ASYMPTOTIC THEORY FOR RANDOM FORESTS

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Random forests have proven themselves to be reliable predictive algorithms in many application areas. Not much is known, however, about the statistical properties of random forests. Several authors have established conditions under which their predictions are consistent, but these results do not provide practical estimates of the scale of random forest errors. In this paper, we analyze a random forest model based subsampling, and show that random forest predictions are asymptotically normal provided that the subsample size scales as \( s(n)/n = o(\log(n)^{-d}) \), where \( n \) is the number of training examples and \( d \) is the number of features. Moreover, we show that the asymptotic variance can consistently be estimated using an infinitesimal jackknife for bagged ensembles recently proposed by Efron (2013). In other words, our results let us both characterize and estimate the error-distribution of random forest predictions. Thus, random forests need not only be treated as black-box predictive algorithms, and can also be used for statistical inference.

1. Introduction. Random forests, introduced by Breiman [6], have become one of the most popular out-of-the-box prediction tools for machine learning. But despite the ubiquity of applications, the statistical properties of random forests are not yet fully understood. Simple questions such as “What is the limiting distribution of random forest predictions as the number of training examples goes to infinity?” and “How can we consistently estimate the sampling variance of random forest predictions?” still remain largely open. This paper provides answers to these questions for a large class of random forest models.

We study random forests with subsampling, defined as follows. Suppose that we have training examples \( Z_i = (X_i, Y_i) \) for \( i = 1, \ldots, n \), a test point \( x \), and a potentially randomized tree predictor \( T \) which makes predictions \( \hat{y} = T(x; Z_1, \ldots, Z_n) \). We can then turn this tree \( T \) into a random forest by averaging it over \( B \) random samples:

\[
RF_s(x; Z_1, \ldots, Z_n) = \frac{1}{B} \sum_{b=1}^{B} T(x; Z_{i1}^*, \ldots, Z_{is}^*) \quad \text{for some } s \leq n,
\]

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where \( \{Z_{b1}, \ldots, Z_{bs}\} \) form a uniformly drawn random subset of \( \{Z_1, \ldots, Z_n\} \).

As explained heuristically by Breiman [6] and more formally by, e.g., Bühlmann and Yu [9], the resampling performed by random forests improves single trees by smoothing their decision thresholds.

Our main result is that, for a large class of base learners \( T \), the predictions made by a random forest of the form (1) are asymptotically normal provided that \( s(n)/n = o(\log(n)^{-d}) \), where \( d \) is the dimension of the feature space. Moreover, under these conditions, we show that the asymptotic variance of the ensemble can be consistently estimated using a simple formula proposed by Efron [14], the infinitesimal jackknife for bagged ensembles. Thus, our results allow us to bring random forest predictions into the realm of classical statistical inference.

1.1. Related Work. Breiman originally described random forests in terms of bootstrap sampling:

\[
\text{RF}(x; Z_1, \ldots, Z_n) = \frac{1}{B} \sum_{b=1}^{B} T(x; Z_{b1}^*, \ldots, Z_{bn}^*),
\]

where the \( Z_{bi}^* \) iid \( \sim \{Z_1, \ldots, Z_n\} \) form a bootstrap sample of the training data.

Random forests of the form (2), however, have proven to be remarkably resistant to classical statistical analysis. As observed by Buja and Stuetzle [10], Chen and Hall [11], Friedman and Hall [16] and others, estimators of this form can exhibit surprising properties even in simple situations. In this paper, we avoid these pitfalls by basing our analysis on subsampling rather than bootstrap sampling.

Subsampling has often been found to be more easily amenable to theoretical analysis than bootstrapping [e.g., 26]. Although Breiman originally built random forests using bootstrap aggregation or bagging [5], subsampled random forests have also been repeatedly studied and found to work well [e.g., 9, 28]. Our present analysis is related to work by Hall and Samworth [18], who study the properties of subsampled \( k \)-nearest neighbors predictors and show that they are consistent provided the subsample size \( s(n) \) grows to infinity slower than \( n \).

Most existing theoretical results about random forests aim to establish the consistency of random forest predictions [2, 3, 7, 25]. There has been much less work, however, on understanding the sampling variance of random forests. One notable exception is a paper by Lin and Jeon [24] that uses an adaptive nearest neighbors analysis of random forests to derive lower bounds for their variance. They then use this result to show that predictors of the form (2) converge slowly in \( n \) if the leaf-size of the trees \( T \) is small.
Our work builds on recent contributions by Duan [13], Sexton and Laake [27] and Wager et al. [30], who sought to move beyond a black-box analysis of random forests by providing variance estimates for their predictions based on ideas like the bootstrap and the jackknife. These papers, however, only gave heuristic and experimental support for their proposed approaches. Here, we provide rigorous results about the asymptotic distribution of random forest predictions.

2. Statistics of Random Forest Predictions. The goal of this paper is to show how random forests can be made amenable to classical statistical analysis. Let \( \hat{y} \) be a prediction made by a random forest trained on \( n \) training examples. We show that, for a large class of random forests, \( \hat{y} \) is consistent as \( n \) grows to infinity and that

\[
\hat{y} \sim \mathcal{N} \left( \mathbb{E}[\hat{y}], \sigma^2 \right),
\]

provided that the random forest is trained using a subsample size \( s(n) \) that is smaller than \( n/\log(n)^d \); here \( d \) is the number of features and \( \mathcal{N} \) is the standard normal density. Moreover, we show that \( \sigma^2 \) can consistently be estimated from data.

We begin by introducing the infinitesimal jackknife estimate for \( \sigma^2 \) below, and show it in action on a real dataset. In Section 2.2, we then describe rigorous conditions under which (3) holds. We give an overview of our proof in Section 3, and provide a simulation study for the accuracy of \( \hat{V}_{IJ} \) in Section 4.

2.1. The Infinitesimal Jackknife for Random Forests. In order to estimate \( \sigma^2 \), we use the infinitesimal jackknife (or non-parametric delta-method) estimator \( \hat{V}_{IJ} \) for bagging introduced by Efron [14]. This estimator can be computed using a particularly simple formula:

\[
\hat{V}_{IJ} = \sum_{i=1}^{n} \text{Cov}_* \left[ T(x; Z_1^*, ..., Z_n^*), N_i^* \right],
\]

where \( N_i^* \) is the number of times \( Z_i \) appears in the subsample used by \( T \) and the covariance is taken with respect to the resampling measure. This formula arises by applying the original infinitesimal jackknife idea of Jaeckel [22] to the resampling distribution.

The estimator \( \hat{V}_{IJ} \) was studied in the context of random forests by Wager et al. [30], who showed empirically that the method worked well for many problems of interest. Wager et al. [30] also emphasized that, when using \( \hat{V}_{IJ} \)...
Fig 1: Random forest predictions on the Boston housing data set [19], along with 95% confidence intervals provided by the $\hat{V}_{IJ}$ estimator. The $x$-axis shows the log-proportion of lower status residents (LSTAT). The LSTAT proportion is the mean of the proportion of residents without some high school education and the proportion of male workers classified as laborers. We selected 337 out of 506 examples for training; the plot shows predictions made on the 169 remaining test examples. The random forest had a subsample size $s = 100$ and $B = 10,000$ replicates; otherwise, we used default settings for the \texttt{randomForest} package in R [23]. The solid line is a smoothing spline with $df = 4$ degrees of freedom.

In practice, it is important to account for Monte Carlo bias; in our case, the appropriate correction is given in (15).

