

Unbiased Measurement of Feature Importance in Tree-Based Methods

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Abstract

We propose a modification that corrects for split-improvement variable importance measures in Random Forests and other tree-based methods. These methods have been shown to be biased towards increasing the importance of features with more potential splits. We show that by appropriately incorporating split-improvement as measured on out of sample data, this bias can be corrected yielding better summaries and screening tools.

1 Introduction

This paper examines split-improvement feature importance scores for tree-based methods. Starting with Classification and Regression Trees (CART; Breiman, 2017) and C4.5 (Quinlan, 2014), decision trees have been a workhorse of general machine learning, particularly within ensemble methods such as Random Forests (RF; Breiman, 2001) and Gradient Boosting Trees (Friedman, 2001). They enjoy the benefits of computational speed, few tuning parameters and natural ways of handling missing values. Recent statistical theory for ensemble methods (e.g. Scornet et al., 2015; Mentch and Hooker, 2016; Wager and Athey, 2017; Zhou and Hooker, 2018) has provided theoretical guarantees and allowed formal statistical inference. For all these reasons, tree-based methods have seen broad applications including in protein interaction models (Meyer et al., 2017) in product suggestions on Amazon (Sorokina and Cantú-Paz, 2016) and in financial risk management (Khaidem et al., 2016).

However, in common with other machine learning models, large ensembles of trees act as “black boxes”, providing predictions but little insight as to how they were arrived at. There has thus been considerable interest in providing tools either to explain the broad patterns that are modeled by these methods, or to provide justifications for particular predictions. This paper examines variable or feature¹ importance scores that provide global summaries of how influential a particular input dimension is in the models’ predictions. These have been among the earliest diagnostic tools for machine learning and have been put to practical use as screening tools, see for example Díaz-Uriarte and De Andres (2006) and Menze et al. (2009). Thus, it is crucial that these feature importance measures reliably produce well-understood summaries.

Feature importance scores for tree-based models can be broadly split into two categories. Permutation methods rely on measuring the change in value or accuracy when the values of one feature are replaced by uninformative noise, often generated by a permutation. These have the advantage of being applicable to any function, but have been critiqued by Hooker (2007); Strobl et al. (2008) for forcing the model to extrapolate. By contrast, in this paper we study the alternative split-improvement scores that are specific to tree-based methods. These naturally aggregate the improvement associated with each node split and can be readily recorded within the tree building process (Breiman, 2017; Friedman, 2001). In Python, split-improvement is the default implementation for almost every tree-based model, including `RandomForestClassifier`, `RandomForestRegressor`, `GradientBoostingClassifier` and `GradientBoostingRegressor` from `scikit-learn` (Pedregosa et al., 2011).

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¹We use “feature”, “variable” and “covariate” interchangeably here to indicate individual measurements that act as inputs to a machine learning model from which a prediction is made.

Despite their common use, split-improvement measures are biased towards features that exhibit more potential splits and in particular towards continuous features or features with large numbers of categories. This was first observed in Strobl et al. (2007)². While this may not be concerning when all covariates are similarly configured, in practice it is common to have a combination of categorical and continuous variables in which emphasizing more complex features may mislead any subsequent analysis. For example, gender will be a very important binary predictor in applications related to medical treatment; whether the user is a paid subscriber is also central to some tasks such as in Amazon and Netflix. But these may be rated as less relevant to age in either case.

We offer an intuitive rationale for this phenomenon and design a simple fix to solve the bias problem. The observed bias is similar to overfitting in training machine learning models, where we should not build the model and evaluate relevant performance using the same set of data. To fix this, split-improvement calculated from a separate test set is taken into consideration. We further demonstrate that this new measurement is unbiased in the sense that features with no predictive power towards target variable will receive an importance score of zero in expectation. These measures can be very readily implemented in tree-based software packages. We believe the proposed measurement provides a more sensible means for evaluating feature importance in practice.

In the following, we introduce some background and notation for tree-based methods in Section 2. In Section 3, split-improvement is described in detail and its bias and limitations are presented. The proposed unbiased measurement is introduced in Section 4. Section 5 applies our idea to real world data sets and we conclude with some discussions and future directions in Section 6. Proofs and some additional simulation results are collected in Appendix A and B respectively.

2 Tree-Based Methods

In this section, we provide a brief introduction and mathematical formulation of tree-based models. We refer readers to relevant chapters in Friedman et al. (2001) for a more detailed presentation that will also serve to introduce our notation.

2.1 Tree Building Process

Decision trees are a non-parametric machine learning tool for constructing prediction models from data. They are obtained by recursively partitioning feature space by axis-aligned splits and fitting a simple prediction function, usually constant, within each partition. The result of this partitioning procedure is represented as a binary tree. Popular tree building algorithms, such as CART and C4.5, may differ in how they choose splits or deal with categorical features. Our introduction in this section mainly reflects how decision tree is implemented in **scikit-learn**.

Suppose our data consists of p inputs and a response, denoted by $z_i = (x_i, y_i)$ for $i = 1, 2, \dots, n$, with $x_i = (x_{i1}, x_{i2}, \dots, x_{ip})$. For simplicity we assume our inputs are continuous³. Labels can be either continuous (regression trees) or categorical (classification trees). Let the data at a node m represented by Q . Consider a splitting variable j and a splitting point s , which results in two child nodes:

$$\begin{aligned} Q_l &= \{(x, y) | x_j \leq s\} \\ Q_r &= \{(x, y) | x_j > s\}. \end{aligned}$$

The impurity at node m is computed by a function H , which acts as a measure for goodness-of-fit and is invariant to sample size. Our loss function for split $\theta = (j, s)$ is defined as the weighted average of the impurity at two child nodes:

$$L(Q, \theta) = \frac{n_l}{n_m} H(Q_l) + \frac{n_r}{n_m} H(Q_r),$$

where n_m, n_l, n_r are the number of training examples falling into node m, l, r respectively. The best split is chosen by minimizing the above loss function:

$$\theta^* = \arg \min_{\theta} L(Q, \theta). \quad (1)$$

²See <https://explained.ai/rf-importance/> for a popular demonstration of this.

³Libraries in different programming languages differ on how to handle categorical inputs. **rpart** and **randomForest** libraries in **R** search over every possible subsets when dealing with categorical features. However, tree-based models in **scikit-learn** do not support categorical inputs directly. Manually transformation is required to convert categorical features to integer-valued ones, such as using dummy variables.

The tree is built by recursively splitting child nodes until some stopping criterion is met. For example, we may want to limit tree depth, or keep the number of training samples above some threshold within each node.

For regression trees, H is usually chosen to be mean squared error, using average values as predictions within each node. At node m with n_m observations, $H(m)$ is defined as:

$$\bar{y}_m = \frac{1}{n_m} \sum_{x_i \in m} y_i,$$

$$H(m) = \frac{1}{n_m} \sum_{x_i \in m} (y_i - \bar{y}_m)^2.$$

Mean absolute error can also be used depending on specific application.

