Scalable and Efficient Hypothesis Testing with Random Forests

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December 10, 2019

Abstract

Throughout the last decade, random forests have established themselves as among the most accurate and popular supervised learning methods. While their black-box nature has made their mathematical analysis difficult, recent work has established important statistical properties like consistency and asymptotic normality by considering subsampling in lieu of bootstrapping. Though such results open the door to traditional inference procedures, all formal methods suggested thus far place severe restrictions on the testing framework and their computational overhead often precludes their practical scientific use. Here we propose a hypothesis test to formally assess feature significance, which uses permutation tests to circumvent computationally infeasible estimates of nuisance parameters. We establish asymptotic validity of the test via exchangeability arguments and show that the test maintains high power with orders of magnitude fewer computations. Importantly, the procedure scales easily to big data settings where large training and testing sets may be employed without the need to construct additional models. Simulations and applications to ecological data where random forests have recently shown promise are provided.

Keywords: Ensemble Methods, Permutation Tests, Variable Importance, Exchangeability

1 Introduction

Advances in computing power and big data collection have produced numerous situations in which complex supervised learning methods can drastically outperform more rigid classical statistical models in terms of predictive accuracy. Despite these advances, many such models and algorithms are largely impenetrable to traditional statistical analysis. The random forests algorithm (Breiman, 2001) is among the relatively few supervised procedures for which formal statistical properties have recently been developed, paving the way for inference procedures. As detailed below, however, methods proposed to this point for assessing variable importance have either been ad hoc and susceptible to producing misleading results even in simple settings or have come with severe restrictions on the testing framework while incurring extreme computational overhead. The primary goal of this paper is to formally develop a statistically valid permutation test approach that maintains high power with orders of magnitude fewer required computations that scales naturally and efficiently to large data settings.

Permutation tests have their roots in the work of Fisher (1937) using contingency tables. The canonical permutation test framework relies on an assumption of exchangeability of observations, at least asymptotically. Given iid samples $\mathbf{X} = X_1, ..., X_n$ and $\mathbf{Y} = Y_1, ..., Y_m$, consider the joined sample, $\mathbf{Z} = \mathbf{X} \uplus \mathbf{Y}$, where \uplus indicates concatenation of datasets and let \mathcal{G} be the group of all permutations of the indices 1, ..., N, for N = m + n. Let $T = r(Z_1, ..., Z_N)$ be a statistic of interest and let T_0 denote the statistic calculated on the original data. A p-value for the hypothesis the null hypothesis $H_0: X \stackrel{d}{=} Y$ is given by

$$p = \frac{1}{|\mathcal{G}|} \sum_{g \in \mathcal{G}} I(|T_0| > |T(g\mathbf{Z})|) := 1 - \hat{J}_N(T_0; \mathbf{Z}) + \hat{J}_N(-T_0; \mathbf{Z})$$

where $\hat{J}_N(\cdot; \mathbf{Z})$ is the permutation distribution function, often referred to as the conditional distribution. To achieve a test with type I error rate α , we reject H_0 if $p < \alpha$. Pesarin and Salmaso (2010) note that this p-value is conditionally unbiased, i.e. $P(p < \alpha | \mathbf{Z}, H_0) \leq \alpha$ and $P(p < \alpha | \mathbf{Z}, H_1) \geq \alpha$. However, this procedure is *not* typically unbiased for more general hypotheses, such as $H_0^f : \mathbb{E}(f(X_1)) = \mathbb{E}(f(Y_1))$ for some integrable function $f(\cdot)$. As such, many permutation procedures are heuristics for hypotheses like H_0^f that may provide some practical use and intuition, but without verified statistical validity.

1.1 Permutation Tests

Classical work on permutation tests from Hoeffding (1952) and Lehmann et al. (1949) demonstrates the convergence of the permutation distribution to the sampling distribution for a wide variety of test statistics. Much of the modern work has focused on extending permutation tests to situations where the data may not be iid or even exchangeable (e.g.

Romano (1990)). Studentization is typically proposed as a means of forcing the sampling distribution of a statistic to converge to a normal distribution to which it is then shown that the permutation distribution also converges. This idea has underpinned results in Neuhaus (1993) and Janssen (2005), who provide various sufficient conditions for the convergence to the unconditional distribution.

Permutation tests are exact tests for hypotheses of equal distribution under the assumption of iid sequences, but as noted above, are not necessarily valid for more general hypotheses. Convergence to the unconditional distribution ensures that the permutation distribution can be used for a finite sample exact test of equality of distribution and an asymptotically valid test for more general hypotheses. In this work, we prove results regarding the asymptotic validity of our procedure for more general hypotheses. The individual models (base learners) in supervised ensembles, such as decision trees in a random forest, naturally lend themselves to the permutation framework by being exchangeable in many practical cases.

1.2 Related Work on Random Forests

Decision trees recursively partition the covariate space and generate predictions by fitting some simple model – often an average or majority vote – within each resulting region. Of particular interest are the classical Classification And Regression Trees (Breiman et al., 1984). CART procedures often have low bias, but can overfit the data without careful pruning. Bagging stabilizes the variance by training many individual learners on bootstrap samples. Random forests (Breiman, 2001) augment the bagging procedure by introducing auxiliary randomness in the construction of each individual learner, leading to trees with a lower degree of dependence but higher individual variances. Since their introduction, random forests have sustained a long track-record of empirical success in terms of predictive accuracy; see Fernández-Delgado et al. (2014) for a recent large-scale comparison in which random forests outperform nearly all competitors.

Extensions of random forests beyond classification/regression forests have also been proposed. Meinshausen (2006) used the weights learned in a regression forest to perform quantile regression. Ishwaran and Lu (2008) suggested survival forests whose consistency properties were recently studied in Cui et al. (2017). Zhu et al. (2015) proposed constructing trees within a reinforcement learning framework. Finally, Athey et al. (2016) proposed the unifying framework of generalized random forests, which use random forests weights for general local parameter estimation.

The flexibility offered by random forests makes rigorous analysis of their statistical properties challenging. Breiman (2001) proposed out of bag (oob) measures for variable importance, though a substantial amount of work since has shown that these importance measures are biased towards inflating the importance of correlated variables (Toloşi and Lengauer, 2011) or variables with many levels (Strobl et al., 2007). Alternative measures

have been proposed, for example, in Altmann et al. (2010); Janitza et al. (2016) but do not come with statistical validity. These procedures also generally involve training many random forests and are thus often computationally intractable. Ishwaran and Lu (2019) provides confidence intervals for the standard oob measures that are valid whenever the random forest is assumed to be L_2 consistent.

Wager et al. (2014) applied the infinitesimal jackknife variance estimate developed in Efron (2014) to produce closed form variance estimates for random forest predictions. Scornet et al. (2015) provided the first consistency results for Breiman's original random forest procedure for additive regression functions. Mentch and Hooker (2016) derived the closed form asymptotic distribution for random forest predictions under restrictions on subsample size. More recently, Wager and Athey (2018) proved both consistency and asymptotic normality for subsampled random forests for potentially larger subsamples whenever trees are restricted to being built according to honesty and regularity conditions and large numbers of trees are constructed.

The asymptotic normality established in Mentch and Hooker (2016) was obtained by casting random forests as incomplete, infinite-order U-statistics. In addition to establishing normality and providing the closed form asymptotic variance, the authors also lay out a formal hypothesis testing procedure for evaluating variable importance. This test, though valid, is quite computationally prohibitive. The hypotheses are presumed to be evaluated at predefined test locations in some test set \mathcal{T} and whenever $|\mathcal{T}| = N_t > 1$, calculating the test statistic involves estimating an $N_t \times N_t$ covariance matrix. Accurate estimation of the covariance necessitates constructing a very large number of trees and becomes computationally infeasible for more than 20-30 test points. Mentch and Hooker (2017) extends the procedure to tests for additivity and provide an alternative approximate test involving random projections that allows the procedure to scale up slightly but with additional computational overhead. Even employing the potentially more efficient infinitesimal jackknife variance estimate utilized in Wager et al. (2014) and Wager and Athey (2018) requires the number of trees constructed be at least on the order of n to be valid.

In contrast, the method we propose here is almost entirely computationally immune to the number of test points. The permutation scheme we employ avoids the need for an explicit covariance estimation and thus does not require a larger number of trees for larger datasets. Instead, our hypothesis tests provide valid p-values for variable importance while maintaining the same order of computational complexity as the original random forest procedure. Put simply, if the size and structure of the available data allows for a random forest model to be constructed, our testing procedure can be readily employed.

The remainder of this paper is laid out as follows. In Section 2, we give an overview of the testing procedure, and further highlight its benefits over existing methods. In Section 3, we present results regarding the statistical properties of the proposed test, namely that it attains validity for the desired hypotheses. In Section 4, we present simulation studies of

the testing procedure for a variety of underlying regression functions. In Section 5, we apply our procedure to multiple ecological datasets where random forests have been successfully employed in applied work. In addition to the main text, all technical proofs are provided in Appendix A, and additional simulations demonstrating the robustness of the proposed procedure are presented in Appendix B.

2 Overview of the Testing Procedure

Consider a sample $\mathcal{D}_n = \{Z_1, Z_2, ..., Z_n\}$, with $Z_i = (\mathbf{X}_i, Y_i)$ consisting of observations on covariates $\mathbf{X} = (X_1, ..., X_p) \in \mathcal{X}$ and a response $Y \in \mathcal{Y}$. In this work, it is assumed that $Z_k \stackrel{iid}{\sim} F$ where F is some distribution with support on $\mathcal{X} \times \mathcal{Y}$. In the regression context, we assume that $Y = m(\mathbf{x}) + \epsilon$ where $m(\mathbf{x}) = \mathbb{E}(Y | \mathbf{X} = \mathbf{x})$ and ϵ is an independent noise process, typically with $\mathbb{E}(\epsilon) = 0$ and $\mathrm{Var}(\epsilon) < \infty$. The goal of the random forest procedure is to accurately estimate $m(\mathbf{x})$. Each tree in a random forest is constructed by drawing subsamples of size $k_n < n$, from \mathcal{D}_n , drawing a randomization parameter ϵ from some distribution ϵ , and constructing the randomized decision tree. This process is repeated ϵ times and the random forest prediction at some ϵ is given by

$$RF_{B,k_n}(\boldsymbol{x}) = \frac{1}{B} \sum_{i=1}^{B} T_{j,k_n}(\boldsymbol{x}; \xi_j; \mathcal{D}_n).$$
(2.1)

We can similarly evaluate the RF prediction accuracy at a single fixed test location \boldsymbol{x} and with true response value y via its mean squared error

$$MSE_{RF}(\boldsymbol{x}; y, \mathcal{D}_n) = \left(\frac{1}{B} \sum_{j=1}^{B} T_{k_n, j}(\boldsymbol{x}) - y\right)^2.$$

For sufficiently large B, Eq. 2.1 can be made arbitrarily close to $\mathbb{E}_{\Xi}(RF_{B,k_n}(\boldsymbol{x})|\mathcal{D}_n)$, where the expectation is taken over the subsampling and randomization distributions, conditional on the data. Eq. 2.1 can be interpreted as a Monte Carlo approximation to the infinite forest. The effect of this approximation is studied in Scornet (2016). In what follows, we use the shorthand $X_n \stackrel{d}{\to} \mathcal{N}(\mu, \sigma^2)$ to mean that $X_n \stackrel{d}{\to} Z$ where $Z \sim \mathcal{N}(\mu, \sigma^2)$.