Our analysis provides theoretical backing to these results, by showing that $\hat{V}_{IJ}$ is in fact a consistent estimate for the variance $\sigma^2$ of random forest predictions. The earlier work on this topic [14, 30] had only motivated the estimator $\hat{V}_{IJ}$ by highlighting connections to classical statistical ideas, but did not establish any formal justification for it.
2.1.1. A First Example. To illustrate our inferential framework, we revisit a classic regression data set: the Boston housing data set [19], with \( d = 13 \) features and \( n = 337 \) training examples. In Figure 1, we plot random forest predictions for median house price against a measure of the proportion of lower status residents (LSTAT), along with 95% confidence intervals provided by our theory.

We see that predictions with middle-range LSTAT values are all huddled near a smoothing spline drawn through the data, while the suburbs with extreme values of LSTAT have more scattered predictions. The error bars provided by \( \hat{V}_{ij} \) corroborate this observation: the size of the error bars roughly scales with the distance of the predictions from the smoothing spline trend line. Note that Figure 1 only shows 1 out of 13 predictors; this is why nearby points on the plot can have very different error bars.

Figure 2 shows the relationship between random forest predictions \( \hat{y} \) and

Fig 2: Estimated standard errors for predictions on the Boston housing data set [19], as a function of the prediction itself. The solid line is a smoothing spline with \( df = 4 \) degrees of freedom, while the dotted line is the line connecting zero with the mean of the data. The experimental setup is described in the caption of Figure 1.
the estimated standard error $\hat{\sigma}$. We might have expected for $\hat{\sigma}$ to scale roughly proportionally to $\hat{y}$. This behavior does in fact hold for large valuations $\hat{y}$. However, at the low end of the range of $\hat{y}$, we see that $\hat{\sigma}$ starts climbing back up; in relative terms, the coefficient of variation grows from 2% to 5%.

2.2. Main Results. Here, we provide a more precise statement of our result (3). We assume throughout that $\text{RF}_s$ is a random forest built by training trees $T$ on subsamples of size $s$ out of $n$ drawn without replacement. Moreover, we always take the number of bootstrap replicates $B$ in (1) to be large enough for Monte Carlo effects not to matter. The effects of Monte Carlo noise on $\hat{V}_{IJ}$ are discussed in [30].

The following theorem summarizes our main contributions, which are described in more detail in Section 3. The consistency result (6) is comparable to theorems of Meinshausen [25], Biau et al. [3], and Biau [2]. We are not aware, however, of any prior results resembling (7) or (8).

**Theorem 1.** Suppose that we have $n$ independent and identically distributed training examples $Z_i = (X_i, Y_i) \in [0, 1]^d \times [-M, M]$. Suppose moreover that the distribution of the $X_i$ admits a density that is bounded away from both zero and infinity, that $E[Y^k | X = x]$ is Lipschitz-continuous in $x$ for $k = 1, 2$, and that we are interested in a test point $x$ at which $\text{Var}[Y | X = x] > 0$.

Given this data-generating process, let $T$ be an honest, regular tree in the sense of Definitions 1 and 2, and let $\text{RF}_{s(n)}$ be a random forest with base learner $T$ and a subsample size $s(n)$. Then, provided that the subsample size $s(n)$ satisfies

$$(5) \quad \frac{1}{s(n)} = o(1) \text{ and } \frac{s(n)}{n} = o \left( \frac{1}{\log(n)^d} \right),$$

the random forest will be consistent:

$$(6) \quad \hat{y} := \text{RF}_{s(n)}(x; Z_1, \ldots, Z_n) \rightarrow_p \mu(x)$$

as $n \rightarrow \infty$, where $\mu(x) = E[Y | X = x]$. Moreover, there exists a sequence $\sigma_n \rightarrow 0$ such that

$$(7) \quad (\hat{y} - E[\hat{y}]) / \sigma_n \Rightarrow N(0, 1),$$

and this sequence can consistently be estimated using the infinitesimal jackknife (4):

$$(8) \quad \hat{V}_{IJ} / \sigma_n^2 \rightarrow_p 1.$$
Here, the choice of subsample size $s$ underlies a bias-variance trade-off. The variance of a random forest is governed by two factors [6, 20]: if the individual trees have variance $v$ and correlation $\rho$, the random forest itself will have variance $\rho v$. By making $s$ small we can reduce the overlap between different subsamples, thus decreasing $\rho$ and bringing down the variance of the ensemble. Conversely, when $s$ is large, the trees can grow deep and get very close to being unbiased.

2.3. Growing Trees. In order for the results described in Theorem 1 to hold, we of course need to put some constraints on the class of trees $T$ that can be used as base learners. We start by stating some regularity conditions below. The stronger and more interesting condition on $T$ is an “honesty” condition described in Definition 2.

**Definition 1.** A tree predictor grown by recursive partitioning is called regular if

(A) At each step of the training algorithm, the probability that the tree splits on variable $j$ is bounded below by some $\pi > 0$ for all $j = 1, \ldots, d$.

(B) Each split leaves at least a fraction $\gamma > 0$ of the available training examples on each side of the split.

(C) The trees are fully grown in the sense given training data $(X_i, Y_i)$, the tree make predictions of the form $T(x) = Y_{i^*(x)}$ for some index $i^*(x)$.

Here, conditions (A) and (B) are technical devices introduced by Meinshausen [25] to make sure that the predictions made by random forests become local as the trees get deep. Meanwhile, (C) is a theoretical convenience that lets us simplify the exposition. In practice, trees are sometimes grown to have terminal node size $k$ rather than 1 for regularization. In our setup, however, we already get regularization by drawing subsamples of size $s$ where $s/n \to 0$ and the regularization effect from using larger leaf sizes is not as important. The conditions (A-C) can usually be ignored in practice without invalidating the spirit of Theorem 1.

Our second requirement is that $T$ be “honest”. It is well known that trees act as adaptive nearest neighbors predictors; this idea is discussed in detail by Lin and Jeon [24]. As stated more formally below, we say that a tree is honest if it does not double-use training labels $Y_i$ for both determining split-points of the tree and for making nearest-neighbor predictions. As far as we know, prior papers on the consistency of random forests [e.g., 2, 3, 25] all require a similar condition.
Definition 2. A fully grown tree is called honest if, conditionally on $X_i$, the distribution of $Y_i$ does not depend on knowing whether $i$ is the selected index $i^*(x)$:

$\mathcal{L} (Y_{i^*(x)} \mid X_{i^*(x)} = x) \overset{d}{=} \mathcal{L} (Y_i \mid X_i = x)$

for all values of $x$.

If we do not require (9), it is easy to construct arbitrarily biased tree classifiers $T$. Suppose, for example, that $Y_i \in \{0, 1\}$ and that we are interested in a specific test point $x$. Then, a dishonest tree $T$ can always predict $\hat{y} = 1$ if there exists even a single test example $(X_i, Y_i)$ such that $Y_i = 1$ and $X_i$ is a potential nearest neighbor (PNN) of $x$, i.e., there are no other test examples in the smallest axis-aligned rectangle containing both $x$ and $X_i$. As shown by Lin and Jeon [24], the expected number of PNNs of $x$ grows to infinity with $n$, and so, in general, for large $n$ we can with high probability find a tree such that $T(x) = 1$.

CART trees are of course not honest in the sense of Definition 2, because they use training labels both to choose splits and make predictions. And, as we show in Figure 3, random forests trained with CART trees are not consistent either even for very simple problems. In this example, we drew $X$ uniformly from $[0, 1]^2$, and $Y \sim \text{Bernoulli}(0.01)$ independently of $X$; thus, $E [Y \mid X = x] = 0.01$ everywhere. CART-based random forests, however, do not consistently learn this constant function, but rather seem to warp up near the edges and down in the middle. At $x = (0, 0)$, the tree was predicting $\hat{y} = 3.5\%$ instead of $1\%$. It appears that the CART trees are trying to aggressively separate the points with $Y_i = 1$ from the rest of the data, and in doing so push the neighborhoods surrounding those points towards the edge of the domain of $X$.

