Abstract
Random forests (RF) are one of the most widely used ensemble learning methods in classification and regression tasks. Despite its impressive performance, its theoretical consistency, which would ensure that its result converges to the optimum as the sample size increases, has been left far behind. Several consistent random forest variants have been proposed, yet all with relatively poor performance compared to the original random forests. In this paper, a novel RF framework named multinomial random forests (MRF) is proposed. In the MRF, an impurity-based multinomial distribution is constructed as the basis for the selection of a splitting point. This ensures that a certain degree of randomness is achieved while the overall quality of the trees is not much different from the original random forests. We prove the consistency of the MRF and demonstrate with multiple datasets that it performs similarly as the original random forests and better than existent consistent random forest variants for both classification and regression tasks.

1. Introduction
Random forests are a popular type of ensemble learning method, where a large number of randomized decision trees are constructed and the results from all trees are combined for the final prediction of the forest. Since its introduction (Breiman, 2001), random forests and its several variants have been widely used in many fields, such as computer vision (Cootes et al., 2012; Kontschieder et al., 2016) and data mining (Bifet et al., 2009; Xiong et al., 2012), because of its excellent performance and fast yet efficient training process.

Despite their great performance and extensive use in practice, some of their theoretical properties, especially the consistency, are not fully established. Due to the inherent bootstrap randomization and the highly greedy data-dependent construction process, it is very difficult to prove the theoretical consistency of random forests.

To address this issue, several random forests variants (Breiman, 2004; Biau et al., 2008; Genuer, 2012; Biau, 2012; Denil et al., 2014; Wang et al., 2018) have been proposed with various type of randomness introduced to the tree building process. The consistency can be established for these approaches. Unfortunately, they all suffer from relatively poor performance compared to Breiman’s original random forests, presumably due to too strong randomness introduced in these approaches. As research continues, the gap between the theoretical consistency and empirical soundness is shrinking while its existence still continuously drives researchers to fill this gap.

In this paper, we propose a novel random forest framework, multinomial random forest (MRF), for both classification and regression. We prove that the MRF is consistent, and demonstrate using multiple datasets that in both classification and regression tasks, its performance is on par with Breiman’s random forest and is better than existent consistent random forest variants. In the original random forest, tree growing is a greedy process and splitting a node has two steps: (1) a set of candidate features is selected, and (2) the best splitting point is determined. In the MRF, we introduce randomness into these steps. First, we add an extra component to the feature selection step: with a small probability $p$ (e.g., $p = 0.01$), we randomly select a single feature as the feature candidate, and with probability $1 - p$, we use the original feature set selection. This introduced randomness is necessary for the consistency because it ensures that every feature has a chance to be the feature for splitting, albeit under a very small probability. Other types of randomness such as Poisson distribution (Denil et al., 2014) are also used for this purpose. Second, we introduce randomness in the selection of a splitting point: All possible splits are considered and the final split is determined according to an impurity-based multinomial distribution. The best split-
Multinomial Random Forests: Fill the Gap between Theoretical Consistency and Empirical Soundness

The main contributions of this paper can be stated as follows: 1) Theoretical consistency of the MRF in both classification and regression is proved; 2) A method of constructing a multinomial distribution using the Softmax function to improve the greedy splitting process is proposed and achieved significant results; 3) A large number of experiments demonstrating the superiority over other consistent random forests and very similar performance as the original RF. With these, the gap between theoretical consistency and empirical soundness has been successfully filled.

2. Related Work

Random forest (Breiman, 2001) is a distinguished ensemble learning algorithm inspired by the random subspace method (Ho, 1998) and random split selection (Dieterich, 2000). In the original method, decision trees are built upon bootstrap datasets from the training set using the CART methodology (Breiman et al., 1984). Its various variants, such as quantile regression forests (Meinshausen, 2006) and deep forests (Zhou & Feng, 2017), have been proposed and used in a wide range of applications (Bifet et al., 2009; Cootes et al., 2012; Xiong et al., 2012; Kontschieder et al., 2016) for their effective training process and great performance.

Despite the widespread use of random forests in practice, theoretical analysis of their success has yet been fully established. Breiman (Breiman, 2001) showed the first theoretical result indicating that the generalization error is bounded by the performance of individual trees and the diversity of the whole forest. After that, the relationship between random forests and a type of nearest neighbor-based estimator has been studied by Lin and Jeon (Lin & Jeon, 2006).