Similarly, we can calculate the MSE of a forest at a collection of test points $\mathcal{T} = [(\boldsymbol{x}_1, y_1), ..., (\boldsymbol{x}_{N_t}, y_{N_t})]$ as $MSE_{RF}(\mathcal{T}) = \frac{1}{N_t} \sum_{\ell=1}^{N_t} MSE_{RF}(\boldsymbol{x}_\ell; Y_\ell, \mathcal{D}_n)$. Let RF^{π} be defined similarly to Eq. 2.1, but with \mathcal{D}_n replaced by \mathcal{D}_n^{π} , where \mathcal{D}_n^{π} replaces some subset of features with an alternate copy drawn independent of Y given the rest of the covariates. To make this concrete, suppose that this subset consists of just a single feature X_j . We can then evaluate whether X_j is important by conducting a test of the following hypotheses

$$H_0^j : \mathbb{E}(MSE_{RF}(\mathcal{T})) = \mathbb{E}(MSE_{RF^{\pi}}(\mathcal{T}))$$

$$H_1^j : \mathbb{E}(MSE_{RF}(\mathcal{T})) < \mathbb{E}(MSE_{RF^{\pi}}(\mathcal{T}))$$
(2.2)

where the expectation is taken over the training data and auxillary randomness, but is conditional on \mathcal{T} . We call X_j important if we are able to reject H_0^j . This definition of importance is model based and therefore less general than alternative definitions such as that utilized in the recent *knockoff* literature (Barber et al., 2015; Candes et al., 2016), where a variable X_j is deemed unimportant if

$$(Y \perp \!\!\!\perp X_i) \mid \boldsymbol{X}_{-i}.$$

It should be noted that the above is neither necessary nor sufficient for H_0^j . However, in practice, the test statistic utilized in the knockoff procedure is generally taken as the difference in importance measures between original and knockoff variables and thus the outcome of the procedure itself remains highly model dependent. We also note that our procedure, while it could use knockoffs, does not require knowledge of the distribution of the covariates.

2.1 Testing Procedure

In general, if two randomized ensemble methods produce predictions that are similarly accurate, then the permutation distribution of discrepancies in accuracy should be centered around 0. In our particular setting for testing feature significance, we compare the accuracy of two random forests built on different data. For a given (original) dataset \mathcal{D}_n , we first construct \mathcal{D}_n^{π} in such a way so as to remove any dependence of response on these features. However, rather than permuting the data and retraining entire random forests, we first train trees on both \mathcal{D}_n and \mathcal{D}_n^{π} separately, record predictions at the test locations, and then permute the predictions between the forests. The new forests formed at each iteration thus consist of some trees built on the original data and some built with the permuted counterpart so that on average. In this light, the testing procedure can be seen as directly analogous to a classic permutation test to evaluate equality in distribution across two groups. This procedure requires only 2B trees, regardless of the size of the test set.

Pseudo-code for the permutation test is provided in Algorithm 1. We use \oplus to denote concatenation of data matrices by column, \oplus to denote concatenation by row, and \ominus to denote the removal of columns from a dataset. In order to prevent p-values exactly equal to 0, we add 1 to the numerator and denominator, ensuring that under H_0 the p-values are stochastically larger than uniform random variables. This suffices to make the testing procedure slightly more conservative, but more amenable to potential p-value transforming procedures; see, for example, Phipson and Smyth (2010) for a more thorough discussion. Crucially, note that this procedure requires no explicit variance estimation of the N_t predictions made by individual forests, thereby providing a dramatic computational speed-up over existing parametric approaches (Mentch and Hooker, 2016, 2017) that require the estimation of a $N_t \times N_t$ covariance matrix.

