Getting Better from Worse: 
Augmented Bagging and a 
Cautionary Tale of Variable Importance

Lucas Mentch and Siyu Zhou

Department of Statistics 
University of Pittsburgh

March 10, 2020

Abstract

As the size, complexity, and availability of data continues to grow, scientists are increasingly relying upon black-box learning algorithms that can often provide accurate predictions with minimal a priori model specifications. Tools like random forest have an established track record of off-the-shelf success and even offer various strategies for analyzing the underlying relationships between features and the response. Motivated by recent insights into random forest behavior, here we introduce the idea of augmented bagging (AugBagg), a procedure that operates in an identical fashion to the classical bagging and random forest counterparts but which operates on a larger space containing additional, randomly generated features. Somewhat surprisingly, we demonstrate that the simple act of adding additional random features into the model can have a dramatic beneficial effect on performance, sometimes outperforming even an optimally tuned traditional random forest. This finding that the inclusion of an additional set of features generated independently of the response can considerably improve predictive performance has crucial implications for the manner in which we consider and measure variable importance. Numerous demonstrations on both real and synthetic data are provided.

Keywords: Regularization, Random Forests, Feature Importance, Ridge Regression

1 Introduction

As data continues to become larger and more complex, scientists and analysts are increasingly relying upon adaptive learning methods in lieu of the more traditional parametric statistical models that require a priori model specification. Among these flexible alternatives, bagging (Breiman, 1996) and random forests (Breiman, 2001) have proven among the
most popular and robust tools available with successful application in nearly every scientific field; for just a few select examples, see Díaz-Uriarte and De Andres (2006); Cutler et al. (2007); Bernard et al. (2007); Mehrmohamadi et al. (2016); Coleman et al. (2017). In a recent study, Fernández-Delgado et al. (2014) compared the performance of 179 classification methods across all datasets then available in the UCI Machine Learning Repository (Dua and Graff, 2017) and found random forests to be the top overall performer. In the previous two decades since their inception, numerous studies have sought to establish their important statistical properties including consistency (Biau and Devroye, 2010; Scornet et al., 2015; Klusowski, 2019), asymptotic normality (Mentch and Hooker, 2016; Wager and Athey, 2018), and rates of convergence (Peng et al., 2019) as well as means by which standard errors (Sexton and Laake, 2009), confidence intervals (Wager et al., 2014; Mentch and Hooker, 2016), and hypothesis testing procedures (Mentch and Hooker, 2016, 2017; Coleman et al., 2019) can be obtained.

Bagging, first introduced in a tree-based setting by Breiman (1996), involves drawing $B$ bootstrap samples from the original training data, refitting the base model (tree) on each, and averaging the individual outputs to obtain the final predictions. When base models are the traditional classification or regression trees (Breiman et al., 1984), at each internal node, the optimal empirical split point is chosen by searching over all features and potential splits. Random forests can thus be seen as a less-greedy alternative, whereby eligible features for splitting are randomly selected at each internal node.

Despite the abundance of forest-related work in recent years, substantially less effort has been devoted to principled studies of the inner workings of random forests that might more fully explain their robust record of success. Recently however, Mentch and Zhou (2019) suggested that the additional randomness utilized in random forests was simply an implicit form of regularization. The $m_{\text{try}}$ parameter in random forests that dictates the number of available features at each split could therefore been seen as akin to the $\lambda$ shrinkage penalty in explicit regularization methods like ridge regression (Hoerl and Kennard, 1970) and lasso (Tibshirani, 1996). Mentch and Zhou (2019) suggested that the random subsampling of features helped the trees to avoid overfitting and that this was particularly beneficial in low signal-to-noise ratio settings. LeJeune et al. (2019) demonstrated a similar effect for ensembles consisting of linear model base learners fit via ordinary least squares (OLS).

The idea that the randomness in random forests serves as a means of regularization not only eliminates some of the mystery of their sustained success but also suggests that alternative modifications to the standard bagging procedure that also induce some means of regularization may also produce similar gains in accuracy. In this work, we propose one
such alternative we refer to as augmented bagging (AugBagg) wherein the original feature space is augmented with additional noise features generated conditionally independent of the response and the standard bagging procedure is then carried out. Surprisingly, we demonstrate throughout the remainder of this paper that this simple and seemingly unintuitive modification can sometimes lead to dramatic gains in accuracy. Like the original random forest procedure, such advantages are most noticeable when the signal-to-noise ratio (SNR) in the data is low. Unlike random forests, however, in some settings, the augmented bagging procedure can be easily amended to produce competitive performance even at larger SNRs by simply correlating the additional noise features with features in the original data.

The remainder of this paper is laid out as follows. In Section 2 we formally introduce the AugBagg procedure and provide some theoretical motivation inspired by recent results established for other learning procedures. Simulations and demonstrations on real data are provided in Section 3. Importantly, these findings have crucial implications for the manner in which feature importance is measured. In particular, our findings suggest quite strongly that hypothesis tests comparing model accuracy when features are included vs. dropped from a model may, with very high probability, reject the null hypothesis that the features are unimportant even when those features are completely independent of the response. Such procedures and more reliable alternatives are discussed in Section 4 before concluding with a discussion in Section 5.

2 Augmented Bagging

Throughout the remainder of this paper, we will assume data of the form \( D_n = \{Z_1, ..., Z_n\} \) where each ordered pair \( Z_i = (X_i, Y_i) \) consists of a feature vector \( X_i = (X_{1,i}, ..., X_{p,i}) \) and response \( Y_i \in \mathbb{R} \). Given \( B \) bootstrap samples of the data, recall that the original bagging procedure (Breiman, 1996) generates a prediction at \( x \) of the form

\[
\hat{y}_{\text{Bagg}} = \frac{1}{B} \sum_{i=1}^{B} T(x; \omega_i, D_n) \tag{1}
\]

where the randomness \( \omega_i \) serves only to select the bootstrap sample on which the \( i^{th} \) tree \( T \) is trained. Whenever the randomness is assumed to select both the bootstrap sample as well as the eligible features at each internal node, the random forest prediction \( \hat{y}_{\text{RF}} \) can be written in the same general form as (1).

The augmented bagging (AugBagg) procedure we introduce here represents a very straightforward extension of classical bagging. Beginning with the original dataset \( D_n \),
we create an augmented dataset $D_n^*$ consisting of additional noise features generated conditionally independent of $Y$. This augmented dataset thus takes the form $D_n^* = \{Z_1^*, ..., Z_n^*\}$ where each $Z_i^*$ now denotes an ordered triplet $(X_i, N_i, Y_i)$ consisting of the original features $X_i$ and response $Y_i$, but also an additional set of noise features $N_i = (N_{1,i}, ..., N_{q,i})$. The original bagging procedure is then performed on this augmented feature space so that the AugBagg output produces predictions of the form

$$\hat{y}_{\text{AugBagg}} = \frac{1}{B} \sum_{i=1}^{B} T((x, n); \omega_i, D_n^*).$$

(2)

where $n$ can be filled in with random draws from the additional noise features.