One important property, consistency, has yet been established for random forests. The consistency of a prediction method ensures that its performance converges to the optimum as the sample size goes to infinity. This property was firstly discussed in Breiman’s mathematical heuristics report (Breiman, 2004). After that, the consistency of two directly simplified random forests was verified by Biau (Biau et al., 2008).

Several variants of random forests have been proposed and shown to be consistent; for example, quantile regression forests (Meinshausen, 2006), random survival forests (Ishwaran & Kogalur, 2010), and an online version of random forests (Denil et al., 2013). Recently, Denil et al. (Denil et al., 2014) developed a version in which a subspace of candidate features is selected according to a Poisson distribution. Wang (Wang et al., 2018) introduced Bernoulli random forests (BRF), in which two Bernoulli distributions are used in the tree construction process. Among all these variants, the performance of the BRF is the closest to that of the original random forest.

3. Multinomial Random Forests

We present the multinomial random forests (MRF) in the classification setting in this section. Their extension to the regression setting will be presented in Section 5. The MRF differs from the original random forest in three aspects. A training set partitioning process (details in 3.1) is used instead of the bootstrap technique. At every internal node, randomness is introduced in feature set selection, and an impurity-based multinomial distribution is used for splitting point selection (details in 3.2). By doing these, we ensure that every feature and every possible splitting point have a chance to be selected. The key is to minimize the negative impact of the randomness, which is needed for consistency, on prediction performance.

Let $D_n$ denotes a data set consisting of $n$ i.i.d. observations. Each observation has the form $(X, Y)$, where $X \in \mathbb{R}^D$ represents the $D$-dimensional features and $Y \in \{1, \cdots, K\}$ is the corresponding label of the observation.

3.1. Training Data Set Partition

To build a tree, the training set is divided randomly into two non-overlapping subsets. The two subsets play different roles in the process. One subset will be used to build the structure of a tree; we call the samples in this subset the structure points. Once a tree is built, the labels of its leaves will be re-determined on the basis of the other subsets; we call the samples in this subset the estimation points. In this process, the structure points are used only to influence the shape of the tree by determining the splitting point in each internal node, while the estimation points are used only for the final prediction of the tree. The partitioning of the training set and the separation of their roles are necessary for ensuring consistency of the tree.

To build another tree, the training set is re-partitioned randomly and independently. The sizes of the two subsets are fixed. The ratio of the two parts is parameterized by partition rate $\gamma = |\text{Structure points}| / |\text{Estimation points}|$.

3.2. Tree Construction

In the proposed MRF, comparing to the original RF, the bootstrap technique is replaced by the training data set partition process. In the procedure of candidate features selection and splitting point selection, we introduced some
randomness in a reasonable way. Note that there are many ways to randomly select the candidate features, as long as it satisfies that every feature can be chosen with a positive possibility at each split. For a more convenient comparison, we discuss the case using the Bernoulli distribution in this paper.

The first alteration in MRF is to randomly choose candidate features. Specifically, for each internal node, we randomly draw from a Bernoulli distribution $B(p)$. If it is 1 we randomly select a feature as the feature set; otherwise we proceed with the original procedure for feature set selection (e.g. randomly select $N(D)$ features, where $N(D) = \sqrt{D}$ or $N(D) = \log D$).

In the classification problem, the impurity decrease caused by splitting point $v$ is denoted by

$$I(v) = T(D^S) - \frac{|D^S_l|}{|D^S|}T(D^S_l) - \frac{|D^S_r|}{|D^S|}T(D^S_r), \quad (1)$$

where $D^S$ is the structure points and $D^S_l, D^S_r$ are two children sets generated by $D^S$ splitting at $v$, $T(\cdot)$ is the impurity criterion (e.g. Shannon entropy or Gini index).

The second alteration is that the splitting point is randomly selected based on a multinomial distribution instead of the deterministic rule. More specifically, in contrast to the original random forests where splitting point $v$ is determined by maximizing $I(v)$, we select splitting points randomly according to a multinomial distribution $M(\phi)$ constructed based on the impurity decrease of all possible points. The specific construction of $M(\phi)$ is as follows:

Let $I = (I_1, \ldots, I_m)$ be the vector of impurity decrease for all possible splitting points and all candidate features. We first normalize it as $\hat{I} = \frac{(I_1 - \min I, \ldots, I_m - \min I)}{(\max I - \min I, \ldots, \max I - \min I)}$, and then compute the probabilities $\phi = (\phi_1, \ldots, \phi_m) = \text{softmax}(B\hat{I})$, where $B > 0$ is a hyperparameter.