In classification, there are several different choices for the impurity function H . Suppose for node m , the target y can take values of $1, 2, \dots, K$, define

$$p_{mk} = \frac{1}{n_m} \sum_{x_i \in m} \mathbb{1}(y_i = k)$$

to be the proportion of class k in node m , for $k = 1, 2, \dots, K$. Common choices are:

1. Misclassification error:

$$H(m) = 1 - \max_{1 \leq k \leq K} p_{mk}.$$

2. Gini index:

$$H(m) = \sum_{k \neq k'} p_{mk} p_{mk'} = 1 - \sum_{k=1}^K p_{mk}^2.$$

3. Cross-entropy or deviance:

$$H(m) = - \sum_{k=1}^K p_{mk} \log p_{mk}.$$

This paper will focus on mean squared error for regression and Gini index for classification.

2.2 Random Forests and Gradient Boosting Trees

Though intuitive and interpretable, there are two major drawbacks associated with a single decision tree: they suffer from high variance and in some situations they are too simple to capture complex signals in the data. Bagging (Breiman, 1996) and boosting (Friedman, 2001) are two popular techniques used to improve the performance of decision trees.

Suppose we use decision tree as a base learner $t(x; z_1, z_2, \dots, z_n)$, where x is the input for prediction and z_1, z_2, \dots, z_n are training examples as before. Bagging aims to stabilize the base learner t by resampling the training data. In particular, the bagged estimator can be expressed as:

$$\hat{t}(x) = \frac{1}{B} \sum_{b=1}^B t(x; z_{b1}^*, z_{b2}^*, \dots, z_{bn}^*)$$

where z_{bi}^* are drawn independently with replacement from the original data (bootstrap sample), and B is the total number of base learners. Each tree is constructed using a different bootstrap sample from the original data. Thus approximately one-third of the cases are left out and not used in the construction of each base learner. We call these *out-of-bag* samples.

Random Forests (Breiman, 2001) are a popular extension of bagging with an additional randomness injected. At each step when searching for the best split, only p_0 features are randomly selected from all p possible features and the best split θ^* must be chosen from this subset. When $p_0 = p$, this reduces to bagging. Mathematically, the prediction is written as

$$\hat{t}^{RF}(x) = \frac{1}{B} \sum_{b=1}^B t(x; \xi_b, z_{b1}^*, z_{b2}^*, \dots, z_{bn}^*)$$

with $\xi_b \stackrel{\text{iid}}{\sim} \Xi$ denoting the additional randomness for selecting from a random subset of available features.

Boosting is another widely used technique by data scientists to achieve state-of-the-art results on many machine learning challenges (Chen and Guestrin, 2016). Instead of building trees in parallel as in bagging, it does this sequentially, allowing the current base learner to correct for any previous bias. In Ghosal and Hooker (2018), the authors also consider boosting RF to reduce bias. We will skip over some technical details on boosting and restrict our discussion of feature importance in the context of decision trees and RF. Note that as long as tree-based models combine base learners in an additive fashion, their feature importance measures are naturally calculated by (weighted) average across those of individual trees.

3 Measurement of Feature Importance

Almost every feature importance measures used in tree-based models belong to two classes: split-improvement or permutation importance. Though our focus will be on split-improvement, permutation importance is introduced first for completeness.

3.1 Permutation Importance

Arguably permutation might be the most popular method for assessing feature importance in machine learning community. Intuitively, if we break the link between a variable X_j and y , the prediction error increases then variable j can be considered as important.

Formally, we view the training set as a matrix X of size $n \times p$, where each row x_i is one observation. Let $X^{\pi,j}$ be a matrix achieved by permuting the j^{th} column according to some mechanism π . If we use $L(y_i, f(x_i))$ as the loss incurred when predicting $f(x_i)$ for y_i , then the importance of j^{th} feature is defined as:

$$\text{VI}_j^\pi = \sum_{i=1}^n L(y_i, f(x_i^{\pi,j})) - L(y_i, f(x_i)) \quad (2)$$

the increase in prediction error when the j^{th} feature is permuted. Variations include choosing different permutation mechanism π or evaluating Equation (2) on a separate test set. In Random Forests, Breiman (2001) suggest to only permute the values of j^{th} variable in the *out-of-bag* samples for each tree, and final importance for the forest is given by averaging across all trees.

There is a small literature analyzing permutation importance in the context of RF. Ishwaran et al. (2007) studied paired importance. Hooker (2007) and Strobl et al. (2008) advocated against permuting features by arguing it emphasizes behavior in regions where there is very little data. More recently, Gregorutti et al. (2017) conducted a theoretical analysis of permutation importance measure for an additive regression model.

3.2 Split-Improvement

While permutation importance measures can generically be applied to any prediction function, split-improvement is unique to tree-based methods, and can be calculated directly from the training process. Every time a node is split on variable j , the combined impurity for the two descendent nodes is less than the parent node. Adding up the weighted impurity decreases for each split in a tree and averaging over all trees in the forest yields an importance score for each feature.

Following our notation in Section 2.1, the impurity function H is either mean squared error for regression or Gini index for classification. The best split at node m is given by θ_m^* which splits at j^{th} variable and results in two child nodes denoted as l and r . Then the decrease in impurity for split θ^* is defined as:

$$\Delta(\theta_m^*) = \omega_m H(m) - (\omega_l H(l) + \omega_r H(r)), \quad (3)$$

where ω is the proportion of observations falling into each node, i.e., $\omega_m = \frac{n_m}{n}$, $\omega_l = \frac{n_l}{n}$ and $\omega_r = \frac{n_r}{n}$. Then, to get the importance for j^{th} feature in a single tree, we add up all $\Delta(\theta_m^*)$ where the split is at the j^{th} variable:

$$\text{VI}_j^T = \sum_{m, j \in \theta_m^*} \Delta(\theta_m^*). \quad (4)$$

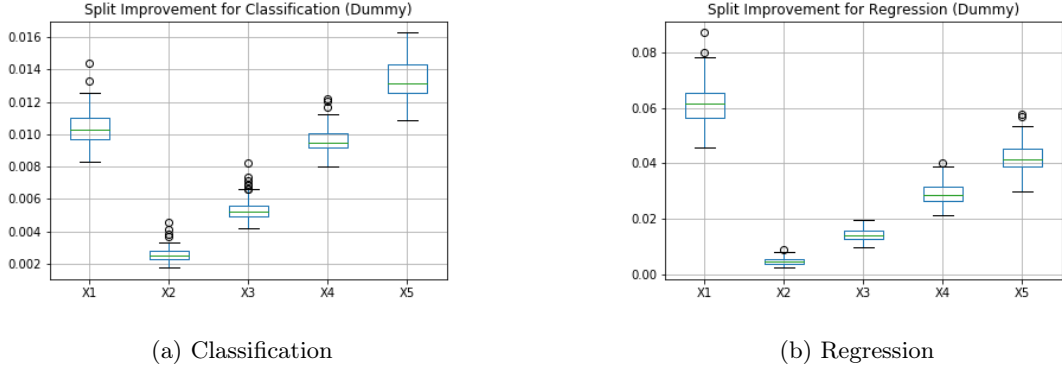


Figure 1: Split-improvement measures on five predictors. Box plot is based on 100 repetitions. 100 trees are built in the forest and maximum depth of each tree is set to 5.

