

# INFFOREST Variable Importance for Random Forests

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# Abstract

Random forests are powerful predictive models but they lack a built-in method for statistical inference. This paper compares several of the most common methods of performing inference on random forests while presenting a new method, INFFOREST variable importance. On simulated data with multicollinearity, the INFFOREST method is able to show significance for four out of five predictors used to generate the response. Existing methods are tested and performed similarly on the simulated data set. INFFOREST variable importance allows claims to be made about the relationship between a predictor and the response, in the context of the rest of the variables in the model. This sets it apart from the exiting methods and creates some interesting implications.



# Dedication

For Nick.





# Chapter 1

## Introduction

### 1.1 Trees and Random Forests

To begin our discussion of trees and random forests, we will first consider the following example using data from a dendrologic study of five orange trees. This study measured two variables for each tree: the age of the tree (recorded in days) and the circumference of the trunk (in cm). These are called, in general terms, the variables recorded by the study. In the dataset below, each column represents a variable and each row represents one set of measurements. There are 2 columns (age and circumference) and 35 rows. The first six rows are displayed in table 1.1.

Suppose we are interested in the following question: knowing only the circumference of the orange tree, can we predict the age of the tree? This question can be translated into a formula. Formulas represent guesses of way the data was generated. We often refer to formulas using the following notation:

$$Age \sim Circumference$$

In this formula, circumference is the predictor and age is the response. Suppose we expanded the study to include the height of the orange trees at various stages of development. Now we can consider both the circumference and the height of the tree when we make our predictions of the age. When we have multiple predictors, we add

Table 1.1: The first six rows of the orange trees data set

age	circumference
118	30
484	58
664	87
1004	115
1231	120
1372	142

them to the notation in the following way:<sup>1</sup>

$$Age \sim Circumference, Height$$

Returning to the original orange tree data set, we can begin to assess the structure in the data set by plotting the data and observing the relationship between the variables (figure 1.1).

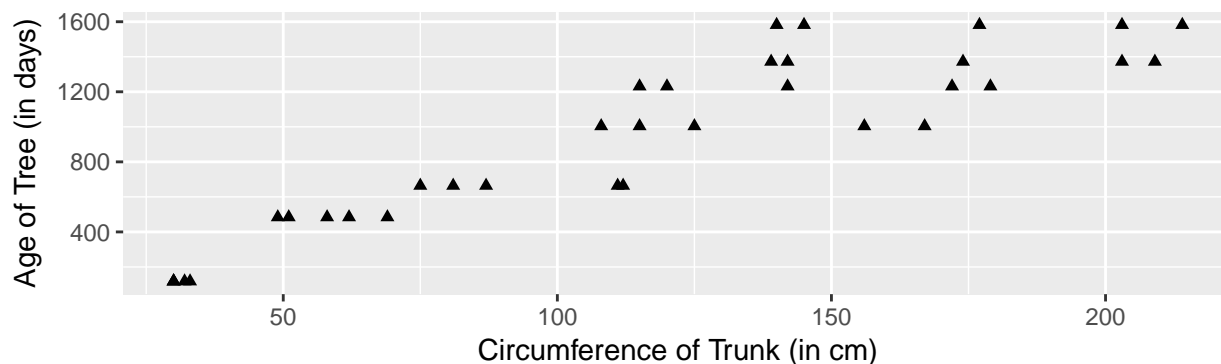


Figure 1.1: The relationship between age and circumference of the trunk of orange trees.

As can be seen in figure 1.1, generally older trees have thicker trunks, and it seems like we are not wrong to suspect that circumference is a good predictor of age. As the data could be reasonably represented by a straight line, we can say that the relationship between trunk circumference and tree age is roughly linear. Now that we have a formula, we can build a model to test it. To create our predictions of age, we fit the formula  $Age \sim Circumference$  to a model. A predictive model is, put simply, a systematic way to make our predictions. The most common type of model is the linear model, which creates predictions from a line through the data.

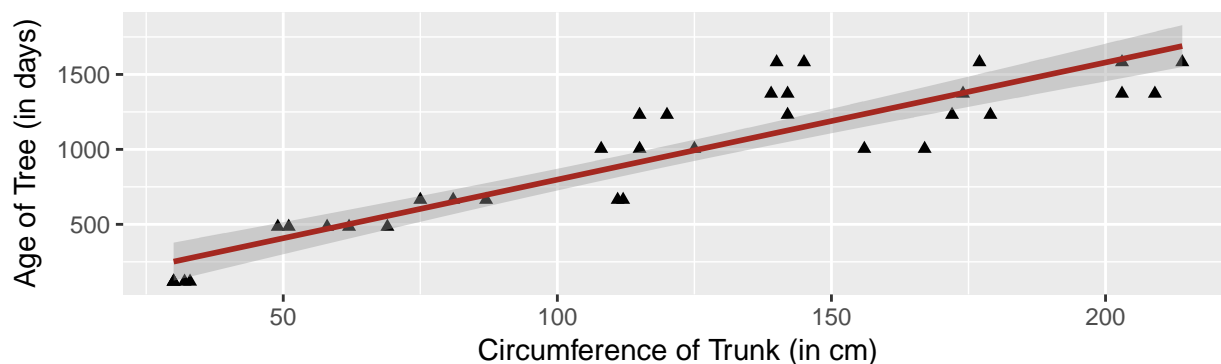


Figure 1.2: A linear model representing age  $\sim$  trunk circumference in orange trees. The shaded area represents a 95% confidence interval around this line.

<sup>1</sup>Often the notation for multiple predictors is written  $Y \sim X + W$  but this assumes an additive, linear relationship between the predictors and the response. This assumption is unnecessary for tree-based models so the notation,  $Y \sim X, W$  is used.

As can be guessed from figure 1.2, the linear model works better on certain data than others. The linear model necessitates several assumptions that may not always be appropriate. We'll return to a brief discussion of the assumptions of the linear model later in this chapter.

This paper discusses at length tree-based models. A tree for the formula  $age \sim circumference$  is similar to the linear model in that it presents a systematic way to make predictions, but the two differ in that the tree is not linear in any fashion. In fact, we can compare the differences between the two models by comparing figures 1.2 and 1.3.



Figure 1.3: A tree modeling the formula  $age \sim trunk\ circumference$  first creates partitions on the predictor, seen as vertical lines, and then predicts the value of the response within that partition, seen as text.

When using the linear model, we make predictions in the following way: given a value of  $X$  (circumference) the corresponding value of  $Y$  (age) on the line is our prediction. The predictions from the tree are gathered similarly: given a value of  $X$  (circumference), our prediction is the average value of  $Y$  (age) within the partition that  $X$  falls into.<sup>2</sup>

Tree methods get their name from a common way of representing them in higher dimensions, when there is more than one predictor. Figure 1.4 shows this method. In this case, given a new value for circumference, one would start their predictions at the top of the tree and, depending on the value of circumference and the instructions at each intersection or split, one would fall down branch by branch before landing on a prediction for age. If the new value for circumference is less than the value stated at the split, we would move down to the branch on the left. If circumference was more than the value for circumference at the split, we would move down to the branch on the right.

<sup>2</sup>While any curve can be approximated in a step-wise manner when the number of steps approaches  $\infty$ , a tree model does not always converge to the linear model as the number of splits approaches the number of observations.

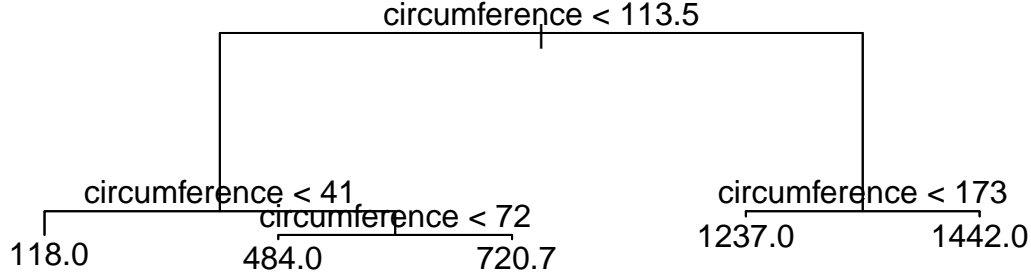


Figure 1.4: A tree representing age  $\sim$  trunk circumference in orange trees.

### 1.1.1 Mathematical notation for trees

Given a data set,  $D$ , and a formula  $Y \sim X$ , where  $Y$  and  $X$  are columns in  $D$ , a tree,  $t$ , is a stepwise function from  $X$  to  $Y$ .  $X$  can also be defined as a set of columns in  $D$ . Recall, that  $X$  is the set of our predictors and  $Y$  is our response. In example in section 1.1, the orange trees data is the data set, the ages of the trees make up our response, and the circumferences are our predictor.

$$t : X \rightarrow Y$$

$t$  is created using some sample of the rows of  $D$ . This sample is called the *training* set. The predictions or the image of  $t$ , are discrete values in the range of  $Y$ . We test the prediction accuracy of  $t$  using the rows of  $D$  that were not in the training set. This set of rows is called the *test* set. Often with trees, we generate the training set from the initial data set  $D$  by *bootstrapping* the  $D$ . “Bootstrapping” means sampling with replacement. This allows us to have large test and training sets without starting with an extra large data set  $D$ . This is valuable because it is more difficult to create good predictive models on small amounts of data relative to the entire population. The orange trees data set is an excellent candidate for bootstrapping, as there are only 35 records from 5 trees in the data set when there are presumably thousands of orange trees in the world at large. Table 1.2 demonstrates a bootstrapped sample of the first six rows of the orange trees data set from table 1.1.

