^{1/2}, \tag{A.18}
$$

which, when combined with (A.14) and (A.17), proves (A.12). Recognizing that \( \| X_1 - X \|_S \leq \sum_{j \in S} | X_1^{(j)} - X^{(j)} | \), we have

$$
\mathbb{E} \left[ \mathbb{I}_{\{X_1 \in A_n\}} \| X_1 - X \|_S | X, \Theta \right]
$$

$$
\leq \sum_{j \in S} \prod_{k \neq j} \lambda(A_{nk}) \mathbb{E}_{X_1^{(j)}} \left[ \mathbb{I}_{\{X_1 \in A_n\}} \| X_1^{(j)} - X^{(j)} \|_S \right]
$$

$$
\leq \frac{1}{2} \sum_{j \in S} \prod_{k \neq j} \lambda(A_{nk}) \lambda^2(A_{nj}) \quad \text{(since } X_1^{(j)} \sim \text{Uniform}(0, 1))
$$

$$
= \frac{1}{2} \lambda(A_n) \sum_{j \in S} \lambda(A_{nj}) \leq 2^{-\log k_n - 1} \sum_{j \in S} \lambda(A_{nj}).
$$

Furthermore, by \( \mathbb{E} [\lambda(A_{nj}) | X] = (1 - p_{nj}/2)^{\log k_n} \), this shows (A.18). Finally, we show (A.13). To see this, note that

$$
\mathbb{E} \left[ \mathbb{E}_{\Theta} [W_{n1}]^2 \Delta_1^2 \right] = \mathbb{E} \left[ \mathbb{E}_{\Theta} [W_{n1}]^2 (f^*(X_{1S}) - f^*(X_{S}))^2 \right]
$$

$$
\leq L^2 \mathbb{E} \left[ \mathbb{E}_{\Theta} [W_{n1}]^2 \| X_1 - X \|_S^2 \right]
$$

$$
= L^2 \mathbb{E} \left[ W_{n1} W_{n1}^\prime \| X_1 - X \|_S^2 \right]. \tag{A.19}
$$

where \( \Theta^\prime \) is an independent copy of \( \Theta \). Next, using similar arguments to show (A.16), we have

$$
\mathbb{E} \left[ W_{n1} W_{n1}^\prime \| X_1 - X \|_S^2 \right] \leq \frac{2k_n \log k_n}{n(n+1)} \mathbb{E} \left[ \mathbb{I}_{\{X_1 \in A_n \cap A_n'\}} \| X_1 - X \|_S^2 \right]. \tag{A.20}
$$
In like fashion for establishing (A.18), we have the inequalities
\[
\mathbb{E} \left[ 1 \{x_i \in A_n \cap A'_n\} \| X_1 - X \|_S^2 \mid X, \Theta, \Theta' \right]
= \sum_{j \in S} \prod_{k \neq j} \lambda(A_{nk} \cap A'_{nk}) \mathbb{E}_{x_i^{(j)}} \left[ 1 \{x_i^{(j)} \in A_{nj} \cap A'_nj\} \| X_1^{(j)} - X^{(j)} \|_S^2 \right]
\]
(\text{since } X^{(j)} \sim \text{Uniform}(0, 1))
\leq \frac{1}{3} \sum_{j \in S} \prod_{k \neq j} \lambda(A_{nk} \cap A'_{nk}) \lambda^3(A_{nj} \cap A'_{nj}) = \frac{1}{3} \lambda(A_n \cap A'_n) \sum_{j \in S} \lambda^2(A_{nj} \cap A'_{nj})
\leq \frac{2^{−\lceil \log_2 k_n \rceil}}{3} \sum_{j \in S} 2^{−K_{nj} - K'_{nj}}. \quad (A.21)

To finish, note that by independence of $K_{nj}$ and $K'_{nj}$ conditionally on $X$ and $[\cdot]$
\[
\mathbb{E} \left[ 2^{−K_{nj} - K'_{nj}} \mid X \right] = \left[ \mathbb{E} \left[ 2^{−K_{nj}} \mid X \right] \right]^2 = (1 - p_{nj}/2)^2 \leq k_n^{2 \log_2(1 - p_{nj}/2)} \quad (A.22)
\]
Combining inequalities (A.19), (A.20), (A.21), and (A.22) proves the claim (A.13). \hfill \square

**Lemma A.4.** Suppose $\text{Var}[Y \mid X] \lesssim \sigma^2$. There exists a universal constant $C > 0$ such that
\[
\mathbb{E} \left[ f_n(X) - \mathbb{E} \left[ f_n(X) \mid X \right] \right]^2 \geq C \sigma^2 \left( \frac{k_n^2}{n} \right) \mathbb{E} \left[ \lambda(A_n(X), \Theta) \cap A_n(X, \Theta') \right].
\]