Here the sum is taken over all non-terminal nodes of the tree, and we use the notation $j \in \theta_m^*$ to denote that the split is based on the j^{th} feature.

The notion of split-improvement for decision trees can be easily extended to Random Forests by taking the average across all trees. Suppose there are B base learners in the forest, we could naturally define

$$VI_j^{\text{RF}} = \frac{1}{B} \sum_{b=1}^B VI_j^{\text{T(b)}} = \frac{1}{B} \sum_{b=1}^B \sum_{m, j \in \theta_m^*} \Delta_b(\theta_m^*). \quad (5)$$

3.3 Bias in Split-Improvement

Strobl et al. (2007) pointed out that the split-improvement measure defined above is biased towards increasing the importance of continuous features or categorical features with many categories. This is because of the increased flexibility afforded by a larger number of potential split points. We conducted a similar simulation to further demonstrate this phenomenon. All our experiments are based on Random Forests which gives more stable results than a single tree.

We generate a simulated dataset so that $X_1 \sim N(0, 1)$ is continuous, and X_2, X_3, X_4, X_5 are categorically distributed with 2, 4, 10, 20 categories respectively. The probabilities are equal across categories within each feature. In particular, X_2 is Bernoulli distribution with $p = 0.5$. In classification setting, the response y is also generated as a Bernoulli distribution with $p = 0.5$, but independent of all the X 's. For regression, y is independently generated as $N(0, 1)$. We repeat the simulation 100 times, each time generating $n = 1000$ data points and fitting Random Forests⁴ using the data set. Here categorical features are encoded into dummy variables, and we sum up importance scores for corresponding dummy variables as final measurement for a specific categorical feature. In Appendix B, we also provide simulation results when treating those categorical features as (ordered) discrete variables.

Box plots are shown in Figure 1a and 1b for classification and regression respectively. The continuous feature X_1 is frequently given the largest importance score in regression setting, and among the four categorical features, those with more categories receive larger importance scores. Similar phenomenon is observed in classification as well, while X_5 appears to be artificially more important than X_1 . Also note that all five features get positive importance scores, though we know that they have no predictive power for the target value y .

We now explore how strong a signal is needed in order for the split-improvement measures to discover important predictors. We generate X_1, X_2, \dots, X_5 as before, but in regression settings set $y = \rho X_2 + \epsilon$ where $\epsilon \sim N(0, 1)$. We choose ρ to range from 0 to 1 at step size 0.1 to encode different levels of signal. For classification experiments, we first make $y = X_2$ and then flip each element of y according to $P(U > \frac{1+\rho}{2})$ where U is Uniform[0, 1]. This way, the correlation between X_2 and y will be approximately ρ . We report the average ranking of all five variables across 100 repetitions for each ρ . The results are shown in Figure 2.

We see that ρ needs to be larger than 0.2 to actually find X_2 is the most important predictor in our classification setting, while in regression this value increases to 0.6. And we also observe

⁴Our experiments are implemented using **scikit-learn**. Unless otherwise noted, default parameters are used.

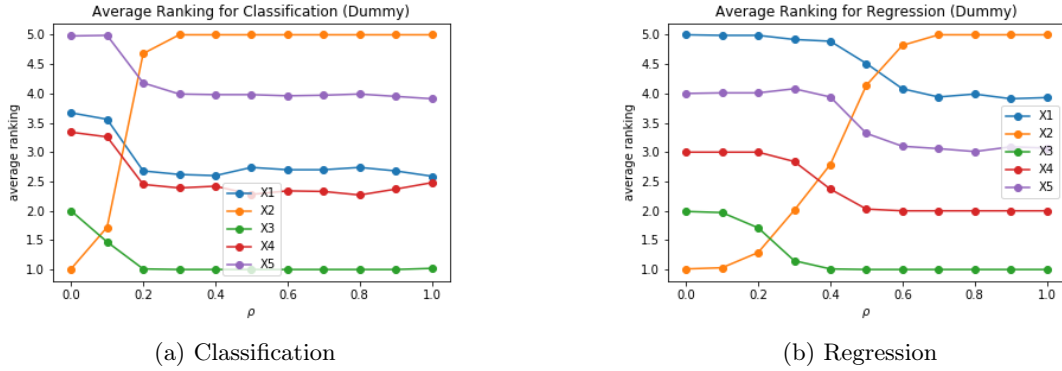


Figure 2: Average feature importance ranking across different signal strengths over 100 repetitions. 100 trees are built in the forest and maximum depth of each tree is set to 5.

that a clear order exists for the remaining (all unimportant) four features.

This bias phenomenon could make many statistical analyses based on split-improvement invalid. For example, gender is a very common and powerful binary predictor in many applications, but feature screening based on split-improvement might think it is not important compared to age. In the next section, we explain intuitively why this bias is observed, and provide a simple but effective adjustment.

4 Unbiased Split-Improvement

When it comes to evaluating the performance of machine learning models, we generally use a separate test set to calculate generalization accuracy. The training error is usually smaller than the test error as the algorithm is likely to "overfit" on the training data. This is exactly why we observe the bias with split-improvement. Each split will favor continuous features or those features with more categories, as they will have more flexibility to fit the training data. The vanilla version of split-improvement is just like using train error for evaluating model performance.

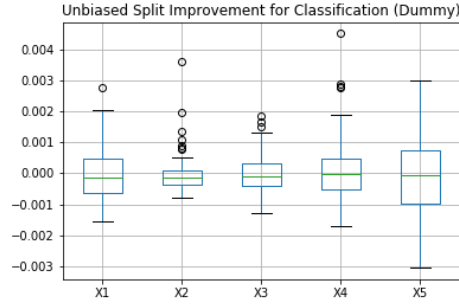
In [Strobl et al. \(2007\)](#), the authors resort to a different algorithm called **cforest** ([Hothorn et al., 2010](#)), which is based on a conditional inference framework ([Hothorn et al., 2006](#)). Below we propose methods to remedy this bias phenomenon by utilizing a separate test set, and prove that for features with no predictive power, we're able to get an importance score of 0 in expectation for both classification and regressions settings. Our method is entirely based on the original framework of RF, requires barely no additional computational efforts, and can be easily integrated into any existing software libraries.

