Statistical Inference on Random Forests

_____

A Thesis

Presented to

The Division of Mathematics and Natural Sciences

Reed College

_____

In Partial Fulfillment

of the Requirements for the Degree

Bachelor of Arts

_____

Aurora Owens

May 2017

Approved for the Division
(Mathematics)

_____

Andrew Bray

Acknowledgements

I want to thank a few people.

Preface

This is an example of a thesis setup to use the reed thesis document class.

Table of Contents

List of Tables

List of Figures

Abstract

The preface pretty much says it all.

Second paragraph of abstract starts here.

Dedication

You can have a dedication here if you wish.

Introduction

Welcome to the *R Markdown* thesis template. This template is based on (and in many places copied directly from) the LaTeX template, but hopefully it will provide a nicer interface for those that have never used TeX or LaTeX before. Using *R Markdown* will also allow you to easily keep track of your analyses in **R** chunks of code, with the resulting plots and output included as well. The hope is this *R Markdown* template gets you in the habit of doing reproducible research, which benefits you long-term as a researcher, but also will greatly help anyone that is trying to reproduce or build onto your results down the road.

Hopefully, you won't have much of a learning period to go through and you will reap the benefits of a nicely formatted thesis. The use of LaTeX in combination with *Markdown* is more consistent than the output of a word processor, much less prone to corruption or crashing, and the resulting file is smaller than a Word file. While you may have never had problems using Word in the past, your thesis is likely going to be about twice as large and complex as anything you've written before, taxing Word's capabilities. After working with *Markdown* and **R** together for a few weeks, we are confident this will be your reporting style of choice going forward.

Why use it?

R Markdown creates a simple and straightforward way to interface with the beauty of LaTeX. Packages have been written in **R** to work directly with LaTeX to produce nicely formatting tables and paragraphs. In addition to creating a user friendly interface to LaTeX, *R Markdown* also allows you to read in your data, to analyze it and to visualize it using **R** functions, and also to provide the documentation and commentary on the results of your project. Further, it allows for **R** results to be passed inline to the commentary of your results. You'll see more on this later.

Who should use it?

Anyone who needs to use data analysis, math, tables, a lot of figures, complex cross-references, or who just cares about the final appearance of their document should use *R Markdown*. Of particular use should be anyone in the sciences, but the user-friendly nature of *Markdown* and its ability to keep track of and easily include figures, automatically generate a table of contents, index, references, table of figures, etc. should make it of great benefit to nearly anyone writing a thesis project.

0.1 Trees and Random Forests

0.1.1 Trees

Decision trees may be familiar to many with a background in the social or medical sciences as convenient ways to represent data and can assist in decision making. Morgan and Sonquist (1963) derived a way for constructing trees motivated by the specific feature space of data collected from interviews and surveys. Unlike, say agricultural data which involves mostly numerical variables like rainfall, the data collected from interviews is mostly categorical. On top of this issue, the datasets Morgan and Sonquist dealt with had few participants, n, and much data collected on them, p. To continue with their list of difficulties, there was reason to believe that there were lurking errors in the variables that would be hard identify and quantify. Lastly, many of the predictors were correlated and Morgan and Sonquist doubted that the additive assumptions of many models would be appropriate for this data. Morgan and Sonquist noted that while many statistical methods would have a difficulty accurately parsing this data, a clever researcher with quite a lot of time could create a suitable model simply by grouping values in the feature space and predicting that the response corresponding to these values would be the mean of the observed responses given the grouped conditions. Their formalization of this procedure in terms of "decision rules" laid the ground work for future research on decision trees.

Later researchers proposed new methods for creating trees that improved upon the Morgan and Sonquist model. Leo Breiman et al 1984 proposed an algorithm called CART, *classification and regression trees*, that would allow trees to be fit on various types of data. An alternative to this method is conditional inference trees. Torsten Hothorn, Kurt Hornik, 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 effect 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.

There is a limit to the predictive capabilities of a single tree as they suffer from high variance. To alleviate this, random forests are often used instead. They function by enlisting the help of many trees, and then by aggregating the responses over all of them but with a subtle trick that ensures the trees will be independent of each other. At each split only m variables are considered as possible candidates.