While the procedure is most straightforward and easily implemented when the additional noise $N$ is assumed independent of all original data $(X, Y)$, we insist only that $N$ be conditionally independent of $Y$ given $X$. This allows for noise to be added that is correlated with the original features $X$ and as demonstrated in Section 3, the manner in which this noise is generated can have a dramatic impact on performance.

2.1 Theoretical Motivation and Analogous Results

Though straightforward, many readers may be skeptical of the potential benefits of the AugBagg procedure outlined above. In the following three subsections, we draw upon recent results on interpolation and implicit regularization in order to provide some theoretical motivation for why the AugBagg procedure may have potential for improving performance in practice.

2.1.1 Randomization as Regularization

In very recent work, Mentch and Zhou (2019) argue that the success of random forests is due in large part to a kind of implicit regularization offered by the $mtry$ parameter governing the features available for splitting at each node. The authors demonstrate that the lower the signal-to-noise ratio (SNR) of the data, the smaller the optimal value of $mtry$. Moreover, the authors demonstrate that this behavior is not tree-specific, but holds for any ensemble consisting of forward-selection-style base learners in which the available features are randomly restricted at each step. Specifically, the authors consider a type of randomized forward selection (RandFS) that proceeds in the same fashion as a standard linear model forward selection process, but where only a randomly selected subset of the remaining features are eligible to be added to the model at each step.
Given data of the form described above, consider a generic regression relationship of the form \( Y = f(X) + \epsilon \) and consider an estimate \( \hat{f}_{RFS} \) formed by averaging over \( B \) individual RandFS models \( \hat{f}_{RFS,1}, \ldots, \hat{f}_{RFS,B} \). Each of the individual RandFS models can be written as

\[
\hat{\beta}_{RFS}^{(b)} = \hat{\beta}_0^{(b)} + X_{(1)}^{(b)} \hat{\beta}_{(1)}^{(b)} + \cdots + X_{(d)}^{(b)} \hat{\beta}_{(d)}^{(b)}
\]

where \( X_{(j)}^{(b)} \) is the feature selected at the \( j^{th} \) step in the \( b^{th} \) model and \( \hat{\beta}_{(j)}^{(b)} \) is the corresponding coefficient estimate. Given an orthogonal design matrix, the authors note that for any given feature \( X_i \), the corresponding coefficient estimate in each model is either 0 if \( X_i \) is not included in the model or the ordinary least squares estimate \( \hat{\beta}_{i,OLS} \) if \( X_i \) is selected. Averaging across \( B \) models of this form thus yields a term in the final model of the form \( \gamma_i \cdot \hat{\beta}_{i,OLS} \) where \( \gamma_i \) corresponds to the proportion of individual RandFS models in which \( X_i \) was included.

In this sense, the ensemblized RandFS procedure can be seen as producing a kind of shrinkage whereby the amount of shrinkage \( \gamma_i \) on each feature depends on both the probability that the feature is made eligible and the probability that the feature is actually selected if made available. While the later probability depends on the particular modeling technique and loss function employed, the probability of being made eligible is a direct function of only \( mtry \).

Now suppose that \( mtry \) is held fixed and that the procedure is repeated on an augmented feature space where more noise variables are added. Under the same setup as above, it’s clear that \( \gamma_i \) decreases as a function of the number of extra noise features \( q \) since each original feature will thus have a lower probability of being made eligible. However, even for large values of \( mtry \), we argue further that the probability of being selected once eligible also decreases as \( q \) increases and that such a decrease can be particularly dramatic for features only weakly related to the response. Put simply, for a given original feature \( X_i \), as more noise features are added to the model, the probability that some of those new features will appear at least as important as \( X_i \) grows with \( q \). Thus, even for large values of \( mtry \) where the procedure begins to resemble that of bagging, the augmented version of the procedure may produce a similar kind of regularization and shrinkage to that offered by traditional random forests.

### 2.1.2 AugBagg and OLS Ensembles

While the recent work of Mentch and Zhou (2019) utilized linear model forward selection settings in order to better illustrate the regularization effect of random forests, in work...
appearing around the same time, LeJeune et al. (2019) provided an alternative analysis focused specifically on standard OLS ensembles wherein each base learner is simply a linear model constructed on a subsample of features and observations with coefficients estimated via ordinary least squares. As in Mentch and Zhou (2019), the authors observe that feature subsampling at the base-learner stage produces a regularization effect, concluding that for optimally-tuned subsampling rates, the asymptotic risk of the OLS ensemble is equal to the asymptotic risk of ridge regression, an explicit regularization procedure. Here we review the setup utilized in LeJeune et al. (2019) and demonstrate that the same procedure applied to an augmented design is equivalent to one in which more shrinkage is applied to the original design.

Assume now that we have data of the form $Z_1, ..., Z_n$ where each $Z_i = (X_i, Y_i)$ and

$$ Y_i = X_i' \beta + \epsilon_i $$

where $Y_i \in \mathbb{R}$ denotes the response, the features $X_i \in \mathbb{R}^p$ are drawn i.i.d. from $\mathcal{N}_p(0_{p \times 1}, \Sigma)$, and the $\epsilon_i$ are i.i.d. with mean 0 and variance $\sigma^2$ and independent of $X$.

To build OLS ensembles, we draw $B$ submatrices by applying row subsampling to the observations and column subsampling on $X = [X_1, \ldots, X_n]'$. Let $S_b$ and $T_b$ denote the sets of column and row indices, respectively, selected in the $b^{th}$ model, while $S_b$ and $T_b$ denote the subsampling matrices obtained by selecting the the columns from $I_p$ and $I_n$ corresponding to the indices in $S_b$ and $T_b$. Let $S$ and $T$ denote the entire collections of all possible $S_b$ and $T_b$, respectively. For each base learner, the OLS minimum-norm estimator is given by

$$ \hat{\beta}^{(b)} = S_b (T_b' X S_b)^+ T_b Y $$

where $(\cdot)^+$ denotes the Moore-Penrose pseudoinverse, so that the estimated coefficients of the ensemble are thus given by

$$ \hat{\beta}^{ens} = \frac{1}{B} \sum_{b=1}^{B} S_b (T_b' X S_b)^+ T_b Y. $$

The risk of $\hat{\beta}^{ens}$

$$ R(\hat{\beta}^{ens}) \triangleq \mathbb{E}_x \left[ (x, \beta - \hat{\beta}^{ens}) \right] = \left( \beta - \hat{\beta}^{ens}, \Sigma(\beta - \hat{\beta}^{ens}) \right) $$