There are many ways to test prediction accuracy of a model, but we will be considering the following two in this paper:  $MSE$  and  $RSS$ .<sup>3</sup>  $MSE$  is the mean squared error and is defined as:

$$MSE(t, Y, X) = \frac{1}{n} \sum_{i=1}^n (Y_i - t(X_i))^2$$

Where  $n$  is the number of rows in  $X$  and  $Y$ .  $RSS$  is the residual sum of squares error and is defined as:

$$RSS(t, X, Y) = \sum_{i=1}^n (Y_i - t(X_i))^2$$

<sup>3</sup>This paper considers only the case of regression with continuous random variables. There are analogous ways to test predictive accuracy for other types of data but they are beyond the scope of this paper.

Table 1.2: The first six rows of the orange trees data set are repeated here (left) with row numbers. The table on the right represent a bootstrapped sample of the data on the left.

age	circumference	row	age	circumference	row
118	30	1	484	58	2
484	58	2	664	87	3
664	87	3	1004	115	4
1004	115	4	1372	142	6
1231	120	5	484	58	2
1372	142	6	1372	142	6

In many cases, we are interested in creating predictive models to use as tools to predict the response in situations where an observed value is missing or difficult to find. We may want to build a model to predict the age of orange trees from trunk circumference because while it is relatively easy to measure the circumference of the trunk, age is often unknown. Then our model could be used to estimate the age of orange trees in situations where only circumference is known. When we generate predictions on new observations of the response, we cannot know how accurate our predictions are. Often  $MSE$  and  $RSS$  are calculated on the test set to create an estimate of how well the model will be able to predict the outcome of a new observation. Then they are referred to as  $MSE_{test}$  and  $RSS_{test}$ , respectively.

### 1.1.2 A brief history of trees

Trees are a convenient way to represent data and assist in decision making. Morgan and Sonquist (1963) derived a way for constructing trees motivated by the specific characteristics of data collected from interviews and surveys. The first difficulty in analyzing this data was that data collected from surveys is mostly categorical, where the observation is that the participant is a member of some discrete group. Some common categorical variables are gender, ethnicity, and education level. Numeric variables, like age, height, and weight are, in general, much easier to work with. On top of this, the data sets Morgan and Sonquist dealt with had few participants (rows) and many variables (columns). To add to their difficulties, there was reason to believe that there were lurking errors in the data that would be hard to identify and quantify. Lastly, many of the predictors were correlated. Morgan and Sonquist doubted that the additive assumptions of many models would be appropriate for this data. They noted that while many statistical methods would have difficulty accurately parsing this data, a clever researcher with quite a lot of time could create a suitable model simply by grouping values of the predictors and predicting that the response corresponding to these values would be an average of the observed responses given the grouped conditions. Their formalization of this procedure in terms of “decision rules” laid the groundwork for future research on decision trees. (Venables & Ripley, 2002) See figure 1.3 for a visualization of this process.

Later researchers proposed new methods for creating trees that improved upon the Morgan and Sonquist model. Leo Breiman et al. proposed an algorithm called CART (Classification And Regression Trees) to fit trees on various types of data (1984). Torsten Hothorn, Kurt Hornik and Achim Zeileis argue in their 2006 paper, *Unbiased Recursive Partitioning: A Conditional Inference Framework*, CART has a selection bias toward variables with either missing values or a great number of possible splits. This bias can affect the interpretability of all tree models fit using this method. As an alternative to CART and other algorithms, Hothorn et al. propose a new method: conditional inference trees. The conditional inference trees algorithm is similar to CART in many ways, but a thorough description is beyond the scope of this paper.

In the 1984 textbook *Classification and Regression Trees*, Breiman, Friedman, Olshen, and Stone described their method for creating, pruning, and testing regression trees. There are essentially three steps: one, decide on a variable to split over, two, partition that variable space in two distinct partitions, and three, set our initial predictions for each partition to be mean value of the response according to the observed responses corresponding to the values in the partitions. Recursively, this process is repeated for each new partition until some stopping condition is reached. This is a top down, greedy algorithm that functions by creating as large a tree as possible (Venables & Ripley, 2002).

Random Forests are generated by fitting a large number of trees, each on a boosted sample of the data. The crucial difference, however, between the trees in CART and the trees in a random forest, is that at each node in a random forest, only a subset of the predictors are considered as candidates for possible splits. This decorrelates each tree from its neighbors, and limits variability of the whole forest (James, Witten, Hastie, & Tibshirani, 2013).

There is a limit to the predictive capabilities of a single tree as they suffer from high variance. (James et al., 2013) These are further explored in chapter 2. To alleviate this, aggregate methods called forests are often used instead. They function by enlisting the help of many trees, and then by aggregating the responses over all of them. The two common types of forests are bagged and random forests.

### 1.1.3 Mathematical notation for bagged and random forests

Given a data set,  $D$ , and a formula  $Y \sim X$ , where  $Y$  and  $X$  are columns in  $D$ , a forest,  $R$ , is a collection of trees from  $X$  to  $Y$ . As  $R$  is a collection of trees from  $X$  to  $Y$ , it is also a stepwise function from  $X$  to  $Y$ .

$$R : X \rightarrow Y$$

The trees in a forest are fit using bootstrapped samples of the original data set  $D$ . The bootstrapped training set for a tree  $t$  is  $B_t$  and the corresponding test set is  $\bar{B}_t$ . These test and training sets are called the *in bag* set and the *out of bag* set. When the  $MSE$  or  $RSS$  is calculated for a tree in a forest, it is done on the out of bag set for that tree and called the OOB (out of bag) error. The predictive accuracy of the

Table 1.3: Estimated linear coefficients, error, and p-values from the model fit in section 1.1 on the orange tree dataset

	Estimate	Std. Error	t value	Pr(> t )
(Intercept)	16.603609	78.1406182	0.2124837	0.8330368
circumference	7.815998	0.6058806	12.9002281	0.0000000

random forest is the average of the out of bag error across all the trees in the forest. The predictions for the random forest,  $R(X)$ , are the average prediction of each tree on  $X$ .

These are *bagged forests*. *Random forests* are a variation on bagged forests, and are the main focus of this paper. There is no difference between bagged and random forests when there is only one predictor in the data set, but, in cases with more than one predictor, the trees are generated in a slightly different way. Usually, to make a split all the predictors are considered.<sup>4</sup> If we had a larger version of the orange tree data set that included the heights of each tree, then the tree would always consider both height and circumference as possible candidates for splits. In a random forest tree, it is possible that only one predictor, height or circumference, would be considered at a time. The splitting procedure is discussed at length in chapter 3 and this property of random forests is discussed in chapter 4. For now only a cursory understanding is needed.

### 1.1.4 Inferential vs Descriptive Statistics

In the earlier sections, we focused on building predictive models, but this paper hopes to use tree-based methods beyond this context. The linear model is a mainstay in social science because it allows for easy and interpretable statistical inference. Return to the orange tree example from section 1.1. The linear model gives us a line with which we can make predictions, but it also gives estimated coefficients and conducts hypothesis tests on the values of the coefficients.

This table provides evidence that not only is trunk circumference a good predictor of age, the relationship between them is the equation of the line:

$$Age = 7.81 \cdot Circumference + 16.6$$

Roughly, for every 1 cm of trunk growth, we would expect the tree to be 7.81 days older. Not only are we provided with a way to describe the relationship between age and circumference, we have conducted statistical tests to make reasonably sure that our estimates, 7.81 and 16.6 in the equation above, are not zero. Inferential claims about the nature of tree age and trunk growth are possible here.

<sup>4</sup>A brief note on uncertainty is needed here. It's true that in this setting we can say that  $V_4$  is actually unimportant to understanding  $Y$ , but in situations with real data this is profoundly more difficult to parse. Often like in the social science situations that Morgan and Sonquist encountered, the real relationship between correlated predictors is complicated and often there is some theoretical backing or other insight that is gained to include variables that may not be important to the model.

It is important to note the difference between inferential and descriptive statistics. Descriptive statistics describe the data at hand without making any reference to a larger data generating system that they come from. It follows that inferential statistics then make claims about the data generating system given the data. The model in figure 1.4 could be used to make descriptive claims about the orange tree data. For example, given the data we have, we expect a sapling with a trunk circumference less than 41 cm to be 118 days old. However, trees are variable; they are very sensitive to changes in the data set. It's entirely possible that if we fit this tree on a new sample of the data, the predictions would change. See chapter 2 for more discussion on the variability of trees. Our claims about the relation between circumference and age in young orange trees can only be descriptive as we have not taken into account the variability in gathering them. This paper's aim is to describe a process of making inferential claims using trees and random forests that employs permutation tests.

As stated in the introduction of the *Chronicle of Permutations Statistical Methods* by KJ Berry et al. 2014, there are two models of statistical inference. One is the population model, where we assume that the data was randomly sampled from one (or more) populations. Under this model, we assume that the data generated follows some known distribution. “Under the population model, the level of statistical significance that results from applying a statistical test to the results of an experiment or a survey corresponds to the frequency with which the null hypothesis would be rejected in repeated random samplings from the same specified population(s)” (Berry, 2014).