That being said, the bias of CART trees seems to be subtle enough that it does not affect the performance of random forests in most situations. Similarly, in our simulation experiments presented in Section 4, we find that the infinitesimal jackknife $\hat{V}_{IJ}$ works well for estimating the variance of random forests with CART base learners. Thus, it seems reasonable to assume that our main results from Theorem 1 still provide useful insight in understanding the behavior of CART random forests as implemented in, e.g., the popular R library randomForest [23]. Seeing whether it is possible to improve the practical performance of CART trees by making them honest and unbiased seems like a promising avenue for further research.

3. Theoretical Development. The ideas used in our proof go back to techniques developed by Hoeffding [21] and Hájek et al. [17] to establish the
Fig 3: Heat map of predictions made by a random forest with \( n = 1,000,000 \) training examples and a subsample size \( s = 1,000 \). The optimal prediction function should be constant, but the random forest systematically makes larger predictions near the edges and small ones in the middle of the domain.

We begin by briefly reviewing their results to give some context to our proof. Given a predictor \( T \) and independent training examples \( Z_1, \ldots, Z_n \), the Hájek projection of \( T \) is defined as

\[
\hat{T} = \mathbb{E}[T] + \sum_{i=1}^{n} (\mathbb{E}[T | Z_i] - \mathbb{E}[T]) .
\]

In other words, the Hájek projection of \( T \) captures the first-order effects in \( T \). This projection has the properties we would expect: in particular \( \text{Var} [\hat{T}] \leq \text{Var} [T] \), and if

\[
\lim_{n \to \infty} \frac{\text{Var} [\hat{T}]}{\text{Var} [T]} = 1, \text{ then } \lim_{n \to \infty} \mathbb{E} \left[ \left\| \hat{T} - T \right\|^2 / \text{Var} [T] \right] = 0.
\]

Since the Hájek projection \( \hat{T} \) is a sum of independent random variables, we should expect it to be asymptotically normal under all but pathological
conditions. Thus whenever the ratio of the variance of $\tilde{T}$ to that of $T$ tends to 1, the theory of Hájek projections almost automatically guarantees that $T$ will be asymptotically normal.$^1$

If $T$ is decision tree, however, the condition from (11) does not apply, and we cannot use the classical theory of Hájek projections directly. Our analysis is centered around a weaker form of this condition, which we call $\alpha$-incrementality. With our definition, predictors $T$ to which we can apply the argument (11) directly are $1$-incremental.

**Definition 3.** The predictor $T$ is $\alpha(s)$-incremental at $x$ if

$$\frac{\text{Var} \left[ \tilde{T} (Z_1, ..., Z_s) \right]}{\text{Var} \left[ T (Z_1, ..., Z_s) \right]} \gtrsim \alpha(s),$$

where $\tilde{T}$ is the Hájek projection of $T$ (10). In our notation,

$$f(s) \gtrsim g(s) \text{ means that } \lim_{s \to \infty} f(s)/g(s) \geq 1.$$

Our argument proceeds in two steps. First we establish lower bounds for the incrementality of regression trees in Section 3.1. Then, in Section 3.2 we show how we can turn weakly incremental predictors $T$ into $1$-incremental ensembles by subsampling, thus bringing us back into the realm of classical theory. We also establish the consistency of the infinitesimal jackknife for random forests.

Our analysis of regression trees is motivated by the “potential nearest neighbors” model for random forests introduced by Lin and Jeon [24]. Meanwhile, the key technical device used in Section 3.2 is the ANOVA decomposition of Efron and Stein [15]. The discussion of the infinitesimal jackknife for random forest builds on results of Efron [14] and Wager et al. [30].

3.1. **Regression Trees and Incremental Predictors.** Analyzing specific greedy tree models such as CART trees can be challenging. We thus follow the lead of Lin and Jeon [24], and analyze a more general class of predictors—potential nearest neighbors predictors—that operate by doing a nearest-neighbor search over rectangles.

**Definition 4.** Consider a set of points $X_1, ..., X_s \in \mathbb{R}^d$ and a fixed $x \in \mathbb{R}^d$. A point $X_i$ is a potential nearest neighbor (PNN) of $x$ if the

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$^1$The moments defined in (10) depend on the data-generating process for the $Z_i$, and so cannot be observed in practice. Thus, the Hájek projection is mostly useful as an abstract theoretical tool. For a review of classical projection arguments, see Chapter 11 of Van der Vaart [29].
The smallest axis-aligned hyperrectangle with vertices \( x \) and \( X_i \) contains no other points \( X_j \). A predictor \( T \) is a PNN predictor if, given a training set \((X_1, Y_1), \ldots, (X_s, Y_s) \in \mathbb{R}^d \times \mathcal{Y}\) and a test point \( x \in \mathbb{R}^d \), \( T \) always outputs \( Y_i \) corresponding to a PNN \( X_i \) of \( x \).

In other words, given a test point \( x \), a PNN classifier is allowed to predict \( Y_i \) only if there exists a rectangle containing \( x \), \( X_i \), and no other test points. All standard decision trees result in PNN predictors.

**Proposition 2** (Lin and Jeon [24]). Any decision tree \( T \) that makes axis-aligned splits and has leaves of size 1 is a PNN predictor. In particular, the base learners originally used by Breiman [6], namely fully grown CART trees [8], are PNN predictors.

Predictions made by PNNs can always be written as

\[
T(x; Z) = \sum_{i=1}^{s} S_i Y_i,
\]

where \( S_i \) is a selection variable that takes the value 1 for the selected index \( i \) and 0 for all other indices. An important property of PNN predictors is that we can often get a good idea about whether \( S_i \) can possibly be 1 even if we only get to see \( Z_i \); more formally, as we show below, the quantity \( n \text{Var}[S_1 | Z_1] \) cannot get too small. Establishing this fact is a key step in showing that PNNs are incremental.

**Lemma 3.** Suppose that the features \( X \) are independently and identically distributed on \([0, 1]^d\) with a density \( f \) that is bounded away from zero and infinity, and let \( T \) be any PNN predictor. Then, there is a constant \( C_f \) depending only on \( f \) and \( d \) such that

\[
s \text{Var}[E[S_1 | Z_1]] \gtrsim C_f/ \log(s)^d,
\]

where \( S_i \) is defined as in (12). When \( f \) is uniform over \([0, 1]^d\), the bound holds with \( C_f = 2^{d+1}/(d-1)! \).

Thanks to this result, we are now ready to show that all honest regular trees are incremental. The proof of the following theorem makes use of an important technical lemma from Meinshausen [25].

**Theorem 4.** Suppose that the conditions of Lemma 3 hold and that \( T \) is an honest regular tree in the sense of Definitions 1 and 2. Suppose
moreover that the moments $\mathbb{E} \left[ Y \mid X = x \right]$ and $\mathbb{E} \left[ Y^2 \mid X = x \right]$ are both finite and Lipschitz continuous functions of $x$, and that $\mathbb{E} \left[ Y^2 \mid X = x \right]$ is uniformly bounded for all $x \in [0, 1]^d$. Finally, suppose that $\text{Var} \left[ Y \mid X = x \right] > 0$. Then $T$ is $\alpha(s)$-incremental with

$$\alpha(s) = C_f / \log(s)^d,$$

where $C_f$ is the constant from Lemma 3.

3.2. Random Forests with Incremental Base Learners. In the previous section, we showed that decision trees are $\alpha$-incremental, in that the Hájek projection $\hat{T}$ of $T$ contains at least some information about $T$. In this section, we show that randomly subsampling $\alpha$-incremental predictors makes them 1-incremental; this then lets us proceed with a classical statistical analysis. The following lemma, which flows directly from the ANOVA decomposition of Efron and Stein [15], provides a first motivating result for our analysis.