is defined as the expected squared error at an independent point $x$ and by the independence between $X$ and $\epsilon$, LeJeune et al. (2019) show that the expected risk over $\epsilon$ can be
decomposed into bias and variance terms as

$$
\mathbb{E}_\mathbf{x} \left[ R(\hat{\beta}^{ens}) \right] = \text{bias}(\hat{\beta}^{ens}) + \text{variance}(\hat{\beta}^{ens}) = \frac{1}{B^2} \sum_{b,c=1}^{B} \text{bias}_{b,c}(\hat{\beta}^{ens}) + \frac{1}{B^2} \sum_{b,c=1}^{B} \text{var}_{b,c}(\hat{\beta}^{ens})
$$

where

$$
\text{bias}_{b,c}(\hat{\beta}^{ens}) = \left\langle \beta' \right\rangle - \left( I_p - S_b (T'_b X S_b) T'_b X \right) \Sigma \left( I_p - S_c (T'_c X S_c) T'_c X \right)
$$

$$
\text{var}_{b,c}(\hat{\beta}^{ens}) = \sigma^2 \left( S_b (T'_b X S_b) T'_b, \Sigma S_c (T'_c X S_c) T'_c \right).
$$

The following assumptions allow us to more precisely evaluate the risk.

**Assumption 1.** (Finite Subsampling) The subsets in the collections $\mathcal{S}$ and $\mathcal{T}$ are selected at random such that $|S_b| < |T_b| - 1$ and that the following hold:

- $\Pr(j \in S_b) = \frac{|S_b|}{p}$ for all $j \in [p] = \{1, 2, \ldots, p\}$
- $\Pr(m \in T_b) = \frac{|T_b|}{n}$ for all $m \in [n]$
- The subsets $S_1, S_2, \ldots, S_B, T_1, \ldots, T_B$ are conditionally independent given the row subsample sizes $|T_b|_{b=1}^B$.

**Assumption 2.** (Asymptotic Subsampling) For some $\alpha, \eta \in [0, 1]$, the subsets in the collections $\mathcal{S}$ and $\mathcal{T}$ are selected randomly such that $|S_b|/p \overset{a.s.}{\rightarrow} \alpha$ as $p \rightarrow \infty$ and $|T_b|/n \overset{a.s.}{\rightarrow} \eta$ as $n \rightarrow \infty$ for all $b \in [B]$.

Furthermore, it is assumed that $\Sigma = I_p$, that $\|\beta\|_2 = 1$, and that $p/n \rightarrow \gamma$ with $\eta > \alpha\gamma$ as $n, p \rightarrow \infty$. Under these assumptions, conditional on the subset sizes, the expected risk of the bias and variance components over $X, \mathcal{S}$ and $\mathcal{T}$ converge almost surely as follows:

$$
\mathbb{E}_{X,\mathcal{S},\mathcal{T}} \left[ \text{bias}_{b,c}(\hat{\beta}^{ens}) \right] \overset{a.s.}{\rightarrow} B(\alpha) := \begin{cases} 
(1 - \alpha)^2 \left( 1 + \frac{\alpha^2}{1 - \alpha^2 \gamma} \right) & \text{if } b \neq c \\
(1 - \alpha) \left( 1 + \frac{\alpha^2}{\eta^2 \alpha^2 \gamma} \right) & \text{if } b = c
\end{cases}
$$

$$
\mathbb{E}_{X,\mathcal{S},\mathcal{T}} \left[ \text{var}_{b,c}(\hat{\beta}^{ens}) \right] \overset{a.s.}{\rightarrow} V(\alpha) := \begin{cases} 
\frac{\sigma^2 \alpha^2}{1 - \alpha^2 \gamma} & \text{if } b \neq c \\
\frac{\sigma^2 \alpha^2}{\eta^2 \alpha^2 \gamma} & \text{if } b = c.
\end{cases}
$$

Thus, for an OLS ensemble built with $\alpha = \alpha_1$ with subsamples drawn such that $|S_b| = \lfloor \alpha_1 p \rfloor$ and $|T_b| = \lfloor \eta \alpha_1 n \rfloor$, $\mathbb{E}_{X,\mathcal{S},\mathcal{T}} \left[ \text{bias}_{b,c}(\hat{\beta}^{ens}) \right]$ and $\mathbb{E}_{X,\mathcal{S},\mathcal{T}} \left[ \text{var}_{b,c}(\hat{\beta}^{ens}) \right]$ will converge almost surely to $B(\alpha_1)$ and $V(\alpha_1)$ respectively.

Now suppose that the same kind of subsampled OLS ensemble is constructed on an augmented feature space where $X$ is augmented with $N = [N_1, \ldots, N_n]' \in \mathbb{R}^{n \times q}$, and
where the \( N_i \) are drawn i.i.d. from \( N_q(0_{q \times 1}, I_q) \). Let \( S_b^* \) and \( T_b^* \) denote the subsampling indices on the \( b^{th} \) model constructed on this augmented design \([X \ N]\) and suppose that the subsampling sizes remain the same as in the OLS ensemble constructed on the original data so that \(|S_b^*| = |S_b| \) and \(|T_b^*| = |T_b| \). Furthermore, suppose that the number of additional features \( q \to \infty \) as \( p \to \infty \) such that \( \frac{q}{p} \to \theta \) for some constant \( \theta > 0 \). Under these assumptions,

\[
\frac{|S_b|}{p + q} \to \frac{\alpha_1}{1 + \theta} = \alpha_1^* < \alpha_1
\]

and so

\[
\mathbb{E}_{X,S,T} \left[ \text{bias}_{b,c} (\hat{\beta}^{\text{ens}}) \right] \quad \text{and} \quad \mathbb{E}_{X,S,T} \left[ \text{var}_{b,c} (\hat{\beta}^{\text{ens}}) \right]
\]

converge to \( B(\alpha_1^*) \) and \( V(\alpha_1^*) \), respectively. Thus, constructing an OLS ensemble on an augmented design has the same effect as constructing the ensemble on the original design with a smaller subsampling rate, thereby producing a more regularized estimator.