The permutation family of methods, on the other hand, only assumes that the observed result was caused by experimental variability. The test statistics are calculated for the observed data, then the data is permuted a number of times. The statistic is calculated after each permutation to derive a distribution of possible values under some null hypothesis. Then the original test statistic is tested against this distribution. If the observed value is exceptionally rare, then there is evidence that our observation did not come from that distribution.

## 1.2 Inference on Random Forests

### 1.2.1 The Problem

Random forests create models with great predictive, but poor inferential capabilities. After Morgan and Sonquist's initial development of decision trees, trees quickly moved to the domain of machine learning and away from statistics. Researchers focused on bettering predictions and improving run times and less on the statistics behind them. In a single tree, descriptive claims may be simple to make, but it is much more difficult to describe the behavior of the whole forest. Inferential statistics with random forests generally falls behind the predictions in importance. This has limited the applications of random forests in certain fields, as to many the question of “why” the data is the way it is is more important than building predictions. There are several means of performing descriptive statistics with random forests that could be interpreted



incorrectly as attempting to answer this but without a statistically backed method for performing inference, the use of random forest is limited to prediction-only settings.

### 1.2.2 Proposed solutions to this problem

Variable importance could be the tree-based analogue to the coefficients of the linear model, in that the variable importance for the predictor  $X_i$  in the model for  $Y \sim X_1, \dots, X_p$  is the amount of predictive accuracy due to  $X_i$ . Breiman proposed a method of permuted variable importance in his paper *Statistical Modeling: The Two Cultures* to answer this problem. Their method compares the variable importance for each variable in a tree-wise manner. For each tree, the permuted variable importance of the variable  $X_j$  is:

$$VI^t(X_j) = \frac{\sum_{i \in |\bar{B}_t|} (y - \hat{y})^2}{|\bar{B}_t|} - \frac{\sum_{i \in |\bar{B}_t^*|} (y - \hat{y}^*)^2}{|\bar{B}_t^*|}$$

Where  $\bar{B}_t$  is the out of bag sample for tree  $t$ ,  $|\bar{B}|$  is the number of observations in that sample,  $\bar{B}_t^*$  is with  $X_j$  permuted,  $\hat{y}$  is the predicted outcome, and  $\hat{y}^*$  is the predicted outcomes after variable  $X_j$  has been permuted. This value is averaged over all the trees. It is important to note that if the variable  $X_j$  is not split on in the tree  $t$ , the tree-wise variable importance will be 0.

Strobl et al from the University of Munich criticize this method in their 2008 technical report *Danger: High Power! – Exploring the Statistical Properties of a Test for Random Forest Variable Importance*. First, this method has the downside of increasing power with increasing numbers of trees in the forest. This is a more or less arbitrary parameter which we would hope would not affect our importance estimates. Second, the null hypothesis under Breiman and Cutler’s strategy is that the variable importance  $VI$  for any variable  $X_j$  is not equal to zero given  $Y$ , the response. Because random forests are most often used in situations with multicollinearity that would make other methods like the linear model difficult, Strobl argues that any variable importance measure worth its salt should not be misled by correlation within the predictors.

The researchers at the University of Munich published a fully fleshed response to the Breiman and Cutler method in 2008, titled *Conditional Variable Importance for Random Forests* that addresses these issues. Strobl et al propose restructuring the Breiman and Cutler algorithm to account for conditional dependence among the predictors. The null hypothesis is that  $VI_\beta(X_j) = 0$  given the predictor  $Y$  and all other predictors  $X_1, \dots, X_n$ . This accounts for interactions between  $X_j$  and the other predictors, while preserving the relationship between  $Y$  and the remaining predictors.

This paper aims to provide a response to this method. The partitions are made from the random forest corresponding to the formula of  $Y \sim X_1, \dots, X_n$  instead of a model of  $X_j \sim X_1, \dots, X_n$ . This ignores the common situation where if the predictors are correlated enough, then they act as stand ins for each other, so that if one variable is heavily influential in a certain tree at predicting  $Y$ , the other variable will be forgotten altogether.



# Chapter 2

## Simulations and Comparisons

Our goal for this chapter is to compare trees, random forests, and linear models. In this chapter, we will use simulated data instead of the orange trees data set. One reason for this is theoretical consistency. One hopes that one's results will not be rendered null and void by any misstep in the data collection that comes to light. This also ensures that these simulations can be repeated by later researchers, but, granted, it does not make for the most exciting analysis. For now, consider  $Y$  to be our response variable. In the first simulation,  $V$  will be the set of our predictors, and  $V_j$  to be a predictor in  $V$ . The formula will be the same for each model:  $Y \sim V$ . In our second simulation, our set of predictors will be denoted as  $X$  and  $X_j$  will be a member of  $X$ . The formula in this case is  $Y \sim X$ . A single row in  $D_1$  will be denoted as  $v$ , and a single row in  $D_2$  as  $x$ .

### 2.1 Simulated Data

Random forests excel in predicting outcomes with correlated predictors, although these situations can make it difficult to perform intelligible inference. In a situation in which the correlated predictors are  $X_1$  and  $X_2$  and the formula we're estimating is  $Y \sim X_1 + X_2$ , it can be difficult to say if  $X_1$  or  $X_2$  is truly the better predictor. To illustrate this idea, compare a few existing methods, and explore methods of inference on tree based models, we will simulate two data sets with different correlation structures. We will focus more on the correlation structure between the predictors than on their relationships with the response and this will be reflected in the simulations.

The first simulated dataset is generated under the same scheme as in (Strobl, Boulesteix, Kneib, Augustin, & Zeileis, 2008). Under this method, the 13 x 1000 data set,  $D_1$ , has 12 predictors,  $V_1, \dots, V_{12}$ , where  $V_j \sim N(0, 1)$ . The first four are block correlated to each other with  $\rho = .9$ . They are related to  $Y$  by the linear equation:

$$Y = 5 \cdot V_1 + 5 \cdot V_2 + 2 \cdot V_3 + 0 \cdot V_4 + -5 \cdot V_5 + -5 \cdot V_6 + 0 \cdot V_7 + 0 \cdot \dots + E, E \sim N(0, \frac{1}{2})$$

Note in table 2.1, the coefficients for  $V_7, \dots, V_{12}$  are all zero.

In the last column of table 2.1, the coefficient "beta", refers to the function used to generate the  $Y$  values. Although  $V_4$  was not included in the model  $Y \sim V_1, \dots, V_{12}$ ,

Table 2.1: Empirical correlations and coefficients of the variables in the first simulated data set

	V1	V2	V3	V4	V5	V6	V7	y	beta
V1	1.000	0.915	0.908	0.907	-0.034	0.006	0.012	0.839	5
V2	0.915	1.000	0.914	0.914	-0.020	-0.001	-0.001	0.838	5
V3	0.908	0.914	1.000	0.903	-0.017	-0.007	0.007	0.818	2
V4	0.907	0.914	0.903	1.000	-0.002	-0.015	0.023	0.800	0
V5	-0.034	-0.020	-0.017	-0.002	1.000	0.044	0.005	-0.392	-5
V6	0.006	-0.001	-0.007	-0.015	0.044	1.000	-0.005	-0.368	-5
V7	0.012	-0.001	0.007	0.023	0.005	-0.005	1.000	0.004	0

its strong correlation with more influential predictors  $V_1, \dots, V_3$  ensures that it still shows a strong, empirical linear correlation with  $Y$ . A linear model would likely *overstate* the effect of  $V_4$  on  $Y$ .<sup>12</sup>

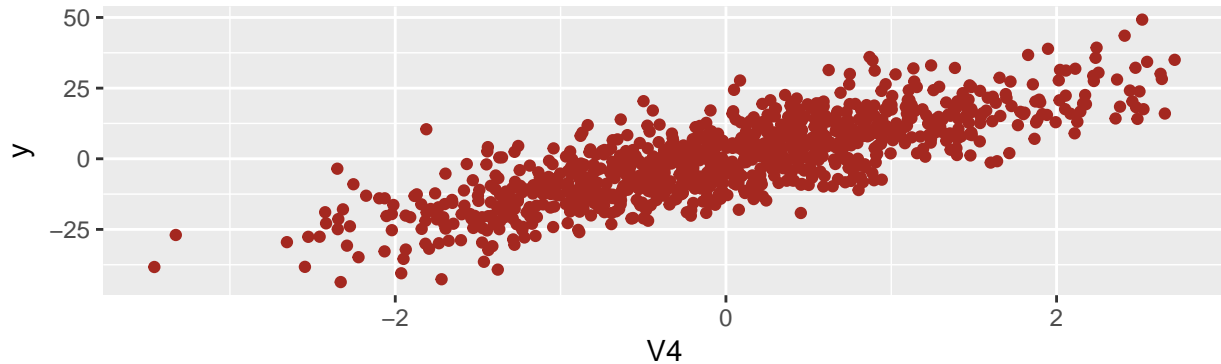


Figure 2.1: Relation between  $V_4$  and  $Y$ . This relation has empirical linear correlation = .789

<sup>1</sup>A brief note on uncertainty is needed here. It's true that in this setting we can say that  $V_4$  is actually unimportant to understanding  $Y$ , but in situations with real data this is profoundly more difficult to parse. Often like in the social science situations that Morgan and Sonquist encountered, the real relationship between correlated predictors is complicated and often there is some theoretical backing or other insight that is gained to include variables that may not be important to the model.