**Lemma 5.** Let $\text{RF}_s$ be a random forest with base learner $T$ as defined in (1), and let $\hat{\text{RF}}_s$ be the Hájek projection of $\text{RF}_s$ (10). Then

$$\mathbb{E} \left[ \left( \text{RF}_s(Z_i) - \hat{\text{RF}}_s(Z_i) \right)^2 \right] \leq \left( \frac{s(n)}{n} \right)^2 \text{Var} \left[ T \right]$$

whenever the variance $\text{Var} \left[ T \right]$ of the base learner is finite.

This technical result paired with Theorem 4 leads to our first main result about random forests.

**Theorem 6.** Let $\text{RF}_{s(n)}$ be a random forest with base learner $T$ trained according the conditions of Theorem 4, with $Y$ restricted to a bounded interval $Y \in [-M, M]$. Suppose, moreover, that the subsample size $s(n)$ satisfies

$$\lim_{n \to \infty} s(n) = \infty \text{ and } \lim_{n \to \infty} s(n) \log(n)^d / n = 0.$$  

Then, the random forest is consistent. Moreover, there exists a sequence $\sigma_n \to 0$ such that

$$(14) \quad \frac{1}{\sigma_n} \left( \text{RF}_{s(n)}(x; Z_1, ..., Z_n) - \mathbb{E} \left[ \text{RF}_{s(n)}(x, Z_1, ..., Z_n) \right] \right) \Rightarrow \mathcal{N}(0, 1),$$

where $\mathcal{N}(0, 1)$ is the standard normal density.
Theorem 6 by itself is just an abstract characterization theorem about random forests. As we show below, however, it is possible to accurately estimate the noise-level $\sigma$ of a random forest using the infinitesimal jackknife for random forests [14, 30]. Thus, our theory allows us to do statistical inference about random forest predictions.

**Theorem 7.** Let $\hat{V}_{IJ}(x; Z_1, ..., Z_n)$ be the infinitesimal jackknife for random forests [14] as defined in (4). Then, under the conditions of Theorem 6,

$$\hat{V}_{IJ}(x; Z_1, ..., Z_n) / \sigma^2 \Rightarrow 1.$$  

4. Simulation Study. In this section we test the result from Theorem 7, namely that the infinitesimal jackknife estimate of variance $\hat{V}_{IJ}$ is a good predictor of the true variance $\sigma^2$ of random forest predictions. The simulations all used a subsample size of $s = [n^{0.7}]$ and $B = 5n$ bootstrap replicates; otherwise, we used default settings for the randomForest package in R [23].

As emphasized by Wager et al. [30], when we only use $B = O(n)$ bootstrap replicates, $\hat{V}_{IJ}$ can suffer from considerable Monte Carlo bias. To alleviate this problem, they propose a Monte Carlo bias correction for $\hat{V}_{IJ}$; in the case of subsampling with subsample size $s$ and $B$ bootstrap replicates, this bias correction is

$$\hat{V}_{BIJ} = \sum_{i=1}^{n} C_i^2 - \frac{s(n-s)}{n} \hat{\nu} B,$$

where

$$C_i = \frac{1}{B} \sum_{b=1}^{B} (N_{bi}^* - s/n) (T_b^* - \bar{T}^*)$$

and

$$\hat{\nu} = \frac{1}{B} \sum_{b=1}^{B} (T_b^* - \bar{T}^*)^2.$$ 

Here, the first term of $\hat{V}_{BIJ}$ is a plug-in formula where $C_i$ acts as a Monte Carlo estimate for $\text{Cov}^* [N_i^*, T_i^*]$, and the second term is a bias correction.

Table 1 shows the performance of $\hat{V}_{IJ}$ on several synthetic distributions. To produce this table, we first drew $K = 100$ random test points $\{x^{(k)}\}_{k=1}^{100}$ from the data-generating distribution. We then constructed $R = 100$ random training sets $\{Z^{(r)}\}_{r=1}^{R}$, and evaluated both the prediction $\text{RF}_k(x^{(k)}; Z^{(r)})$ and the variance estimate $\hat{V}_{IJ}(x^{(k)}; Z^{(r)})$ for each test point $x^{(k)}$. The num-
| Distr. | d | n  | Bias^2 | Variance | MSE    | Bias^2 | Variance | MSE    |
|-------|---|----|--------|----------|--------|--------|----------|--------|
| Cosine | 2 | 200| 0.13   | 0.08     | 0.21   | 1.23E-03 | 7.76E-04 | 2.00E-03 |
| Cosine | 2 | 1000| 0.04   | 0.08     | 0.11   | 3.97E-05 | 8.52E-05 | 1.24E-04 |
| Cosine | 2 | 5000| 0.03   | 0.05     | 0.08   | 6.44E-06 | 1.17E-05 | 1.80E-05 |
| Cosine | 10 | 200 | 0.10   | 0.07     | 0.17   | 7.60E-04 | 5.63E-04 | 1.32E-03 |
| Cosine | 10 | 1000 | 0.10   | 0.04     | 0.14   | 1.31E-04 | 5.06E-05 | 1.81E-04 |
| Cosine | 10 | 5000 | 0.04   | 0.03     | 0.07   | 4.42E-06 | 3.28E-06 | 7.66E-06 |
| AND   | 20 | 200 | 0.08   | 0.09     | 0.17   | 6.92E-03 | 7.35E-03 | 1.42E-02 |
| AND   | 20 | 1000| 0.22   | 0.07     | 0.29   | 2.06E-03 | 6.54E-04 | 2.71E-03 |
| AND   | 20 | 5000| 0.65   | 0.27     | 0.92   | 3.01E-04 | 1.26E-04 | 4.26E-04 |
| AND   | 100 | 200 | 0.07   | 0.18     | 0.24   | 2.15E-03 | 5.69E-03 | 7.78E-03 |
| AND   | 100 | 1000| 0.07   | 0.11     | 0.18   | 3.27E-04 | 5.00E-04 | 8.23E-04 |
| AND   | 100 | 5000| 0.07   | 0.25     | 0.33   | 4.40E-05 | 1.49E-04 | 1.92E-04 |
| XOR   | 5  | 200 | 0.10   | 0.07     | 0.17   | 7.08E-03 | 4.51E-03 | 1.16E-02 |
| XOR   | 5  | 1000| 0.05   | 0.04     | 0.10   | 4.66E-04 | 3.95E-04 | 8.56E-04 |
| XOR   | 5  | 5000| 0.06   | 0.02     | 0.08   | 5.38E-05 | 2.38E-05 | 7.73E-05 |
| XOR   | 20 | 200 | 0.12   | 0.07     | 0.19   | 7.58E-03 | 3.97E-03 | 1.15E-02 |
| XOR   | 20 | 1000| 0.06   | 0.04     | 0.09   | 5.38E-04 | 3.27E-04 | 8.62E-04 |
| XOR   | 20 | 5000| 0.04   | 0.02     | 0.06   | 4.53E-05 | 2.56E-05 | 7.07E-05 |

Table 1

Performance of the infinitesimal jackknife for random forests on synthetic distributions.

The “absolute” metrics describe the accuracy of \( \hat{V}_{IJ} \), while the “relative” metrics describe the accuracy of \( \hat{V}_{IJ} / \sigma^2 \), where \( \bar{\sigma}^2 \) is the average of \( \sigma^2 \) over the test set. All examples have a subsample size of \( s = \lfloor n^{0.7} \rfloor \) and use \( B = 5n \) bootstrap replicates.

The \( \sigma^2 \) was estimated based on the variance and mean-squared error (MSE) columns were computed analogously. In the “absolute” columns we show the raw metrics as is, while for the “relative” columns we divided the metrics by the average of \( \sigma^2 (x^{(k)})^2 \) over the test points.