0.2 What We Mean When We Talk About Inference

0.2.1 Inferential vs Descriptive Statistics

A note should be made of the difference between inferential and descriptive statistics. This paper's aim is to describe a process of making inferential claims using

random forests, not descriptive ones. 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 at hand.

—Frequentist vs Bayesian—

—There is some debate about interpreting inferential statistics. On one hand, we have the Bayesian model—

Need a better way to discuss inference than Bayes/frequentist

0.3   Permutations and Populations

As stated in the introduction of the **Chronical 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 et al, 2014).

The permutation family of methods, on the other hand, only assumes that the observed result was caused by experimental variability. The test statistics is first calculated for the observed data, then the data is permuted a number of times. The statistic is calculated after each permutation to dervive a distribution of possible values. Then the original test statistic is tested against this distribution. If it is exceptionally rare, then there is evidence that our observation was not simply experimental variability.

0.4   Inference on Random Forests

0.4.1   The Problem

Random forests create models with great predictive-, but poor inferential capabilities. After Morgan and Sonquist initial development of decision trees, they quickly moved to the domain of machine learning and away from statistics, thus, researchers focused on bettering predictions and improving run times and less on the statistics behind them. Inferential statistics with random forests is usually treated as a variable selection problem, and 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 just, if not more, important as the predictions. There are several means of performing descriptive statistics with random forests that could be interpreted incorrectly as attempting to answer this, namely base variable importance, but without a statistically backed method for performing variable importance, the use of random forest is limited to prediction-only settings.

0.4.2 Proposed solutions to this problem

Statisticians Breiman and Cutler proposed a method of permuted variable importance 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:

$$PV^t(x_j) = \frac{\sum_{i \in |B|} y - \hat{y}^t}{|B|} - \frac{\sum_{i \in |*B|} y - \hat{*y}^t}{|*B|}$$

Where B is the matrix representing the feature space, $|B|$ is the number of observations, $*B$ is the matrix of predictors but with X_j permuted, $\hat{y}$ is the predicted outcome, and $\hat{*y}^t$ is the predicted outcomes after variable X_j has been permuted. This value is averaged over all the trees. It's 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.

Creating a permutation-based method is certainly an attractive solution to our problem. One, it allows us to estimate the distribution of variable importance and generate a Z score under the null hypothesis that $PV = 0$.

$$PV(x_j) = \frac{\sum_1^n treePV^t(x_j)}{\frac{\hat{\sigma}}{\sqrt{ntree}}}$$

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**. One, 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. Secondly, the null hypothesis under Breiman and Cutler's strategy is that the variable importance V for any variable X_j is not equal to zero given Y, the response. Because random forests are most often used in situations with multicolinearity that would make other methods like the linear model difficult, Strobl argues that any variable importance measure worth its salt should not be mislead 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 address these issues. Strobl et al propose restructuring the Breiman and Cutler algorithm to account for conditional dependence among the predictors. Their algorithm looks like this:

1. Fit a random forest to the model, R_0, and calculate base variable importance for each variable V
2. For every predictor $X_j \in X_1, ..., X_n$:

- 2a. Conditionally permute X_j given the splits found in R_0
- 2b. Fit a new random forest R_j with the permuted data
- 2c. Calculate a new variable importance $\hat{V}_j$

3. For every variable $X_1, ..., X_n$,

$$CV(X_j) = \hat{V}_j - V_j$$

The null hypothesis is that $CV(X_j) = 0$ given the predictor Y *and all other predictors* $X_1, ..X_n$. This accounts for interactions between X_j and the other predictors. Using the simulated data from the previous example, here's an implementation of the algorithm outlined here as it is in the `party` package.

This paper aims to provide a response to this method. One the conditional permutation algorithm is notoriously slow with any dataset of a size that is appropriate for a random forest. Two, the partitions are made from the random forest corresponding to the formula of Y $X_1, ..., X_n$ instead of a model of X_j $X_1, ..., X_n$.