<sup>2</sup>Another point that could be said is that, no  $V_4$  is not unimportant,  $V_1, V_2$ , and  $V_3$  are just stand ins for the real star,  $V_4$ , as they are nearly the same ( $\rho \sim 1$ ). Then the real relationship represented here is  $Y \sim (5 + 5 + 2) \cdot V_4 + -5 \cdot V_5 + -5 \cdot V_6 + -2 \cdot V_7$ . This model is not unsuccessful in capturing the structure of the data, and this is typically the practice used to model data with highly correlated predictors. If this seems philosophically satisfying to you, the rest of this thesis may seem a bit inconsequential.

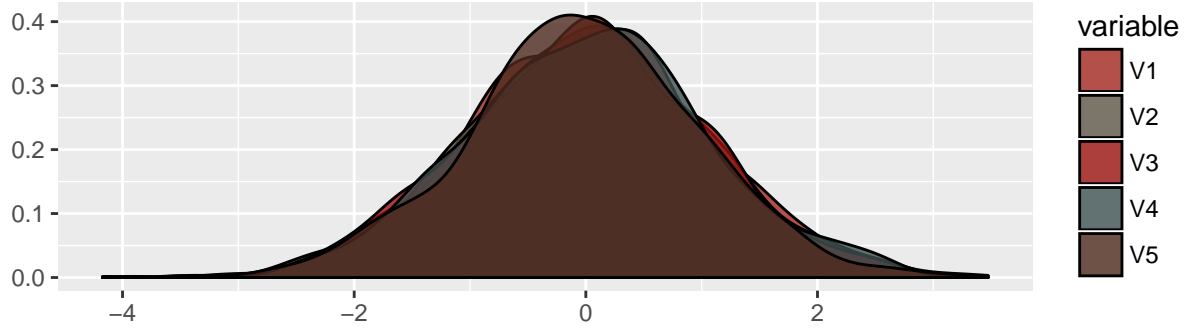


Figure 2.2: Empirical densities for V1 through V4

The densities of  $V_1, \dots, V_4$  in figure 2.2 are all very similar due to the way they were generated.  $D_1$  represents the case where some of the predictors are linearly correlated with each other, but that is not the only possible correlation structure. The data set  $D_2$  is simulated similarly to  $D_2$  in that  $D_2$  contains twelve predictors and one response variable. The first four variables are generated in the following way:

$$X_1 \sim N(0, 1)$$

$$X_2 = \log(X_1) + E, E \sim N(0, 1)$$

$$X_3 = \log(X_2) + E, E \sim N(0, 1)$$

$$X_4 = \log(X_4) + E, E \sim N(0, 1)$$

This simulation scheme leads to the first four variables having an obvious relationship between each other, but relatively low linear correlations, as seen in figure 2.3. Predictors are sampled by  $X_5, \dots, X_{12} \sim N(0, 1)$ . The  $Y$  values are generated according to the following formula:

$$Y = 5 \cdot (X_1)^2 + 5 \cdot (X_2)^2 + 2 \cdot (X_3)^2 + 0 \cdot X_4 + -5 \cdot X_5 + -5 \cdot X_6 + 0 \cdot X_7 + 0 \cdot \dots + E, E \sim N(0, \frac{1}{2})$$

Table 2.2: Empirical correlations and coefficients of the first seven predictors and the response using the second simulated dataset

	X1	X2	X3	X4	X5	X6	X7	y	beta
X1	1.000	0.013	0.044	0.002	-0.012	-0.012	-0.044	-0.003	5
X2	0.013	1.000	-0.520	-0.272	0.073	0.004	0.006	-0.697	5
X3	0.044	-0.520	1.000	-0.004	0.030	-0.013	0.023	0.271	2
X4	0.002	-0.272	-0.004	1.000	-0.031	0.022	-0.002	0.352	0
X5	-0.012	0.073	0.030	-0.031	1.000	0.010	-0.030	-0.099	-5
X6	-0.012	0.004	-0.013	0.022	0.010	1.000	-0.088	-0.022	-5
X7	-0.044	0.006	0.023	-0.002	-0.030	-0.088	1.000	0.013	0

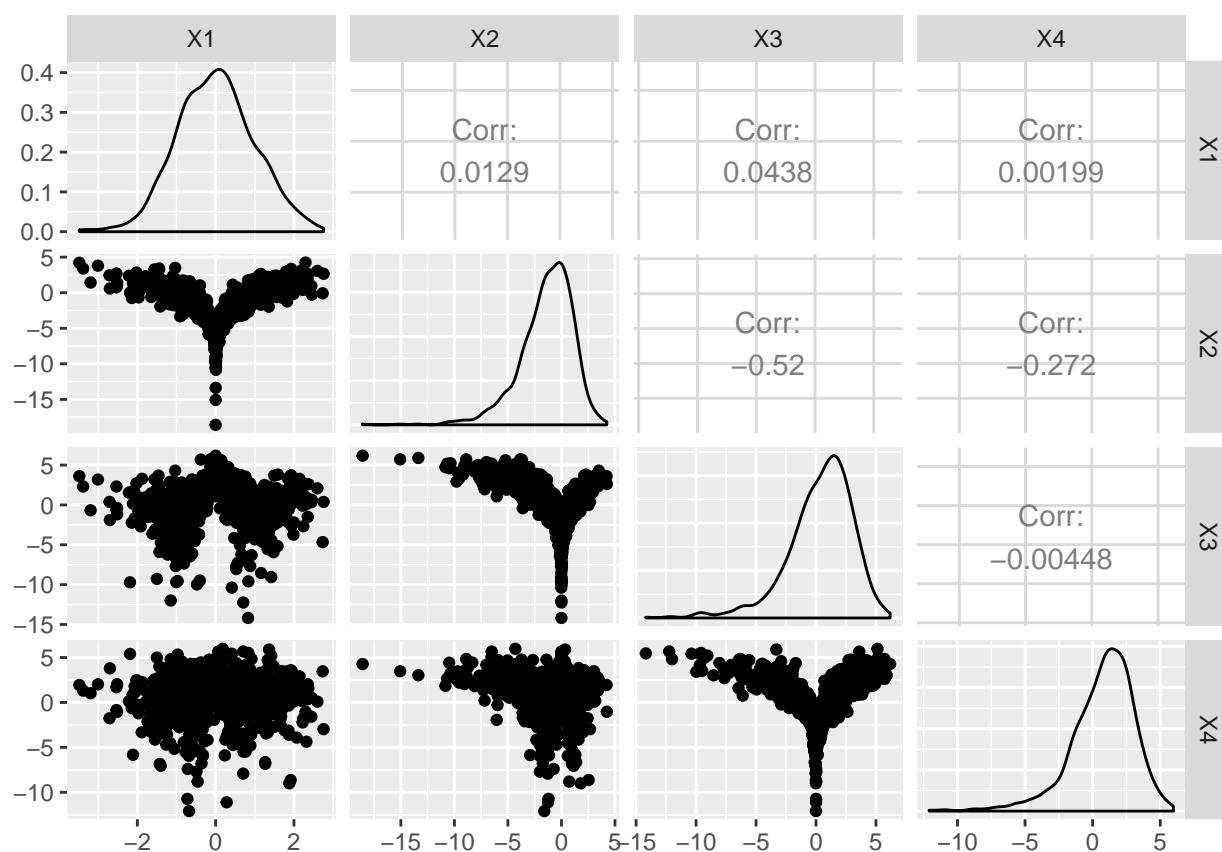


Figure 2.3: Correlation structure of the first four variables in  $D_2$

The correlation structure in  $D_2$  is much more difficult to capture with a single line. The relationships between the first four predictors form striking, symmetrical scatter plots in figure 2.3. This information is considered again in table 2.2, where the empirical correlations of the first seven variables are presented along with their observed correlations with  $Y$  and their simulation coefficients.

## 2.2 Models and Comparisons

### CART: Regression Trees

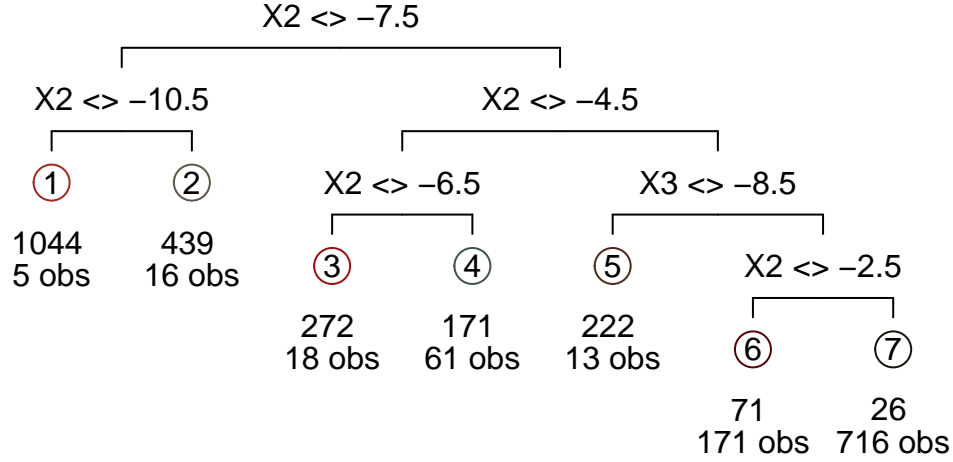


Figure 2.4: CART representing  $Y \sim X$ , from  $D_2$

The CART tree representing the model  $Y \sim X$  in figure 2.4 is easy enough to understand. Starting at the very top of the tree, predictions can be made based on the values of the leaves (or ending nodes) given the requirements of the path to get there. Trees can be quite variable, so to get a better idea of the differences between the methods let's run a simulation. This simulation scheme will take advantage of the non linearity present in  $D_2$ .