The main ingredient of the proposed method is to calculate the impurity function H using additional information provided from test data. In the context of RF, we can simply take *out-of-bag* samples for each individual tree. Our experiments below are based on this strategy. In the context of the honest trees proposed in [Wager and Athey \(2017\)](#) that divide samples into a partition used to determine tree structures and a partition used to obtain leaf values, the latter could be used as our test data below. In boosting, it is common not to sample, but to keep a test set separate to determine a stopping time. Since the choice of impurity function H is different for classification and regression, in what follows we will treat them separately.

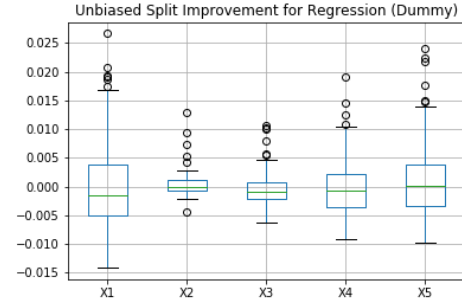
Figure 3 and 4 shows the results on previous classification and regression tasks when our unbiased method is applied. Feature scores for all variables are spread around 0, though continuous features and categorical features with more categories tend to exhibit more variability. In the case where there is correlation between X_2 and y , even for the smallest $\rho = 0.1$, we can still find the most informative predictor, whereas there are no clear order for the remaining noise features.

4.1 Classification

Consider a root node m and two child nodes, denoted by l and r respectively. The best split $\theta_m^* = (j, s)$ was chosen by Formula (1) and Gini index is used as impurity function H .

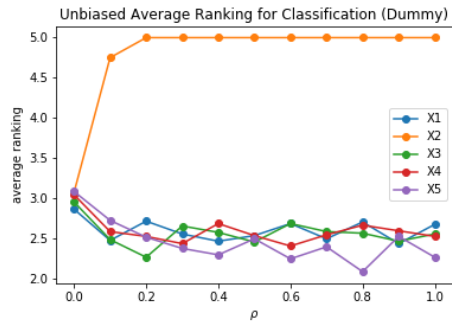


(a) Classification

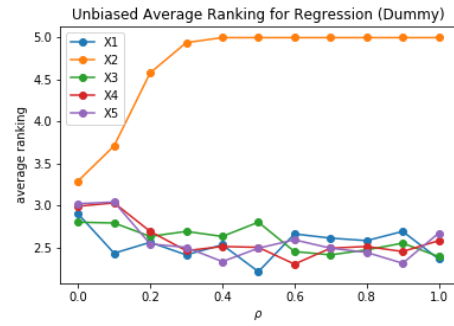


(b) Regression

Figure 3: Unbiased split-improvement. Box plot is based on 100 repetitions. 100 trees are built in the forest and maximum depth of each tree is set to 5. Each tree is trained using bootstrap samples and *out-of-bag* samples are used as test set.



(a) Classification



(b) Regression

Figure 4: Unbiased feature importance ranking across different signal strengths averaged over 100 repetitions. 100 trees are built in the forest and maximum depth of each tree is set to 5. Each tree is trained using bootstrap samples and *out-of-bag* samples are used as test set.

For simplicity, we focus on binary classification. Let p denote class proportion within each node. For example, $p_{r,2}$ denotes the proportion of class 2 in the right child node. Hence the Gini index for each node can be written as:

$$\begin{aligned} H(m) &= 1 - p_{m,1}^2 - p_{m,2}^2, \\ H(l) &= 1 - p_{l,1}^2 - p_{l,2}^2, \\ H(r) &= 1 - p_{r,1}^2 - p_{r,2}^2. \end{aligned}$$

The split-improvement for a split at j^{th} feature when evaluated using only the training data is written as in Equation (3). This value is always positive no matter which feature is chosen and where the split is, which is exactly why a selection bias will lead to overestimate of feature importance.

If instead, we have a separate test set available, the predictive impurity function for each node is modified to be:

$$\begin{aligned} H'(m) &= 1 - p_{m,1}p'_{m,1} - p_{m,2}p'_{m,2}, \\ H'(l) &= 1 - p_{l,1}p'_{l,1} - p_{l,2}p'_{l,2}, \\ H'(r) &= 1 - p_{r,1}p'_{r,1} - p_{r,2}p'_{r,2}, \end{aligned} \tag{6}$$

where p' is class proportion evaluating on the test data. And similarly,

$$\begin{aligned} \Delta'(\theta_m^*) &= \omega_m H'(m) - (\omega_l H'(l) + \omega_r H'(r)) \\ &= \omega_l (H'(m) - H'(l)) + \omega_r (H'(m) - H'(r)). \end{aligned} \tag{7}$$

Using these definitions, we first demonstrate that an individual split is unbiased in the sense that if y has no bivariate relationship with X_j , $\Delta'(\theta_m^*)$ will have expectation 0.

Lemma 1. *In classification settings, for a given feature X_j , if y is marginally independent of X_j within the region defined by node m , then*

$$E\Delta'(\theta_m^*) = 0$$

when splitting at the j^{th} feature.

Proof. See Appendix A. □

Similar to Equation (4), split-improvement of x_j in a decision tree is defined as:

$$VI_j^{T,C} = \sum_{m,j \in \theta_m^*} \Delta'(\theta_m^*). \tag{8}$$

We can now apply Lemma 1 to provide a global result so long as X_j is always irrelevant to y .

Theorem 2. *In classification settings, for a given feature X_j , if y is independent of X_j in every hyper-rectangle subset of the feature space, then we always have*

$$EVI_j^{T,C} = 0.$$

Proof. The result follows directly from Lemma 1 and Equation (8). □

This unbiasedness result can be easily extended to the case of RF by (5), as it's an average across base learners. We note here that our independence condition is designed to account for relationships that appear before accounting for splits on other variables, possibly due to relationships between X_j and other features, and afterwards. It is trivially implied by the independence of X_j with both y and the other features. Our condition may also be stronger than necessary, depending on the tree-building process. We may be able to restrict the set of hyper-rectangles to be examined, but only by analyzing specific tree-building algorithms.

4.2 Regression

In regression, we use mean squared error as the impurity function H :

$$\bar{y}_m = \frac{1}{n_m} \sum_{x_i \in m} y_i,$$

$$H(m) = \frac{1}{n_m} \sum_{x_i \in m} (y_i - \bar{y}_m)^2.$$

If instead the impurity function H is evaluated on a separate test set, we define

$$H'(m) = \frac{1}{n'_m} \sum_{i=1}^{n'_m} (y'_{m,i} - \bar{y}_m)^2$$

and similarly

$$\Delta'(\theta_m^*) = \omega_m H'(m) - (\omega_l H'(l) + \omega_r H'(r)).$$

Note that here $H'(m)$ measures mean squared error within node m on test data with the fitted value \bar{y}_m from training data. If we just sum up Δ' as feature importance, it will end up with negative values as \bar{y}_m will overfit the training data and thus make mean squared error much larger deep in the tree. In other words, it *over-corrects* the bias. For this reason, our unbiased split-improvement is defined slightly different from the classification case (8):

$$\text{VI}_j^{\text{T,R}} = \sum_{m, j \in \theta_m^*} (\Delta(\theta_m^*) + \Delta'(\theta_m^*)). \quad (9)$$

Notice that although Equation (8) and (9) are different, they originate from the same idea by correcting bias using test data. Unlike Formula (6) for Gini index, where we could design a predictive impurity function by combining train and test data together, it's hard to come up with a counterpart in regression setting.