Chapter 1

Simulations and Comparisons

In 1984, Breiman et al introduces a revolutionary new algorithm for trees. **Need to acquire** *Classification and Regression Trees* **to make sure the method discused in MASS is the same that Breiman uses/is used in** `randomForest`

Tree Algorithm CART?

Begin by considering the entire feature space $X_1, ..., X_n$. Then:

1. Consider every possible pair of partitions of this feature space, P_1, P_2, so that if $X_1 = x_1, X_2 = x_2, ..., X_n = x_n$ where $x_1, ..., x_n \in P_1$ then our prediction is the mean value of y given $x_1, .., x_n \in P_1$.

2. Choose the partitions that minimize RSS

3. For each new partition, repeat steps 1 and 2 until some stopping condition is reached.

CI trees 1. For case weights w test the global null hypothesis of independence between any of the m covariates and the response. Stop if this hypothesis cannot be rejected. Otherwise select the j_{th} covariate Xj with strongest association to Y.

2. Choose a set $A \subset X_j$ in order to split X_j into two disjoint sets A and X_j A. The case weights w_{left} and w_{right} determine the two subgroups with $w_{left,i} = w_i I(X_{j \cdot i} \in A)$ and $w_{right,i} = w_i I(X_{ji} \in A)$ for all $i = 1, ..., n$ ($I(\mathring{u})$ denotes the indicator function).

3. Recursively repeat steps 1 and 2 with modified case weights $w_l eft$ and $w_r ight$, respectively.

from `https://eeecon.uibk.ac.at/~zeileis/papers/Hothorn+Hornik+Zeileis-2006.pdf`

After step 1 is completed, any goodness of fit method can be used to generate the split and choose the set A. Note that in this method the splitting is done separately from the variable selection.

Chapter 2

Permuatations Tests Theory and Application to Conditional Variable Importance

Chapter 3

Implementation of Our Method

Conclusion

If we don't want Conclusion to have a chapter number next to it, we can add the `{.unnumbered}` attribute. This has an unintended consequence of the sections being labeled as 3.6 for example though instead of 4.1. The LaTeX commands immediately following the Conclusion declaration get things back on track.

More info

And here's some other random info: the first paragraph after a chapter title or section head *shouldn't be* indented, because indents are to tell the reader that you're starting a new paragraph. Since that's obvious after a chapter or section title, proper typesetting doesn't add an indent there.

Appendix A

The First Appendix

This first appendix includes all of the R chunks of code that were hidden throughout the document (using the `include = FALSE` chunk tag) to help with readibility and/or setup.

In the main Rmd file:

```r
# This chunk ensures that the reedtemplates package is
# installed and loaded. This reedtemplates package includes
# the template files for the thesis and also two functions
# used for labeling and referencing
if(!require(devtools))
  install.packages("devtools", repos = "http://cran.rstudio.com")
if(!require(reedtemplates)){
  library(devtools)
  devtools::install_github("ismayc/reedtemplates")
}
library(reedtemplates)
```

In :

```r
# This chunk ensures that the reedtemplates package is
# installed and loaded. This reedtemplates package includes
# the template files for the thesis and also two functions
# used for labeling and referencing
if(!require(devtools))
  install.packages("devtools", repos = "http://cran.rstudio.com")
if(!require(dplyr))
    install.packages("dplyr", repos = "http://cran.rstudio.com")
if(!require(ggplot2))
    install.packages("ggplot2", repos = "http://cran.rstudio.com")
```

```r
if(!require(reedtemplates)){
  library(devtools)
  devtools::install_github("ismayc/reedtemplates")
  }
library(reedtemplates)
#flights <- read.csv("data/flights.csv")
```

Appendix B

The Second Appendix, for Fun

References

Angel, E. (2000). *Interactive computer graphics : A top-down approach with opengl.* Boston, MA: Addison Wesley Longman.

Angel, E. (2001a). *Batch-file computer graphics : A bottom-up approach with quicktime.* Boston, MA: Wesley Addison Longman.

Angel, E. (2001b). *Test second book by angel.* Boston, MA: Wesley Addison Longman.