Algorithm 1: Permutation test pseudocode for variable importance

```
Data: Training data \mathcal{D}_n test sample (\mathcal{T} = [(\boldsymbol{x}_1, y_1), ..., (\boldsymbol{x}_{N_t}, y_{N_t})]), specified feature(s) of interest, \boldsymbol{X}_S, N_0 number of permutations to evaluate

Result: p-value, \tilde{p} for importance of \boldsymbol{X}_S at points in \mathcal{T}_n

SET number of permutations n_{perm}, subsample size k_n, and n_{tree} = B;

DEFINE \boldsymbol{X}_S^\pi by permuting the rows of \mathcal{D}_n and selecting the columns corresponding to \boldsymbol{X}_S;

DEFINE \mathcal{D}_n^\pi = \mathcal{D}_n \ominus \boldsymbol{X}_S \oplus \boldsymbol{X}_S^\pi;

for i in \{1, ..., B\} do

SAMPLE k_n rows from \mathcal{D}_n: \mathcal{D}_i^* = \{Z_{i,1}^*, ..., Z_{i,k_n}^*\};

SAMPLE k_n rows from \mathcal{D}_n^\pi: \mathcal{D}_i^{**} = \{Z_{i,1}^*, ..., Z_{i,k_n}^*\};

PREDICT at \mathcal{T}_n using T_i, T_i^\pi, generating T_i = [T_i(\boldsymbol{x}_1), ..., T_i(\boldsymbol{x}_{N_t})] and T_i^\pi = [T_i^\pi(\boldsymbol{x}_1), ..., T_i^\pi(\boldsymbol{x}_{N_t})] end

CALCULATE MSE_0 = \frac{1}{N_t} ||\frac{1}{B}\sum_{i=1}^B T_i - \boldsymbol{y}||_2^2 and MSE_0^\pi = \frac{1}{N_t} ||\frac{1}{B}\sum_{i=1}^B T_i^\pi - \boldsymbol{y}||_2^2;

for j in \{1, ..., N_0\} do

SAMPLE T_{j,1}^*, ..., T_{j,B}^* from \{T_1, ...T_B, T_1^\pi, ..., T_B^\pi\} without replacement, call the B remaining trees T_{j,1}^{**\pi}, ..., T_{j,B}^{**\pi};

CALCULATE MSE_j^* = \frac{1}{N_t} ||\frac{1}{B}\sum_{l=1}^B T_{j,l}^* - \boldsymbol{y}||_2^2 and MSE_j^{*\pi} = \frac{1}{N_t} ||\frac{1}{B}\sum_{l=1}^B T_{j,l}^{*\pi} - \boldsymbol{y}||_2^2 end

CALCULATE \tilde{p} = \frac{1}{N_t} ||\frac{1}{B}\sum_{l=1}^{B} T_{j,l}^* - \boldsymbol{y}||_2^2 and MSE_j^{*\pi} = \frac{1}{N_t} ||\frac{1}{B}\sum_{l=1}^B T_{j,l}^{*\pi} - \boldsymbol{y}||_2^2 end
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3 Theoretical Justification

We now develop the theoretical backing for the hypothesis testing procedure outlined above. In subsection 3.1, we make explicit the connection between bagged-models and exchangable random variables. Then, in subsection 3.2, we use these results establish asymptotic normality for subsampled random forest predictions, under mild conditions. Next, in subsection 3.3, we extend these results to the fixed-test set MSE, establishing a CLT for this quantity. To use these distributions directly is unwieldy - there is no obvious consistent estimator of the variance parameters available. Thus, in subsection 3.4, we prove that the proposed permutation test is asymptotically equivalent to the computationally infeasible parametric test, building on recent arguments from Chung and Romano (2013). For readability, most proofs are reserved for Appendix A.

3.1 Exchangeable Random Variables & Permutation Tests

Recall that a sequence of random variables $X_1, X_2, ...$ is exchangeable if $(X_{i_1}, X_{i_2}, ..., X_{i_k}) \stackrel{d}{=} (X_{\pi(1)}, X_{\pi(2)}, ..., X_{\pi(k)})$ for every finite sub-collection indexed by $i_1, ..., i_k$ and every permutation of the indices $\pi(\cdot)$, see Aldous (1985) for a thorough review.

Permutation tests naturally lend themselves to exchangeable data by providing a means of

evaluating the hypothesis that the joint distribution of a collection of random variables is invariant under permutations. They maintain exactness for the null hypothesis whenever $X_i \stackrel{iid}{\sim} P$ and independently $Y_j \stackrel{iid}{\sim} Q$ because the joint measure of the data factorizes as

$$\mu(\boldsymbol{X}, \boldsymbol{Y}) = \prod_{i=1}^{n} P(X_i) \prod_{j=1}^{m} Q(Y_j)$$

which is invariant to permutations of observations if and only if P = Q.

Modern work for permutation tests has focused largely on modifications needed to account for violations of the exchangeability assumption. Chung and Romano (2013) propose a studentization of the permutation test statistic when conducting inference a functional of two distributions. Consider, for example a two sample problem, with $X_1, ..., X_n \stackrel{iid}{\sim} P_X = \mathcal{N}(0,5)$ and independently let $Y_1, ..., Y_m \stackrel{iid}{\sim} P_Y = \mathcal{N}(0,1)$. Clearly, median $(P_X) = \text{median}(P_Y)$, but the data are no longer exchangeable and so an unstudentized permutation test of H_0 : median $(P_X) = \text{median}(P_Y)$ is no longer valid at a pre-specified level (see Chung and Romano (2013) for details). However, note that exchangeability is violated only because the data are no longer identically distributed; permutation tests can remain valid for data that are correlated but identically distributed so long as the pairwise dependence is constant.

Theorem 1. Denote a sequence of (potentially randomized) subsampled trees as $\{T_k(\cdot)\}_1^{\infty}$. Under the conditions outlined above, the residuals at $\mathbf{Z}^* = (\mathbf{X}^*, Y^*) \sim F$ given by

$$r_k = T_k(\boldsymbol{X}^*) - Y^*$$

form an infinitely exchangeable sequence of random variables.

In the case of a single random forest, exchangeability is readily apparent as the order in which trees are trained has no bearing on their structure. Indeed, Theorem 1 can be extended to any bagged learning method.

The primary goal of this work is to identify covariates that produce statistically significant improvements in model accuracy. To assess this, we consider building two forests, one on the original dataset \mathcal{D}_n and another on a second dataset \mathcal{D}_n^{π} wherein the covariate(s) of interest X_S are rendered independent of Y, conditional on the rest of the features. This muting can be achieved in various ways:

- Outright exclusion: X_S is simply removed from the second training dataset.
- Random permutation: Each covariate in X_S is randomly shuffled so that X_S is replaced by some permuted alternative X_S^{π} in the second training dataset.
- Knockoffs: Each covariate in X_i in X_S is replaced by some knockoff alternative X_i^{π} sampled from the distribution of $X_i|X_{-i}$ so that X_S is replaced by a randomized alternative X_S^{π} in the second training dataset. See Candes et al. (2016) for details.

Given two samples \mathcal{D}_n^1 and \mathcal{D}_n^2 drawn independently from the same population and a collection of subsampled trees, say T_1 and T_2 , trained on each, $T_1 \stackrel{d}{=} T_2$, but the trees are no longer exchangeable because the conditioning random vector (i.e. the training data) is different. In general, the within sample dependence between trees will be higher than the between sample correlation. In practice, the trees are approximately exchangeable - higher within sample dependence tends to die out when the subsample size grows slower than n. More specifically, provided the tree distributions converge weakly to some distribution, we can establish the notion of asymptotic exchangeability. This idea is well studied, if rarely explicitly mentioned, with necessary conditions provided, for example, in Romano (1990); Chung and Romano (2013); Good (2002). Recall also that the original motivation for inserting the additional randomness in random forests was to reduce between-tree correlation, further dampening the effect.

In practical terms, this implies that replacing the covariates under investigation with a randomized counterpart – either a permutation or knock-off – leads to a procedure with more desirable properties than when those covariates are simply dropped, creating a lower-dimensional covariate space. In particular, to attain near-exchangeability under the null hypothesis, the individual trees should be constructed in a near-identical fashion by building trees on data with the same dimension feature space, on the same subsample size, and with other various tree-specific parameters controlled.

Given a dataset \mathcal{D}_n with $n \times p$ design matrix X, let $S \subset \{1, ..., p\}$ and define $X_S = \{X_j : j \notin S\}$ where we take X_S to be the covariates of interest. We then create a randomized version of X_S independent of Y, denoted by X_S^{π} . Note in particular that when the entire joint density P(X) of the covariates is known, Algorithm 1 of Candes et al. (2016) can be used to generate the knockoffs that make up X_S^{π} which then ensures that $[X_{-S}, X_S] \stackrel{d}{=} [X_{-S}, X_S^{\pi}]$. By construction, $X_S^{\pi} \perp \!\!\!\perp Y | X_{-S}$ and consequently, if we now replace X_S with X_S^{π} in the design matrix to form a new training dataset \mathcal{D}_n^{π} , then the trees trained on \mathcal{D}_n^{π} inherit the conditional independence so that $T(x; \mathcal{D}_n^{\pi}) \perp \!\!\!\perp Y | X_{-S}$.

Assuming X_{-S} are the only predictively important covariates, we would expect predictions from trees trained on \mathcal{D}_n to have the same distribution as those generated from trees trained on \mathcal{D}_n^{π} . As such, the trees should be asymptotically exchangeable between forests and it follows that we can test this exchangeability assumption via a permutation test.

3.2 Asymptotic Behavior of Trees

Within-forest exchangeability is not sufficient to justify the proposed testing procedure at the nominal level. Instead, we need to establish sufficient conditions to justify exchanging trees between forests. An important step in this direction is to establish the existence of a limiting sequence of subsampled trees that behave like an iid sequence. Condition 1. There exists a random function T_{∞} such that $\lim_{n\to\infty} T_{k_n} \stackrel{d}{=} T_{\infty}$

In subsubsection 3.3.1 we provide sufficient conditions for this to be satisfied. Note that this condition is similar in spirit to Assumption 15.7.1 in Lehmann and Romano (2006), which is fundamental to the validity of subsampling based intervals for model parameters.

In practice, we would like to establish results for random forests trained on growing subsamples. If we insist that the subsample size k_n grow slower than \sqrt{n} , we obtain the following intuitive result.

Lemma 1. Consider a collection of B_n trees built from a training dataset of size n on subsamples of size k_n , say $\{T_{j,k_n}\}_{j=1}^{B_n}$, satisfying Condition 1. Then, as long as $k_n/\sqrt{n} \to 0$ and

$$\binom{B_n}{2} \log \left[\frac{\binom{n-k_n}{k_n}}{\binom{n}{k_n}} \right] \to 0$$

the infinite sample sequence of trees, $\{T_{1,\infty,k_{\infty}},...,T_{B,\infty,k_{\infty}},...\}$, is an infinite sequence of pairwise independent random functions.

The condition on the number of trees B_n is likely not of much practical importance. For finite B_n , the probability sequence has the form of a_n^K , so because $a_n \to 1$, a_n^K also converges to 1. However, if we let B_n grow with n, the number of trees may overwhelm the independence induced by subsampling. Thus, we must let the log probability of an individual pair being independent go to 0 faster than $\binom{B_n}{2} \approx B_n^2/2$ goes to infinity.

Lemma 1 establishes asymptotic pairwise independence, but not that the limiting sequence is iid. For this, we turn to a result from Aldous (1985).

Lemma 2. (Aldous, 1985) Let $Z_1, Z_2, ...$ be an infinitely exchangeable sequence. If $Z_i \perp \!\!\! \perp Z_j, i \neq j$, then $Z_1, Z_2, ...$ is a sequence of iid random variables.

An immediate consequence of the preceding lemmas is the following corollary.

Corollary 1. Let $\{T_{j,k_n}\}_{j=1}^{B_n}$ be a collection of B_n trees trained on subsamples from \mathcal{D}_n , satisfying the conditions of Lemma 1. Then, $\{T_{j,\infty}\}_{j=1}^{\infty} := \lim_{n\to\infty} \{T_{j,k_n}\}_{j=1}^{B_n}$ is an iid sequence of functions.