The hyperparameter $B$ plays a role in regulating the probabilities for selecting the splitting point. The larger $B$, the greater probability that the point with largest impurity decrease will be selected. When $p \to 0$ and $B = 0$, for the splitting point selection process, the MRF becomes a completely random forests (Liu et al., 2008) (since every possible point is selected in the same probability); When $p \to 0$ and $B \to +\infty$, the MRF becomes Breiman’s random forests.

Through the two processes above, one feature and its corresponding splitting value as a splitting point is chosen to grow the tree. Note that the tree construction is only influenced by structure points while the prediction only involves the estimation points. The splitting process is repeated until the given stopping criteria are satisfied.

Similar to original random forests, MRF’s stopping condition also relates to the minimum leaf size. More specifically, in each leaf, the number of estimation points is required to be larger than $k_n$ where $k_n \to \infty$ and $k_n/n \to 0$ as $n \to \infty$.

**Algorithm 1 Decision Tree Training in MRF: $MTree()$**

1. **Input:** Structure points $D^S$, Estimation points $D^E$, parameter $k_n, p, B$, and function $N(D)$.
2. **Output:** The decision tree $T$ in MRF.
3. **if** $|D^E| > k_n$ **then**
4. Select candidate features: Draw a value from a Bernoulli distribution $B(p)$. If it is 1, randomly choose a feature. If it is 0, choose a set of $N(D)$ random features.
5. Calculate the normalized vector $\hat{I}$ of impurity decrease, and the probabilities $\phi = \text{softmax}(B\hat{I})$.
6. Select the splitting point randomly according to the multinomial distribution $M(\phi)$.
7. The structure and estimation points are correspondingly split into two child nodes, called $D^S_l, D^S_r$ and $D^E_l, D^E_r$.
8. $T.leftchild \leftarrow MTree(D^S_l, D^E_l, k_n, p, B)$
9. $T.rightchild \leftarrow MTree(D^S_r, D^E_r, k_n, p, B)$
10. **end if**
11. **Return:** A decision tree $T$ in MRF

### 3.3. Prediction

Once a tree has been grown using the structure points as described above, we re-determine the predicted values for the leaves using the estimation points.

Suppose the unlabeled sample is $x$ and $h$ denotes a decision tree in MRF. The probability that the sample $x$ with label $c (c \in \{1, \ldots, K\})$ evaluated by this tree is

$$\eta^c(x) = \frac{1}{|N^E_h(x)|} \sum_{(x, y) \in N^E_h(x)} \mathbb{I}\{Y = c\}, \quad (2)$$

and the prediction is given by maximizing $\eta^c(x)$:

$$\hat{y} = h(x) = \arg \max_c \{\eta^c(x)\}, \quad (3)$$

where $N^E_h(x)$ denotes the number of estimation points in the node containing $x$, $\mathbb{I}(\cdot)$ is the indicator function.

The final prediction from the MRF is based on the majority vote:

$$\bar{y} = h^{\hat{M}}(x) = \arg \max_c \sum_{i=1}^M \mathbb{I}\{h^{(i)}(x) = c\}, \quad (4)$$

where $M$ is the number of individual trees in MRF.
4. Consistency

Consistency is a fundamental theoretical property of a learning algorithm which guarantees that the output of the algorithm converges to optimum as the data size goes to infinity. In this section, we provide some necessary Lemmas and prove the consistency of the proposed MRF.

4.1. Preliminaries

**Definition 1.** When the data set $D_n$ is given, for a certain distribution of $(X,Y)$, a sequence of classifiers $\{h\}$ are consistent if the error probability $L$ satisfies

$$E(L) = \mathbb{P}(h(X,Z,D_n) \neq Y) \to L^*, \tag{5}$$

where $L^*$ denotes the Bayes risk, $Z$ denotes the randomness involved in the construction of the tree, such as the selection of candidate features.

**Lemma 1.** The voting classifier $\widehat{h}(M)$ which takes the majority vote over $M$ copies of $h$ with different randomizing variables has consistency if those classifiers $\{h\}$ have consistency.

**Lemma 2.** Suppose a series of classifiers $\{h\}$ are consistent on condition $I$ for a distribution on $(X,Y)$:

$$\mathbb{P}(h(X,Z,I) \neq Y \mid I) \to L^*, \tag{5}$$

where $I$ denotes the event that the training data set is randomly partitioned. If acceptable structure points and estimation points created by partitioning produces with probability $I$, $\{h\}$ are unconditionally consistent:

$$\mathbb{P}(h(X,Z,I) \neq Y) \to L^*. \tag{5}$$

**Lemma 3.** Suppose that $\eta(c|x) = \mathbb{P}(Y = c \mid X = x)$ is the posterior estimation for class $c$, and that these estimates are each consistent. The classifier

$$h(x) = \arg \max_c \{\eta(c|x)\} \tag{6}$$

is also consistent.