### 2.1.3 Implicit Regularization and Ridge Regression

In addition to the work described above, an intriguing collection of work has emerged within the last couple of years focused around the so-called “double-descent” phenomenon coined in Belkin et al. (2019), whereby the generalizability error of models may sometimes continue to improve beyond the point of interpolation where training error vanishes. Hastie et al. (2019) followed up this work with an impressive and thorough analysis on the behavior of minimum norm interpolation for high-dimensional least squares estimators. While this work focused on the “ridgeless” setting, interesting related results have also been established for ridge and kernel ridge regression. Kobak et al. (2019) showed that for a standard ridge estimator of the form

\[
\hat{\beta}_\lambda = (X'X + \lambda I)^{-1}X'Y
\]

the optimal penalty \( \lambda \) can be 0 or negative even when \( p \gg n \). In particular, this may happen when the majority of signal comes from a small subset of high-variance features due to an implicit regularization effect offered by a larger collection of relatively low-variance noise features. In very recent work, Jacot et al. (2020) consider ridge estimators acting on a (possibly larger) transformed feature space consisting of Gaussian random features and show that such an estimator with ridge penalty \( \lambda \) is close to a kernel ridge regression estimator with effective penalty \( \tilde{\lambda} \) where \( \tilde{\lambda} > \lambda \). d’Ascoli et al. (2020) consider a similar random feature setup in investigating the double descent behavior of neural networks and provide a thorough review of much of the recent work on interpolation where we would refer interested readers.
In motivating the AugBagg procedure proposed above, we turn to a key result from Kobak et al. (2019). As above, assume we have (original) training data of the form \((X, Y)\) where \(y = x'\beta + \epsilon\) and let \(\hat{\beta}_\lambda\) denote the ridge estimator of \(\beta \in \mathbb{R}^p\). Now consider a new estimator \(\hat{\beta}_q\) formed by performing minimum norm least squares and taking only the first \(p\) elements after augmenting \(X\) with \(q\) additional i.i.d. noise features, each with mean 0 and variance \(\lambda/q\). The theorem below shows that augmenting the original design with low-variance noise features produces an equivalent regularization effect to ridge regression.

**Theorem 1.** [Kobak et al. (2019)] Under the setup described above,

\[
\hat{\beta}_q \xrightarrow{a.s. \; q \to \infty} \hat{\beta}_\lambda.
\]

Furthermore, for any \(x\), let \(\hat{y}_\lambda = x'\hat{\beta}_\lambda\) denote the ridge prediction and let \(\hat{y}_{\text{Aug}}\) be the prediction generated by the augmented model that includes the additional \(q\) parameters using \(x\) extended with \(q\) random elements generated in the same fashion. Then

\[
\hat{y}_{\text{Aug}} \xrightarrow{a.s. \; q \to \infty} \hat{y}_\lambda.
\]

Now suppose we build ensembles of estimators of the kind in Theorem 1 by drawing \(B\) subsamples, constructing the estimators on each subsample, and averaging. Similar to the setup used above in LeJeune et al. (2019), let \(T_b \subseteq [n]\) be the set of indices of selected observations in the \(b^{th}\) subsample and let \(T_b\) be the \(n \times |T_b|\) matrix obtained by selecting columns from \(I_n\) corresponding to the indices in \(T_b\). Construct \(\hat{\beta}^{(b)}_q\) as above based on \(T_b'X\) and \(T_b'Y\), which denote the design matrix and response, respectively, corresponding to the observations selected in \(b^{th}\) subsample. The final ensemble coefficient estimate formed by averaging the augmented minimum norm estimators is given by

\[
\hat{\beta}_{\text{ens}} = \frac{1}{B} \sum_{b=1}^B \hat{\beta}^{(b)}_q
\]

where, by Theorem 1,

\[
\hat{\beta}_{\text{ens}} = \frac{1}{B} \sum_{b=1}^B \hat{\beta}^{(b)}_q \xrightarrow{a.s. \; q \to \infty} \frac{1}{B} \sum_{b=1}^B \hat{\beta}_\lambda
\]

with

\[
\hat{\beta}_\lambda^{(b)} = (X'T_bT_b'X + \lambda I_p)^{-1}X'T_bT_b'Y.
\]

Now consider a simple setting where \(p = n\) and \(X = I_n\) and let \(\eta\) denote the subsampling rate so that \(|T_b|/n \to \eta \in (0, 1]\). Let \(N\) be a \(n \times n\) diagonal matrix where \(N_{ii}\) is the number
of times that the $i^{th}$ observation appears in the $B$ subsamples and let $\lambda_q = \frac{1+\lambda-\eta}{\eta} \geq \lambda$.

Then we have

$$\hat{\beta}_{\text{ens}} \xrightarrow{a.s.}{\lambda_q \to \infty} \frac{1}{B} \sum_{b=1}^{B} \hat{\beta}_\lambda^{(b)} = \frac{1}{B} \sum_{b=1}^{B} (T_bT_b' + \lambda I_p)^{-1}T_bY = \frac{1}{1 + \lambda B} NY \xrightarrow{B \to \infty} \frac{\eta}{1 + \lambda} Y = \frac{1}{1 + \lambda} Y = \hat{\beta}_\lambda$$

Thus, in this simple case, an ensemble of minimum-norm least squares estimators constructed on an augmented design produces an estimate equivalent to one produced via ridge regression on the original design. Furthermore, the shrinkage produced by the ensemble is stronger than that of each individual base model.

### 3 Simulations and Real Data Examples

The above results provide some theoretical motivation for the idea that the AugBagg procedure may induce a kind of implicit regularization similar to that induced by the feature subsampling in a traditional random forest. We now present a number of simulation studies to demonstrate the effectiveness of the procedure in practice. To begin, we consider a standard linear model of the form $Y = X\beta + \epsilon$, with $n \times p$ design matrix, the rows of which are i.i.d. multivariate normal $N_p(0, \Sigma)$ where $\Sigma \in \mathbb{R}^{n \times p}$ has entry $(i, j) = \rho^{|i-j|}$ with $\rho = 0.35$. The form of this covariance corresponds to that utilized frequently in the recent work by Mentch and Zhou (2019) and to the ‘beta-type 2’ setup utilized in Hastie et al. (2017). The original data was chosen to include $n = 100$ observations, $p = 5$ original signal features with $\beta_1 = \cdots = \beta_5 = 1$, and $q$ additional i.i.d. noise features sampled from $N(0, 1)$ independent of $X$ were then added with $q$ ranging from 1 to 250. As in Mentch and Zhou (2019) and Hastie et al. (2017), the noise term $\epsilon$ was sampled from $N(0, \sigma^2_\epsilon)$ with $\sigma^2_\epsilon$ chosen to satisfy a particular SNR given by $\beta^T \Sigma \beta / \sigma^2_\epsilon$.