---

#### Algorithm 1 Simulation Scheme 2.1

---

- 1: **for**  $i \leq 1000$  **do**
  - 2:   Randomly sample  $\frac{2}{3}$  of the observations in  $D_2$  to a training set,  $D_{2,train}^i$ . The other observations,  $x \in D_2, x \notin D_{2,train}^i$  form the testing set  $D_{2,test}^i$
  - 3:   Fit a tree,  $T^i$ , to the data under the model  $Y \sim X_1, \dots, X_2$  using the observations in  $D_2^i$
  - 4:   Calculate the  $MSE_{test}$  of the model using the equation:  $MSE_{test} = \frac{1}{n} \sum (y_j - \hat{y}_j)^2$
  - 5: **end for**
- 

Note that  $n$  is the number of observations in  $D_{1,test}^i$ ,  $y_j \in D_{2,test}^i$ ,  $\hat{y}_j \in T^i(D_{2,test}^i)$  for  $1 \leq j \leq n$ . This produces one distribution of  $MSE_{test}$  for CART. This simulation scheme will be repeated for the linear model and the random forest and the  $MSE_{test}$  distributions are compared in figure 2.5.<sup>3</sup> Note that the scales on the x-axis are drastically different for each of these models. The  $MSE_{test}$  distribution for the random forest has such low variance, and low  $MSE_{test}$  it would be difficult to display it on the same plot as the other two.

---

<sup>3</sup>Recall that we only allow splits to take place that split the data into two groups, each with more than five members.

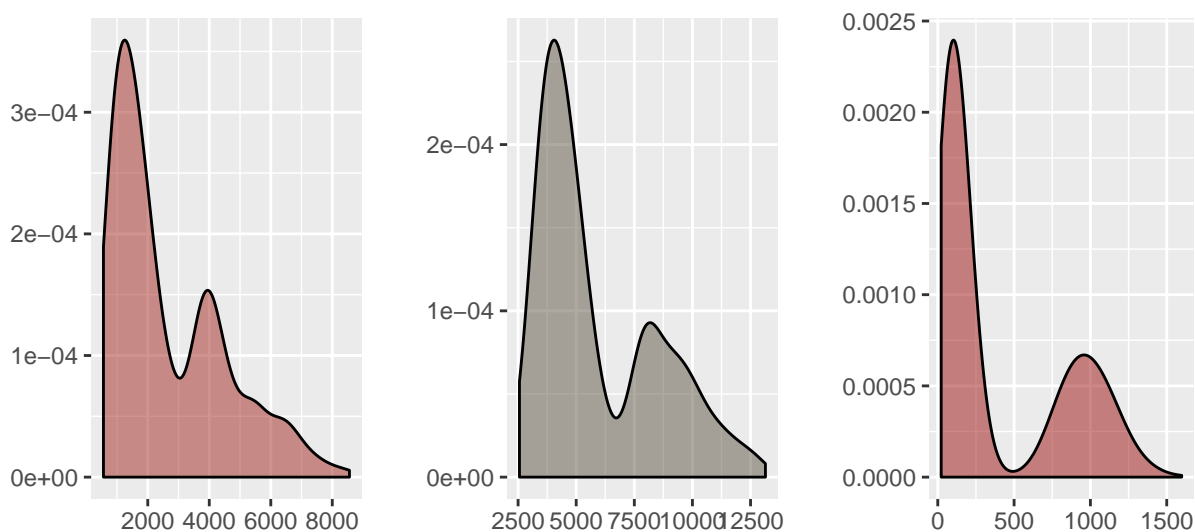


Figure 2.5: The simulated MSE distributions of CART, linear model, and the random forest on D2

The linear model is characteristically less flexible and less prone to over-fitting than either of the tree-based methods, CART and random forests, and has a  $MSE_{test}$  distribution that is quite peaked. CART is flexible and suffers from high variance. The random forest models perform much better on average than either the CART or the linear model, due to both the non-linear relationships between  $Y$  and the predictors and the random forest's ability to decorrelate each of the trees by restricting the variables available on each split. See chapter 3 for more discussion on the enforced heterogeneity of trees in the random forest. As  $MSE_{test}$  is a test of *predictive* accuracy it is not surprising that the random forest performed admirably. On a certain level, that is what they are designed to do. Highly predictive models are good at *predicting* outcomes, but not necessarily good evidence that the data was generated in a similar way to that model. The linear model is not always popular in predictive situations but it is ubiquitous in inferential ones.



## Chapter 3

# Random Forest Variable Importance

To implement the various variable importance measures discussed in this chapter and in chapter 4, functions for creating trees, random forests, and their importance measures were created. The trees were fit using the standard two-part CART-like algorithm. The function chooses a variable to split on with linear correlation with respect to  $Y$ , but instead of looking for correlations above a certain threshold which is common, it chooses the variable with the highest correlation when compared to its peers. This alleviates the situation where a variable with a non-linear relationship would be passed over again and again. The splitting is then done via minimization of the following function with respect to  $i$ :

$$RSS_{node}(i, X, Y) = RSS_{leaf}(Y|X < i) + RSS_{leaf}(Y|X \geq i)$$

$$RSS_{leaf} = \sum_{y \in Y} (y - \hat{y})^2$$

Note that  $\hat{y}$  is the mean value of  $Y$ . This function considers the regression case only, and only numeric predictors. Leaves are created when the resultant split would be unsatisfactory, i.e. at least one of these cases applies: one daughter node would have five members or less, the split on the chosen variable would not result in a decrease in RSS, or the response contained in the node, or the predictor considered for the split, are already homogeneous. This generates very large trees: a quality that is not an issue in random forests but may be problematic in a single-tree setting.

There are several ways to display a tree, but when it is displayed as in table 3.1 it is read in the following way: each row corresponds to a node of the tree which contains a certain number, **n** observations. This number of observations, or rows in the data set is naturally a subset of both the original data set and the subsets above the node on the tree. Here our predictions, **ypred**, are the mean of the  $Y$  values included in the node. If there is an optimal and allowable split,<sup>1</sup> then the chosen variable, **var**,

---

<sup>1</sup>Recall that we only allow splits to take place that split the data into two groups, each with more than five members.

Table 3.1: t, a home-grown tree grown on the first four columns and the first 140 rows of D2

var	n	dev	ypred	split.cutleft
X2	140	234791.36	49.79	-4.52
X4	127	92293.01	33.49	0.64
X4	60	59974.42	49.64	3.86
leaf	6	4827.51	96.24	0.00
X3	54	39569.87	44.46	1.91
leaf	21	21874.78	65.75	0.00
leaf	33	17695.09	30.91	0.00
X3	67	12473.55	19.03	1.45
leaf	7	2562.75	45.24	0.00
X3	60	7608.15	15.97	-0.18
X2	32	4033.15	21.77	1.05
leaf	10	1486.19	31.31	0.00
leaf	22	2546.96	17.43	0.00
X2	28	1678.22	9.35	-0.47
leaf	13	631.76	14.20	0.00
X2	15	660.31	5.15	-0.88
leaf	6	330.90	-1.07	0.00
leaf	9	329.41	9.29	0.00
leaf	13	112843.76	208.98	0.00

and the  $RSS_{node}$ , `dev`, are recorded.<sup>2</sup> The value of the variable in question that acts as the split point is recorded as `split.cutleft`. If there is no split on the node in question, then `var` will be recorded as `<leaf>` and the `dev` value will be the value of  $RSS_{leaf}$  at this node.

The tree output is read roughly from top to bottom, with a coda in the middle. The first row corresponds to the first node, or the node that includes the entire data set. The second row is the beginning of the right subtree or the right daughter of the first node. This pattern continues, favoring the right daughter, until a leaf is reached. The left daughter of the first node is found after all of the splits off of the right daughter have finished but is easily identified as the row with a value of `n` that is exactly the difference between the `n` values of the first two rows. In the case where the right daughter contained many more observations of the original data set, there may be a node within the right subtree that contains the same number of observations as the left daughter of the first node.<sup>3</sup> In this case, the left daughter is simply the second row with this property. The pattern of following the right daughter until a leaf is reached continues with the left subtree.

## 3.1 Breiman et al. Introduce Permuted Variable Importance (1984)

### 3.1.1 Variable Importance on a Single Tree

Breiman et al. in *Classification and Regression Trees* (1984) propose a method for variable importance for individual trees that stems from their definition of  $\tilde{s}$ , a surrogate split. Surrogate splits help Breiman et al. deal with several common problems: missing data, masking, and variable importance. They are defined using logic that resembles that behind random forests.