**Remark 1.** The value of $P_2$ relates to the specific candidate features selection strategy. If it’s through Bernoulli($\nu$) as in (Wang et al., 2018), $P_2 = \frac{1}{\nu^2}$; if Poisson($\lambda$) is used as in (Denil et al., 2013; 2014), $P_2 = \frac{1}{\nu^2} e^{-\lambda}$.

**Lemma 4.** Suppose that features are all supported on $[0,1]$, once a feature $A$ is selected to split, if this feature is divided into $N$ equal partitions $A_1, \cdots, A_N$ from small to large, for the splitting point $v$,

$$\exists P_2 > 0, \text{ s.t. } \mathbb{P}\left(v \in \bigcup_{i=2}^{N-1} A_i \mid A\right) \geq P_2. \tag{5}$$

**Proof.** Recall that the impurity decrease vector $I$ is normalized before multiplying the parameter $B$, i.e., $I \in [0,1]^n$ where $n$ is the number of possible points. When the normalized impurity decrease vector $\hat{I} = (1, 0, \cdots, 0)$, the probability that the first possible point is selected for splitting is the largest, and when $\hat{I} = (0, 1, \cdots, 1)$, the probability reaches smallest.

Thus for all possible splitting point $v$, the probability that it is selected for splitting satisfies the following restriction:

$$\frac{1}{1 + (n-1)e^B} \leq \mathbb{P}(v) \leq \frac{e^B}{e^B + (n-1)}. \tag{8}$$

In this case,

$$\mathbb{P}\left(v \in \bigcup_{i=2}^{N-1} A_i \mid A\right) = \frac{\int_{A_1 \cap \bigcup_{i=2}^{N-1} A_i} f(v)dv}{\int_{A_i} f(v)dv} \geq \lim_{n \to +\infty} \left( \frac{\int_{A_1 \cap \bigcup_{i=2}^{N-1} A_i} 1 + (n-1)e^B dv}{\int_{A_i} e^B + (n-1) dv} \right) \tag{9}$$

$$= \lim_{n \to +\infty} \frac{N-2}{N} e^{2B} \triangleq P_2.$$
Theorem 1. Suppose that $X$ is supported on $[0, 1]^D$ and have non-zero density almost everywhere, the cumulative distribution function of the splitting points is right-continuous at 0 and left-continuous at 1. MRF is consistent if $k_n \to \infty$ and $k_n/n \to 0$ as $n \to \infty$.

Proof. Firstly, since MRF requires $|N^E(X)| \geq k_n$ where $k_n \to \infty$ as $n \to \infty$, $|N^E(X)| \to \infty$ when $n \to \infty$ is trivial.

Let $V_m(a)$ denotes the size of the $a$-th feature of $N_m(X)$ where $X$ falls into the node $N_m(X)$ at $m$-th level. To prove $\text{diam}(N(X)) \to 0$ in probability, we only need to show that $\mathbb{E}(V_m(a)) \to 0$ for all $a \in \{1, \cdots, K\}$.

For a given feature $a$, let $V^*_m(a)$ denotes the largest size of feature $a$ among all the children nodes of node $N_{m-1}(X)$. By Lemma 5,

$$\mathbb{E}(V^*_m(a)) \leq (1 - P_2)V_{m-1}(a) + P_2 \frac{N - 1}{N} V_{m-1}(a) = \left(1 - \frac{1}{N} P_2\right) V_{m-1}(a).$$

By Proposition 1,

$$\mathbb{E}(V_m(a)) \leq (1 - P_1)V_{m-1}(a) + P_1 \mathbb{E}(V^*_m(a)) = \left(1 - \frac{1}{N} P_1 P_2\right) V_{m-1}(a).$$

Since $V_0(a) = 1$,

$$\mathbb{E}(V_m(a)) \leq \left(1 - \frac{1}{N} P_1 P_2\right)^m. \quad (10)$$

Unlike the deterministic rule in the Breiman, the splitting point rule in our proposed MRF has randomness, therefore the final selected splitting point can be regarded as a random variable $W_i(i \in \{1, \cdots, m\})$, whose cumulative distribution function is denoted by $F_{W_i}$.