Figure 1 shows the performance of the AugBagg procedure against that of traditional bagging and random forests built on the original data consisting of only the first $p = 5$ features. Here we measure performance by relative test error, defined simply as the test MSE scaled by $\sigma^2_\epsilon$. Each plot corresponds to a different SNR – 0.01, 0.05, 0.09, or 0.14 – and shows the test error as calculated on an independent, randomly generated test set.
Figure 1: Performance of Augmented Bagging as \( q \) additional noise covariates are added to the model as compared with random forests and traditional bagging on the original data. At low SNRs, we see a dramatic improvement over even the optimal random forest model as \( q \) grows.

containing 1000 observations. Each point in each plot corresponds to the average error calculated over 500 iterations. Horizontal lines in each plot correspond to the accuracy of a random forest constructed with a particular value of \( \texttt{mtry} \) and we see that in each case the random forest error grows as \( \texttt{mtry} \) increases. At the lowest SNR of 0.01, AugBagg appears to continually improve with \( q \), easily surpassing the best random forest at around \( q = 25 \). The results are similar, though less dramatic, when the SNR is increased to 0.05. When the SNR is increased to 0.09, the performance of AugBagg appears to level-off around \( q = 50 \), never achieving that of the optimal random forest with \( \texttt{mtry} = 1 \). Finally, when the SNR is 0.14, the additional noise features appear to help until approximately \( q = 50 \), after which point the performance begins to deteriorate.
Figure 2: Performance of AugBagg compared against bagging and random forests as additional noise variables are added to the procedure. Different colored lines in each plot correspond to different correlation strengths between the original and noisy additional features.

The results in Figure 2 expand these simulations. The data and model setup remain the same but the results are explored over a wider range of 8 SNRs ranging from 0.01 to 2.07. Furthermore, in addition to the additional noise features sampled independently of $X$, here we consider the addition of noisy features that are correlated with one of the first 5 signal features. In a similar fashion to knockoffs (Barber et al., 2015; Candes et al., 2018), such noise features are thus independent of the response $Y$ given $X$. To generate such features, we first select an original feature $X$ at random and generate a standard normal $Z \sim N(0, 1)$. For a given level of correlation $r$, each of the additional $q$ features then take the form

$$N = rX + \sqrt{(1 - r)^2}Z.$$  \hfill (3)

In each of the plots in Figure 2 we consider correlations of $r = 0, 0.2, 0.7,$ and 0.99 for batches of additional features ranging in size from 1 to 250. Performance is measured in the same fashion and estimates are averaged over 500 replications for each point in each plot. In the following discussion, we will use the shorthand $AB(q, r)$ to denote an AugBagg model with $q$ additional noise features, each of which has correlation $r$ with one of the features in the original dataset.
Figure 3: RTE on real datasets with additional noise injected to the response. Left: low dimensional datasets. Right: high dimensional datasets.

Figure 2 presents a very interesting and telling story in terms of how the additional noise features are influencing performance and how that influence changes across different SNR levels. At the lowest SNRs of 0.01 and 0.05, we see that in every case, the AugBagg models are improving with the number of extra noise features $q$. Once $q > 50$, all AugBagg models begin to outperform even the best random forest, with the exception of $AB(q, 0.99)$ where very highly correlated noise features are added. At SNR = 0.09, much the same story is present but now only $AB(q, 0.7)$ outperforms the optimal random forest and again this transition happens around $q = 50$. At SNR = 0.14 we begin to see an interesting shift where the performance of the independent noise model $AB(q, 0)$ begins to deteriorate with $q$. When the SNR grows to 0.42 and 0.71, this effect is much more pronounced with $AB(q, 0)$ and $AB(q, 0.2)$ both deteriorating with $q$. At the largest SNRs of 1.22 and 2.07, $AB(q, 0.99)$ is now the only model not deteriorating substantially with $q$.

3.1 Experiments on Real World Data

The previous simulations demonstrate that the AugBagg procedure can lead to substantial gains in accuracy over the baseline bagging procedure on synthetic datasets. Following a very similar setup to Mentch and Zhou (2019), we now investigate its performance on real data taken from the UCI Machine Learning Repository (Dua and Graff, 2017). Data summaries are provided in Table 1; a total of nine low-dimensional ($p < n$) and five high-dimensional ($p > n$) datasets are included.

In implementing the AugBagg procedure, we consider tuning both the number of ad-
ditional noise features $q$ as well as the level of correlation $r$. Since different datasets have different numbers of original features, $q$ is tuned over $p/2$, $p$, $3p/2$ and $2p$. The correlation strength $r$ is tuned over 0, 0.1, 0.4, 0.7 and 0.9. In datasets with mixed feature types, each additional noise feature is chosen to be correlated with one randomly selected continuous feature from the original data. As in Mentch and Zhou (2019), we inject further noise of the form $\epsilon \sim N(0, \sigma^2_\epsilon)$ into the response where $\sigma^2_\epsilon$ is chosen as some proportion of the variance of the original response. Performance is measured in terms of relative test error (RTE), defined as
\[
\text{RTE} = \frac{\tilde{E}\text{rr}(\text{bagging}) - \tilde{E}\text{rr}(\text{AugBag})}{\tilde{\sigma}^2_y} \times 100\% \quad (4)
\]
with positive values indicating superior performance by AugBagg.

Results are shown in Figure 3. In every case, the performance of the tuned AugBagg procedure increases as the SNR decreases as demonstrated by the positive slope displayed for each dataset. In 12 of the 14 datasets, AugBagg quickly begins to outperform bagging on the original data with substantial improvements occurring as more noise is injected. Furthermore, it is interesting to note that in the 2 cases where traditional bagging remains superior, both datasets (AquaticTox and mtp2) are high-dimensional and, in fact, contain the largest number of original features out of all datasets considered ($p = 468$ and 1142,

| Dataset | $p$ | $n$ |
|---------|-----|-----|
| Abalone Age [abalone] Waugh (1995) | 8 | 4177 |
| Bike Sharing [bike] Fanaee-T and Gama (2014) | 11 | 731 |
| Bioston Housing [boston] Harrison Jr and Rubinfeld (1978) | 13 | 506 |
| Concrete Compressive Strength [concrete] Yeh (1998) | 8 | 1030 |
| CPU Performance [cpu] Ein-Dor and Feldmesser (1987) | 7 | 209 |
| Conventional and Social Movie [csm] Ahmed et al. (2015) | 10 | 187 |
| Facebook Metrics [fb] Moro et al. (2016) | 7 | 499 |
| Servo System [servo] Quinlan (1993) | 4 | 167 |
| Solar Flare [solar] Li et al. (2000) | 10 | 1066 |
| Aquatic Toxicity [AquaticTox] He and Jurs (2005) | 468 | 322 |
| Molecular Descriptor Influencing Melting Point [mtp2] Bergström et al. (2003) | 1142 | 274 |
| Weighted Holistic Invariant Molecular Descriptor [pah] Todeschini et al. (1995) | 112 | 80 |
| Adrenergic Blocking Potencies [phen] Cammarata (1972) | 110 | 22 |
| PDGFR Inhibitor [pdgfr] Guha and Jurs (2004) | 320 | 79 |

Table 1: Summary of UCI datasets utilized.
**Algorithm 1** Random Forest Permutation Test (Coleman et al., 2019)

**Require:** Original training set $D_n$, test set $D_{test}$, number of permutations $P$

1. Create alternative data $D_n^*$
2. Build ensemble $RF$ with $D_n$ and predict at $D_{test}$
3. Build ensemble $RF^*$ with $D_n^*$ and predict at $D_{test}$
4. Compute difference in errors $d_0 = MSE(RF^*) - MSE(RF)$
5. for $i$ in $1 : P$ do
   a. Randomly shuffle base models between ensembles to form $RF_i$ and $RF_i^*$
   b. Compute permuted difference in errors $d_i = MSE(RF_i^*) - MSE(RF_i)$
6. Calculate p-value $p = \frac{1}{P+1} \left[ 1 + \sum_{i=1}^{P} I(d_0 > d_i) \right]$

respectively). In these cases, it is quite possible that many of the original features are themselves noisy and thus the additions we make are of no further benefit.