**Proof.** First, note that by [Biau, 2012, Section 5.2, p. 1083-1084]
\[
\mathbb{E} \left[ f_n(X) - \mathbb{E} \left[ f_n(X) \mid X \right] \right]^2
= n \sigma^2 \mathbb{E} \left[ \mathbb{E}_{\Theta}[W_{n1}] \right]
= \mathbb{E} \left[ \frac{n \sigma^2 1 \{x_i \in A_n \cap A'_n\}}{\left(1 + \sum_{i=2}^n 1 \{x_i \in A_n\}\right)\left(1 + \sum_{i=2}^n 1 \{x_i \in A'_n\}\right)} \right]
= \mathbb{E} \left[ \frac{n \sigma^2 \lambda(A_n \cap A'_n)}{\left(1 + \sum_{i=2}^n 1 \{x_i \in A_n\}\right)\left(1 + \sum_{i=2}^n 1 \{x_i \in A'_n\}\right)} \right],
\]
where $\Theta'$ is an independent copy of $\Theta$. Thus, it remains to lower bound
\[
\mathbb{E} \left[ \frac{1}{\left(1 + \sum_{i=2}^n 1 \{x_i \in A_n\}\right)\left(1 + \sum_{i=2}^n 1 \{x_i \in A'_n\}\right)} \mid X, X_1, \Theta, \Theta' \right],
\]
which can be done via Jensen’s inequality:
\[
\mathbb{E} \left[ \left(1 + \sum_{i=2}^n 1 \{x_i \in A_n\}\right)\left(1 + \sum_{i=2}^n 1 \{x_i \in A'_n\}\right) \mid X, X_1, \Theta, \Theta' \right].
\]
Next, we use linearity of expectation to write
\[
\mathbb{E} \left[ \left(1 + \sum_{i=2}^n 1 \{x_i \in A_n\}\right)\left(1 + \sum_{i=2}^n 1 \{x_i \in A'_n\}\right) \mid X, X_1, \Theta, \Theta' \right]
= 1 + 2(n - 1)2^{−\lceil \log_2 k_n \rceil} + (n - 1)(n - 2)2^{−2\lceil \log_2 k_n \rceil}
+ (n - 1)\lambda(A_n \cap A'_n)
\leq 1 + 3(n - 1)2^{−\lceil \log_2 k_n \rceil} + (n - 1)(n - 2)2^{−2\lceil \log_2 k_n \rceil},
\]

25
where the last inequality follows from $\lambda(A_n \cap A_n') \leq 2^{-|\log_2 k_n|}$. \hfill \Box

**Lemma A.5.** Let $(M_1, \ldots, M_k)$ be a multinomial distribution with $m$ trials and event probabilities $(p_1, \ldots, p_k)$, all bounded away from zero. Let $(M'_1, \ldots, M'_k)$ be an independent copy. Then,

$$
\mathbb{E}
\left[
2^{-\frac{1}{2} \sum_{j=1}^{k} |M_j - M'_j|}
\right]
\leq
\frac{8^{k-1}}{\sqrt{m^{k-1} p_1 \cdots p_k}}.
$$

(A.23)

Furthermore, if $m$ is large compared to the maximum among $1/p_{nj}$, then there exists a universal constant $C > 0$ such that

$$
\mathbb{E}
\left[
2^{-\frac{1}{2} \sum_{j=1}^{k} |M_j - M'_j|}
\right]
\geq
\frac{C^{k-1}}{\sqrt{m^{k-1} p_1 \cdots p_k}}.
$$

(A.24)

**Proof.** First, note that

$$
\mathbb{E}
\left[
2^{-\frac{1}{2} \sum_{j=1}^{k} |M_j - M'_j|}
\right]
= 
\sum_{w_1 \geq 0, \ldots, w_{k-1} \geq 0}
\mathbb{P}
\left[
\bigcap_{j=1}^{k-1} \{ |M_j - M'_j| = w_j \}
\right]
2^{-\frac{1}{2} \sum_{j=1}^{k} w_j}
\leq 
\sum_{w_1 \geq 0, \ldots, w_{k-1} \geq 0}
\sum_{\tau \in \{-1,1\}^{k-1}}
\mathbb{P}
\left[
\bigcap_{j=1}^{k-1} \{ \tau_j (M_j - M'_j) = w_j \}
\right]
2^{-\frac{1}{2} \sum_{j=1}^{k} |\tau_j w_j|}
\leq 
\sum_{\tau \in \{-1,1\}^{k-1}}
\sum_{w_1 \geq 0, \ldots, w_{k-1} \geq 0}
\mathbb{P}
\left[
\bigcap_{j=1}^{k-1} \{ \tau_j (M_j - M'_j) = w_j \}
\right]
2^{-\frac{1}{2} \sum_{j=1}^{k} |\tau_j w_j|},
$$