Rather encouragingly, we see that \( \hat{V}_{IJ} \) is overall quite accurate, and gets more accurate as \( n \) gets larger. For the “Cosine” and “XOR” distributions, the relative MSE also decays with \( n \), as predicted by Theorem 7. The “AND” distribution appears to have been the most difficult distribution: although the error of \( \hat{V}_{IJ} \) decays with \( n \), we have not yet entered the regime where it decays faster than \( \sigma^2 \). The fact that the “AND” distribution would be the most difficult one is not surprising, as it has the highest dimensionality \( d \).

We also tested \( \hat{V}_{IJ} \) on some parametric bootstrap simulations based on
Table 2

| Distr. | d  | n   | Relative Bias | Variance | MSE   | Absolute Bias | Variance | MSE   |
|--------|----|-----|---------------|----------|-------|---------------|----------|-------|
| Auto   | 7  | 314 | 0.09          | 0.10     | 0.19  | 5.30E-03      | 5.90E-03 | 1.11E-02 |
| Fires  | 12 | 344 | 0.10          | 0.15     | 0.25  | 4.73E-04      | 6.90E-04 | 1.16E-03 |
| Housing| 13 | 337 | 0.09          | 0.14     | 0.23  | 2.46E-02      | 4.05E-02 | 6.46E-02 |

Performance of the infinitesimal jackknife for random forests on the auto, forest fires and Boston housing data sets from the UCI repository [1]. The “absolute” metrics describe the accuracy of $\hat{V}_{1,1}$, while the “relative” metrics describe the accuracy of $\hat{V}_{1,1}/\bar{\sigma}^2$, where $\bar{\sigma}^2$ is the average of $\sigma^2$ over the test set. All examples have a subsample size of $s = \lfloor n^{0.7} \rfloor$ and use $B = 5n$ bootstrap replicates.

classic data sets from the UCI machine learning repository [1]; results are shown in Table 2. The “forest fires” and “housing” data sets are originally due to [12, 19]; with the forest fires data set, we predicted log-area of the fire. For these experiments, we divided the original data set into a test set and a training set, and then used the training set to construct a parametric bootstrap distribution. From there, we proceeded as with the synthetic distributions from Table 1. The infinitesimal performed quite well here, despite the small sample size.

4.1. Synthetic Data-Generating Distributions. To generate the data used in Table 1, we first drew features $X \sim U ([0, 1]^p)$ and then generated the labels $Y$ using the following rules:

- **Cosine:** $Y = 3 \cdot \cos (\pi \cdot (X_1 + X_2)) + \varepsilon$
- **XOR:** $Y = 5 \cdot [\text{XOR} (X_1 > 0.6, X_2 > 0.6) + \text{XOR} (X_3 > 0.6, X_4 > 0.6)] + \varepsilon$
- **AND:** $Y = 10 \cdot \text{AND} (X_1 > 0.3, X_2 > 0.3, X_3 > 0.3, X_4 > 0.3) + \varepsilon$.

Here, $\varepsilon$ is standard Gaussian noise, while XOR and AND are treated as 0/1-valued functions. Similar distributions were also used for simulation experiments in [30].

5. Discussion. Following Breiman’s lead, random forests have mostly been studied in terms of black-box metrics like cross-validation error or test-set error. Although measuring test-set error is of course important, a pure black-box evaluation can miss out on much of the richness of a more careful statistical analysis. It cannot answer questions like: are there some points at which the random forest is more stable than others?, or how much might the predictions change if we gathered more training data?

In this paper, we studied a random forest model based on subsampling with a subsample size satisfying $s/n = o(\log(n)^{-d})$. We established results
about the asymptotic normality of random forest predictions, and showed that their asymptotic variance can be accurately estimated from data. Thus, our results open the door to a more complete and nuanced statistical understanding of random forest models.

6. Proofs.

6.1. Proofs about the Incrementality of Regression Trees.

**Proof of Lemma 3.** Here, we focus on the case where \( f \) is constant; the result can then be generalized to other densities \( f \) using similar arguments as used by Lin and Jeon [24].

Consider the quantities \( W_i \), which indicate whether \( X_i \) is a PNN of \( x \). Because \( T \) is a PNN predictor, the feature vector \( X_i \) for the selected index \( i \) must be a PNN of \( x \). Thus, \( W_i \) is an upper bound for \( S_i \) and, in particular,

\[
\mathbb{E} [ S_1 | Z_1 ] \leq \mathbb{E} [ W_1 | Z_1 ].
\]

The bulk of the proof involves showing that

\[
P \left[ \mathbb{E} [ W_1 | Z_1 ] \geq \frac{1}{s^2} \right] \lesssim \frac{2^{d+1} \log (s)^d}{(d-1)!} \frac{1}{s};
\]

by the above argument, this relationship also holds for \( S_i \). Now, we also know that \( \mathbb{E} [ \mathbb{E} [ S_1 | Z_1 ] ] = 1/s \), and so

\[
P \left[ \mathbb{E} [ S_1 | Z_1 ] \geq \frac{1}{s^2} \right] \mathbb{E} \left[ \mathbb{E} [ S_1 | Z_1 ] | \mathbb{E} [ S_1 | Z_1 ] \geq \frac{1}{s^2} \right] \sim \frac{1}{s}.
\]

By Jensen’s inequality, we then see that

\[
\mathbb{E} \left[ \mathbb{E} [ S_1 | Z_1 ]^2 \right] \geq P \left[ \mathbb{E} [ S_1 | Z_1 ] \geq \frac{1}{s^2} \right] \mathbb{E} \left[ \mathbb{E} [ S_1 | Z_1 ] | \mathbb{E} [ S_1 | Z_1 ] \geq \frac{1}{s^2} \right]^2
\]

\[
\sim \frac{s^{-2}}{P \left[ \mathbb{E} [ S_1 | Z_1 ] \geq \frac{1}{s^2} \right]}
\]

which, paired with (18), implies that

\[
\mathbb{E} \left[ \mathbb{E} [ S_1 | Z_1 ]^2 \right] \geq \frac{(d-1)!}{2^{d+1} \log (s)^d} \frac{1}{s}.
\]

This is equivalent to (13) because \( \mathbb{E} [ \mathbb{E} [ S_1 | Z_1 ] ]^2 = 1/s^2 \) is negligibly small.
We now return to establishing (18). Recall that $X_1, ..., X_s$ are independently and uniformly distributed over $[0, 1]^d$, and that we are trying to find points that are PNNs a prediction point $x$. For now, suppose that $x = 0$. We know that $X_1$ is a PNN of 0 if and only if there is no other $X_i$ such that $X_{ij} \leq X_{1j}$ for all $j = 1, ..., d$ (because the $X$ have a continuous density, there will almost surely be no ties). Thus,

$$E_{x=0} [W_1 \mid Z_1] = \left( 1 - \prod_{j=1}^{d} X_{1j} \right)^{s-1}.$$

We can check that $X_{1j} = e^{-E_j}$ where $E_j$ is a standard exponential random variable, and so

$$E_{x=0} [W_1 \mid Z_1] = \left( 1 - \exp \left[ - \sum_{j=1}^{d} E_j \right] \right)^{s-1}.$$

Thus,

$$P_{x=0} \left[ E [W_1 \mid Z_1] \geq \frac{1}{s^2} \right] = P \left[ \exp \left[ - \sum_{j=1}^{d} E_j \right] \leq 1 - \left( \frac{1}{s^2} \right)^{\frac{1}{s-1}} \right] = P \left[ \sum_{j=1}^{d} E_j \geq - \log \left( 1 - \exp \left[ -2 \frac{\log (s)}{s-1} \right] \right) \right].$$