Before we discuss surrogate splits, let's cover an obvious definition of variable importance for a single tree. In the tree represented by table 3.1, define variable importance as the number of splits on each variable. This would allow us to answer the question: how useful (important) was variable  $X_i$  in constructing our model for  $Y$ ? Just by counting the splits on that variable, we would arrive at the following ranking:

There are several downfalls to this method. One, trees are variable. If we were to resample this data and fit another tree, it's likely that this ranking would change. Two, in the case where two variables are close enough to each other that they could act as stand-ins for one another, these rankings are much less interesting. We are lucky in this case to know without doubt that  $X_1$  has a rich relationship with  $X_2$  and the other predictors included in this model (see chapter 2, section 1). This leads us to believe that while  $X_1$  is left out of these rankings, it just as easily could have been

<sup>2</sup>It's the convention to call the  $RSS_{node}$  the deviance at a node  $N$ , but, of course, this only makes sense when the node is a leaf.

<sup>3</sup>This occurs when the variable in question has a group of values that are, 1) larger in magnitude than the mean, and 2) are separated from the general trend. Essentially this occurs when we have unscaled data with outliers.

Table 3.2: The number of splits on each variable in the tree T.

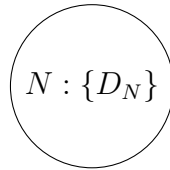
variable	appearances.in.tree
X2	4
X3	3
X4	2
X1	0

included instead of  $X_2$ , or one of the other predictors.  $X_1$  had bad luck by not being in this model and it wouldn't make sense to say that the  $X_1$  is the least important predictor of  $Y$  when it is very nearly identical to  $X_2$ . However, it's possible that the tree algorithm would only pick one of the correlated predictors to be included in a model at a time. Is it possible that we can grasp this relationship by only fitting one tree?

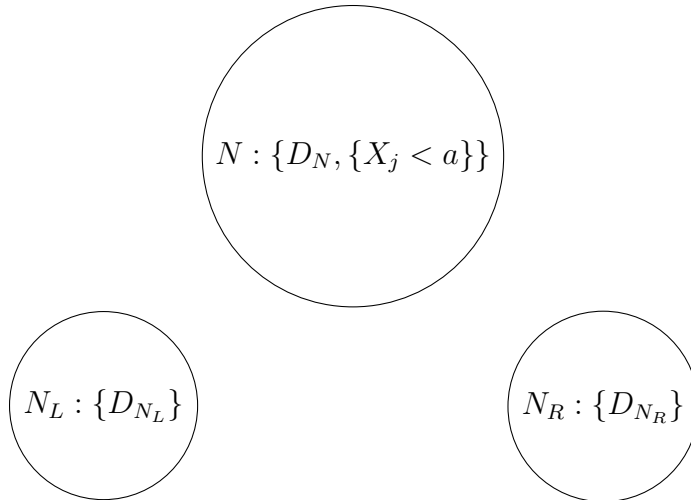
This dilemma is solved by surrogate splits. To set the stage for surrogate splitting, imagine a CART tree,  $t$ , fit on some data set  $D$  according to the formula  $Y \sim X$  where  $X_i \in X$ ,

if

$i \in 1 : p$ . Now say that we're only considering a single node,  $N$ , in  $t$ . The node  $N$  contains the subset of the rows in the original data set  $D$ ,  $D_N$ .  $D_N$  is determined by the previous nodes and splits in the tree.



On that node, we have the split on  $X_j$  where  $X_j < a$ . This gives us two daughter nodes to  $N$ ,  $N_L$  and  $N_R$ .



The data sets  $D_{N_L}$  and  $D_{N_R}$  are subsets of  $D_N$  and when combined, they equal  $D_N$ . They are determined by the rule: if a row of observations has a value of

$X_j < a$  then it is a member of  $D_{N_L}$ , if the value of  $X_j$  in that row is greater than or equal to  $a$  then it belongs to  $D_{N_R}$ .  $X_j$  was chosen to split on in node  $N$  because the correlation between the subsets of  $X_j$  and  $Y$  in  $D_N$  was stronger than the correlations between  $Y$  and any of the other predictors in that subset of the original data. Imagine, however, that split on  $X_i$  would lead to very similar<sup>4</sup> left and right daughter nodes to the daughter nodes generated by the split on  $X_j$ . This occurs even though  $X_i$  and  $Y$  had a lower correlation than  $Y$  and  $X_j$ . This would be considered a surrogate split for our original split on  $N$ . Now define variable importance for a predictor  $X_j$  across the tree  $t$  as the decrease in  $RSS_{node}$  according to the split on  $X_j$ , whether *surrogate* or not. This allows  $X_j$  and  $X_i$  to share the importance measure, if both  $X_j$  and  $X_i$  would have provided a similar, valuable split on node  $N$ . In *Classification and Regression Trees*, Breiman et al, outline several potential problems with this method that they do not attempt to solve. First, that this is only one of a number of reasonable ways to define variable importance. Second, the variable importances for variables  $X_1, \dots, X_p$  can be affected by outliers or random fluctuations within the data. (Ch 5.3). The second problem is mitigated when we move from single trees to a random forest, but the first is a problem with variable importance in general.

### 3.1.2 Variable Importance for a Random Forest

One way to define variable importance for a random forest follows directly from Breiman et al's definition for a single tree. Recall that each tree in a random forest is fit to a bootstrapped sample of the original observations. To estimate the test error, therefore no cross validation is needed - each tree is simply tested against the test set of observations that were not in that tree's training, or in bag, set. Additionally, we may be interested in defining variable importance for a predictor  $X_j$  by considering the predictive capabilities of the other  $p - 1$  predictors. Recall: a random forest is a set of trees that are de-correlated with each other because at each split on each tree, less than half of the predictors are not even considered as possible candidates for splitting. To estimate the importance of  $X_j$  given the other variables  $X_{-j}$  and their relationship with  $Y$ , we can consider the "test" RSS of the set of trees that did not ever split on  $X_j$ . These values are then averaged over the subset forest that did not include  $X_j$ . A large value would imply that in trees that included  $X_j$ , the predictive capabilities were increased.

To formalize that idea, let's refer to the set of trees that did not consider  $X_j$ ,  $t_{-X_j}^c$ . Now,  $t_{X_j}^c \subset R$ , the random forest. The subset of the original data that will be tested on each tree,  $t$ , is  $\bar{B}_t$ . The dimensions of  $\bar{B}_t$  are  $\nu_t \times p$ , where  $p$  is the number of predictors and  $\nu_t \leq n$ . The number of trees in  $t_{x_j}^c$  is  $\mu$  where  $\mu \leq ntree$

Now, base variable importance is:

---

<sup>4</sup>This is intentionally vague. The level of similarity considered "similar enough" depends on the properties of the data set and there's no guarantee that suitable surrogate splits exist. (Breiman et al., 1984)

$$VI_\alpha(X_j, R) = \sum_{t \in t_{x_j}^c} \frac{1}{\nu_t} RSS(t, \bar{B}_t)$$

However, this method poses some problems. Namely, while variable importance for random forests is more stable than for the variable importance values for CART (this is because the model is less variable in general), it is lacking the traditional inferential capabilities of other regression models. In an effort to derive a p-value for variable importance values, Breiman (2001b) describes a *permuted variable importance* or  $VI_\beta$  that does not utilize  $t_{x_j}^c$ .

---

**Algorithm 2** Permuted Variable Importance for Random Forests,  $VI_\beta$ 


---

```

Fit a random forest,  $R$  on the data set  $D$  estimating the model  $Y \sim X_1, \dots, X_p$ .
for each  $X_j \in X_1, \dots, X_p$  do
  for each  $t \in R$  do
    Calculate:  $\Phi_o = \frac{1}{\nu_t} RSS(t, \bar{B}_t)$ 
    Permute  $X_j$ . Now find  $\Phi^* = \frac{1}{\nu_t} RSS(t, \bar{B}_t^*)$ 
    The difference between these values,  $\Phi^* - \Phi_o$ , is the variable importance for
     $X_j$  on  $t$ ,
  end for
end for

```

---

In other words, we start with one tree in the random forest,  $t_u$ , and one variable,  $X_j$ , where  $1 \leq u \leq ntree$  and  $1 \leq j \leq p$ . There are two subsets of the original data associated with  $t_u$ , one is the subset used to generate the tree  $B^t$  and the other is the rest of the original data set, notated as  $\bar{B}_t$ . We calculate the residual sum of squares for  $t_u$  on the new (to  $t_u$ ) data,  $\bar{B}_t$ . Then we alter  $\bar{B}_t$  by randomly shuffling  $X_j$ . This means that in one row of  $\bar{B}_t$ , the values are the same as they were before, except the values for  $X_j$  may be interchanged with the values in other rows. Then RSS is calculated again and compared with the RSS before the shuffling took place. As each tree in the random forest is fit to a bootstrapped sample of the original data set and splits on a fraction of the possible predictors, the tree-wise computation gives an estimate of the distribution of  $VI_\beta(X_j)$ .