Let $M_1 = \min(W_1, 1 - W_1)$ denotes the size of the root smallest child, we have

$$\mathbb{P}(M_1 \geq \sigma^{1/m}) = \mathbb{P}(\sigma^{1/m} \leq M_1 \leq 1 - \sigma^{1/m}) = F_{W_i}(1 - \sigma^{1/m}) - F_{W_i}(\sigma^{1/m}).$$

WLOG, we normalize the values of all attributes to the range $[0, 1]$ for each node, then after $m$ splits, the smallest child at the $m$-th level have the size at least $\sigma$ with the probability at least

$$\prod_{i=1}^m \left(F_{W_i}(1 - \sigma^{1/m}) - F_{W_i}(\sigma^{1/m})\right). \quad (11)$$

Since $F_{W_i}$ is right-continuous at 0 and left-continuous at 1, $\forall \epsilon_1 > 0$, $\exists \sigma > 0$ s.t.

$$\prod_{i=1}^m \left(F_{W_i}(1 - \sigma^{1/m}) - F_{W_i}(\sigma^{1/m})\right) > (1 - \epsilon_1)^m > 1 - \epsilon.$$ 

In other words, after $m$ splits, the probability of a node with size $\sigma$ is greater than $1 - \epsilon$.

Since the distribution of $X$ has a non-zero density, each node has a positive measure with respect to $\mu_X$.

Defining

$$p = \min_{\mathcal{N}: \text{ node at } m\text{-th level}} \mu_X(N),$$

we know $p > 0$ since the minimum is over finitely many nodes and each node contains a set of positive measure.

Suppose the data set with size $n$, the number of data points falling in the node $A$, where $A$ denotes the $m$-th level node with measure $p$, follows Binomial$(n, p)$. Note that this node $A$ is the one containing the smallest expected number of samples. WLOG, considering the partition rate = 1, the expectation number of estimation points in $A$ is $np/2$.

From Chebyshev’s inequality, we know that

$$\mathbb{P}\left(|\mathcal{N}^E(X)| < k_n\right) = \mathbb{P}\left(|\mathcal{N}^E(X)| - \frac{np}{2} < k_n - \frac{np}{2}\right) \leq \mathbb{P}\left(|\mathcal{N}^E(X)| - \frac{np}{2} > |k_n - \frac{np}{2}|\right) \leq \frac{1}{k_n - \frac{np}{2}}, \quad (12)$$

where the first inequality holds since $k_n - \frac{np}{2}$ is negative as $n \to \infty$ and the second one is by Chebyshev’s inequality.

Since the right hand side goes to zero as $n \to \infty$, the node contains at least $k_n$ estimation points in probability. According to the stopping condition, the tree will grow infinitely often in probability, i.e.,

$$m \to \infty. \quad (13)$$

By (10) and (13), the theorem is proved.

\[\square\]

5. Extension to Regression Problem

5.1. The MRF Algorithm for Regression

The construction process of MRF and its consistency of classification tasks have been demonstrated in Section 3 and Section 4 respectively. MRF also has consistency for the regression problem, which will be discussed in this section.

Just like the classification task, a Bernoulli distribution and a multinomial distribution are also used for the splitting point selection. The main differences between regression and classification tasks are reflected in two main aspects:
the calculation of impurity decrease and the prediction of the model.

Let \( D_n \) denote a data set consisting of \( n \) i.i.d. observations. Each observation has the form \((X, Y)\), where \( X \in \mathbb{R}^D \) and \( Y \in \mathbb{R} \). In regression problems, impurity is defined as a mean square error (MSE):

\[
MSE(D^S) = \frac{1}{|D^S|} \sum_{(X,Y) \in D^S} (Y - \hat{Y})^2,
\]

where \(|D^S|\) is the number of structure points contained in node \( D \) and \( \hat{Y} \) denotes the empirical mean of the structure points in \( D \).

In this case, the impurity decrease caused by splitting point \( v \), the \( I(v) \), is now

\[
I(v) = MSE(D^S) - MSE(D^{S_l}) - MSE(D^{S_r}),
\]

where \( D^{S_l}, D^{S_r} \) are two children sets of structure points generated by \( D^S \) splitting at \( v \).