The infinite sequence of subsampled trees enjoys many properties that the finite sequence does not. In particular, we can obtain the following pointwise central limit theorem.

Corollary 2. Let $\{T_{j,k_n}\}_{j=1}^{B_n}$ be a sequence of trees on subsamples from \mathcal{D}_n , satisfying the conditions of Lemma 1 and Condition 1. Further, assume $\mathbf{x} \in \mathcal{X}$ is such that $0 < Var(T_{\infty}(\mathbf{x})) = \sigma^2(\mathbf{x}) < \infty$. Then as $n \to \infty$

$$\sqrt{B_n} \left[\frac{1}{B_n} \sum_{i=1}^{B_n} T_{i,k_n}(\boldsymbol{x}) - \mathbb{E} \left(\frac{1}{B_n} \sum_{i=1}^{B_n} T_{i,k_n}(\boldsymbol{x}) \right) \right] \stackrel{d}{\to} \mathcal{N}(0, \sigma^2(\boldsymbol{x}))$$
(3.1)

Corollary 2 follows directly from applying the Central Limit Theorem to the sequence of univariate random variables $\{T_{j,\infty}(\boldsymbol{x})\}_{j=1}^{\infty}$, which are iid by Corollary 1.

Remark. For a collection of test points, $\boldsymbol{x}_1, ..., \boldsymbol{x}_{N_t}$, we can also consider the sequence of vectors $\boldsymbol{T}_{i,k_n} = [T_{i,k_n}(\boldsymbol{x}_1), ..., T_{i,k_n}(\boldsymbol{x}_{N_t})]^T$, which are iid by Corollary 1. If we assume that $\Sigma = \mathbb{E}[(\boldsymbol{T}_{i,k_n} - \mathbb{E}(\boldsymbol{T}_{i,k_n}))(\boldsymbol{T}_{i,k_n} - \mathbb{E}(\boldsymbol{T}_{i,k_n}))^T]$ has finite entries, the multivariate central limit theorem gives that as $n \to \infty$

$$\sqrt{B_n} \left[\frac{1}{B_n} \sum_{i=1}^{B_n} \mathbf{T}_{i,k_n} - \mathbb{E} \left(\frac{1}{B_n} \sum_{i=1}^{B_n} \mathbf{T}_{i,k_n} \right) \right] \stackrel{d}{\to} \mathcal{N}(0,\Sigma).$$

Remark. We can generalize the independence results to a collection of two sets of trees. In particular, suppose that we now train $B_n/2$ trees on $\mathcal{D}_n = \{Z_i\}_{i=1}^n$ and $\mathcal{D}_n^{\pi} = \{Z_i^{\pi}\}_{i=1}^n$, where $Z_i^{\pi} = ([\boldsymbol{X}_{\mathcal{S}}, \boldsymbol{X}_{-\mathcal{S}}^{\pi}]_i, Y_i)$. Note that $Z_i^{\pi} \perp \!\!\!\perp Z_j, \forall i \neq j$, so there is the same independence structure between the datasets as within. Thus, the probability that a pair of trees trained on subsamples of size k_n , one from \mathcal{D}_n and one from \mathcal{D}_n^{π} , are independent is the same as the probability that a pair of trees within forest are independent. As such, $\{T_{i,k_n}(\boldsymbol{x})\}_{i=1}^{B_n}$ and $\{T_{i,k_n}^{\pi}(\boldsymbol{x})\}_{i=1}^{B_n}$, where B_n, k_n satisfy the conditions of Lemma 1, behave like two independently iid samples.

We intentionally leave $\sigma(x)$ as an abstraction since estimation of $\sigma(x)$ is not straightforward. Instead, this result will be used as the basis for asymptotic validity of our permutation test which, uncharacteristically, is far more computationally efficient. Going forward, we consider the asymptotic case, so that the sequence of tree predictions behaves like an iid sequence. Further, in the infinite sample case, the number of trees can be made arbitrarily large, and so we allow B to go to infinity with the understanding that it does so in such a way that respects the requirements of Lemma 1. This is largely a matter of notational convenience; we could explicitly include the dependence on n in each of the following statements and stress that the limiting distributions only hold as $n \to \infty$.

3.3 Asymptotic Distribution of MSEs

Unfortunately, the MSE is not a linear function of exchangeable random variables and thus requires more careful attention before being used as a test statistic in a permutation test. In this subsection we establish the asymptotic normality of the MSE which we then utilize to show that the difference in MSEs between two forests is asymptotically normal. To begin, consider a single test point (x, y). We can write the MSE as

$$MSE_{RF}(\boldsymbol{x};y) = g\left(\frac{1}{B}\sum_{i=1}^{B}T_{i}(\boldsymbol{x}), y\right)$$
 (3.2)

where $g(a,b) = (a-b)^2$. In what follows, we suppress the dependence on y, writing just $MSE_{RF}(\boldsymbol{x};y) = g(RF_B(\boldsymbol{x}))$. We derive the asymptotic distribution of the MSE via the

delta method, which we belabor here for its intuitive value. We can then appeal to the mean value theorem to say

$$g(RF_B(\boldsymbol{x})) = g(\mathbb{E}RF_B(\boldsymbol{x})) + g'(\tilde{R}_B(\boldsymbol{x}))[RF_B(\boldsymbol{x}) - \mathbb{E}RF_B(\boldsymbol{x})]$$

where $\tilde{R}_B(\boldsymbol{x})$ is a random quantity bounded between $RF_B(\boldsymbol{x})$, $\mathbb{E}RF_B(\boldsymbol{x})$. The law of large numbers gives that $RF_B(\boldsymbol{x}) = \mathbb{E}RF_B(\boldsymbol{x}) + o_P(1)$ and further $\tilde{R}_B(\boldsymbol{x}) \stackrel{p}{\to} \mathbb{E}RF_B(\boldsymbol{x})$. Next, continuity of g' gives that $g'(\tilde{R}_B(\boldsymbol{x})) \stackrel{p}{\to} g(\mathbb{E}RF_B)$. Thus,

$$\sqrt{B} \left[g(RF_B(\boldsymbol{x})) - g(\mathbb{E}RF_B(\boldsymbol{x})) \right] = g'(\tilde{R}_B(\boldsymbol{x})) \sqrt{B} \left[RF_B(\boldsymbol{x}) - \mathbb{E}RF_B(\boldsymbol{x}) \right]
\stackrel{d}{\to} \mathcal{N} \left(0, g'(\mathbb{E}RF_B(\boldsymbol{x}))^2 \sigma^2 \right)
\stackrel{d}{=} \mathcal{N} \left(0, 4(\mathbb{E}RF_B(\boldsymbol{x}) - y)^2 \sigma^2 \right) \text{ for } g(x) = (x - y)^2.$$

The calculation above is more informative - we see that the MSE is asymptotically a linear function of the random forest prediction. An issue is that the above quantity is centered around $g(\mathbb{E}RF_B(\mathbf{x}))$ rather than $\mathbb{E}g(RF_B(\mathbf{x}))$, which we now address. In particular, suppose we begin by centering around $\mathbb{E}g(RF_B(\mathbf{x}))$ rather than $g(\mathbb{E}RF_B(\mathbf{x}))$. Then,

$$\sqrt{B} \left[g \left(RF_B(\boldsymbol{x}) \right) - \mathbb{E}g \left(RF_B(\boldsymbol{x}) \right) \right] =$$

$$\sqrt{B} \left[g \left(RF_B(\boldsymbol{x}) \right) - g (\mathbb{E}RF_B(\boldsymbol{x})) \right] + \sqrt{B} \left[g \left(\mathbb{E}RF_B(\boldsymbol{x}) \right) - \mathbb{E}g \left(RF_B(\boldsymbol{x}) \right) \right]$$
(3.3)

so that if $\sqrt{B} [g(\mathbb{E}RF_B(\boldsymbol{x})) - \mathbb{E}g(RF_B(\boldsymbol{x}))] = o(1)$, then the same distributional result holds. This is shown in Lemma 3.

Lemma 3. Assume the conditions needed from Corollary 2. Additionally, assume that g has at least k derivatives for some $k \geq 3$, and that $g^{(k)}(x) < \infty$ for all x. Further, assume that $\mathbb{E}|T_i(x)|^k < \infty$. Then,

$$\sqrt{B} \left[\mathbb{E} g(RF_B(\boldsymbol{x})) - g(\mathbb{E} RF_B(\boldsymbol{x})) \right] = \frac{g''(\mathbb{E} RF_B(\boldsymbol{x}))\sigma^2}{2\sqrt{B}} + o(B^{-3/2}) = o(1)$$

Since the MSE function defined as $g(RF_B(\mathbf{x})) = (RF_B(\mathbf{x}) - y)^2$ satisfies the conditions posited by Lemma 3, we can conclude that

$$\sqrt{B}\left[g\left(RF_B(\boldsymbol{x})\right) - \mathbb{E}g\left(RF_B(\boldsymbol{x})\right)\right] \stackrel{d}{\to} \mathcal{N}\left(0, g'(\mathbb{E}RF_B(\boldsymbol{x}))^2\sigma^2\right).$$

Application of the mean value theorem requires that $g'(\mathbb{E}RF_B(\boldsymbol{x})) \neq 0$ if and only if $\mathbb{E}RF_B \neq y$. The expected prediction can be written as $\mathbb{E}RF_B(\boldsymbol{x}) = m(\boldsymbol{x}) + \delta(\boldsymbol{x})$, where $\delta(\boldsymbol{x})$ is the pointwise bias of the random forest. Recalling that the response is given by $Y = m(\boldsymbol{x}) + \epsilon$, if it holds for all \boldsymbol{x} that $P(\epsilon \neq \delta(\boldsymbol{x})) = 1$, then the result holds for the squared error calculated with respect to almost all Y and thus is trivially satisfied for continuous errors. A similar result could be applied to any continuously differentiable loss function $g(\cdot, \cdot)$, again under the condition that g' is almost surely non zero.

Remark. This CLT result does not depend on Corollary 2. In fact, a similar argument could be used to justify the asymptotic normality of the MSE for any random forest who satisfies a central limit theorem and a law of large numbers (with respect to its own expectation), such as the results in Mentch and Hooker (2016) and Wager and Athey (2018).

We can extend this result to the two forest case, where we compare the MSE of $RF_B(\mathbf{x})$ against that of $RF_B^{\pi}(\mathbf{x})$. In particular, if $\mathbb{E}MSE_{RF}(\mathbf{x};y) = \mathbb{E}MSE_{RF^{\pi}}(\mathbf{x};y)$, we see that

$$\sqrt{B}\left[MSE_{RF}(\boldsymbol{x};y) - MSE_{RF^{\pi}}(\boldsymbol{x};y)\right] \stackrel{d}{\to} \mathcal{N}\left(0, g'(\mathbb{E}RF_B(\boldsymbol{x}))^2\sigma^2 + g'(\mathbb{E}RF_B^{\pi}(\boldsymbol{x}))^2\sigma_{\pi}^2\right)$$
(3.4)

where $\sigma_{\pi}^2 = \text{Var}(T^{\pi}(\boldsymbol{x}))$. This extension uses a similar argument as before to justify centering around the expected MSE instead of the MSE of the expected forest.

Now consider a test set with many points, denoted $\mathcal{T} = [(\boldsymbol{x}_1, y_1), ..., (\boldsymbol{x}_{N_t}, y_{N_t})]^T$. Given the vector of random forest predictions, $RF_B(\mathcal{T})$, we can calculate the pointwise squared errors as $MSE_{RF}(\mathcal{T}) = [(RF_B(\boldsymbol{x}_i) - y_i)^2]_{i=1}^{N_t}$. We now introduce some additional notation to establish joint asymptotic normality of this quantity. Let $g_m : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}^m$ be defined as $g_m([(a_1, b_1), ..., (a_m, b_m)]^T) = [g(a_1, b_1), ..., g(a_m, b_m)]^T$ for some continuously differentiable function $g(\cdot, \cdot)$. In particular, we can write the MSE vector as $MSE_{RF}(\mathcal{T}) = g_{N_t}([(RF_B(\boldsymbol{x}_1), y_1), ..., (RF_B(\boldsymbol{x}_{N_t}), y_{N_t})])$. Then, recalling that a multivariate CLT was shown to hold, we can again appeal to the mean value theorem to write

$$\sqrt{B}\left(MSE_{RF}(\mathcal{T}) - \mathbb{E}MSE_{RF}(\mathcal{T})\right) = \sqrt{B}\nabla g_{N_t}(\tilde{R}_B(\mathcal{T}))\left(RF_B(\mathcal{T}) - \mathbb{E}RF_B(\mathcal{T})\right)$$

where $\tilde{R}_B(\mathcal{T})$ is some point in the hyper-rectangle defined by $\bigotimes_{i=1}^{N_t} [RF_B(\boldsymbol{x}_i), \mathbb{E}RF_B(\boldsymbol{x}_i)],$ where the intervals are understood to begin at $\min\{RF_B(\boldsymbol{x}_i), \mathbb{E}RF_B(\boldsymbol{x}_i)\}$ and \bigotimes is the cartesian product. Note that the area of this rectangle vanishes, so that $\sqrt{B}\left(MSE_{RF}(\mathcal{T}) - \mathbb{E}MSE_{RF}(\mathcal{T})\right)$ is also asymptotically a linear rescaling of the random forest prediction. Therefore, the multipoint MSE satisfies

$$\sqrt{B} \left(MSE_{RF}(\mathcal{T}) - \mathbb{E}MSE_{RF}(\mathcal{T}) \right) \stackrel{d}{\to} \mathcal{N} \left(0, \left[\nabla g_{N_t}(\mathbb{E}RF_B(\mathcal{T})) \right]^T \Sigma \left[\nabla g_{N_t}(\mathbb{E}RF_B(\mathcal{T})) \right] \right)$$

as $B \to \infty$ where Σ is the covariance induced by the proximity of the test points in \mathcal{T} . Then, let $1/N_t$ be the $N_t \times 1$ vector of the quantity $1/N_t$, so that as $B \to \infty$, the limiting distribution of the MSE of a subsampled random forest is given by

$$\sqrt{B}(\mathbf{1}/\mathbf{N}_{t}^{T}MSE_{RF}(\mathcal{T}) - \mathbf{1}/\mathbf{N}_{t}^{T}\mathbb{E}MSE_{RF}(\mathcal{T}))) \stackrel{d}{\to} \\
\mathcal{N}\left(0, \mathbf{1}/\mathbf{N}_{t}^{T}[\nabla g_{N_{t}}(\mathbb{E}RF_{B}(\mathcal{T}))]^{T}\Sigma[\nabla g_{N_{t}}(\mathbb{E}RF_{B}(\mathcal{T}))]\mathbf{1}/\mathbf{N}_{t}\right) \quad (3.5)$$

where we have appealed to the Cramér-Wold theorem in the above.

Finally, to connect back to the testing procedure proposed earlier, we now derive the asymptotic distribution of the differences in MSE between two forests. Let $MSE_{RF}(\mathcal{T})$