Just as in the classification case, we could show the following unbiasedness results:

Lemma 3. *In regression settings, for a given feature X_j , if y is marginally independent of X_j within the region defined by node m , then*

$$E(\Delta(\theta_m^*) + \Delta'(\theta_m^*)) = 0$$

when splitting at the j^{th} feature.

Proof. See Appendix A. □

Theorem 4. *In regression settings, for a given feature X_j , if y is independent of X_j in every hyper-rectangle subset of the feature space, then we always have*

$$E \text{VI}_j^{\text{T,R}} = 0.$$

5 Real World Data

In this section, we apply our method to two real world data sets. The first data set examined is the prediction of C-to-U edited sites in plant mitochondrial RNA. This task was studied statistically in [Cumplings and Myers \(2004\)](#), where the authors applied Random Forests and used the original split-improvement as feature importance. Later, [Strobl et al. \(2007\)](#) demonstrated the performance of **cforest** on this data set.

RNA editing is a molecular process whereby an RNA sequence is modified from the sequence corresponding to the DNA template. In the mitochondria of land plants, some cytidines are converted to uridines before translation ([Cumplings and Myers \(2004\)](#)).

We use the *Arabidopsis thaliana* data file⁵ as in [Strobl et al. \(2007\)](#). The features are based on the nucleotides surrounding the edited/non-edited sites and on the estimated folding energies of those regions. After removing missing values and one column which will not be used, the data file consists of 876 rows and 45 columns:

⁵The data set could be downloaded from [BMC Bioinformatics](#).

Attribute	Description
age	continuous
workclass	categorical (7)
fnlwgt	continuous
education	categorical (16)
education-num	continuous
marital-status	categorical (7)
occupation	categorical (14)
relationship	categorical (6)
race	categorical (5)
sex	binary
capital-gain	continuous
capital-loss	continuous
hours-per-week	continuous
random	continuous

Table 1: Attribute description for adult data set.

- the response (binary).
- 41 nucleotides at positions -20 to 20 relative to the edited site (categorical, one of A, T, C or G).
- the codon position (also 4 categories).
- two continuous variables based on the estimated folding energies.

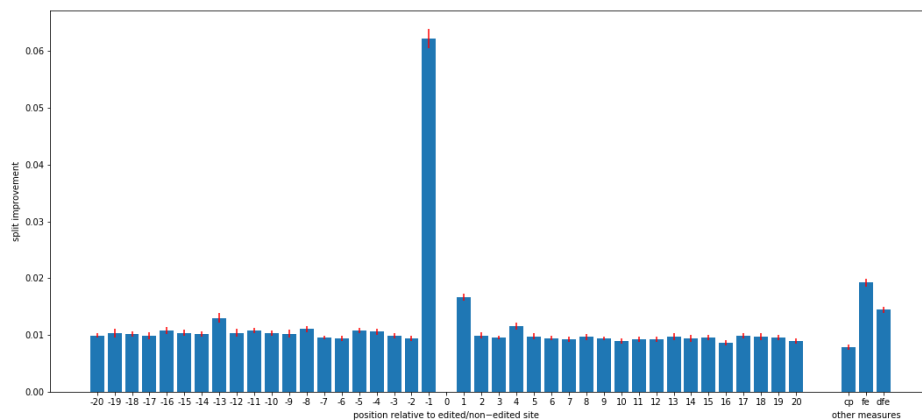
For implementation, we create dummy variables for all categorical features, and build forest using 100 base trees. We do not set the maximum depth for this data set as the number of potential predictors is large. For feature importance, we take the sum of importance across all dummy variables corresponding to a specific feature.

Figure 5a shows the result when using the original split-improvement measure, which is similar to the corresponding figure in Cummings and Myers (2004). Red error bars depict one standard deviation when the experiments are repeated 10 times. Except several apparently dominant predictors (nucleotides at position -1 and 1, and two continuous features fe and dfe), the importance for the remaining nearly 40 features are indistinguishable. Our unbiased split-improvement is displayed in Figure 5b. Although both methods agree on top three features being the nucleotides at position -1 and 1, and the continuous one fe , there are some noticeable differences. Another continuous feature dfe is originally ranked at the fourth place in Figure 5a, but its unbiased split-improvement is close to 0. This decrease in importance agrees with the result of Strobl et al. (2007), corroborating their identification of bias in the original method. Furthermore, we see a large portion of predictors with feature importance close to 0, and it makes subsequent tasks like feature screening easier.

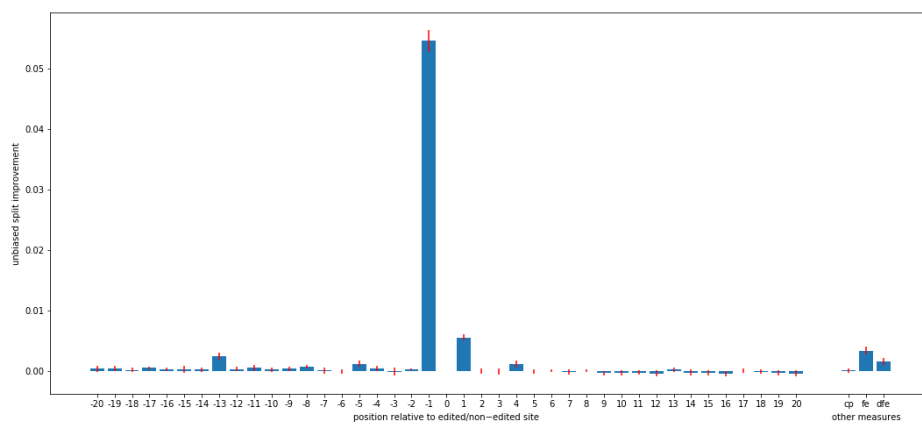
As a second example, we will use the Adult Data Set from UCI Machine Learning Repository⁶. The task is to predict whether income exceeds \$50K/yr based on census data. We remove all entries including missing values, and only focus on people from Unites States. In total, we have 27504 training samples and Table 1 describes relevant feature information. Notice that we add a standard normal random variable, which is shown in the last row.