Notice that this quantity goes to zero as $s$ gets large. The sum of $d$ standard exponential random variables has a gamma distribution with shape $d$ and scale 1, and

$$P \left[ \sum_{j=1}^{d} E_j \geq c \right] = \frac{\Gamma (d, c)}{(d - 1)!},$$

where $\Gamma$ is the upper incomplete gamma function. It is well known that

$$\lim_{c \to \infty} \frac{\Gamma (d, c)}{c^{d-1} e^{-c}} = 1,$$

and so

$$P_{x=0} \left[ E [W_1 \mid Z_1] \geq \frac{1}{s^2} \right] \sim \frac{\left( - \log \left( 1 - \exp \left[ -2 \frac{\log (s)}{s-1} \right] \right) \right)^{d-1} \left( 1 - \exp \left[ -2 \frac{\log (s)}{s-1} \right] \right)}{(d - 1)!}.$$
We can check that
\[ 1 - \exp \left[ -2 \log \left( \frac{s}{s - 1} \right) \right] \sim 2 \frac{\log (s)}{s}, \]
letting us simplify the above expression to

\[ P_{x=0} \left[ E \left[ W_1 \mid Z_1 \right] \geq \frac{1}{s^2} \right] \sim \frac{2}{(d-1)!} \frac{\log (s)^d}{s}. \tag{19} \]

We thus have obtained a tight expression for our quantity of interest for a prediction point at \( x = 0 \).

In the case \( x \neq 0 \), the ambient space around \( x \) can be divided into \( 2^d \) quadrants. In order to check whether \( X_i \) is a PNN, we only need to consider other points in the same quadrant, as no point in a different quadrant can prevent \( X_i \) from being a PNN. Now, index the quadrants by \( k = 1, \ldots, 2^d \), and let \( v_k \) be the volume of the \( k \)-th quadrant. By applying (19) on the \( k \)-th quadrant alone, we see that the probability of \( E \left[ W_1 \mid Z_1 \right] \geq \frac{1}{s^2} \) given that \( X_1 \) is in the \( k \)-the quadrant is asymptotically equal to

\[ \frac{2}{(d-1)!} \frac{\log (s)^d}{v_k s}. \]

Summing over all quadrants, we find that

\[ P_{x=0} \left[ E \left[ W_1 \mid Z_1 \right] \geq \frac{1}{s^2} \right] \sim \sum_{\{k: v_k > 0\}} v_k \frac{2}{(d-1)!} \frac{\log (s)^d}{v_k s} \]
\[ = \left| \{k: v_k > 0\} \right| \frac{2}{(d-1)!} \frac{\log (s)^d}{s} \]
\[ \leq \frac{2^{d+1}}{(d-1)!} \frac{\log (s)^d}{s}, \]

thus establishing (18).

**Proof of Theorem 4.** Without loss of generality, \( E \left[ T (x; Z) \right] = 0 \); let \( S_i \) be defined as in (12). Now, by Lemma 2 of Meinshausen [25], the regularity conditions (A) and (B) from Definition 1 imply that \( \| X_{i^* (x)} - x \|_2 \) converges in probability to 0. Thus, because \( T \) is honest (9) we can use the assumed Lipschitz continuity conditions and the uniform bound of \( E \left[ Y^2 \mid X = x \right] \) to show that

\[ E \left[ Y_{i^* (x)} \mid X_{i^* (x)} \right] \rightarrow_p E \left[ Y \mid X = x \right], \text{ and} \]
\[ E \left[ Y_{i^* (x)}^2 \mid X_{i^* (x)} \right] \rightarrow_p E \left[ Y^2 \mid X = x \right]. \]
In particular, we see that \( \text{Var} \{ T (x; Z) \} \) converges to \( \text{Var} \{ Y \mid X = x \} \).

Moving forward, we can decompose the first-order effects of \( T \) as

\[
\mathbb{E} \left[ T (x; Z) \mid Z_1 \right] = \mathbb{E} \left[ S_1 Y_1 \mid Z_1 \right] + \sum_{k=1}^{s} \mathbb{E} \left[ S_k Y_k \mid Z_1 \right] \\
= \mathbb{E} \left[ S_1 Y_1 \mid Z_1 \right] + (s - 1) \mathbb{E} \left[ S_2 Y_2 \mid Z_1 \right].
\]

Our goal is to obtain a lower bound for \( \text{Var} \left[ \mathbb{E} \left[ T (x; Z) \mid Z_1 \right] \right] \). By the above argument, we see that

\[
\text{Var} \left[ \mathbb{E} \left[ S_1 Y_1 \mid Z_1 \right] \right] = \text{Var} \left[ \mathbb{E} \left[ S_1 \mid X_1 \right] Y_1 \right] \\
\sim \text{Var} \left[ \mathbb{E} \left[ S_1 \mid X_1 \right] \right] \text{Var} \left[ Y \mid X = x \right] \\
+ \text{Var} \left[ \mathbb{E} \left[ S_1 \mid X_1 \right] \right] \mathbb{E} \left[ Y \mid X = x \right]^2 \\
+ \mathbb{E} \left[ S_1 \right]^2 \text{Var} \left[ Y \mid X = x \right].
\]

Here, the \( \mathbb{E} \left[ S_1 \right]^2 \text{Var} \left[ Y \mid X = x \right] \) is \( O \left( 1/s^2 \right) \) and can be effectively ignored. Meanwhile,

\[
(s - 1) \text{Cov} \left[ \mathbb{E} \left[ S_1 Y_1 \mid Z_1 \right], \mathbb{E} \left[ S_2 Y_2 \mid Z_1 \right] \right] \\
\sim (s - 1) \mathbb{E} \left[ Y \mid X = x \right]^2 \text{Cov} \left[ \mathbb{E} \left[ S_1 \mid Z_1 \right], \mathbb{E} \left[ S_2 \mid Z_1 \right] \right] \\
\sim \mathbb{E} \left[ Y \mid X = x \right]^2 \text{Cov} \left[ \mathbb{E} \left[ S_1 \mid Z_1 \right], 1 - \mathbb{E} \left[ S_1 \mid Z_1 \right] \right] \\
= -\mathbb{E} \left[ Y \mid X = x \right]^2 \text{Var} \left[ \mathbb{E} \left[ S_1 \mid Z_1 \right] \right].
\]

Combining all this with with Lemma 3, we find that

\[
(21) \quad \text{Var} \left[ \mathbb{E} \left[ T (x; Z) \mid Z_1 \right] \right] \gtrsim \text{Var} \left[ \mathbb{E} \left[ S_1 \mid Z_1 \right] \right] \text{Var} \left[ Y \mid X = x \right] \\
\gtrsim \frac{\alpha (s)}{s} \text{Var} \left[ Y \mid X = x \right].
\]

Thus finally

\[
\frac{\text{Var} \left[ T (x; Z) \right]}{\text{Var} \left[ T (x; Z) \right]} \sim \frac{s \text{Var} \left[ \mathbb{E} \left[ T (x; Z) \mid Z_1 \right] \right]}{\text{Var} \left[ Y \mid X = x \right]} \gtrsim \alpha (s),
\]

as claimed.