## 4 Implications for Variable Importance

Within any kind of black-box supervised learning framework, determining valid means of measuring the importance of features utilized in the model is often of utmost importance. Indeed, in such non-parametric regimes where model fit and behavior remain largely hidden from view, understanding how features contribute information to the prediction is essential in many settings for scientists and practitioners. In the context of bagging and random forests specifically, Breiman’s original out-of-bag (oob) (Breiman, 2001) importance scores are one such popular measure, though many issues such as a preference for correlated features and those with many categories have been noted in the years following their introduction (Strobl et al., 2007; Nicodemus et al., 2010; Toloşi and Lengauer, 2011).

Recently, however, Mentch and Hooker (2016) proposed a formal hypothesis testing procedure for measuring feature importance in random forests. Given a generic relationship of the form $y = f(x) + \epsilon$, the authors consider partitioning the original set of features $X$ into two groups, $X_0$ and $X_{test}$, where the latter group contains the features of interest so that a null hypothesis of the form

$$H_0 : f(X_0, X_{test}) = f_0(X_0) \quad (5)$$

may be rejected whenever the features in $X_{test}$ make a significant contribution to the response. Importantly, the authors propose to evaluate the hypothesis in (5) by constructing two separate random forest models: one constructed on the original data and one
constructed on an altered dataset where the features in $\mathbf{X}_{\text{test}}$ are either substituted for randomized replacements independent of the response or dropped from the model entirely. Predictions from each forest are then computed at a number of test points and the differences are combined to form an appropriate test statistic. Coleman et al. (2019) recently proposed a more computationally efficient and scalable permutation test alternative that involves exchanging trees between the two forests. An outline of this test is given in Algorithm 1.

Crucially, the tests described above rely on measuring the difference between either raw predictions or predictive accuracy between two tree-based ensembles constructed on different training sets. Both papers advocate for replacing the features under investigation with randomized alternatives, noting that the tests can potentially produce spurious results when features are instead dropped from the second model, though neither provides a detailed explanation as to why this occurs. Elsewhere in the literature, alternative tests specifically propose to evaluate feature importance by measuring the drop in performance when the features in question are removed from the model. Such is the case, for example, with the Leave-Out-Covariates (LOCO) measure proposed recently by Lei et al. (2018) in the context of conformal inference. Furthermore, though often done informally, it is also common throughout the broader scientific literature for authors to argue for the importance of particular variables based on decreases in model performance when such variables are removed.

The results presented in the sections above present a substantial concern with such measures. In particular, if model performance can be improved simply by adding randomly generated covariates that are (at least conditionally) independent of the response, then observing a significant improvement in accuracy when a particular set of features is included does not imply that any relationship to the response or even the other covariates need exist. To emphasize this point, we implement the ensemble-based permutation test recently developed in Coleman et al. (2019) and investigate its behavior under simulated settings similar to those used in the previous sections.

To begin, we utilize the same linear model setup as in Section 3 with $p = 5$ original signal features, adjusting the model errors to produce a pre-specified SNR, and consider adding $q$ additional noise features to test for importance. Thus, relative to the sort of generic null hypothesis specified in (5), our default set of features consist of the original signals so that $\mathbf{X}_0 = (X_1, ..., X_5)$ and the features under investigation are those additional noise features being added, $\mathbf{X}_{\text{test}} = (N_1, ..., N_q)$. To carry out the test, we constructed two random forests: one built using all features $\mathbf{X}_0$ and $\mathbf{X}_{\text{test}}$ and the other using only
those default baseline (signal) features in $X_0$. A total of 500 trees were constructed in each forest and 1000 permutations were used to compare predictive differences after swapping trees between the two ensembles. The entire procedure was repeated 500 times, each time recording whether the null hypothesis that the additional features are not important was rejected at level $\alpha = 0.05$. In rejecting the null hypothesis, we would conclude that the additional features are important.

Figure 4 shows the probability of rejecting $H_0$ and concluding the additional noise features are important across various SNRs, sample sizes, noise distributions, and numbers of additional features $q$. The plots in the top row of Figure 4 correspond to the case where the additional noise features are sampled independently from a standard normal with a
sample size of $n = 100$ on the left and $n = 500$ on the right. The bottom row shows the same setup except that the additional noise features are correlated with a randomly selected (signal) feature in $X_0$ at a strength of $r = 0.7$. Examining these four plots, it is clear that at low SNRs this test is extremely likely to reject even at small values of $q$ and especially when the additional noise features are correlated with the original signal features. Looking at the bottom-right plot in Figure 4 for example, we see that even when the SNR is 1, the test rejects about 50% of the time at $q = 100$.

Though perhaps a bit troubling, these results are not at all surprising given the empirical results in Section 3 that showed strong evidence of improved performance when additional noise features are added to the model. Tests such as those proposed in Mentch and Hooker (2016) and Coleman et al. (2019), however, claim to offer a more robust procedure whenever those features under investigation are replaced by randomly generated substitutes rather than being dropped from the model entirely. Thus, we now turn our attention to investigating the improvement offered by this alternative setup.

Figure 5 compares the performance of such tests under the same linear model setting as above where $n = 500$ and $p = 5$ in every case. The top row shows the performance of the tests when the alternative dataset replaces the features under investigation with randomized replacements compared with that which drops them from the model entirely. In the top-left plot the additional noise features are independent and in the top-right plot they follow the same correlation scheme as above with $r = 0.7$. One characteristic immediately noticeable in both plots is the more consistent behavior of the replacement test across a range of SNRs: in both cases, the rejection probabilities appear to decrease slowly as $q$ increases but maintain rejection probabilities between approximately 0.2 and 0.4. At low SNRs, these probabilities are far smaller than observed for the test that compares predictions between models where features are dropped but larger for large SNRs.