Similarly for previous example, we create dummy variables for all categorical features. Considering the large volume of data, the forest is built using 20 base trees. The results are shown in Figure 6. Notice the random normal feature we added (marked in yellow) is actually ranked the second most important for the original split-improvement measure. This is not surprising as most of the features are categorical, and even for some continuous features, a large portion of the values are actually 0 (such as *capital-gain* and *capital-loss*). For the unbiased measurement we proposed, the random feature is assigned an importance score close to 0 just as expected. Another feature with big discrepancy is *fnlwgt*, which is ranked among top three originally but is almost the least significant for the proposed method. *fnlwgt* represents final weight, the number of units

⁶<https://archive.ics.uci.edu/ml/datasets/adult>

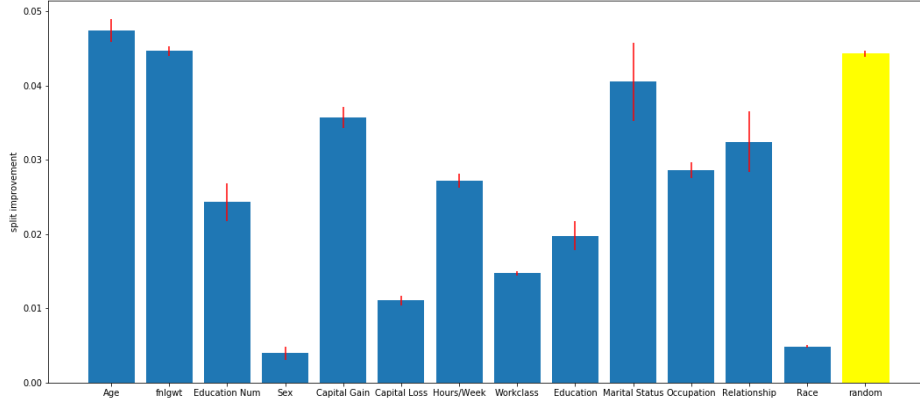


(a) original split-improvement

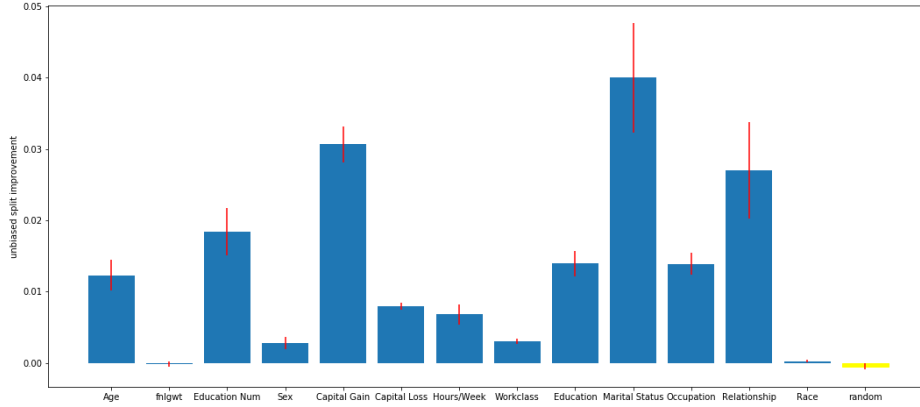


(b) unbiased split-improvement

Figure 5: Feature importance for RNA sequence data. 100 trees are built in the forest. Red error bars depict one standard deviation when the experiments are repeated 10 times.



(a) original split-improvement



(b) unbiased split-improvement

Figure 6: Feature importance for adult data. 20 trees are built in the forest. Red error bars depict one standard deviation when the experiments are repeated 10 times.

in the target population that the responding unit represents. Thus it is unlikely to have strong predictive power for the response. For this reason, some analyses deleted this predictor before fitting models⁷. Based on these observations, we believe our proposed unbiased split-improvement provides a better measurement of feature importance.

6 Discussions

Tree-based methods are widely employed in many applications. One of the many advantages is that these models come naturally with feature importance measures, which practitioners rely on heavily for subsequent analysis such as feature ranking or screening. It is important that these measurements are trustworthy.

We show empirically that split-improvement, as a popular measurement of feature importance in tree-based models, is biased towards continuous features, or categorical features with more categories. This phenomenon is akin to overfitting in training any machine learning model. We propose a simple fix to this problem and demonstrate its effectiveness both theoretically and empirically. Though our examples are based on Random Forests, the adjustment can be easily

⁷http://scg.sdsu.edu/dataset-adult_r/

extended to any other tree-based model.

The original version of split-improvement is the default and only feature importance measure for Random Forests in **scikit-learn**, and is also returned as one of the measurements for **random-Forest** library in R. Statistical analyses utilizing these packages will suffer from the bias discussed in this paper. Our method can be easily integrated into existing libraries, and require almost no additional computational burden. As already observed, while we have used *out-of-bag* samples as a natural source of test data, alternatives such as sample partitions – thought of as a subsample of *out-of-bag* data for our purposes – can be used in the context of honest trees, or a held-out test set will also suffice. The use of subsamples fits within the methods used to demonstrate the asymptotic normality of Random Forests developed in [Mentch and Hooker \(2016\)](#). This potentially allows for formal statistical tests to be developed based on the unbiased split-improvement measures proposed here. Similar approaches have been taken in [Zhou et al. \(2018\)](#) for designing stopping rules in approximation trees.

However, feature importance itself is very difficult to define exactly, with the possible exception of linear models, where the magnitude of coefficients serves as a simple measure of importance. There are also considerable discussion on the subtly introduced when correlated predictors exist, see for example [Strobl et al. \(2008\)](#); [Gregorutti et al. \(2017\)](#). We think that clarifying the relationship between split-improvement and the topology of the resulting function represents an important future research direction.

Acknowledgements

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A Proofs of Lemma 1 and 3

Proof of Lemma 1. We want to show that for independent X_j and y within node m , $\Delta'(\theta_m^*)$ should ideally be zero when splitting on the j^{th} variable. Rewriting $H'(m)$ defined in Equation (6) and we get:

$$\begin{aligned} H'(m) &= 1 - p_{m,1}p'_{m,1} - p_{m,2}p'_{m,2} \\ &= 1 - p_{m,1}p'_{m,1} - (1 - p_{m,1})(1 - p'_{m,1}) \\ &= p_{m,1} + p'_{m,1} - 2p_{m,1}p'_{m,1}. \end{aligned}$$

Using similar expressions for $H'(l)$, we have:

$$H'(m) - H'(l) = (p_{m,1} + p'_{m,1} - 2p_{m,1}p'_{m,1}) - (p_{l,1} + p'_{l,1} - 2p_{l,1}p'_{l,1}).$$