be the MSE of a random forest at a set of test points \mathcal{T} and let $MSE_{RF^{\pi}}(\mathcal{T})$ denote the MSE of a forest trained on the partially randomized data. By the results above, under the hypothesis that $\mathbb{E}MSE_{RF}(\mathcal{T}) = \mathbb{E}MSE_{RF^{\pi}}(\mathcal{T})$, we have that as $B \to \infty$,

$$\sqrt{B}\mathbf{1}/N_{t}^{T}(MSE_{RF}(\mathcal{T}) - MSE_{RF^{\pi}}(\mathcal{T})) \stackrel{d}{\rightarrow} \mathcal{N}(0, \tau^{2})$$

for some $\tau^2 > 0$ that does not necessarily have a form that is amenable to analysis. To calculate τ^2 , first note that for each MSE $g_j(RF_B(\mathbf{X}_j)) = (RF_B(\mathbf{X}_j) - Y_j)^2$, by continuity, $g'_i(\tilde{R}_B(\mathbf{X}_j)) = g'_i(\mathbb{E}RF_B(\mathbf{X}_j)) + o_P(1)$. Thus, we see that

$$MSE_{RF}(\mathcal{T}) - \mathbb{E}MSE_{RF}(\mathcal{T}) = \frac{1}{N_t} \sum_{j=1}^{N_t} MSE_{RF}(\mathbf{X}_j, Y_j)$$

$$= \frac{1}{N_t} \sum_{j=1}^{N_t} g_j'(\mathbb{E}RF_B(\mathbf{X}_j)) \left[RF_B(\mathbf{X}_j) - \mathbb{E}RF_B(\mathbf{X}_j) \right] + o_P(1)$$

$$= \frac{1}{N_t} \sum_{j=1}^{N_t} g_j'(\mathbb{E}RF_B(\mathbf{X}_j)) \left[\frac{1}{B} \sum_{i=1}^{B} \left[T_i(\mathbf{X}_j) - \mathbb{E}RF_B(\mathbf{X}_j) \right] \right] + o_P(1)$$

$$= \frac{1}{B} \sum_{i=1}^{B} \underbrace{\frac{1}{N_t} \sum_{j=1}^{N_t} g_j'(\mathbb{E}RF_B(\mathbf{X}_j)) \left[T_i(\mathbf{X}_j) - \mathbb{E}RF_B(\mathbf{X}_j) \right] + o_P(1)}_{T_i}$$

where $g_j(\cdot)$ is used to suggest that the squared difference is calculated with respect to Y_j . \bar{T}_i is an iid sequence, so that $\sqrt{B}[MSE_{RF}(\mathcal{T}) - \mathbb{E}MSE_{RF}(\mathcal{T})]$ is asymptotically an iid sum with mean 0 and variance $\sigma_{\bar{T}}^2$ given by

$$\sigma_{\bar{T}}^2 = \frac{1}{N_t} \sum_{j=1}^{N_t} \sigma_j^2 \left(g_j'(\mathbb{E}RF_B(\boldsymbol{X}_j)) \right)^2 + \frac{2}{N_t} \sum_{i < j} g_j'(\mathbb{E}RF_B(\boldsymbol{X}_j)) g_i'(\mathbb{E}RF_B(\boldsymbol{X}_i)) \rho_{ij}$$
(3.6)

where $\rho_{ij} = \text{Cov}(T(\boldsymbol{X}_i), T(\boldsymbol{X}_j))$ and $\sigma_j^2 = \text{Var}(T(\boldsymbol{X}_j))$. We can obtain a similar variance $(\sigma_{T^{\pi}}^2)$ for $MSE_{RF^{\pi}}(\mathcal{T})$, so that under the hypothesis that $\mathbb{E}MSE_{RF}(\mathcal{T}) = \mathbb{E}MSE_{RF^{\pi}}(\mathcal{T})$, τ^2 can be seen to be

$$\tau^2 = \sigma_{\bar{T}}^2 + \sigma_{\bar{T}^{\pi}}^2.$$

That the \bar{T}_i and \bar{T}_i^{π} are iid follows from Lemma 2. Independence of the two samples follows from a similar argument to the second remark after Corollary 2. Crucially, there are many complicated quantities in this Eq. 3.6, i.e. $\sigma_j^2, \sigma_{\pi,j}^2, \rho_{ij}, \rho_{ij}^{\pi}$, for which there are not obvious estimators available and thus this result alone is not clearly practical. In the next following sections, we verify the validity of our proposed permutation procedure, which avoids the necessary explicit estimation of these quantities.

3.3.1 Tree-specific results

Until now, our discussion has remained largely agnostic to the type of base-learners employed, subject to the regularity conditions needed for asymptotic normality. We now argue that the trees typically grown in a random forest satisfy such conditions. The following result follows a similar strategy as Lemma 2 in Meinshausen (2006) with regularity conditions similar to those imposed in Wager and Athey (2018).

Proposition 1. Assume that $Y = m(\mathbf{X}) + \epsilon$, where $m(\cdot)$ is continuous on the unit cube. Let $\mathcal{X} = [0,1]^p$, and assume that $X_{i,j} \stackrel{iid}{\sim} Unif(0,1)$ for i = 1, ..., n and j = 1, ..., p. Then, let $T_n(\mathbf{x})$ be a tree trained on iid pairs $(\mathbf{X}_1, Y_1), ..., (\mathbf{X}_n, Y_n)$ such that each leaf of the tree contains a single observation. Further, assume the trees satisfy the following two conditions:

- (i) $\exists \gamma > 0$ such that $P(variable \ j \ is \ split \ on) > \gamma \ for \ j \in \{1,...,p\}$
- (ii) Each split leaves at least γn observations in each node.

Then, for each $x \in \mathcal{X}$

$$T_n(\boldsymbol{x}) \stackrel{d}{\to} Y | \boldsymbol{X} = \boldsymbol{x} \text{ as } n \to \infty.$$

The tree predictions thus asymptotically behave like the conditional samples of Y and as a result, should have finite non zero variance. Note that Breiman (2001) recommends building trees to full depth in which case Condition 1 is automatically satisfied.

3.4 Extension to Permutation Tests

In subsection 3.3 we established that the sampling distribution of MSE differences between forests was asymptotically Gaussian, but with a computationally intractable variance. Here we show that the permutation distribution converges to that sampling distribution. We begin by restating a classical theorem from Hoeffding.

Theorem 2. (Hoeffding, 1952) For a sequence of data $\{X_i\}_{i=1}^N$ and a statistic $S: \mathbb{R}^N \to \mathbb{R}$, define the permutation distribution function as

$$\hat{J}_N(t) = \frac{1}{|\mathcal{G}_N|} \sum_{\pi \in \mathcal{G}_N} I\{S(X_{\pi(1)}, ..., X_{\pi(N)}) \le t\}$$

where \mathcal{G}_N is the group of all permutations of $\{1, ..., N\}$. Let π, π' be two permutations drawn independently and uniformly over \mathcal{G}_N , and suppose that as $N \to \infty$

$$(S(X_{\pi(1)}, ..., X_{\pi(N)}), S(X_{\pi'(1)}, ..., X_{\pi'(N)})) \stackrel{d}{\to} (S, S')$$
 (3.7)

where S, S' are iid with cdf $R(\cdot)$. Then for all t at which $R(\cdot)$ is continuous, $\hat{J}_N(t) \stackrel{p}{\to} R(t)$.

Direct application of Theorem 2 is often challenging. Suppose $\{X_i\}_{i=1}^n \stackrel{iid}{\sim} P_X$ and independently $\{Y_i\}_{i=1}^m \stackrel{iid}{\sim} P_Y$, and we calculate the statistic $\sqrt{n+m} [S(X_1,...,X_n) - S(Y_1,...,Y_m)]$, and further define $p = \lim_{n \to \infty} \frac{n}{n+m}$. Theorem 2.1 of Chung and Romano (2013) states that if there exists a function ψ_{P_Z} (which may depend on the distribution of the data, P_Z) such that

$$\sqrt{N}\left[S(Z_1, ..., Z_N) - \mathbb{E}S(Z_1, ..., Z_N)\right] = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \psi_{P_Z}(Z_i) + o_{P_Z}(1)$$
(3.8)

(i.e. the statistic is asymptotically linear), then the permutation distribution of the aforementioned statistic is asymptotically normal with mean 0 and variance given by

$$\tau^{2} = \frac{1}{p(1-p)} \operatorname{Var}(\psi(Z) \mid Z \sim pP_{X} + (1-p)P_{Y})$$

$$= \frac{1}{p(1-p)} \left[p \operatorname{Var}(\psi(X)) + (1-p) \operatorname{Var}(\psi(Y)) \right]. \quad (3.9)$$

A key challenge is that τ^2 is often not equal to the variance of the unconditional distribution without additional assumptions on P_X and P_Y . A canonical example of this phenomenon is the permutation distribution of the difference in sample means. Given two independent iid samples $X_1, ..., X_n$ and $Y_1, ..., Y_m$, with $\text{Var}(X) = \sigma_X^2 < \infty$, $\text{Var}(Y) = \sigma_Y^2 < \infty$, and $\mathbb{E}X = \mathbb{E}Y$, the central limit theorem gives that $\sqrt{n+m}\left(\bar{X}_n - \bar{Y}_m\right) \stackrel{d}{\to} \mathcal{N}\left(0, \frac{1}{p}\sigma_X^2 + \frac{1}{1-p}\sigma_Y^2\right)$ where $p = \lim_{n \to \infty} \frac{n}{n+m}$. The conclusion of Eq. 3.9, however, is that the permutation distribution of the statistic $\sqrt{n+m}\left(\bar{X}_n - \bar{Y}_m\right)$ approaches a normal disribution with mean 0 and variance $\frac{1}{1-p}\sigma_X^2 + \frac{1}{p}\sigma_Y^2$ (Lehmann and Romano, 2006). Thus, unless $\sigma_X^2 = \sigma_Y^2$ or $p = \frac{1}{2}$, the permutation distribution fails to match the unconditional distribution.

The goal here is thus to provide a general result combining the delta method with the results of Chung and Romano (2013). First, we note that the finite forest centered MSE is equal to the original difference rescaled by $g'(\tilde{R}_B(\mathbf{x})) = g'(\mathbb{E}RF_B(\mathbf{x})) + o_P(1)$, so that

$$\sqrt{B}\left[MSE_{RF}(\boldsymbol{x};y) - \mathbb{E}MSE_{RF}(\boldsymbol{x};y)\right] = \sqrt{B}g'(\mathbb{E}RF_B(\boldsymbol{x}))\left[RF_B(\boldsymbol{x}) - \mathbb{E}RF_B(\boldsymbol{x})\right] + o_P(1)$$

and therefore the MSE at a single point satisfies Eq. 3.8 for

$$\psi(T(\boldsymbol{x})) = g'(\mathbb{E}RF_B(\boldsymbol{x})) [T(\boldsymbol{x}) - \mathbb{E}RF_B(\boldsymbol{x})]$$
$$\psi^{\pi}(T^{\pi}(\boldsymbol{x})) = g'(\mathbb{E}RF_B^{\pi}(\boldsymbol{x})) [T^{\pi}(\boldsymbol{x}) - \mathbb{E}RF_B^{\pi}(\boldsymbol{x})].$$

Thus, the single point MSE satisfies the conditions needed to apply Theorem 2.1 of Chung and Romano (2013). The calculation of the permutation distribution variance follows immediately from Eq. 3.9; the permutation distribution of the statistic $\sqrt{2B} \left[MSE_{RF}(\boldsymbol{x};y) - MSE_{RF^{\pi}}(\boldsymbol{x};y) \right]$ converges to a normal distribution with mean 0 and variance

$$\tau^2 = \frac{1}{1/4} \left[\frac{1}{2} \operatorname{Var}(g'(\mathbb{E}RF_B(\boldsymbol{x}))T(\boldsymbol{x})) + \frac{1}{2} \operatorname{Var}(g'(\mathbb{E}RF_B^{\pi}(\boldsymbol{x}))T^{\pi}(\boldsymbol{x})) \right].$$

This is double the variance of Eq. 3.4, but that in that case the variance was calculated for a \sqrt{B} rescaling, and so the conditional and unconditional variances agree. Because the forest sizes used in Algorithm 1 are assumed to be the same, $p = \frac{1}{2}$, so that the permutation test for equivalence of forest predictions is automatically valid in the sense of matching the permutation and unconditional distributions. This argument is formalized in the following result.

Theorem 3. Let $T_{1,k_n}, ..., T_{B,k_n}$ and $T_{1,k_n}^{\pi}, ..., T_{B,k_n}^{\pi}$ be two collections of trees satisfying the conditions of Lemma 1 and Lemma 3, and fix a test point with location X and response Y. Consider a test of the null hypothesis

$$H_0: \mathbb{E}\left[MSE_{RF}(\boldsymbol{X};Y) \middle| \boldsymbol{X}, Y\right] = \mathbb{E}\left[MSE_{RF^{\pi}}(\boldsymbol{X};Y) \middle| \boldsymbol{X}, Y\right]$$

using the statistic $\hat{\Delta} = MSE_{RF}(\mathbf{X};Y) - MSE_{RF^{\pi}}(\mathbf{X};Y)$. Then under H_0 , the permutation distribution of $\sqrt{B}\hat{\Delta}$ converges to a normal distribution with mean 0 and variance

$$\tau^2 = g'(\mathbb{E}RF_B(\boldsymbol{x}))^2 \sigma^2 + g'(\mathbb{E}RF_B^{\pi}(\boldsymbol{x}))^2 \sigma_{\pi}^2$$

which is also the variance of the unconditional distribution of $\sqrt{B}\hat{\Delta}$, as $n \to \infty$. Thus, the permutation test attains the asymptotic Type I error rate.

Proof. The only claim that remains to be verified is that the permutation test attains the Type I error rate. Let $\Phi(\cdot)$ be the standard normal cdf, and let $\hat{J}_B(t)$ be the (random) cdf of the permutation distribution, with corresponding quantile function $\hat{J}_B^{-1}(q)$. By the argument preceding the theorem statement, we have that $\sup_t |\hat{J}_B(t) - \Phi(t/\tau)| \stackrel{p}{\to} 0$. Then, by Lemma 11.2.1 of Lehmann and Romano (2006), for any number $q \in (0,1)$, $\hat{J}_B^{-1}(q) \stackrel{p}{\to} \tau \Phi^{-1}(q)$. In particular, for a given significance level α , the 1-sided permutation test of H_0 at the level α has a critical value $\hat{J}_B^{-1}(1-\alpha)$ which converges in probability to $\tau \Phi^{-1}(1-\alpha)$. Thus, as $B \to \infty$,

$$P(\sqrt{B}\hat{\Delta} \ge \hat{J}_B^{-1}(1-\alpha)|H_0) \to P(\sqrt{B}\hat{\Delta} \ge \tau\Phi^{-1}(1-\alpha)|H_0) \to \alpha.$$