The bottom row of Figure 5 compares the performance of these tests whenever noise features of one kind are replaced by noise features of another kind. On the left, the original noise features are randomly correlated with an original signal feature at $r = 0.7$ and these features are replaced with independent noise features in carrying out the test. While this setting is likely most representative of what might often happen in practice, for completeness, we consider the opposite setting in the plot on the bottom-right where independent noise features are replaced with ones correlated with a randomly selected feature in $X_0$. Here again we notice a troubling trend: in the bottom-left plot where correlated features are replaced by independent noise, the test has a very high probability of rejecting across all but the lowest SNRs and this probability appears to increase with $q$. Perhaps even
Figure 5: Top row: Rejection probabilities for tests based on removing vs replacing features in question. Noise features are independent in the left plot and correlated with $r = 0.7$ in the right. Bottom Left: Rejection probabilities when noisy features in the original data are substituted for independent replacements. Bottom Right: Rejection probabilities when independent noisy features are replaced by correlated replacements with $r = 0.7$.

worse is the fact that the rejection probabilities appear to be increasing at a faster rate at higher SNRs. Thus, even in “good data” settings, it appears that such tests are very likely to cause correlated noise features to appear important whenever testing against the performance of a model using only independent noise as a substitute. In the opposite case (bottom-right) we see the opposite trend. Here the rejection probabilities appear small for all but the lowest SNRs and also appear to be shrinking as $q$ grows.
4.1 Bad Tests or Bad Interpretations?

Given these results, one may be tempted to conclude that tests of the style proposed in work such as Mentch and Hooker (2016), Lei et al. (2018), and Coleman et al. (2019) are simply “bad” because the outcomes are “wrong” far too often. Indeed, if rejecting the null hypothesis in these types of procedures taken to mean that the features in question are “important” and “important” is taken to mean that those features possess some unique explanatory power for the response not captured by the other features available, then certainly such tests would appear to be highly problematic as the rejection rates in the above settings very often lie far above the nominal level of $\alpha = 0.05$.

In our view, however, such an understanding is too naive. The demonstrations above do not necessarily imply that anything is wrong with the tests themselves. Rejecting the null hypotheses in such tests means only that there is evidence that the features in question improve model performance when included. The simulations in Section 3, however, suggest that even the inclusion of additional noise features can improve model performance, sometimes to a dramatic degree.

This situation highlights the crucial need for precise language in discussions of feature importance. While “predictive improvement” intuitively feels like a natural proxy, it seems quite unlikely that features independent of the response (at least conditionally) ought to ever be considered “important” for most practical purposes. Certainly this is the case whenever scientists argue that particular features must be collected in order to construct the optimal predictive model or when arguing that features generated by a new piece of technology can lead to further improved model performance over those that were previously available.

In situations such as these, it seems that what is really being sought is not a measure of how “important” certain features may be, but rather how “essential” they are. Even when additional variables improve model performance, we really seek to determine whether they do so meaningfully or significantly more than randomized alternatives. The results in the preceding section also highlight the potential issues with replacing features by randomized replacements from a different distribution and thus might suggest some promise for procedures involving knockoff variables (Barber et al., 2015; Candes et al., 2018) that explicitly attempt to generate randomized replacements from the same distribution as the original features. In practice however, even these procedures require estimating the conditional distributions of features in order to generate the replacements.
5 Discussion

The work in the preceding sections introduced the idea of augmented bagging (AugBagg), a simple procedure identical to traditional bagging except that additional noise features, conditionally independent of the response, are first added to the feature space. Surprisingly, we showed that this simple modification to bagging can lead to drastic improvements in model performance, sometimes even outperforming well-established alternatives like an optimally-tuned random forest. Performance gains appear most dramatic at low SNRs, though the introduction of correlated noise features can continue to improve performance even at higher SNRs. The fact that performance can sometimes be dramatically improved by simply adding conditionally-independent features into the model has important implications for variable importance measures and especially in interpreting the results from tests of variable importance.

Though AugBagg may sometimes produce predictions substantially more accurate than an alternative baseline like random forests, we stress that the procedure should not be seen as replacing or superseding more efficient procedures like random forests. As detailed in the introduction, random forests have a long documented history of off-the-shelf success and depending on the size of the data at hand, may be much more computationally feasible to implement in practice. Indeed, while random forests reduce the number of features considered at each node, AugBagg, by construction, explicitly increases this computational burden. Furthermore, while recent work by Mentch and Zhou (2019) suggests that the \texttt{mtry} parameter in random forests be tuned, moderate success can often be found at default values whereas a generic implementation of AugBagg involves tuning both the number of additional features and their correlation with the original features and we are not able to offer default values of these likely to be successful across a broad range of data settings.

Acknowledgements

This research was supported in part by the University of Pittsburgh Center for Research Computing through the resources provided.

References

Ahmed, M., M. Jahangir, H. Afzal, A. Majeed, and I. Siddiqi (2015). Using crowd-source based features from social media and conventional features to predict the movies pop-
ularity. In 2015 IEEE International Conference on Smart City/SocialCom/SustainCom (SmartCity), pp. 273–278. IEEE.

Barber, R. F., E. J. Candès, et al. (2015). Controlling the false discovery rate via knockoffs. *The Annals of Statistics* 43(5), 2055–2085.

Belkin, M., D. Hsu, S. Ma, and S. Mandal (2019). Reconciling modern machine-learning practice and the classical bias–variance trade-off. *Proceedings of the National Academy of Sciences* 116(32), 15849–15854.

Bergström, C. A., U. Norinder, K. Luthman, and P. Artursson (2003). Molecular descriptors influencing melting point and their role in classification of solid drugs. *Journal of chemical information and computer sciences* 43(4), 1177–1185.

Bernard, S., S. Adam, and L. Heutte (2007). Using random forests for handwritten digit recognition. In *Ninth International Conference on Document Analysis and Recognition (ICDAR 2007)*, Volume 2, pp. 1043–1047. IEEE.

Biau, G. and L. Devroye (2010). On the layered nearest neighbour estimate, the bagged nearest neighbour estimate and the random forest method in regression and classification. *Journal of Multivariate Analysis* 101(10), 2499–2518.

Breiman, L. (1996). Bagging predictors. *Machine Learning* 24, 123–140.

Breiman, L. (2001). Random Forests. *Machine Learning* 45, 5–32.

Breiman, L., J. Friedman, C. J. Stone, and R. Olshen (1984). *Classification and Regression Trees* (1st ed.). Belmont, CA: Wadsworth.

Cammarata, A. (1972). Interrelation of the regression models used for structure-activity analyses. *Journal of medicinal chemistry* 15(6), 573–577.

Candes, E., Y. Fan, L. Janson, and J. Lv (2018). Panning for gold: model-xknockoffs for high dimensional controlled variable selection. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 80(3), 551–577.

Coleman, T., L. Mentch, D. Fink, F. La Sorte, G. Hooker, W. Hochachka, and D. Winkler (2017). Statistical inference on tree swallow migrations with random forests. *arXiv preprint arXiv:1710.09793*.