Given that the test data is independent of the training data and the independence between X_j and y , then in expectation, we should have $E(p'_{m,1}) = E(p'_{l,1}) = p'_1$. Thus,

$$\begin{aligned} E(H'(m) - H'(l)) &= (E(p_{m,1}) + E(p'_{m,1}) - 2E(p_{m,1}p'_{m,1})) - (E(p_{l,1}) + E(p'_{l,1}) - 2E(p_{l,1}p'_{l,1})) \\ &= (E(p_{m,1}) + E(p'_{m,1}) - 2E(p_{m,1})E(p'_{m,1})) - (E(p_{l,1}) + E(p'_{l,1}) - 2E(p_{l,1})E(p'_{l,1})) \\ &= (E(p_{m,1}) + p'_1 - 2E(p_{m,1})p'_1) - (E(p_{l,1}) + p'_1 - 2E(p_{l,1})p'_1) \\ &= (E(p_{m,1}) - E(p_{l,1}))(1 - 2p'_1). \end{aligned}$$

Similarly,

$$E(H'(m) - H'(r)) = (E(p_{m,1}) - E(p_{r,1}))(1 - 2p'_1).$$

Combined together into Equation (7),

$$\begin{aligned} E(\Delta'(\theta_m^*)) &= \omega_l(H'(m) - H'(l)) + \omega_r(H'(m) - H'(r)) \\ &= \omega_l(E(p_{m,1}) - E(p_{l,1}))(1 - 2p'_1) + \omega_r(E(p_{m,1}) - E(p_{r,1}))(1 - 2p'_1) \\ &= (1 - 2p'_1)(\omega_m E(p_{m,1}) - \omega_l E(p_{l,1}) - \omega_r E(p_{r,1})) \\ &= (1 - 2p'_1) \times 0 \\ &= 0, \end{aligned}$$

since we always have

$$\omega_m \times p_{m,1} = \omega_l \times p_{l,1} + \omega_r \times p_{r,1}.$$

□

Proof of Lemma 3. Rewriting the expression of $H(m)$:

$$\begin{aligned} H(m) &= \frac{1}{n_m} \sum_{i=1}^{n_m} (y_{m,i} - \bar{y}_m)^2 \\ &= \frac{1}{n_m} \left(\sum_{i=1}^{n_m} y_{m,i}^2 - n_m \bar{y}_m^2 \right). \end{aligned}$$

Thus,

$$\begin{aligned} \Delta(\theta_m^*) &= \omega_m H(m) - (\omega_l H(l) + \omega_r H(r)) \\ &= \omega_m \frac{1}{n_m} \sum_{i=1}^{n_m} (y_{m,i}^2 - n_m \bar{y}_m^2) - (\omega_l \frac{1}{n_l} \sum_{i=1}^{n_l} (y_{l,i}^2 - n_l \bar{y}_l^2) + \omega_r \frac{1}{n_r} \sum_{i=1}^{n_r} (y_{r,i}^2 - n_r \bar{y}_r^2)) \\ &= \frac{1}{n} \sum_{i=1}^{n_m} (y_{m,i}^2 - n_m \bar{y}_m^2) - \left(\frac{1}{n} \sum_{i=1}^{n_l} (y_{l,i}^2 - n_l \bar{y}_l^2) + \frac{1}{n} \sum_{i=1}^{n_r} (y_{r,i}^2 - n_r \bar{y}_r^2) \right) \\ &= \frac{1}{n} \left(\sum_{i=1}^{n_m} (y_{m,i}^2 - n_m \bar{y}_m^2) - \sum_{i=1}^{n_l} (y_{l,i}^2 - n_l \bar{y}_l^2) - \sum_{i=1}^{n_r} (y_{r,i}^2 - n_r \bar{y}_r^2) \right) \\ &= \frac{1}{n} \left(\sum_{i=1}^{n_m} y_{m,i}^2 - \sum_{i=1}^{n_l} y_{l,i}^2 - \sum_{i=1}^{n_r} y_{r,i}^2 \right) - \frac{1}{n} (n_m \bar{y}_m^2 - n_l \bar{y}_l^2 - n_r \bar{y}_r^2) \\ &= \frac{1}{n} (n_l \bar{y}_l^2 + n_r \bar{y}_r^2 - n_m \bar{y}_m^2) \\ &= \omega_l \bar{y}_l^2 + \omega_r \bar{y}_r^2 - \omega_m \bar{y}_m^2. \end{aligned}$$

By Cauchy–Schwarz inequality,

$$(n_l \bar{y}_l^2 + n_r \bar{y}_r^2)(n_l + n_r) \geq (n_l \bar{y}_l + n_r \bar{y}_r)^2 = (n_m \bar{y}_m)^2,$$

thus

$$\Delta(\theta_m^*) = \frac{1}{n} (n_l \bar{y}_l^2 + n_r \bar{y}_r^2 - n_m \bar{y}_m^2) \geq 0$$

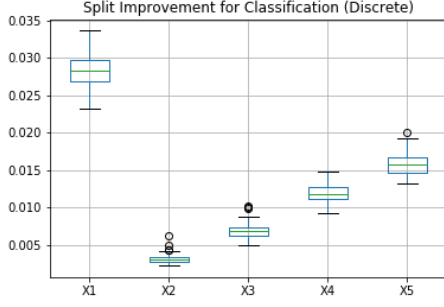
unless $\bar{y}_l = \bar{y}_r = \bar{y}_m$.

Similarly for $H'(m)$:

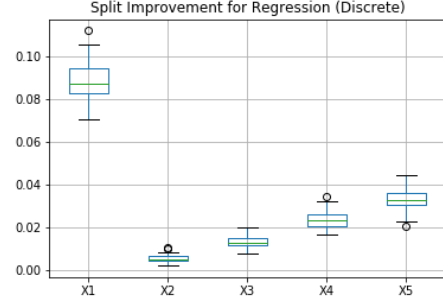
$$\begin{aligned} H'(m) &= \frac{1}{n'_m} \sum_{i=1}^{n'_m} (y'_{m,i} - \bar{y}_m)^2 \\ &= \frac{1}{n'_m} \sum_{i=1}^{n'_m} y'^2_{m,i} - 2 \frac{1}{n'_m} \sum_{i=1}^{n'_m} y'_{m,i} \bar{y}_m + \frac{1}{n'_m} \sum_{i=1}^{n'_m} \bar{y}_m^2 \\ &= \frac{1}{n'_m} \sum_{i=1}^{n'_m} y'^2_{m,i} - 2 \bar{y}'_m \bar{y}_m + \bar{y}_m^2 \end{aligned}$$