Again, once a tree has been grown using the structure points, we re-determine the predicted values for the leaves using the estimation points. The predicted value from a tree \( h \) at feature \( x \) is now

\[
\hat{y} = h(x) = \frac{1}{|\mathcal{N}_h(x)|} \sum_{(x,Y) \in \mathcal{N}_h(x)} Y,
\]

where \( \mathcal{N}_h(x) \) is the set of estimation points in the node containing \( x \). The final prediction from the MRF is the average predicted values from all trees:

\[
\bar{y} = \frac{1}{M} \sum_{i=1}^{M} h^{(i)}(x),
\]

where \( M \) is the number of individual trees in the MRF.

5.2. Proof of Consistency of the MRF for Regression

For the regression problem, the definition of consistency is as follows.

**Definition 2.** Given the data set \( D_n \), a sequence of regression estimators \( \{h\} \) are consistent for a certain distribution of \((X, Y)\) if the risk function \( R(h) \) satisfies

\[
R(h) = \mathbb{E} \left[ (h(X, Z, D_n) - f(X))^2 \right] \to 0 \text{ as } n \to \infty,
\]

where \( f(X) = \mathbb{E}[Y | X] \) is the (unknown) regression function.

Corresponding to Lemma 1 – 4 in classification, some necessary lemmas for the proof of consistency in regression are as follows.

**Lemma 6.** The empirical averaging estimator \( \bar{h}^{(M)} \) obtained by averaging over \( M \) copies of \( h \) with different randomizing variables is consistent if all estimators \( \{h\} \) are consistent.

**Lemma 7.** Suppose a sequence of the estimator \( \{h\} \) are conditionally consistent for a specified distribution on \((X, Y)\), i.e.

\[
\lim_{n \to \infty} \mathbb{E} \left[ (h(X, Z, D_n) - h(X))^2 | \mathcal{I} \right] \to 0,
\]

where \( \mathcal{I} \) represents the event that the data point is partitioned randomly. If the random partitioning produces acceptable structure and estimation points with a probability of 1, and \( h \) is bounded, then \( \{h\} \) are unconditionally consistent, i.e.

\[
\lim_{n \to \infty} \mathbb{E} \left[ (h(X, Z, D_n) - h(X))^2 \right] \to 0.
\]

**Lemma 8.** Considering a regression estimator which builds a prediction by averaging method in each leaf node. If the leaf predictors are fitted by the data which have no effect on the structure of the tree, and \( \mathbb{E}[Y^2] < \infty \), then the partitioning regression function estimate is consistent on the condition that

1. The diameter of \( \mathcal{N}(X) \to 0 \) as \( n \to \infty \) in probability,
2. \(|\mathcal{N}^{CE}(X)| \to \infty \) as \( n \to \infty \) in probability.

Below is a sketch proof of consistency: Similar to the classification problem, according to Lemma 6 to Lemma 8 (Biau et al., 2008; Denil et al., 2014; Győrfi et al., 2006), the consistency of MRF in regression task will also be ensured if leaves in the tree are all sufficiently small yet contain infinite number of estimation points.

By the normalization procedure, \( \mathcal{I} \in [0,1]^n \) holds, therefore Lemma 5 are still preserved. Accordingly, the consistency in regression tasks can be proved follows the same process as Theorem 1.

6. Comparison of Different Random Forests

In this section, we describe the similarities and differences between the MRF and two recently proposed consistent variants of random forest, Denil14 (Denil et al., 2014) and BRF (Wang et al., 2018). For reference, we also include Breiman’s original random forest (Breiman, 2001).

All three consistent RF variants – Denil14, BRF and MRF – have the same procedure of partitioning the training set into two subsets to be used separately for tree construction and for prediction. This is necessary for the proof of consistency according to Lemma 4 and Lemma 8. This is in contrast to the original random forest, where a bootstrap dataset is used for both tree construction and prediction.
When selecting candidate features, all three consistent RF variants have a procedure to ensure that every feature has a chance to be the splitting variable, which is necessary for proving consistency. In Denil14, a Poisson distribution is used to achieve this by selecting min (1 + Poisson(λ), D) features. In both BRF and MRF, a simple Bernoulli distribution is used, as described in Section 3. In contrast, in the original random forest, multiple candidate features are selected to compete in the selection of splitting point.

When determining the splitting point, all three consistent RF variants have some level of randomness to ensure that every splitting point has a chance to be used, which is again necessary for proving consistency. However, all the methods except the MRF involve a greedy step, in which the final selection is deterministic. That is, whenever there is a pool of multiple candidate splitting points, those methods always select the “best” one that has the largest impurity decrease. Specifically, in Denil14, a pool of randomly selected candidate splitting points is created and then searched for the “best” one. In BRF, a Bernoulli distribution is used so that with a small probability, the split is based on a single randomly selected point, and with a large probability, the choice is the same as in the original random forest, that is, the “best” among all possible splitting points.