(A.25)

where, in each summand, $M_k - M'_k = -\sum_{j=1}^{k-1} \tau_j w_j$ and $w_k = |\sum_{j=1}^{k-1} \tau_j w_j|$.

If $z = (z_1, \ldots, z_{k-1})$ is a complex vector in $\mathbb{C}^{k-1}$, then the complex-valued probability generating function of $(\tau_1(M_1 - M'_1), \ldots, \tau_{k-1}(M_{k-1} - M'_{k-1}))$ is

$$
\phi(z) = (\sum_{j=1}^{k} p_j z_j)^m (\sum_{j=1}^{k} p_j z_j^{-1})^m,
$$

where we additionally define $z_k = \tau_k = 1$. By the multivariate version of Cauchy's integral formula [Scheidemann 2005, Theorem 1.3.3],

$$
\mathbb{P}
\left[
\bigcap_{j=1}^{k-1} \{ \tau_j (M_j - M'_j) = w_j \}
\right]
= \frac{1}{(2\pi i)^{k-1}} \int_{T_1 \times \cdots \times T_{k-1}} \frac{\phi(z)}{z_1^{w_1+1} \cdots z_{k-1}^{w_{k-1}+1}} dz,
$$

(A.26)

where each $T_j$ is the positively oriented unit circle in the complex plane $\mathbb{C}$. Replacing the probabilities in (A.25) with (A.26) and interchanging summation and integration, we have
that \((A.25)\) is equal to
\[
\frac{1}{(2\pi i)^{k-1}} \sum_{w_1 \geq 0, \ldots, w_{k-1} \geq 0} \int_{T_1 \times \cdots \times T_{k-1}} \frac{2^{-\frac{1}{2}} \sum_{j=1}^{k-1} w_j \phi(z)}{z_1^{w_1+1} \cdots z_{k-1}^{w_{k-1}+1}} \, dz.
\]

Let \(z_j = e^{i\theta_j}, j = 1, \ldots, k - 1, \) and \(\theta_k = 0.\) For notational brevity, let us write \(e^{i\theta} = (e^{i\theta_1}, \ldots, e^{i\theta_{k-1}}).\) Then the integral \((A.27)\) is equal to
\[
\frac{1}{(2\pi)^{k-1}} \int_{[-\pi, \pi]^{k-1}} \phi(e^{i\theta}) \prod_{j=1}^{k-1} \left( \frac{\sqrt{2}}{\sqrt{2}z_j - 1} \right) \, d\theta,
\]
which is bounded in modulus by
\[
\frac{(2 + \sqrt{2})^{k-1}}{(2\pi)^{k-1}} \int_{[-\pi, \pi]^{k-1}} |\phi(e^{i\theta})| \, d\theta. \tag{A.28}
\]

Next, note that
\[
\left| \sum_{j=1}^{k} p_j e^{i\theta_j} \right|^2 = \left( \sum_{j=1}^{k} p_j \cos(\tau_j \theta_j) \right)^2 + \left( \sum_{j=1}^{k} p_j \sin(\tau_j \theta_j) \right)^2
\]
\[
= \sum_{jj'} p_j p_{j'} [\cos(\tau_j \theta_j) \cos(\tau_{j'} \theta_{j'}) + \sin(\tau_j \theta_j) \sin(\tau_{j'} \theta_{j'})]
\]
\[
= \sum_{jj'} p_j p_{j'} \cos(\tau_j \theta_j - \tau_{j'} \theta_{j'})
\]
\[
= 1 - 2 \sum_{jj'} p_j p_{j'} \sin^2((\tau_j \theta_j - \tau_{j'} \theta_{j'})/2). \quad \text{(since } \sum_{j=1}^{k} p_j = 1) \tag{A.29}
\]

Using the inequality \(1 - x \leq e^{-x}\) for real \(|x| \leq 1,\) we have that
\[
|\phi(e^{i\theta})| \leq \exp \left\{ -2m \sum_{jj'} p_j p_{j'} \sin^2((\tau_j \theta_j - \tau_{j'} \theta_{j'})/2) \right\}.
\]