To visualize the output, the permuted variable importance distribution, of this algorithm on a random forest we will fit a random forest to the data set  $D_1$  from the chapter 2. When fitting a random forest, one considers the formula, the data, the number of trees to fit, (*ntree*), and the number of variables to consider at each split, (*mtry*). We have fit the random forest for the formula  $Y \sim V$  on the data set  $D_1$ , with *mtry* = 7 and *ntree* = 300. The distributions of permuted variable importance in figure 3.1 are for the first six variables in  $D_1$ . Recall that these were the only variables used to create  $Y$ . The permuted variable importance values for variables  $V_7, V_8, V_{10}, V_{11}, V_{12}$  are zero for each of the 300 trees.

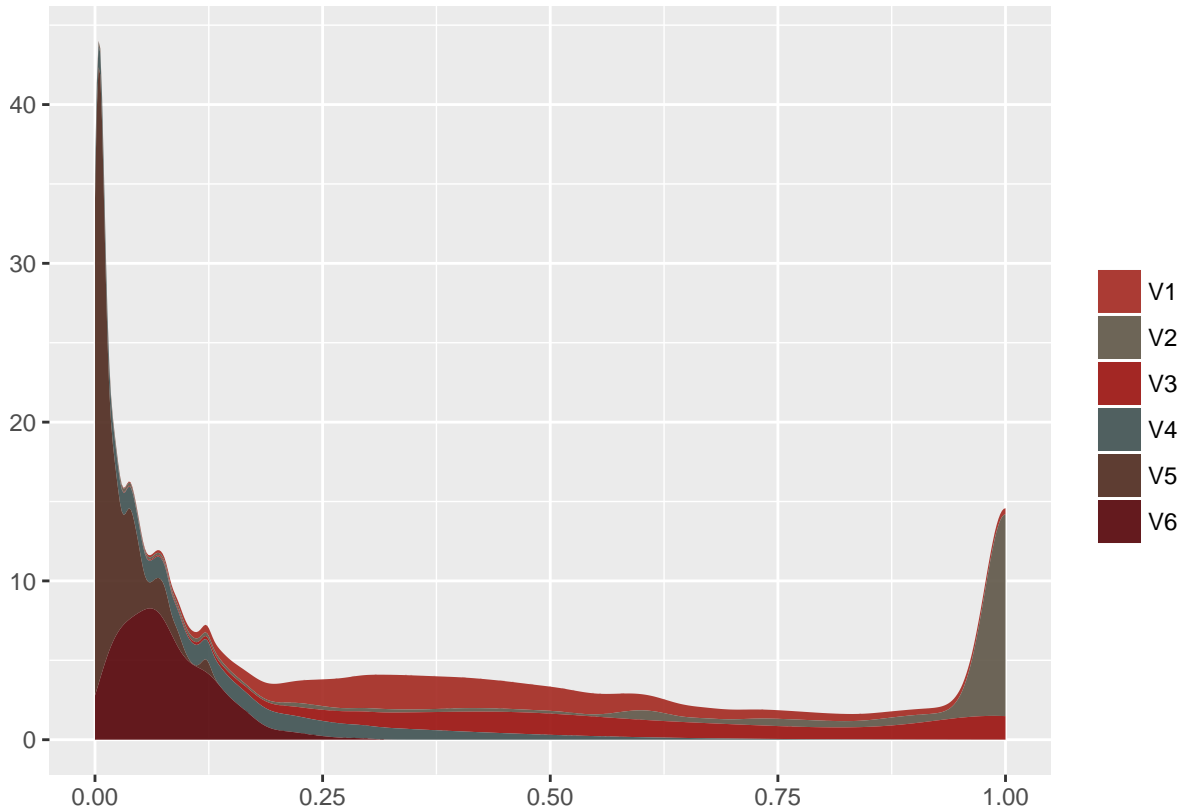


Figure 3.1: The distribution of permuted variable importance for the first six variables in D1.

## 3.2 Strobl et al Respond (2008)

Strobl et al respond to Breiman's method with one main argument: the null hypothesis implied by the permutation distribution utilized in permuted variable importance is that  $X_i$  is independent of  $Y$  **and** the rest of the predictors so the null hypothesis will be rejected in the case where  $X_j$  is independent of  $Y$  but not some subset of the other predictors. As correlation among the predictors is very common in data sets that are used for random forests, this is a large problem for Breiman's method. To alleviate this difficulty, Strobl et al propose a permutation scheme under the null hypothesis that  $X_j$ , given its relationship with the other predictors, is independent of  $Y$ .

This method is fairly similar to permuted variable importance, but there are a few key differences. Given a tree  $t_u$  and a variable  $X_j$ , first we find the out of bag RSS, then we permute. In this case, however, our permutations or shuffling of  $X_j$  is not always done blindly. If  $X_j$  has no (or low) empirical correlation with each of its fellow predictors, then  $X_j$  is shuffled exactly as in permuted variable importance. If that is not the case, then we select the set,  $Z$ , of the predictors with the strongest empirical correlation<sup>5</sup> to  $X_j$ . Recall that our tree  $t_u$  contains many nodes, and each

<sup>5</sup>The authors behind Strobl et al. (2008) recommend constructing the set  $Z$  from prior information about the data or as the set of predictors where each one has empirical correlation greater than or

**Algorithm 3** Conditional Variable Importance for Random Forests,  $VI_\gamma$ 


---

```

1: Fit a random forest,  $R$  on the data set  $D$  fitting the model  $Y \sim X_1, \dots, X_p$ .
2: for each  $t \in R$  do
3:   Calculate:  $\Psi_o = \frac{1}{\nu_t} RSS(t, \bar{B}_t)$ 
4:   for each  $X_i \in X_1, \dots, X_p$  do
5:     Select  $Z \subset \{X_1, \dots, X_{i-1}, X_{i+1}, \dots, X_p\}$  to condition on when permuting  $X_j$ 
6:     Use the cutpoints on each variable in  $Z$  to create a grid on  $X_j$ 
7:     Permute  $X_j$  with respect to this grid
8:     Now find  $\Psi^* = \frac{1}{\nu_t} RSS(t, \bar{B}_t^*)$ 
9:     The difference between these values,  $\Psi^* - \Psi_o$ , is the variable importance
       for  $X_j$  on  $t$ ,
10:   end for
11: end for

```

---

node contains a subset of the data along with a split that determines the subsets of the daughter nodes. We feed the out of bag sample for  $t_u$  into  $t_u$  and look at all the subsets of data in nodes that split on a predictor in  $Z$ . This time when we shuffle  $X_j$  it will only be in these subsets. The union of these subsets is called  $\bar{B}_t^*$  and is used to calculate the permuted RSS.

To visualize the output from algorithm ??, conditional permuted variable importance was calculated for the same random forest from 3.1. The distribution of conditional permuted variable importance on the random forest fit on  $D_1$ , is represented in 3.2.

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equal to .2 with  $X_j$ .



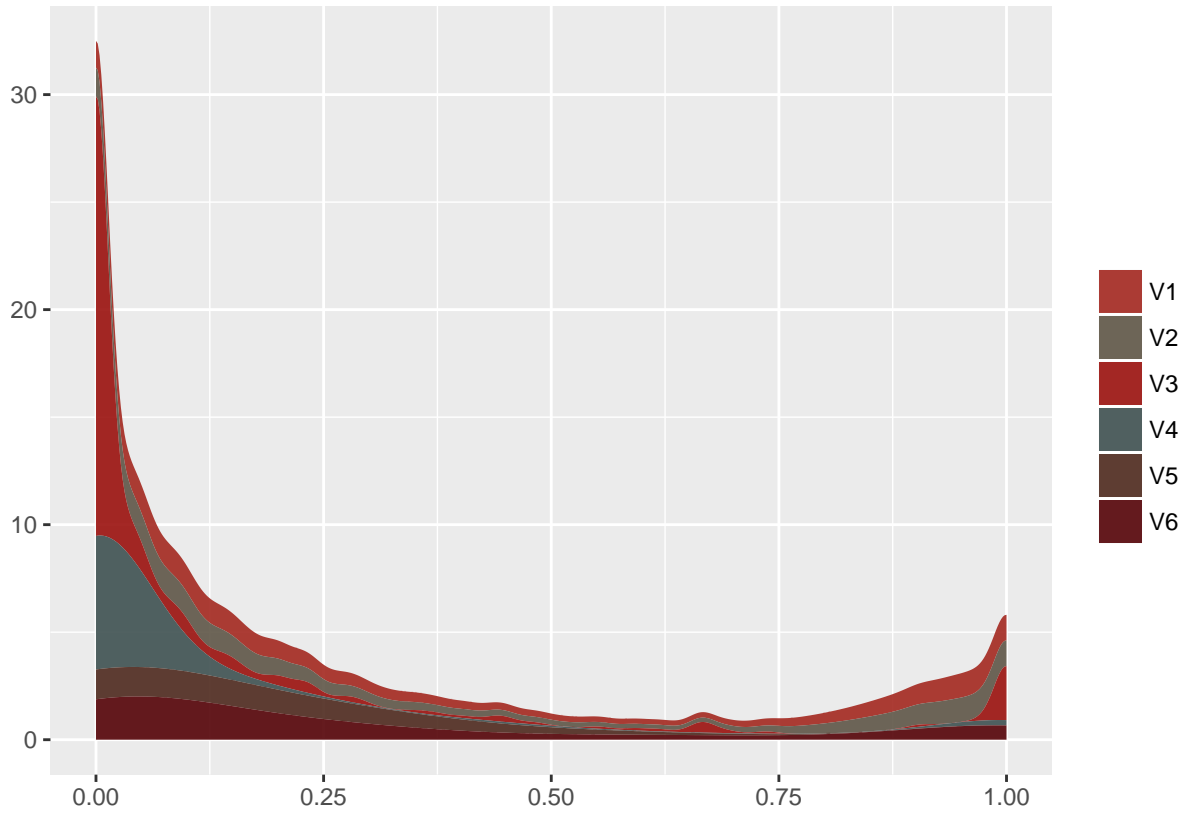


Figure 3.2: The distribution of conditional permuted variable importance for the first six variables in D1.