In contrast, the MRF has a non-greedy selection process, in which a splitting point is chosen randomly according to an impurity-based multinomial distribution. This way, the “best” splitting point has the highest probability to be chosen, but other candidate splitting points that are nearly as good as the “best” one will also have a good chance to be selected. This flexibility in splitting point selection in the MRF may partially explain its good performance to be shown in the next section.

The greedy approach of choosing the “best” splitting point at every node may be too exclusive. This is especially true when a node has a small number of observations and there are several candidate splitting points that are not significantly different from each other. In this case, it may not be a good strategy to choose whichever one that happens to have the largest impurity decrease while ignoring all others that are nearly as good. This issue is solved by the non-greedy approach in the MRF. This non-greedy approach also leads to more diversity in the trees, which may further help improve the ensemble performance of the MRF.

### 7. Experiments

#### 7.1. Data Set Description

All datasets used in our evaluations are listed in Table 1. They were obtained from the UCI repository (Asuncion & Newman, 2017). Those data sets include low, moderate, and high dimensional attributes therefore sufficiently representative to demonstrate and evaluate the performance of different algorithms.

| DATA SET    | INSTANCES | FEATURES | TYPES |
|-------------|-----------|----------|-------|
| ECHO        | 132       | 12       | C     |
| VEHICLE     | 946       | 18       | C     |
| CAR         | 1728      | 6        | C     |
| IMAGE       | 2310      | 19       | C     |
| CHESS       | 3196      | 36       | C     |
| CONNECT-4   | 67557     | 42       | C     |
| YACHT       | 308       | 7        | R     |
| ENERGY      | 768       | 8        | R     |
| WIKI        | 913       | 52       | R     |
| FLARE       | 1389      | 10       | R     |
| AIRFOIL     | 1503      | 6        | R     |
| SKILLCRAFT  | 3395      | 20       | R     |

C: classification; R: regression.

#### 7.2. Experimental Settings

We evaluated the performance of three consistent variants of random forest – Denil14, BRF and MRF – in comparison to Breiman, the original random forest (Breiman, 2001). We carried out 10 times 10-fold cross validation to reduce the effect of randomness.

All forests had $M = 100$ trees, $N(D) = \sqrt{D}$ for candidate feature selection, and minimum leaf size $k_n = 5$ as suggested by (Breiman, 2001). The Gini index was used as the impurity measure in classification problems. For methods that require partitioning the training set, the partition rate was set as 1. Other parameters include: $p = 0.05$ and $B = 10$ for the MRF; $p_1 = p_2 = 0.05$ for the two Bernoulli distributions in BRF. For Denil14, the hyperparameter $m$ for determining the search range was set as 100 according to Denil et al. (2014).

Besides, we also carried out Wilcoxon signed-rank test (Demšar, 2006) to test for difference between the results from the MRF and those from one of the other three methods at significance level 0.05.

#### 7.3. Performance Analysis

Table 2 shows the accuracy for classification problems. Table 3 shows the MSE for regression problems. Among the three consistent algorithms, the one with the best performance (highest accuracy or lowest MSE) is indicated in boldface. Those that had a statistically significant difference from the MRF are marked with “•”.

The MRF had a remarkable improvement over both Denil14 and BRF, with significantly better performance for all the datasets we evaluated. The improvement in the regression problems is particularly significant, where the
We now evaluate the effects of two critical hyperparameters, $B$ and $p$, in the MRF. Specifically, we considered a range of \{0, 1, 2, \cdots, 15\} for $B$ when $p = 0.05$, and a range of \{0.01, 0.02, \cdots, 0.1\} for $p$ when $B = 10$. The other hyperparameters were set as before (i.e., $M = 100$, $N(D) = \sqrt{D}$, $k_n = 5$). Ten times 10-fold cross validation was performed. The results are in Figures 1 and 2. Due to a wide range of MSE values across the datasets, we only show the results of four datasets in Figure 2; the other two datasets have similar trends.

Figure 1(a) and Figure 2(a) demonstrate that when $p$ is small enough (i.e., $p < 0.1$), the MRF is not sensitive to $p$, at least for the datasets we evaluated. Similarly, Figure 1(b) and Figure 2(b) show that when $B$ is big enough (i.e., $B \geq 10$), the MRF is also not very sensitive to $B$. However, when $B$ is too small, the resulting multinomial distribution would allow too much randomness. This would lead to individual trees with poor performance, which would have a negative impact on the performance of the MRF. The results also indicate that classification tasks may be more sensitive to the choice of $B$ than regression tasks, that the optimal value of $B$ may depend on the specific characteristics of a dataset such as the outcome scale and the dimension of the impurity decrease vector.