6.2. Proofs about Subsampling Incremental Base Learners. The results presented in this section rely heavily on the Efron-Stein ANOVA decomposition, summarized here for convenience. Suppose we have any symmetric function \( T : \Omega^n \to \mathbb{R} \), and suppose that \( Z_1, ..., Z_n \) are independent and
identically distributed on $\Omega$ such that $\text{Var} [Z_1, \ldots, Z_n] < \infty$. Then Efron and Stein [15] show that there exist functions $T_1, \ldots, T_n$ such that

$$T (Z_1, \ldots, Z_n) = \mathbb{E} [T] + \sum_{i=1}^{n} T_1 (Z_i) + \sum_{i<j} T_2 (Z_i, Z_j) + \ldots + T_n (Z_1, \ldots, Z_n),$$

and that all $2^n - 1$ random variables on the right side of the above expression are all mean-zero and uncorrelated. It immediately follows that

$$\text{Var} [T] = \sum_{k=1}^{n} \binom{n}{k} V_k, \quad \text{where} \quad V_k = \text{Var} [T_k (Z_1, \ldots, Z_k)].$$

For our purposes, it is also useful to note that the Hájek projection $\hat{T}$ can be written as

$$\hat{T} (Z_1, \ldots, Z_n) = \mathbb{E} [T] + \sum_{i=1}^{n} T (Z_i), \quad \text{and} \quad \text{Var} [\hat{T}] = n V_1.$$

Thus, the ANOVA decomposition provides a convenient abstract framework for analyzing our quantities of interest.

**Proof of Lemma 5.** In the absence of Monte Carlo noise, our random forest is defined as

$$\text{RF}_s (Z_1, \ldots, Z_n) = \binom{n}{s}^{-1} \sum_{i_1 < \ldots < i_s} T (Z_{i_1}, \ldots, Z_{i_s}).$$

Applying the ANOVA decomposition to the individual trees $T$, we see that this forest can equivalently be written as

$$\text{RF}_s (Z_1, \ldots, Z_n) = \mathbb{E} [T] + \binom{n}{s}^{-1} \binom{n-1}{s-1} \sum_{i=1}^{n} T_1 (Z_i)$$

$$+ \binom{n-2}{s-2} \sum_{i<j} T_2 (Z_i, Z_j) + \ldots + \sum_{i_1 < \ldots < i_s} T_s (Z_{i_1}, \ldots, Z_{i_s}).$$

The above formula holds because each training point $Z_i$ appears in $\binom{n-1}{s-1}$ out of $\binom{n}{s}$ possible subsamples of size $s$, each pair $(Z_i, Z_j)$ appears is $\binom{n-2}{s-2}$ subsets, etc.

Now, we can also show that the Hájek projection of $\text{RF}_s$ is

$$\hat{\text{RF}}_s (Z_1, \ldots, Z_n) = \mathbb{E} [T] + \frac{s}{n} \sum_{i=1}^{n} T_1 (Z_i).$$
As with all projections \cite{29},

\[ \mathbb{E} \left[ \left( RF_s - \bar{RF}_s \right)^2 \right] = \text{Var} \left[ RF_s - \bar{RF}_s \right]. \]

Recall that the \( T_k (\cdot) \) are all pairwise uncorrelated. Thus, using the notation \( s_k = s \cdot (s - 1) \cdots (s - k) \) it follows that

\[ \mathbb{E} \left[ \left( RF_s - \bar{RF}_s \right)^2 \right] = \sum_{k=2}^{s} \left( \frac{s_k}{n_k} \right)^2 \binom{n}{k} V_k, \]

\[ = \sum_{k=2}^{s} \frac{s_k}{n_k} \binom{s}{k} V_k, \]

\[ \leq \frac{s^2}{n^2} \sum_{k=2}^{s} \binom{s}{k} V_k, \]

\[ \leq \frac{s^2}{n^2} \text{Var} \left[ T \right], \]

where on the last line we used (23). We recover the stated result by noticing that \( s^2/n^2 \leq s^2/n^2 \) for all \( 2 \leq s \leq n \).

**Proof of Theorem 6.** The statement about consistency follows directly from Lemma 5 together with (20). Now, using notation from the previous lemma, let \( \sigma_n^2 = \frac{s(n)^2}{n} V_1 \) be the variance of \( \bar{RF}_{s(n)} \). We know that

\[ \sigma_n^2 = \frac{s(n)^2}{n^2} n V_1 \leq \frac{s(n)^2}{n^2} \text{Var} \left[ T \right], \]

and so \( \sigma_n \to 0 \) as desired. Now, by Theorem 4 combined with Lemma 5, we find that

\[ \frac{1}{\sigma_n^2} \mathbb{E} \left[ \left( RF_s (Z_i) - \bar{RF}_s (Z_i) \right)^2 \right] \leq \left( \frac{s(n)}{n} \right)^2 \frac{\text{Var} [T]}{\sigma_n^2} \]

\[ = \frac{s(n)}{n} \text{Var} [T] / \text{Var} [\bar{T}] \]

\[ \leq \frac{s(n)}{n} \log (s(n)) \frac{d}{C_f} \]

\[ \to 0 \]

by hypothesis. Thus, by Slutsky’s lemma, it suffices to show that (14) holds for the Hájek projection of the random forest \( RF_{s(n)} \).
By our definition of \( \sigma_n \), all we need to do is check that \( {RF}_{s(n)} \) is asymptotically normal. One way to do so is using the Lindeberg central limit theorem [e.g., 4]. Since

\[
{RF}_{s(n)} = \frac{s}{n} \sum_{i=1}^{n} \left( \mathbb{E} \left[ T \mid Z_i \right] - \mathbb{E} [T] \right)
\]

is a sum of independent and identically distributed random variables, it suffices to show that for any \( \varepsilon > 0 \)

\[
\lim_{n \to \infty} \frac{\mathbb{E} \left[ (\mathbb{E} \left[ T \mid Z_1 \right] - \mathbb{E} [T])^2 \mid (\mathbb{E} \left[ T \mid Z_1 \right] - \mathbb{E} [T])^2 > \tau_n \right]}{\mathbb{E} \left[ (\mathbb{E} \left[ T \mid Z_1 \right] - \mathbb{E} [T])^2 \right]} = 0,
\]

where \( \tau_n = \varepsilon \cdot n \cdot \mathbb{Var} \left[ \mathbb{E} \left[ T \mid Z_1 \right] \right] \).

We know from Theorem 4 that

\[
s(n) \cdot \mathbb{Var} \left[ \mathbb{E} \left[ T \mid Z_1 \right] \right] \geq \frac{C_f}{\log (n)^q}.
\]

Thus, we can check that

\[
\varepsilon \cdot n \cdot \mathbb{Var} \left[ \mathbb{E} \left[ T \mid Z_1 \right] \right] \geq \varepsilon \cdot \frac{n}{s(n) \log (s(n))^q},
\]

the right-hand-side of which converges to infinity by hypothesis as \( n \to \infty \). But, we assumed that \( Y \)—and thus also \( T \)—is bounded, and so for large enough \( n \) the quantity \( (\mathbb{E} \left[ T \mid Z_1 \right] - \mathbb{E} [T])^2 \) can never be greater than \( n / s(n) \log (s(n))^d \). Thus, Lindeberg’s condition holds and \( {RF}_{s(n)} \) makes asymptotically normal predictions.

**Proof of Theorem 7.** Let \( F \) denote the distribution from which we drew \( Z_1, ..., Z_n \). Then, the variance \( \sigma_n^2 \) of the Hájek projection of \( {RF}_{s(n)} \) is

\[
\sigma_n^2 = \sum_{i=1}^{n} \left( \mathbb{E}_{Z \sim F} \left[ {RF} \mid Z_i \right] - \mathbb{E}_{Z \sim F} \left[ {RF} \right] \right)^2
\]

\[
= \frac{s(n)^2}{n^2} \sum_{i=1}^{n} \left( \mathbb{E}_{Z \sim F} \left[ T \mid Z_i \right] - \mathbb{E}_{Z \sim F} \left[ T \right] \right)^2,
\]

whereas Efron [14] showed that

\[
\hat{V}_{IJ} = \frac{n}{n-1} \cdot \frac{s(n)^2}{n^2} \sum_{i=1}^{n} \left( \mathbb{E}_{Z^* \sim \hat{F} \mid Z_i^* = Z_i} \left[ T \mid Z_i^* = Z_i \right] - \mathbb{E}_{Z^* \sim \hat{F}} \left[ T \right] \right)^2,
\]
where $\hat{F}$ is the empirical distribution on \{\(Z_1, \ldots, Z_n\)\}. Recall that we are sampling the $Z^*$ from $\hat{F}$ without replacement.