We now must extend this result to multipoint test sets. However, Theorem 2.1 of Chung and Romano (2013) deals only with the scalar case. As such, recall that the multipoint MSE can be broken down into a sum of iid components. In particular, letting \mathcal{T} be a test set consisting of N_t points, it was shown in subsection 3.3 that

$$\sqrt{B}\left[MSE_{RF}(\mathcal{T}) - \mathbb{E}MSE_{RF}(\mathcal{T})\right] = \frac{1}{\sqrt{B}} \sum_{i=1}^{B} \bar{T}_i + o_P(1)$$

where \overline{T}_i is an iid sequence of random variables, each with mean 0 and variance presented in Eq. 3.6. Thus, the scaled and centered MSE satisfies the linearity condition presented

in Eq. 3.8. In particular, $\bar{T}_1, ..., \bar{T}_B \stackrel{iid}{\sim} P$ and $\bar{T}_1^{\pi}, ..., \bar{T}_B^{\pi} \stackrel{iid}{\sim} P^{\pi}$, and we are testing H_0 : $\mathbb{E}\bar{T}_i = \mathbb{E}\bar{T}_i^{\pi}$. Thus, because each is calculated with B trees, the same results hold and the test is asymptotically valid at multiple test points. This leads naturally to the following culminating theorem, the proof of which follows an identical argument to that of Theorem 3, and is therefore omitted.

Theorem 4. Let $T_{1,k_n},...,T_{B,k_n}$ and $T_{1,k_n}^{\pi},...,T_{B,k_n}^{\pi}$ be two collections of trees satisfying the conditions of Lemma 1 and Lemma 3, and fix a collection of test points \mathcal{T} . Consider a test of the null hypothesis

$$H_0: \mathbb{E}\left[MSE_{RF}(\mathcal{T}) \mid \mathcal{T}\right] = \mathbb{E}\left[MSE_{RF^{\pi}}(\mathcal{T}) \mid \mathcal{T}\right]$$

using the statistic $\hat{\Delta} = MSE_{RF}(\mathcal{T}) - MSE_{RF^{\pi}}(\mathcal{T})$. Then, assuming H_0 , the permutation distribution of $\sqrt{B}\hat{\Delta}$ converges to a normal distribution with mean 0 and variance given by Eq. 3.6 which is also the variance of the unconditional distribution of $\sqrt{B}\hat{\Delta}$, as $n \to \infty$. Thus, the permutation test attains the asymptotic Type I error rate.

3.4.1 Beyond the iid Approximation

We note that the conditions of Lemma 1 are likely far stronger than needed to attain the result in Theorem 4. The proofs of validity for the permutation tests rely on projecting the random forest (which is a correlated sum $\frac{1}{B}\sum_{i=1}^{B}T_{i}(\boldsymbol{x})$) onto a sum of iid random variables, $\sum_{i=1}^{n}\psi_{n}(Z_{i})$ for some function ψ_{n} , to which a central limit theorem can then apply. Indeed, this is exactly the approach of the Hájek projection and H-decomposition used respectively by Mentch and Hooker (2016) and Wager and Athey (2018). In these works, it is roughly shown that, under constraints on the forest construction, the random forest prediction at a point \boldsymbol{x} satisfies

$$\frac{1}{\sqrt{B}}\sum_{i=1}^{B}\left[T_{i}(\boldsymbol{x})-\mathbb{E}RF_{B}(\boldsymbol{x})\right]=\sum_{i=1}^{n}\psi_{n}(Z_{i})+o_{P}(1).$$

For example, if the Hájek projection is used, $\psi_n(Z_i) = \sqrt{B}\mathbb{E}\left[RF_B(\boldsymbol{x}) \mid T_i(\boldsymbol{x})\right] - \mathbb{E}RF_B(\boldsymbol{x})$. Moreover, as mentioned in the remark following Lemma 3, the fact that the MSE is asymptotically linear is independent of the iid approximation, and thus the MSE for these forests is also asymptotically linear.

4 Simulations

We now apply our testing procedure in a number of settings with varying regression functions and covariate structures. We simulate data from four models summarized in Table 1, with covariate structures summarized in Table 2. For each of our simulations, we train

random forests using the randomForest package in R (Liaw and Wiener, 2002) using the default mtry parameters.

Model #	Data Generating Model	Covariate Structure
1	$Y = \beta X_1 + \beta I(X_6 = 2) + \epsilon$	M1
2	$Y = \beta \sin(\pi I(X_7 = 2)X_1) + 2\beta(X_305)^2 + \beta X_4 + \beta X_2 + \epsilon$	M1
3	$P(Y = 1 \mathbf{X}) = \operatorname{expit}\left[\beta \sum_{j=2}^{5} X_j\right]$	M2
4	$Y = RF_{\mathtt{eBird}}(oldsymbol{X}) + \epsilon$	eBird

Table 1: Distributions of Y|X for each model. $\exp(z) = \frac{1}{1+e^z}$.

Model #	Covariate Structure
M1	$X_1,, X_5 \stackrel{iid}{\sim} Unif(0, 1), X_6,, X_{10} \stackrel{iid}{\sim} \text{Multinomial}(1, [\frac{1}{3}, \frac{1}{3}, \frac{1}{3}]^T)$
M2	$X_1,, X_{500} \sim AR_1(0.15)$
eBird	Data from Coleman et al. (2017) - 12 variables + 2 proxy variables

Table 2: Distribution of X for various simulation studies.

Model 1 is a standard ANCOVA model, which is intended to include both an important discrete and continuous predictor, to demonstrate the robustness of the proposed procedure to covariate type. Here we test the importance of (X_1, X_6, X_2, X_7) where X_1, X_6 are important, X_1, X_2 are continuous, and X_6, X_7 are categorical. Model 2 resembles the MARS data generating model (Friedman, 1991) commonly used in random forest studies, but with a modification to include an important discrete covariate. In both settings, we draw n = 2000 points from the joint distribution of (\mathbf{X}, Y) , subsample sizes of $k_n = n^{0.6} \approx 95$, and build B = 125 trees in each forest. Predictions were made at $N_t = 100$ test points, each drawn from the same joint distribution as the training data. Note that the null hypothesis, as defined in Eq. 2.2, is conditional on the test points used. These simulations change the null hypothesis each time, because the validation set changes. Thus, the simulations mimic the common practice of random splitting the data into a training and validation fold.

For Models 1 and 2, we focus on a marginal signal to noise ratio, which is controlled by the parameters β and σ . We fix $\beta = 10$ across all simulations let $\sigma = 10/j$ where j takes 9 equally spaced values between 0.005 and 2.25 so that for small k, the signal to noise ratio (SNR) is small. The results are shown in Figure 1. We see that the test maintains the nominal type I error rate and attains high power for marginal SNRs near 1 for all variables except X_7 in Model 2. Note also that the type I error rate appears insensitive to the covariate structure. In the MARS model, we see that the test has more power against X_3 than X_7 , because X_7 is only important insofar as it interacts with X_1 .

Model 3 is an adaptation of the model used in Candes et al. (2016) for high-dimensional correlated data. Here we test for the significance of X_2 , which is important, and also X_1 and

 X_{500} , which are unimportant, but X_1 is highly correlated with X_2 and X_{500} is much more weakly correlated. Candes et al. (2016) demonstrated that the standard logistic regression p-values in this situation are far from uniform under H_0 , so that standard parametric inference may not be valid. Random forests, on the other hand, have been shown (Biau, 2012; Scornet et al., 2015) to be largely insensitive to the dimension of the ambient feature space, and instead sensitive only to the "strong" feature space. This setting helps to explore the utility of our method in the high dimensional sparse signal case.

We limit n=600 so that p/n is not small, though the dimension of the strong features is still small relative to n. We let $k_n=n^{0.6}\approx 46$, B=125, $N_t=100$, and vary the β coefficient according to 8 equally spaced values between 0.01 and 2.5 and also for 7 equally spaced values between 5 and 20. The results are shown in the bottom panel of Figure 1. Note that the test resolves the biased p-value issue associated with the standard glm procedure and is still able to attain reasonable power for the effect of X_2 . The power is likely limited by the fact that for large β , the change in the marginal effect of each covariate only changes P(Y=1|X) slightly due to the rapidly decaying first derivative of the expit(z) function.

Finally, we turn to Model 4 where the true data generating model is a random forest. We utilize a dataset from Coleman et al. (2017) describing the occurrence of tree swallows and to construct $RF_{\tt eBird}$, we draw 5000 points from the data, and train $RF_{\tt eBird}$, a random forest with $\tt mtry = 9$ and 1000 total trees. To simulate from this model, we draw (without replacement) samples of size n from the remaining 20727 points, predict at them using $RF_{\tt eBird}$, and add Gaussian noise. We test for the effect of two variables: eff.hours, which corresponds to the number of hours a user expended upon a hike, and dfs, which is a fractional measurement of day of year. We further include two proxy variables (not used to train $RF_{\tt eBird}$), defined as eff.hours.proxy = $\frac{\tt eff.hours+Z_{0.5}}{\sqrt{{\rm Var}(\tt eff.hours)+0.5}}$ and dfs.proxy =

 $\frac{\text{dfs}+Z_{0.025}}{\sqrt{\text{Var}(\text{dfs})}+0.025}$ where Z_{σ} is a standard normal random variable with variance σ^2 . The purpose of this construction is that the proxy variables' relationship with Y is solely dictated by their dependence on their original copy.

In Model 4, we let n = 2000, $k_n = n^{0.6}$, B = 125, $N_t = 100$, and let $\sigma = e^{-j}$ for 10 values of j equally spaced between 1 and 5. The results of this simulation are show in Figure 1. We see that again the test maintains the nominal type I error rate with modest power for signal variables. Moreover, the procedure correctly identifies the true variables as important over their proxies.

5 Applications to Ecological Data

We now apply our testing procedure on two ecological datasets where random forests have been shown to perform well in recent work.

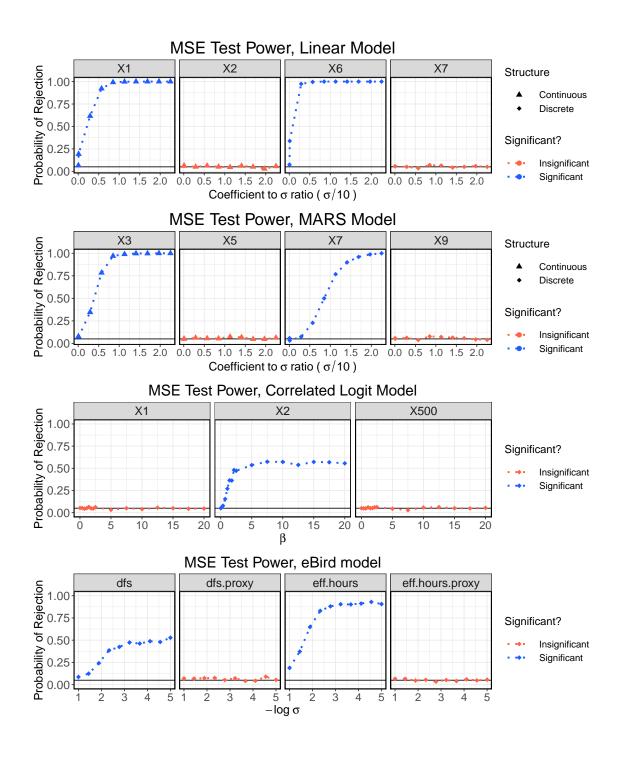


Figure 1: Simulation results for each of the models from Table 1. Black line corresponds to $\alpha = 0.05$, the nominal level

eBird: We first consider the eBird data described in the previous section to construct a simulated random forest model. Here we utilize the original data as considered in Coleman et al. (2017). The standard task is to predict tree swallow occurrence during the fall migration season in a particular geographic area referred to as Bird Conservation Region (BCR) 30. This is a Citizen Science project where observers submit reports detailing when and where they recorded observations. The response in each row of the data is either 0 or 1 corresponding to whether a tree swallow was observed during that particular outing. Features include information about latitude, longitude, time of year, as well as observer, environmental, temperature, and land cover characteristics. The data consists of n = 25727 observations on 23 features, gathered between 2008 and 2013. Coleman et al. (2017) carry out a testing procedure based on the parametric approach in Mentch and Hooker (2016) but due to the limitations described in previous sections, are limited to a test sample of only 25 points.

We first apply Algorithm 1 to test the importance of any variables in predicting occurrence, analogous to an overall F-test in multiple linear regression. Here we select 15% of the available observations (≈ 3800 points) uniformly at random to serve as the test set where the hypotheses will be evaluated. The random forests were trained with the ranger package using the default mtry = 4, subsamples of size $k_n = n^{0.6}$, and consisting of B = 250 trees in each. The results are shown on the left hand side of Figure 2. There is clear evidence for signal in the data, with an overall p-value of p < 0.0001. Next, to produce an output similar to the out-of-bag importance scores traditionally computed, we repeat the testing procedure for each covariate individually, recording the marginal importance for each as the number of standard deviations away that the original MSE difference is from the center of the permutation distribution. The results are shown in the right hand side of Figure 2. We see that dfs, which corresponds to the day of the year, eff. hours, which corresponds to a users' effort (in time), and aster.elev, which corresponds to elevation, are the most important features. Time of year (dfs) and elevation (aster.elev) have an intuitive relationship with occurrence, serving as proxies for climate conditions. Larger eff.hours suggest that a user spent more time out in the field on a particular day, meaning they were more likely to observe a tree swallow because of increased birding time.