Introduce the change of variable \(u_j = \tan(\theta_j/4), j = 1, \ldots, k - 1\) and \(u_k = 0.\) Then 
\(d\theta_j = \frac{4}{1+u_j^2} \, du_j\) and
\[
\sin^2((\theta_j - \theta_{j'})/2) = \frac{4(u_j - u_{j'})^2(1 + u_j u_{j'})^2}{(1 + u_j^2)^2(1 + u_{j'}^2)^2}
\]
\[
\geq \frac{1}{4} (u_j - u_{j'})^2(1 + u_j u_{j'})^2,
\]
for all $u_j$ and $u_{j'}$ in $[-1, 1]$. Thus,

\[
\int_{[-\pi, \pi]^{k-1}} \exp \left\{ -2m \sum_{jj'} p_j p_{j'} \sin^2 \left( \frac{(\tau_j \theta_j - \tau_{j'} \theta_{j'})}{2} \right) \right\} \, d\theta
\]

\[
= \int_{[-\pi, \pi]^{k-1}} \exp \left\{ -2m \sum_{jj'} p_j p_{j'} \sin^2 \left( \frac{(\theta_j - \theta_{j'})}{2} \right) \right\} \, d\theta
\]

\[
\leq 4^{k-1} \int_{[-1,1]^{k-1}} \exp \left\{ -\frac{m}{2} \sum_{jj'} p_j p_{j'} (u_j - u_{j'})^2 (1 + u_j u_{j'})^2 \right\} \, du. \tag{A.30}
\]

Note that if we could lower bound the factor $1 + u_j u_{j'}$ by $1/2$ in the exponent of the integrand of (A.30), then the whole exponent could be bounded above by $-\frac{1}{4} \sum_{jj'} p_j p_{j'} (u_j - u_{j'})^2 = \frac{1}{2} u^T \Sigma^{-1} u$, where $\Sigma^{-1}$ is a $(k - 1) \times (k - 1)$ positive definite matrix defined by $[\Sigma^{-1}]_{jj'} = p_j (1 - p_j)$ if $j = j'$ and $[\Sigma^{-1}]_{jj'} = -p_j p_{j'}$ if $j \neq j'$ for $j, j' = 1, \ldots, k - 1$. In particular, $\det(\Sigma^{-1}) = p_1 \cdots p_k$. Interpreting (A.30) as approximately an unnormalized Gaussian integral with zero mean vector and covariance matrix $\frac{1}{m} \Sigma$, we have that

\[
\int_{\mathbb{R}^{k-1}} \exp \left\{ -\frac{m}{2} u^T \Sigma^{-1} u \right\} \, du = \frac{(2\pi)^{(k-1)/2}}{\sqrt{m^{k-1} p_1 \cdots p_k}}.
\]

Unfortunately, this factor cannot be avoided and we must use a cruder approximation,

\[
\int_{[-1,1]^{k-1}} \exp \left\{ -\frac{m}{2} \sum_{jj'} p_j p_{j'} (u_j - u_{j'})^2 (1 + u_j u_{j'})^2 \right\} \, du
\]

\[
\leq \int_{[-1,1]^{k-1}} \exp \left\{ -mp_k \sum_{j=1}^{k-1} p_j u_j^2 \right\} \, du
\]

\[
\leq \int_{\mathbb{R}^{k-1}} \exp \left\{ -mp_k \sum_{j=1}^{k-1} p_j u_j^2 \right\} \, du
\]

\[
= \frac{(2\pi)^{(k-1)/2}}{\sqrt{2^{k-1} m^{k-1} p_1 \cdots p_{k-1} p_k^{k-1}}}. \tag{A.31}
\]
Putting everything together, it follows that

\[
\mathbb{E}\left[2^{-\frac{1}{2}} \sum_{j=1}^{k} |M_j - M'_j| \right] 
\leq \sum_{\tau \in \{-1,+1\}^{k-1}} \sum_{w_1,\ldots,w_{k-1} \geq 0} P\left( \bigcap_{j=1}^{k-1} \{ \tau_j (M_j - M'_j) = w_j \} \right) 2^{-\frac{1}{2}} \sum_{j=1}^{k-1} w_j
\leq \sum_{\tau \in \{-1,+1\}^{k-1}} \sqrt{m^{k-1} p_1 \cdots p_k p_{k-1}^{k-1}} \left( \frac{2(2+\sqrt{2})}{\sqrt{\pi}} \right)^{k-1} \left( \frac{1}{8} \right) \sum_{j=1}^{k-1} w_j
\leq \sqrt{m^{k-1} p_1 \cdots p_k p_{k-1}^{k-1}}.
\]

Thus, we have shown (A.23).