It is useful to write our expression of interest $\hat{V}_{IJ}$ using the Hájek projection $\hat{T}$ of $T$:

$$\hat{V}_{IJ} = \frac{n}{n-1} \cdot \frac{s(n)^2}{n^2} \cdot \sum_{i=1}^{n} (A_i + R_i)^2,$$

where

$$A_i = \mathbb{E}_{Z^* \subset \hat{F}} \left[ \hat{T} \mid Z^*_1 = Z_i \right] - \mathbb{E}_{Z^* \subset \hat{F}} \left[ \hat{T} \right] \quad \text{and}$$

$$R_i = \mathbb{E}_{Z^* \subset \hat{F}} \left[ T - \hat{T} \mid Z^*_1 = Z_i \right] - \mathbb{E}_{Z^* \subset \hat{F}} \left[ T - \hat{T} \right].$$

As we show in Lemma 8, the main effects $A_i$ give us $\sigma^2_n$, in that

$$1 - \frac{2}{n} \frac{s(n)^2}{n^2} \sum_{i=1}^{n} A_i^2 \rightarrow_p 1. \quad (25)$$

Meanwhile, Lemma 9 establishes that the $B_i$ all satisfy

$$\mathbb{E} \left[ R_i^2 \right] \leq \frac{2}{n} \text{Var} \left[ T (x; Z_1, \ldots, Z_{s(n)}) \right], \quad (26)$$

and so

$$\mathbb{E} \left[ \frac{s(n)^2}{n^2} \sum_{i=1}^{n} R_i^2 \right] \leq \frac{2}{n} \frac{s(n)^2}{n^2} \text{Var} \left[ T (x; Z_1, \ldots, Z_{s(n)}) \right] \leq \frac{2}{n} \frac{s(n)^2}{n^2} \log(n)^d \sigma^2_n.$$

Because all terms are positive and $s(n)/n \log(n)^d$ goes to zero by hypothesis, Markov’s inequality implies that

$$1 - \frac{s(n)^2}{n^2} \sum_{i=1}^{n} R_i^2 \rightarrow_p 0. \quad (25)$$

Using Cauchy-Schwarz to bound the cross terms of the form $A_i R_i$, we can thus conclude that $\hat{V}_{IJ}$ is consistent for $\sigma^2_n$.

**Lemma 8.** Under the conditions of Theorem 7, (25) holds.

**Proof.** We can write

$$A_i = \mathbb{E}_{Z^* \subset \hat{F}} \left[ \hat{T} \mid Z^*_1 = Z_i \right] - \mathbb{E}_{Z^* \subset \hat{F}} \left[ \hat{T} \right]$$

$$= \left(1 - \frac{s(n)}{n}\right) T_1 (Z_i) + \left( \frac{s(n)}{n} - \frac{n-1}{n^2} \right) \sum_{j \neq i} T_1 (Z_j),$$
and so our sum of interest is asymptotically unbiased for $\sigma^2_n$:

$$
\mathbb{E} \left[ \frac{n}{n-1} \frac{s(n)^2}{n^2} \sum_{i=1}^{n} A_i^2 \right] \sim \frac{s(n)^2}{n} \mathbb{E} \left[ T_1(Z)^2 \right] \\
= \frac{s(n)}{n} \text{Var} \left[ \hat{T}(Z_1, ..., Z_n) \right] \\
= \sigma^2_n.
$$

Thus, it only remains to show that this sum has a coefficient of variation that converges to zero. Since the $A_i$ are only weakly correlated, it suffices to show that

$$
\frac{1}{\sqrt{n} \text{Var} [A_i^2]} \to_p 0.
$$

Because $|Y_i| \leq M$, we must have $0 \leq A_i^2 \leq 4M^2$. In the worst case

$$
\frac{\mathbb{E} [A_i^2]}{\text{Var} [A_i^2]} \leq 16M^4,
$$

and to coefficient of variation in fact converges to zero. \(\square\)

**Lemma 9.** Under the conditions of Theorem 7, (26) holds.

**Proof.** Without loss of generality, we establish (26) for $R_1$. Using the ANOVA decomposition (22), we can write our term of interest as

$$
R_1 = \mathbb{E}_{Z^* \subset \hat{F}} \left[ T - \hat{T} | Z_1^* = Z_1 \right] - \mathbb{E}_{Z^* \subset \hat{F}} \left[ T - \hat{T} \right] \\
= \left( \frac{s-1}{n-1} - \binom{s}{2} / \binom{n}{2} \right) \sum_{i=2}^{n} T_2(Z_1, Z_i) \\
+ \left( \binom{s-1}{2} / \binom{n-1}{2} - \binom{s}{2} / \binom{n}{2} \right) \sum_{2 \leq i < j \leq n} T_2(Z_i, Z_j) \\
+ \left( \binom{s-1}{2} / \binom{n-1}{2} - \binom{s}{3} / \binom{n}{3} \right) \sum_{2 \leq i < j \leq n} T_3(Z_1, Z_i, Z_j) \\
+ \left( \binom{s-1}{3} / \binom{n-1}{3} - \binom{s}{3} / \binom{n}{3} \right) \sum_{2 \leq i < j < k \leq n} T_3(Z_i, Z_j, Z_k) \\
+ \ldots
$$
Because all the terms in the ANOVA expansion are mean-zero and uncorrelated, we see using notation from (23) that

\[
\mathbb{E} \left[ R_1^2 \right] = (n - 1) \left( \frac{s - 1}{n - 1} - \left( \frac{s}{2} / \left( \frac{n}{2} \right) \right) \right)^2 V_2 \\
+ \left( \frac{n - 1}{2} \right) \left( \left( \frac{s - 1}{2} / \left( \frac{n - 1}{2} \right) \right) - \left( \frac{s}{2} / \left( \frac{n}{2} \right) \right) \right)^2 V_2 \\
+ \left( \frac{n - 1}{2} \right) \left( \left( \frac{s - 1}{2} / \left( \frac{n - 1}{2} \right) \right) - \left( \frac{s}{3} / \left( \frac{n}{3} \right) \right) \right)^2 V_3 \\
+ \left( \frac{n - 1}{3} \right) \left( \left( \frac{s - 1}{3} / \left( \frac{n - 1}{3} \right) \right) - \left( \frac{s}{3} / \left( \frac{n}{3} \right) \right) \right)^2 V_3 \\
+ \ldots
\]

Recall that

\[
\sum_{k=1}^{s} \left( \begin{array}{c} s \\ k \end{array} \right) V_k = \text{Var} \left[ T \left( Z_1, ..., Z_s \right) \right].
\]

The above sum is maximized when all the variance is contained in second-order terms, and \( \left( \begin{array}{c} s \\ 2 \end{array} \right) V_2 = \text{Var} \left[ T \right] \). This implies that

\[
\mathbb{E} \left[ R_1^2 \right] \lesssim (n - 1) \left( \frac{s - 1}{n - 1} - \left( \frac{s}{2} / \left( \frac{n}{2} \right) \right) \right)^2 \left( \frac{s}{2} \right)^{-1} \text{Var} \left[ T \left( Z_1, ..., Z_s \right) \right] \\
\sim \frac{2}{n} \text{Var} \left[ T \left( Z_1, ..., Z_s \right) \right],
\]

thus completing the proof. \( \square \)
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