8. Conclusion

In this paper, we proposed a new random forest framework, multinomial random forest (MRF), with proved theoretical consistency and great empirical performance for both classification and regression tasks. In the MRF, we proposed an impurity-based multinomial distribution for the selection of splitting points. Experiments and comparisons demonstrate that the MRF remarkably surpasses existing consistent random forests, and its performance is very close to or even surpasses Breiman’s original random forest. The results are not sensitive to the default MRF hyperparameter values that were used in our evaluations.

Besides, this reasonably constructed multinomial distribution based random selection process instead of greedy rule based process, can be easily extended to other similar circumstance. Overall, MRF already filled the gap between
theoretical consistency and empirical soundness of random forests in both classification and regression.

References

Asuncion, A. and Newman, D. UCI machine learning repository, 2017. URL http://archive.ics.uci.edu/ml.

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

Biau, G., Devroye, L., and Lugosi, G. Consistency of random forests and other averaging classifiers. *Journal of Machine Learning Research*, 9:2015–2033, 2008.

Bifet, A., Holmes, G., Pfahringer, B., Kirkby, R., and Gavaldà, R. New ensemble methods for evolving data streams. In *Proceedings of the 15th ACM SIGKDD international conference on Knowledge discovery and data mining*, pp. 139–148. ACM, 2009.

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

Breiman, L. Consistency for a simple model of random forests. Technical Report 670, Statistical Department, University of California at Berkeley, 2004.

Breiman, L., Friedman, J., Stone, C. J., and Olshen, R. *Classification and Regression Trees*. CRC Press, 1984.

Cootes, T. F., Ionita, M. C., Lindner, C., and Sauer, P. Robust and Accurate Shape Model Fitting Using Random Forest Regression Voting. Springer Berlin Heidelberg, 2012.

Demšar, J. Statistical comparisons of classifiers over multiple data sets. *Journal of Machine learning research*, 7 (Jan):1–30, 2006.

Denil, M., Matheson, D., and Freitas, N. Consistency of online random forests. In *International Conference on Machine Learning*, pp. 1256–1264, 2013.

Denil, M., Matheson, D., and De Freitas, N. Narrowing the gap: Random forests in theory and in practice. In *International conference on machine learning*, pp. 665–673, 2014.

Devroye, L., Györfi, L., and Lugosi, G. *A probabilistic theory of pattern recognition*, volume 31. Springer Science & Business Media, 2013.

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

Genuer, R. Variance reduction in purely random forests. *Journal of Nonparametric Statistics*, 24(3):543–562, 2012.

Györfi, L., Kohler, M., Krzyzak, A., and Walk, H. *A distribution-free theory of nonparametric regression*. Springer Science & Business Media, 2006.

Ho, T. K. The random subspace method for constructing decision forests. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 20(8):832–844, 1998.

Ishwaran, H. and Kogalur, U. B. Consistency of random survival forests. *Statistics & probability letters*, 80(13-14):1056–1064, 2010.

Kontschieder, P., Fiterau, M., Criminisi, A., and Bulo, S. R. Deep neural decision forests. In *IEEE International Conference on Computer Vision*, pp. 1467–1475, 2016.

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

Liu, F. T., Kai, M. T., Yu, Y., and Zhou, Z. H. Spectrum of variable-random trees. *Journal of Artificial Intelligence Research*, 32(1):355–384, 2008.

Meinshausen, N. Quantile regression forests. *Journal of Machine Learning Research*, 7(Jun):983–999, 2006.

Wang, Y., Xia, S. T., Tang, Q., Jia, W., and Zhu, X. A novel consistent random forest framework: Bernoulli random forests. *IEEE Transactions on Neural Networks & Learning Systems*, 29(8):3510–3523, 2018.

Xiong, C., Johnson, D., Xu, R., and Corso, J. J. Random forests for metric learning with implicit pairwise position dependence. In *Proceedings of the 18th ACM SIGKDD international conference on Knowledge discovery and data mining*, pp. 958–966. ACM, 2012.

Zhou, Z.-H. and Feng, J. Deep forest: towards an alternative to deep neural networks. In *Proceedings of the 26th International Joint Conference on Artificial Intelligence*, pp. 3553–3559. AAAI Press, 2017.