Forest Fires: Cortez and Morais (2007) sought to predict $\log(1+\text{area})$ burned by several fires in northern Portugal using covariate information on location, time of year, and local weather characteristics. The data contains n=537 observations on 13 features. Cortez and Morais (2007) found that a naive mean predictor attained the lowest RMSE - suggesting that there is weak signal in the data. We carry out our testing procedure in exactly the same fashion as the eBird data, using mtry = 12 and $k_n = n^{0.6} \approx 43$, B = 250 trees for the importance test and B = 500 trees for the overall test; results are shown in Figure 3. The overall test suggests that there is signal in the data (p = 0.0040), albeit a weaker effect than in the preceding eBird case study. The importance procedure suggests that only wind – the wind speed at the location of the fire – is significant at the 0.05 level.

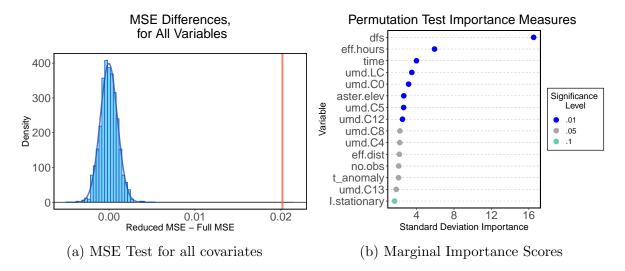


Figure 2: Results on the eBird data from (Sullivan et al., 2009, 2014). Red line indicates observed value, and histograms of differences in MSE after permutation are overlayed by an estimated normal density.

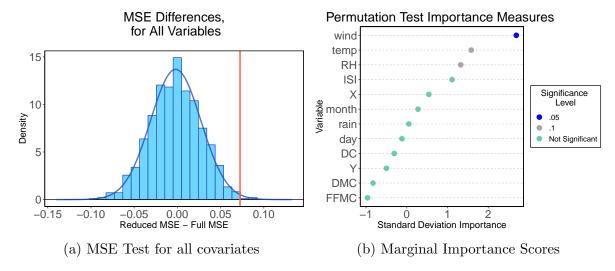


Figure 3: Results on the forest fire data from Cortez and Morais (2007). Red line indicates observed value, and histograms of differences in MSE after permutation are overlayed by an estimated normal density.

6 Discussion

The work here presents a formal hypothesis testing framework for evaluating the predictive significance of covariates in a random forests model which, unlike existing approaches, is both computationally efficient and statistically valid, placing hypothesis tests with random forests firmly within the grasp of applied researchers. Previously suggested parametric approaches are computationally prohibitive and place severe restrictions on where the hypotheses can be evaluated while the popular heuristic out-of-bag (oob) approaches are easily computed but also easily fooled by correlated and/or categorical covariates. We note further that while the ensemble nature of random forests presents a natural context for such tests, much of the theoretical backing for this procedure is largely agnostic to the particular class of base-learner models being constructed.

Besides its feasibility, this permutation approach also offers some flexibility in the kinds of problems open to investigation by practitioners. Consider, for example, the mediator detection problem arising frequently in medical studies wherein a covariate X_1 is a mediator for another covariate X_2 whenever the effect of X_2 on the response is nullified (or substantially lessened) by including X_1 in the model. The same two-step process often employed with linear models can be carried out with random forests using the tests developed here: first determine whether X_2 is significant without X_1 in the model, then test whether the significance of X_2 disappears whenever X_1 is included.

One potential criticism of the approach presented here may be that it becomes more computationally burdensome whenever one wishes to evaluate the significance of all available covariates one at a time. Note however that by construction, we need only build relatively few trees to conduct each test and thus in small or even moderate dimensions, simply repeating our permutation approach p times is still more computationally efficient than carrying out even a single parametric test. Finally, we note that the validity of our approach was verified by arguing that the random forest trees behave like an iid sequence asymptotically. As argued in subsection 3.4, random forest predictions are often near an iid sum, so that the linearity condition of Chung and Romano (2013) may be applicable in many wider cases.

SUPPLEMENTARY MATERIAL

R code for implementing the testing procedure as well as all simulation examples is provided here and publicly available.

ACKNOWLEDGEMENTS

This research was supported in part by the University of Pittsburgh Center for Research Computing through computing resources. We specifically acknowledge the assistance of Kim Wong. LM was supported in part by NSF DMS-1712041. We thank the thousands

of eBird participants for their contributions and support for eBird from The Wolf Creek Foundation and the National Science Foundation (ABI sustaining: DBI-1356308; computing support from CNS-1059284). We also thank Giles Hooker for useful feedback.

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A Proofs of Technical Results

We now provide the technical details and proofs for theoretical discussion in Section 3. For completeness, theorems and lemmas are restated.

Theorem 1. Under the exchangeability conditions outlined in Section 3.1, denote a sequence of (potentially randomized) trees trained on subsamples from \mathcal{D}_n as $\{T_k(\cdot)\}_1^{\infty}$. Moreover, consider an independently drawn test point, $\mathbf{Z}^* = (\mathbf{X}^*, Y^*) \sim F$. Then, the residuals

$$r_k = T_k(\boldsymbol{X}^*) - Y^*$$

form an infinitely exchangeable sequence of random variables.

Proof. Let Ξ be the distribution of randomization parameters, and let $S_{k_n}(\mathcal{D}_n)$ be the distribution of subsamples of size k_n drawn uniformly from the original data. Then, to construct a tree, we have the following procedure:

- 1. Draw $\mathcal{D}_{k_n}^* \sim \mathcal{S}_{k_n}(\mathcal{D}_n)$
- 2. Draw $\xi \sim \Xi$
- 3. Draw $Z^* \sim F$
- 4. Construct a tree according to some combining function, say ϕ , of ξ , $\mathcal{D}_{k_n}^*$, i.e. $T = \phi(\xi, \mathcal{D}_{k_n}^*)$.

Each draw is done independent of the other draws. Repeating (1) and (2) independently gives iid sequences $\{\mathcal{D}_{l,k_n}^*\}_{l=1}^{\infty}$ and $\{\xi_j\}_{j=1}^{\infty}$. Then, the sequence

$$T_1 = \phi(\xi_1, \mathcal{D}_{1,k_n}^*), \ T_2 = \phi(\xi_2, \mathcal{D}_{2,k_n}^*), \dots$$

is a mixture of iid sequences, where the mixture is directed (in the sense of Aldous (1985)) by \mathcal{D}_n . So, $\{T_l \mid \mathcal{D}_n\}$ is exactly an iid sequence of functions. Further, $\{r_l \mid \mathcal{D}_n, \mathbf{Z}^*\}$ is an iid sequence of random variables, and thus the conclusion follows from the converse of DeFinetti's Theorem.

See Aldous (1985) page 29 for more details on this construction.

We turn now to Lemma 1 from Section 3.2, which establishes asymptotic pairwise independence.

Lemma 1. Consider a collection of B_n trees built from a training dataset of size n on subsamples of size k_n , say $\{T_{j,k_n}\}_{j=1}^{B_n}$, satisfying Condition 1. Then, as long as $k_n/\sqrt{n} \to 0$ and

$$\binom{B_n}{2} \log \left[\frac{\binom{n-k_n}{k_n}}{\binom{n}{k_n}} \right] \to 0$$

the infinite sample sequence of trees, $\{T_{1,\infty,k_{\infty}},...,T_{B,\infty,k_{\infty}},...\}$ is an infinite sequence of pairwise independent random functions.

Proof. Condition 1 guarantees the existence of a limiting random variable.

It is sufficient to show that asymptotically, the trees are trained using independent training samples, because we have assumed that our original data are iid. Define the indices of a subsample in the following way:

$$\operatorname{ind}(\mathcal{D}_{k_n}^*) := \{ j \in \{1, ..., n\} : Z_j \in \mathcal{D}_{k_n}^* \}.$$

Then, by the assumption that the Z_k are independent,

$$\mathcal{D}_{k_n,j}^* \perp \!\!\! \perp \mathcal{D}_{k_n,l}^* \iff |\operatorname{ind}(\mathcal{D}_{k_n,j}^*) \cap \operatorname{ind}(\mathcal{D}_{k_n,l}^*)| = 0$$

so, it is sufficient to show that

$$\lim_{n \to \infty} P(|\operatorname{ind}(\mathcal{D}_{k_n,j}^*) \cap \operatorname{ind}(\mathcal{D}_{k_n,l}^*)| = 0) = 1, \ \forall \ j \neq l.$$

Note that if $k_n \ge n/2$, this event has probability 0, so choose n so that $n > 2k_n$. Then

$$P(|\operatorname{ind}(\mathcal{D}_{k_n,j}^*) \cap \operatorname{ind}(\mathcal{D}_{k_n,l}^*)| = 0) = \frac{\binom{n-k_n}{k_n}}{\binom{n}{k_n}}$$

$$= \frac{((n-k_n)!)^2}{n!(n-2k_n)!}$$

$$= \frac{(n-k_n)!}{n!} \times \frac{(n-k_n)!}{(n-2k_n)!}$$

$$= \frac{(n-k_n)(n-k_n-1)...(n-2k_n+1)}{n(n-1)...(n-k_n+1)}.$$

There are k_n terms in both the numerator and denominator here, so we can separate the

product in the term above as

$$P(|\operatorname{ind}(\mathcal{D}_{k_n,j}^*) \cap \operatorname{ind}(\mathcal{D}_{k_n,l}^*)| = 0) = \frac{n - k_n}{n} \times \frac{n - k_n - 1}{n - 1} \times \dots \times \frac{n - 2k_n + 1}{n - k_n + 1}.$$

$$\geq \left(\frac{n - 2k_n + 1}{n}\right)^{k_n}$$

$$= \left(1 - \frac{2k_n + 1}{n}\right)^{k_n}$$

$$= \exp\left[k_n \log\left(1 - \frac{2k_n + 1}{n}\right)\right]$$

$$\approx \exp\left[k_n \left(-\frac{2k_n + 1}{n}\right) - \frac{k_n}{2}\left(\frac{2k_n + 1}{n}\right)^2\right]$$

$$\approx \exp\left[-\frac{2k_n^2 + k_n}{n}\right]$$

$$\approx 1$$

where $a_n \approx b_n$ means that $\lim_{n\to\infty} a_n/b_n = 1$, and we have used the Taylor expansion of $\log(1-x)$ in the above.

This means that two pre-specified subsamples will be independent in the limit. Next, we need to ensure that this holds for all subsamples, i.e.

$$P\bigg(\bigcap_{j\neq l}\{|\operatorname{ind}(\mathcal{D}_{k_n,j}^*)\cap\operatorname{ind}(\mathcal{D}_{k_n,l}^*)|=0\}\bigg)\to 1.$$

For B_n trees, there are $\binom{B_n}{2}$ subsample pairings, each drawn independently. Thus

$$P\bigg(\bigcap_{j\neq l} \{|\operatorname{ind}(\mathcal{D}_{k_n,j}^*) \cap \operatorname{ind}(\mathcal{D}_{k_n,l}^*)| = 0\}\bigg) = \prod_{j\neq l} P(|\operatorname{ind}(\mathcal{D}_{k_n,j}^*) \cap \operatorname{ind}(\mathcal{D}_{k_n,l}^*)| = 0)$$
$$= \bigg(\frac{\binom{n-k_n}{k_n}}{\binom{n}{k_n}}\bigg)^{\binom{B_n}{2}}.$$

Next, by assumption,

$$\log P\left(\bigcap_{j\neq l} \{|\operatorname{ind}(\mathcal{D}_{k_n,j}^*) \cap \operatorname{ind}(\mathcal{D}_{k_n,l}^*)| = 0\}\right) = \binom{B_n}{2} \log \left[\frac{\binom{n-k_n}{k_n}}{\binom{n}{k_n}}\right] \to 0$$

so that the probability of this event goes to 1.

After Lemma 1, we next need to prove Lemma 3, whose purpose is to show that the observed MSE is asymptotically centered around its own expectation.

Lemma 3 Assume the conditions needed from Corollary 2. Additionally, assume that g has at least k derivatives for some $k \geq 3$, and that $g^{(k)}(x) < \infty$ for all x. Further, assume that $\mathbb{E}|T_i(x)|^k < \infty$. Then,

$$\sqrt{B} \left[\mathbb{E} g(RF_B(\boldsymbol{x}) - g(\mathbb{E} RF_B(\boldsymbol{x})) \right] = \frac{g''(\mathbb{E} RF_B(\boldsymbol{x}))\sigma^2}{2\sqrt{B}} + o(B^{-3/2}).$$

Proof. We rely on a result presented in Oehlert (1992), which states that under the conditions presented in the lemma statement,

$$\mathbb{E}g(RF_B(\boldsymbol{x})) = g(\mathbb{E}RF_B(\boldsymbol{x})) + \frac{g''(\mathbb{E}RF_B(\boldsymbol{x}))\sigma^2}{2B} + o(B^{-2}). \tag{A.1}$$

Thus, the result follows from multiplying both sides of Eq. A.1 by \sqrt{B} and rearranging terms.

Next, we move on to the proof of Proposition 1 from subsubsection 3.3.1, which gives that the trees typically utilized in a random forest obey the necessary regularity conditions for Corollary 2.