# Chapter 4

## Conclusion

### 4.1 INFFOREST Comparisons With Other Methods

As discussed in the beginning of chapter 4, each type of permuted variable importance, permuted, conditionally permuted, and INFFOREST, operates on a slightly different null hypothesis. This explains the differences in the results when each method is run on the same random forest.

INFFOREST variable importance is not alone in methods that conduct statistical inference on random forests. To compare the results from INFFOREST, conditional variable importance, and permuted variable importance, a random forest was generated on the first 200 rows of the data set  $D_1$ , following the formula  $Y \sim V$ . This random forest considered 7 of the 12 predictors at each split and contained 200 trees. Then the INFFOREST, conditional permuted, and permuted variable importance distributions were calculated for each variable. These distributions are represented below in figure 4.1.

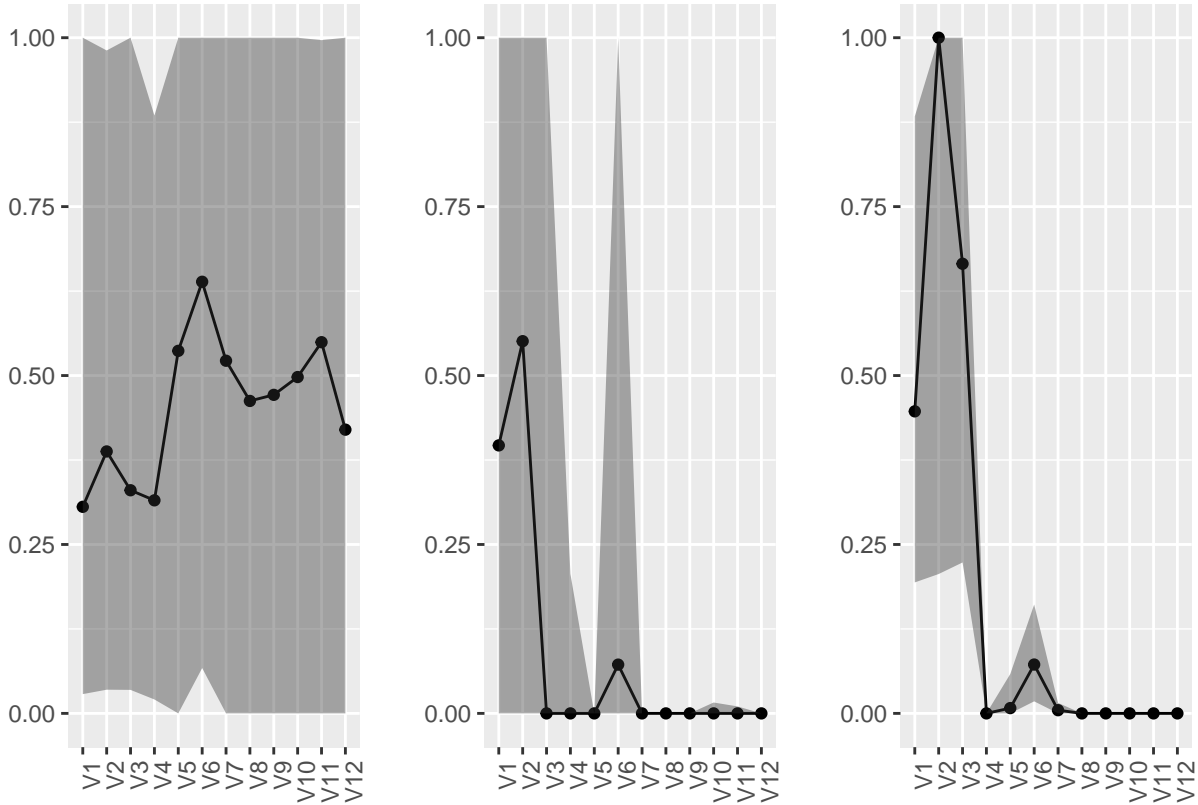


Figure 4.1: Median Values of INFFOREST, Conditionally Permuted, and Permuted Variable Importance

Mimicking the construction of the plot in chapter 4, the ribbon surrounding the average values is the 95% confidence interval constructed around the average importance values. The first main difference visible between INFFOREST and the other methods in figure 4.1 is that the median INFFOREST values are above zero, even for the variables that are not considered significant. The random forest is conducted in such a way that even predictors that may not be important in the overall model are important in a few trees. These are three different methods, following three different permutation schemes, and they are based on three different null hypotheses.

## 4.2 INFFOREST Conclusions

Using INFFOREST variable importance, we were able to demonstrate significance for all of the five predictors used to generate the response. More precisely, we were able to demonstrate that the INFFOREST values for  $V_1, \dots, V_6$  were significantly different from zero. Given the null hypothesis we considered, this allows us to claim that  $V_1, \dots, V_6$  are significant predictors of  $Y$ , given the other variables included in the model. We found one predictor to be significant,  $V_4$ , when it was not used to generate  $Y$ , and so did not quite achieve the original goal. For comparisons, these are the predictors deemed significant by the analogous linear model:

Table 4.1: The estimated coefficients and p-values for a linear model on the formula  $Y \sim V$ ,  $D_1$

	Estimate	Std. Error	t value	$\Pr(> t )$
(Intercept)	-0.01	0.04	-0.42	0.68
V1	4.83	0.11	44.85	0.00
V2	5.20	0.12	44.44	0.00
V3	2.07	0.10	19.91	0.00
V4	-0.09	0.09	-0.95	0.34
V5	-5.02	0.04	-131.79	0.00
V6	-5.01	0.04	-131.10	0.00
V7	0.03	0.03	1.05	0.30
V8	-0.04	0.04	-1.10	0.27
V9	0.07	0.04	1.84	0.07
V10	-0.01	0.03	-0.22	0.83
V11	0.04	0.03	1.28	0.20
V12	-0.05	0.04	-1.31	0.19

These results may not be as surprising as one would think. The response in the data set  $D_1$  was generated linearly from the predictors. The relationship between the response and the predictors is better represented by the linear model, as it is a linear relationship. When the same procedure is repeated on  $D_2$ , seen in the table below, we do not find that the linear model is a better fit,<sup>1</sup> as the structure in  $D_2$  is not linear.

There is clearly work to be done to recover the inferential and interpretable properties of the linear model in machine learning. As mentioned briefly in the introduction, random forests of CART trees may be biased. Hothorn et al. demonstrated that CART is biased toward variables with a great number of possible splits. An interesting follow up to this paper would be to apply INFFOREST variable importance to forests of the unbiased conditional inference trees, as discussed in Hothorn et al. As the **party** package in R created by Hothorn et al. that implements conditional inference trees, contains functions for accessing and creating custom random forests, this could be relatively simple.

On a theoretical level it would be interesting to see a proof that in the case where the linear model is appropriate, that CART does or does not approximate the linear model. From my reading and from my simulations, it does not seem like CART fits linear data very well, but a formalization of this phenomenon would be welcome.

Another area for further study is testing the INFFOREST code on situations with lots of data and lots of trees in the random forest. As  $ntree$  and  $n$ , the number of rows in the data set, increase, variance in the INFFOREST distribution seems to

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### 4.2.1 Areas for further study

Table 4.2: INFFOREST Variable Importance (left) for a random forest on the data set D2 with 300 trees is compared to the coefficients of the linear model (right)

	median	pval	Estimate	Std. Error	t value	Pr(> t )
V1	0.54	0.13	-4.54	3.45	-1.32	0.19
V2	0.40	0.00	-13.98	1.94	-7.22	0.00
V3	0.41	0.02	2.59	1.60	1.62	0.11
V4	0.43	0.01	6.48	1.46	4.44	0.00
V5	0.54	0.07	-5.88	3.45	-1.71	0.09
V6	0.47	0.11	-8.94	3.28	-2.72	0.01
V7	0.52	0.09	-4.72	3.27	-1.44	0.15
V8	0.50	0.10	-6.39	3.47	-1.84	0.07
V9	0.49	0.14	2.06	3.38	0.61	0.54
V10	0.50	0.11	-0.56	3.14	-0.18	0.86
V11	0.55	0.10	-1.50	3.70	-0.41	0.69
V12	0.56	0.06	4.46	3.36	1.33	0.19

decrease. When  $n$  is increased, the average tree size increases. When  $ntree$  is increased, the size of our forests is increased. As it is written now, however, the random forest object requires quite a lot of memory and the code to perform operations on the trees is quite intensive. This would most likely require rewriting significant parts of the code, potentially in a language other than R. A full look at this property was unfortunately not possible in the given time frame due to these constraints.

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