and thus

$$\begin{aligned} \Delta'(\theta_m^*) &= \omega_m H'(m) - (\omega_l H'(l) + \omega_r H'(r)) \\ &= \omega_m \left(\frac{1}{n'_m} \sum_{i=1}^{n'_m} y'^2_{m,i} - 2 \bar{y}'_m \bar{y}_m + \bar{y}_m^2 \right) - \omega_l \left(\frac{1}{n'_l} \sum_{i=1}^{n'_l} y'^2_{l,i} - 2 \bar{y}'_l \bar{y}_l + \bar{y}_l^2 \right) - \omega_r \left(\frac{1}{n'_r} \sum_{i=1}^{n'_r} y'^2_{r,i} - 2 \bar{y}'_r \bar{y}_r + \bar{y}_r^2 \right) \\ &= \left(\omega_m \frac{1}{n'_m} \sum_{i=1}^{n'_m} y'^2_{m,i} - \omega_l \frac{1}{n'_l} \sum_{i=1}^{n'_l} y'^2_{l,i} - \omega_r \frac{1}{n'_r} \sum_{i=1}^{n'_r} y'^2_{r,i} \right) + (\omega_m \bar{y}_m^2 - \omega_l \bar{y}_l^2 - \omega_r \bar{y}_r^2) - 2(\omega_m \bar{y}'_m \bar{y}_m - \omega_l \bar{y}'_l \bar{y}_l - \omega_r \bar{y}'_r \bar{y}_r) \\ &= \left(\omega_m \frac{1}{n'_m} \sum_{i=1}^{n'_m} y'^2_{m,i} - \omega_l \frac{1}{n'_l} \sum_{i=1}^{n'_l} y'^2_{l,i} - \omega_r \frac{1}{n'_r} \sum_{i=1}^{n'_r} y'^2_{r,i} \right) - \Delta(\theta_m^*) - 2(\omega_m \bar{y}'_m \bar{y}_m - \omega_l \bar{y}'_l \bar{y}_l - \omega_r \bar{y}'_r \bar{y}_r). \end{aligned}$$

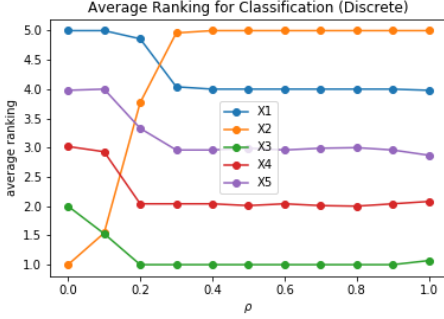


(a) Classification

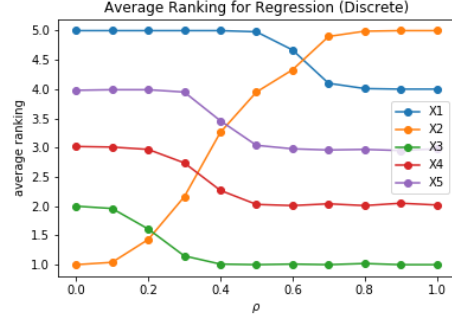


(b) Regression

Figure 7: Split-improvement measures on five predictors, where we treat categorical features as ordered discrete values. Box plot is based on 100 repetitions. 100 trees are built in the forest and maximum depth of each tree is set to 5.



(a) Classification



(b) Regression

Figure 8: Average feature importance ranking across different signal strengths over 100 repetitions, where we treat categorical features as ordered discrete values. 100 trees are built in the forest and maximum depth of each tree is set to 5.

By the independence assumptions, we have

$$E \frac{1}{n'_m} \sum_{i=1}^{n'_m} y_{m,i}'^2 = E \frac{1}{n'_l} \sum_{i=1}^{n'_l} y_{l,i}'^2 = E \frac{1}{n'_r} \sum_{i=1}^{n'_r} y_{r,i}'^2,$$

and

$$E \bar{y}_m' = E \bar{y}_l' = E \bar{y}_r'.$$

We can conclude that

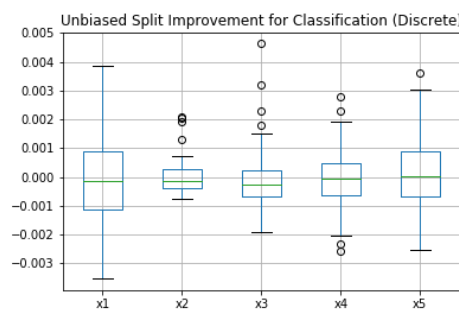
$$E(\Delta(\theta_m^*) + \Delta'(\theta_m^*)) = 0.$$

□

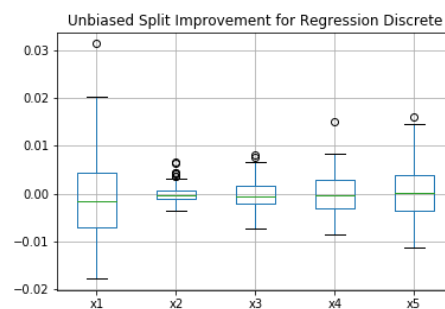
B Additional Simulation Results

Our simulation experiments in Section 3 and 4 operate by creating dummy variables for categorical features. It would be interesting to see the results if we instead treat those as ordered discrete values.

Figure 7 and 8 show the original version of split-improvement corresponding to Figure 1 and 2. Similar phenomenon is again observed: it over estimates importance of continuous features and categorical features with more categories. It is worth noticing that the discrepancy between continuous and categorical features is even larger in this case. Unlike in Figure 1a, X_1 is always ranked the most important. This results from the fact that by treating categorical features as ordered discrete ones, it limit the number of potential splits compared to using dummy variables.

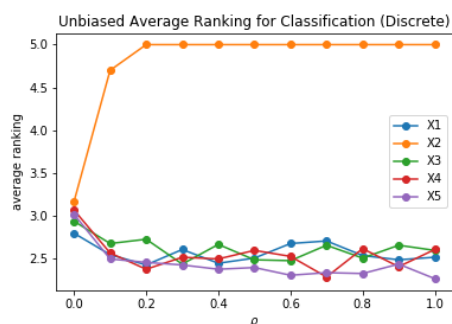


(a) Classification

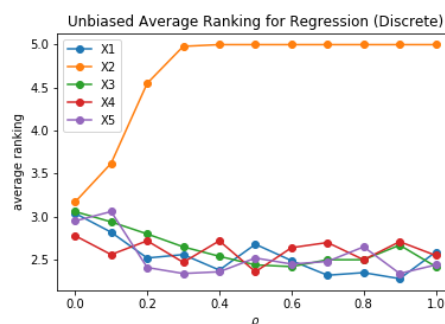


(b) Regression

Figure 9: Unbiased split-improvement, where we treat categorical features as ordered discrete values. Box plot is based on 100 repetitions. 100 trees are built in the forest and maximum depth of each tree is set to 5. Each tree is trained using bootstrap samples and *out-of-bag* samples are used as test set.



(a) Classification



(b) Regression

Figure 10: Unbiased feature importance ranking across different signal strengths averaged over 100 repetitions, where we treat categorical features as ordered discrete values. 100 trees are built in the forest and maximum depth of each tree is set to 5. Each tree is trained using bootstrap samples and *out-of-bag* samples are used as test set.

Not surprisingly, our proposed method work well in declaring all five features have no predictive power or finding the most informative one, as shown in Figure 9 and 10.

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