Proposition 1. Assume that $Y = m(\mathbf{X}) + \epsilon$, where $m(\cdot)$ is continuous on the unit cube. Let $\mathcal{X} = [0,1]^p$, and assume that $X_{i,j} \stackrel{iid}{\sim} Unif(0,1)$ for i = 1, ..., n and j = 1, ..., p. Then, let $T_n(\mathbf{x})$ be a tree trained on iid pairs $(\mathbf{X}_1, Y_1), ..., (\mathbf{X}_n, Y_n)$ such that each leaf of the tree contains a single observation. Further, assume the trees satisfy the following two conditions:

- (i) $\exists \gamma > 0$ such that $P(variable \ j \ is \ split \ on) > \gamma \ for \ j \in \{1,...,p\}$
- (ii) Each split leaves at least γn observations in each node.

Then, for each $x \in \mathcal{X}$

$$T_n(\boldsymbol{x}) \stackrel{d}{\to} Y | \boldsymbol{X} = \boldsymbol{x} \text{ as } n \to \infty$$

Proof. Each tree divides \mathcal{X} into a partition of rectangular subspaces, corresponding to leaves of the tree. Following Meinshausen (2006), for each point \boldsymbol{x} (with coordinates $[x_1,...,x_p]$), let $\ell(\boldsymbol{x})$ denote the unique leaf of the tree containing \boldsymbol{x} . Let $R_{\ell}(\boldsymbol{x})$ be the rectangular subspace of $[0,1]^p$ corresponding to a particular leaf $\ell(\boldsymbol{x})$. The rectangular nature of the subspaces means that for each input feature, R_{ℓ} can be expressed as

$$R_{\ell}(\boldsymbol{x}) = \bigotimes_{i=1}^{p} [a(\boldsymbol{x}, i), b(\boldsymbol{x}, i)]$$

where $0 \le a(\boldsymbol{x}, i) \le x_i \le b(\boldsymbol{x}, i) \le 1$ are scalars inducing an interval in dimension i. Then, the tree (by the existence of the requisite γ) satisfies the conditions of Lemma 2 in

Meinshausen (2006), so that $\max_i |a(\boldsymbol{x},i) - b(\boldsymbol{x},i)| \stackrel{p}{\to} 0$. Let $\boldsymbol{a}(\boldsymbol{x}) = [a(\boldsymbol{x},1),...,a(\boldsymbol{x},p)]$ and similarly define $\boldsymbol{b}(\boldsymbol{x})$, so that the previous sentence implies: $\boldsymbol{a}(\boldsymbol{x}) \stackrel{p}{\to} \boldsymbol{b}(\boldsymbol{x})$. We therefore also see that $a(\boldsymbol{x},i),b(\boldsymbol{x},i) \stackrel{p}{\to} x_i$ for all i.

The trees are fully grown, so the tree prediction at the point x is given by

$$T_n(\boldsymbol{x}) = \sum_{k=1}^n I(\boldsymbol{X}_k \in R_\ell(\boldsymbol{x})) Y_k$$

i.e. the response for the observation whose leaf contains \boldsymbol{x} . As such, let k^* be the index corresponding to the observation who shares a leaf with \boldsymbol{x} , so that $T_n(\boldsymbol{x}) = Y_{k^*}$. We can deconstruct the event $\boldsymbol{X}_{k^*} \in R_{\ell}(\boldsymbol{x})$ as

$$\{ \boldsymbol{X}_{k^*} \in R_{\ell}(\boldsymbol{x}) \} = \bigcap_{i=1}^{p} \{ a(\boldsymbol{x}, i) \le X_{i, k^*} \le b(\boldsymbol{x}, i) \}.$$

Thus, in the limit, $a(\boldsymbol{x},i), b(\boldsymbol{x},i) \xrightarrow{p} X_{i,k^*}$, and so $X_{i,k^*} \xrightarrow{p} x_i$ for all i. Further, continuity of m yields that $m(\boldsymbol{X}_{k^*}) \xrightarrow{p} m(\boldsymbol{x})$. Thus, we see that, in the limit

$$Y_{k^*} = m(\boldsymbol{x}) + \epsilon_{k^*} \stackrel{d}{=} m(\boldsymbol{x}) + \epsilon \stackrel{d}{=} Y | \boldsymbol{X} = \boldsymbol{x}$$

because ϵ_{k^*} is independent of the location of X.

B Additional Simulations

We include some additional simulations here to demonstrate the following points.

- 1. The accuracy of the permutation distribution approximation of the Gaussian. The theory outlined in Section 3 establishes that the difference in MSEs between forests is asymptotically Gaussian but the difficulty in estimating the resulting variance largely restricts its direct usage in practical settings. We go on to demonstrate that the permutation distribution approaches this distribution, thereby circumventing the need for a direct variance estimate. The simulations below present empirical evidence that this approximation is reasonable in practical settings.
- 2. The instability of the variance estimation procedures laid out in Wager et al. (2014) and Mentch and Hooker (2016). Clearly variance estimation is useful for developing confidence intervals about random forest predictions, which in the case of pointwise consistency (as in the honest trees proposed by Wager and Athey (2018)), are also valid for the underlying regression function. However, in the hypothesis testing framework, these estimates are useful only insofar as they allow for calculation of a test statistic. These variance estimates, such as the infinitesmal jackknife of Wager et al.

- (2014), recommend building $B = \mathcal{O}(n^{\beta})$ trees where $\beta \geq 1$. We demonstrate that this recommendation cannot be violated.
- 3. The robustness (and potential weaknesses) of the proposed procedure to different random forest implementations. In particular, we want to study the effect of larger subsamples/more trees. The theoretical results presented in Section 3 rely on treating the tree predictions as iid. Clearly, this is never true in practice, and some theoretical justification for the effects of this being small were presented in Section 6.

B.1 Normality of Permutation Distributions

Here we provide a concise simulation demonstrating the accuracy of the permutation distribution approximation of the Gaussian in a practical setting. We simulate n=2000 training observations from Model 2 with covariate structure M1 as described in Section 4. Specifically, we consider the model $Y = \beta \sin(\pi I(X_7 = 2)X_1) + 2\beta(X_3 - .05)^2 + \beta X_4 + \beta X_2 + \epsilon$ where we sample covariates according to $X_1, ..., X_5 \stackrel{iid}{\sim} Unif(0,1)$ and $X_6, ..., X_{10} \stackrel{iid}{\sim} \text{Multionimial}(1, [\frac{1}{3}, \frac{1}{3}, \frac{1}{3}]^T)$. Here we use $\beta = 10, \sigma = 10$, along with $N_t = 100$ test observations and apply our procedure to test for the significance of X_3 (important) and X_5 (unimportant). The random forests each consist of B = 200 trees trained on subsamples of size $k_n = n^{0.6}$, with mtry = 3. The resulting permutation distributions are shown in Figure 4.

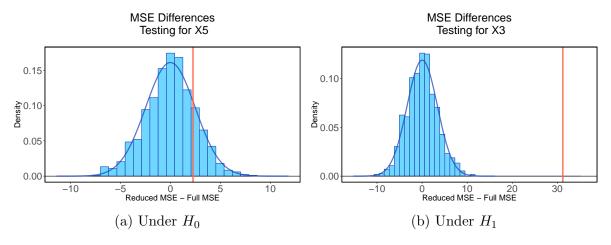


Figure 4: Permutation distributions of Δ_B . Red line indicates observed value, and histograms are overlayed by an estimated normal density.

These plots demonstrate that the permutation distributions do approximate a Gaussian distribution. Moreover, in the null case, the observed Δ_B lies squarely in the center of the

distribution, while in the alternative case, Δ_B lies far away from the center. Next, we more formally investigate the power/validity of the testing procedure.

B.2 Variance Estimation Instability

Here, we use the infinitesmal jackknife (IJ), as implemented in the ranger package (Wright and Ziegler, 2015), to estimate the variance of a random forest prediction at a given point. In particular, we simulate data from Model 2 from Table 1, train a subsampled random forest, and record the IJ variance estimate of random forest prediction at $X_1 = ... = X_5 = 0.5$ and $X_6 = ... = X_{10} = 2$. We use n = 2000, $k_n = n^{0.5} \approx 44$, and vary the number of trees. Often times, the IJ variance estimate is negative, leading to a NaN output from the IJ software. These instances represent a case when the IJ estimate is useless to a practitioner, and as such, we report the percentage of times that a NaN output is returned for each number of trees. For each number of trees, we repeat the simulation 100 times, and results are shown in Figure 5.

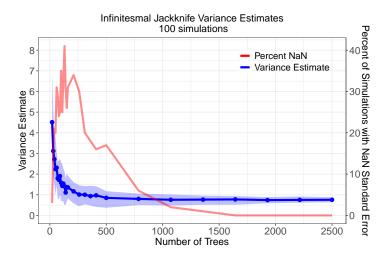


Figure 5: ranger IJ variance estimate. Blue ribbon plot indicates central 90% of variance estimates (corresponds to left axis), and red line (corresponds to right axis) represents percentage of runs that return NaN.

The IJ estimate provides overwhelmingly large variance estimates for small numbers of trees, leading to overly conservative confidence intervals and tests with exceptionally low power. Moreover, the ribbon remains quite wide until around B=2000 trees, suggesting that at least $\mathcal{O}(n)$ trees are necessary to attain a stable variance estimate. A similar number of trees is necessary to ensure that a NaN is never returned. We should note that this is the simplest possible case of variance estimation, i.e. the estimation is only at a single point. The problem grows exponentially more complex as more test points are

considered and covariance estimates are needed. Mentch and Hooker (2016) note that the procedure is infeasible for more than 20-30 test points. The authors demonstrate in follow-up work (Mentch and Hooker, 2017) that an approximate test can be produced by utilizing random projections which allows for slightly larger test sets but at the cost added computational strain. In contrast, besides the minimal overhead required to form the additional predictions, the testing procedure proposed here is almost entirely immune to the number of points in the test set. Once the initial predictions are formed, the only remaining work is to shuffle predictions (trees) and re-compute the difference in MSE between forests.

B.3 Test Robustness

We now present more figures similar to the power curves presented in Section 4. The goal here is to present the proposed procedure's robustness to the number of trees B and the subsample size k_n . To do so, we modify the simulation study plotted in the second panel of Figure 1. Here, we fix the error variance at $\sigma^2(\epsilon) = 16$, and again simulate n = 2000 training observations and $N_t = 100$ test observations. First, we vary the number of trees built, according to

$$B \in \big\{20, 50, 75, 125, 250, 375, 500, 750, 1000\big\}$$

and let $k_n = n^{0.6}$. The resulting simulations are plotted in Figure 6.

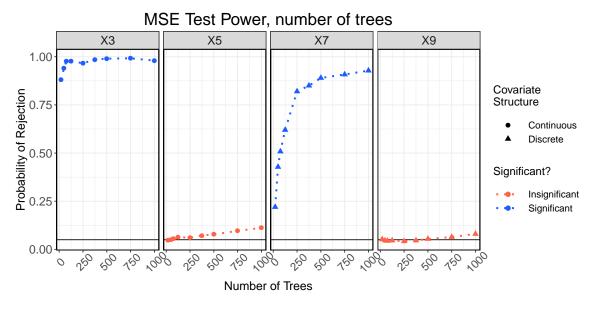


Figure 6: Model 2 power curves for 500 simulations, by number of trees. The Y-axis represents $P(\tilde{p} \le \alpha)$ where $\alpha = 0.05$ and is shown as the horizontal line across the bottom of the plots.

Two clear patterns are clear in the figure - the power and type I error rate of the test both increase as the number of trees grows. However, the rate of growth for each of them is markedly different - the test attains high power around $B\approx 250$ trees, but deviations from the nominal level are only noticeable around $B\approx 500$ trees. Even when B=1000, the observed level is still within nearly 5% of the baseline. Thus, while the level of the test may be slightly inflated for large numbers of trees, the procedure remains valid for limited, but realistic tree sizes.

Recall that the subsample size is a key limiting factor of Lemma 1 - it is required that $k_n = o(\sqrt{n})$ - to establish asymptotic normality. Other work (Wager and Athey, 2018) weakens these conditions, but places explicit restrictions on the types of trees allowed in the ensemble. We now examine the behavior of our procedure under larger sample sizes. We use the same simulation parameters as in Figure 6, but now fix B = 125 and let $k_n = n^p$, and we vary p at 10 equally spaced values between 0.1 and 0.99.

The resulting simulation is shown in Figure 7. We see that for $p \leq 0.75$, the Type I error rate is maintained, but for larger subsamples, we begin to see a severe deviation. Though severe, this is not necessarily surprising as such large subsampling rates correspond directly to a more severe violation of the iid approximation.

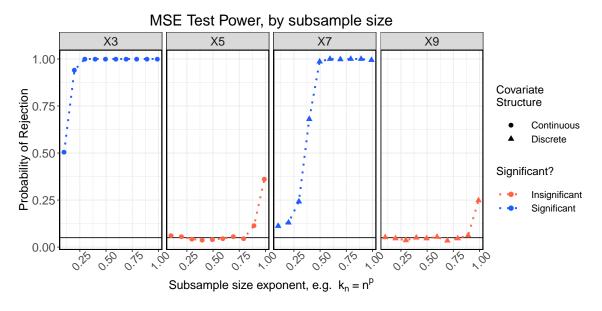


Figure 7: Model 2 power curves for 500 simulations, by subsample exponent. The Y-axis represents $P(\tilde{p} \leq \alpha)$ where $\alpha = 0.05$ and is shown as the horizontal line across the bottom of the plots.