Coleman, T., W. Peng, and L. Mentch (2019). Scalable and efficient hypothesis testing with random forests. *arXiv preprint arXiv:1904.07830*.
Cutler, D. R., T. C. Edwards Jr, K. H. Beard, A. Cutler, K. T. Hess, J. Gibson, and J. J. Lawler (2007). Random forests for classification in ecology. *Ecology* 88(11), 2783–2792.

d’Ascoli, S., M. Refinetti, G. Biroli, and F. Krzakala (2020). Double trouble in double descent: Bias and variance (s) in the lazy regime. *arXiv preprint arXiv:2003.01054*.

Díaz-Uriarte, R. and S. A. De Andres (2006). Gene selection and classification of microarray data using random forest. *BMC bioinformatics* 7(1), 3.

Dua, D. and C. Graff (2017). UCI machine learning repository.

Ein-Dor, P. and J. Feldmesser (1987). Attributes of the performance of central processing units: A relative performance prediction model. *Communications of the ACM* 30(4), 308–318.

Fanaee-T, H. and J. Gama (2014). Event labeling combining ensemble detectors and background knowledge. *Progress in Artificial Intelligence* 2(2-3), 113–127.

Fernández-Delgado, M., E. Cernadas, S. Barro, and D. Amorim (2014). Do we need hundreds of classifiers to solve real world classification problems? *The Journal of Machine Learning Research* 15(1), 3133–3181.

Guha, R. and P. C. Jurs (2004). Development of linear, ensemble, and nonlinear models for the prediction and interpretation of the biological activity of a set of pdgfr inhibitors. *Journal of Chemical Information and Computer Sciences* 44(6), 2179–2189.

Harrison Jr, D. and D. L. Rubinfeld (1978). Hedonic housing prices and the demand for clean air. *Journal of environmental economics and management* 5(1), 81–102.

Hastie, T., A. Montanari, S. Rosset, and R. J. Tibshirani (2019). Surprises in high-dimensional ridgeless least squares interpolation. *arXiv preprint arXiv:1903.08560*.

Hastie, T., R. Tibshirani, and R. J. Tibshirani (2017). Extended comparisons of best subset selection, forward stepwise selection, and the lasso. *arXiv preprint arXiv:1707.08692*.

He, L. and P. C. Jurs (2005). Assessing the reliability of a qsar model’s predictions. *Journal of Molecular Graphics and Modelling* 23(6), 503–523.

Hoerl, A. E. and R. W. Kennard (1970). Ridge regression: Biased estimation for nonorthogonal problems. *Technometrics* 12(1), 55–67.
Jacot, A., Şimşek, F. Spadaro, C. Hongler, and F. Gabriel (2020). Implicit regularization of random feature models. *arXiv preprint arXiv:2002.08404*.

Klusowski, J. M. (2019). Sharp analysis of a simple model for random forests. *arXiv preprint 1805.02587v6*.

Kobak, D., J. Lomond, and B. Sanchez (2019). Optimal ridge penalty for real-world high-dimensional data can be zero or negative due to the implicit ridge regularization. *liver 1*, 1–2.

Lei, J., M. GSell, A. Rinaldo, R. J. Tibshirani, and L. Wasserman (2018). Distribution-free predictive inference for regression. *Journal of the American Statistical Association 113*(523), 1094–1111.

LeJeune, D., H. Javadi, and R. G. Baraniuk (2019). The implicit regularization of ordinary least squares ensembles. *arXiv preprint arXiv:1910.04743*.

Li, J., G. Dong, and K. Ramamohanarao (2000). Instance-based classification by emerging patterns. In *European Conference on Principles of Data Mining and Knowledge Discovery*, pp. 191–200. Springer.

Mehrmohamadi, M., L. K. Mentch, A. G. Clark, and J. W. Locasale (2016). Integrative modelling of tumour dna methylation quantifies the contribution of metabolism. *Nature communications 7*, 13666.

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

Mentch, L. and G. Hooker (2017). Formal hypothesis tests for additive structure in random forests. *Journal of Computational and Graphical Statistics 26*(3), 589–597.

Mentch, L. and S. Zhou (2019). Randomization as regularization: A degrees of freedom explanation for random forest success. *arXiv preprint arXiv:1911.00190*.

Moro, S., P. Rita, and B. Vala (2016). Predicting social media performance metrics and evaluation of the impact on brand building: A data mining approach. *Journal of Business Research 69*(9), 3341–3351.

Nicodemus, K. K., J. D. Malley, C. Strobl, and A. Ziegler (2010). The behaviour of random forest permutation-based variable importance measures under predictor correlation. *BMC bioinformatics 11*(1), 110.
Peng, W., T. Coleman, and L. Mentch (2019). Asymptotic distributions and rates of convergence for random forests and other resampled ensemble learners. arXiv preprint arXiv:1905.10651.

Quinlan, J. R. (1993). Combining instance-based and model-based learning. In Proceedings of the tenth international conference on machine learning, pp. 236–243.

Scornet, E., G. Biau, J.-P. Vert, et al. (2015). Consistency of random forests. The Annals of Statistics 43(4), 1716–1741.

Sexton, J. and P. Laake (2009). Standard errors for bagged and random forest estimators. Computational Statistics & Data Analysis 53(3), 801–811.

Strobl, C., A.-L. Boulesteix, A. Zeileis, and T. Hothorn (2007). Bias in random forest variable importance measures: Illustrations, sources and a solution. BMC bioinformatics 8(1), 25.

Tibshirani, R. (1996). Regression shrinkage and selection via the lasso. Journal of the Royal Statistical Society: Series B (Methodological) 58(1), 267–288.

Todeschini, R., P. Gramatica, R. Provenzani, and E. Marengo (1995). Weighted holistic invariant molecular descriptors. part 2. theory development and applications on modeling physicochemical properties of polyaromatic hydrocarbons. Chemometrics and Intelligent Laboratory Systems 27(2), 221–229.

Toloşi, L. and T. Lengauer (2011). Classification with correlated features: unreliability of feature ranking and solutions. Bioinformatics 27(14), 1986–1994.

Wager, S. and S. Athey (2018). Estimation and inference of heterogeneous treatment effects using random forests. Journal of the American Statistical Association 113(523), 1228–1242.

Wager, S., T. Hastie, and B. Efron (2014). Confidence intervals for random forests: The jackknife and the infinitesimal jackknife. The Journal of Machine Learning Research 15(1), 1625–1651.

Waugh, S. G. (1995). Extending and benchmarking Cascade-Correlation: extensions to the Cascade-Correlation architecture and benchmarking of feed-forward supervised artificial neural networks. Ph. D. thesis, University of Tasmania.

25
Yeh, I.-C. (1998). Modeling of strength of high-performance concrete using artificial neural networks. *Cement and Concrete research* 28(12), 1797–1808.