To show (A.24), first note that

\[
\mathbb{E}\left[2^{-\frac{1}{2}} \sum_{j=1}^{k} |M_j - M'_j| \right] \geq P\left( \bigcap_{j=1}^{k-1} \{ M_j = M'_j \} \right),
\]

and by (A.26),

\[
P\left( \bigcap_{j=1}^{k-1} \{ M_j = M'_j \} \right) = \frac{1}{(2\pi)^{k-1}} \int_{\mathbb{T}^{k-1}} \frac{\phi(z)}{z_1 \cdots z_{k-1}} dz 
= \frac{1}{(2\pi)^{k-1}} \int_{[-\pi,\pi]^{k-1}} \phi(e^{i\theta}) d\theta
\]

Next, let us use the inequalities \( \sin^2(x) \leq x^2 \) for all real \( x \) and \( 1 - x \geq e^{-2x} \) for all real \( |x| \leq 1/2 \) so that

\[
\phi(e^{i\theta}) = \left( 1 - 2 \sum_{jj'} p_{jj'} \sin^2((\theta_j - \theta_{j'})/2) \right)^m \quad \text{(by (A.29))}
\geq \left( 1 - \frac{1}{2} \sum_{jj'} p_{jj'} (\theta_j - \theta_{j'})^2 \right)^m
\geq \exp \left\{ -m \sum_{jj'} p_{jj'} (\theta_j - \theta_{j'})^2 \right\},
\]

for all \( \theta_j \) and \( \theta_{j'} \) in \([-1/2,1/2]\]. This shows that

\[
\mathbb{E}\left[2^{-\frac{1}{2}} \sum_{j=1}^{k} |M_j - M'_j| \right] \geq \frac{1}{(2\pi)^{k-1}} \int_{[-1/2,1/2]^{k-1}} \exp \left\{ -m \sum_{jj'} p_{jj'} (\theta_j - \theta_{j'})^2 \right\} d\theta
= \frac{1}{(2\pi)^{k-1}} \int_{[-1/2,1/2]^{k-1}} \exp \left\{ -2m \mathbf{\theta}^\top \mathbf{\Sigma}^{-1} \mathbf{\theta} \right\} d\theta.
\]
Finally, introduce the change of variables $v = \sqrt{m} \Sigma^{-1/2} \theta$ so that (A.32) is equal to

$$\frac{1}{(2\pi)^{k-1} \sqrt{m^{k-1}p_1 \cdots p_k}} \int_V \exp \{-2v^\top v\} \, dv,$$

where $V = \{v = \sqrt{m} \Sigma^{-1/2} \theta : \theta \in [-1/2, 1/2]^{k-1}\}$. The conclusion follows from noting that

$$\int_V \exp \{-2v^\top v\} \, dv \to \int_{\mathbb{R}^{k-1}} \exp \{-2v^\top v\} \, dv = \left(\frac{\pi}{2}\right)^{(k-1)/2}, \quad \text{as } m \to +\infty.$$

\[ \square \]

**Remark A.5.** We can also justify (A.23) for $k = 2$ heuristically using normal approximations. For example, when $m$ is sufficiently large, $\frac{M_1-M_1'}{\sqrt{2mp_1p_2}}$ is well approximated by a standard normal distribution. Similarly, $\frac{M_1-M_1'}{\sqrt{2mp_1p_2}}$ is well approximated by a standard normal distribution. Thus, we have the approximation

$$E \left[ 2^{-\frac{1}{2} \sum_{j=1}^{2} |M_j-M_j'|} \right] = E \left[ 2^{-|M_1-M_1'|} \right] \approx E \left[ 2^{-\sqrt{2mp_1p_2}|Z|} \right], \quad Z \sim N(0, 1). \quad (A.33)$$

The last expectation in (A.33) is equal to the moment generating function $M_{|Z|}(t) = 2\mathbb{P}[Z \leq t] e^{t^2/2}$ of $|Z|$ evaluated at $t = -\log 2\sqrt{2mp_1p_2}$. By the asymptotic expression for Mills’s ratio, we have that

$$M_{|Z|}(-t) \sim \frac{2}{\sqrt{2\pi t}}, \quad t \to \infty.$$

Thus, we expect that

$$E \left[ 2^{-|M_1-M_1'|} \right] \approx \frac{1}{\log 2\sqrt{\pi mp_1p_2}},$$

for large $m$. Note that this asymptotic expression is within a constant factor of the rigorously established bound in (A.23).