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Big Data and Better Decisions
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Module 12: Tree – Based Methods

1. INTRODUCTION

Tree based methods involve stratifying or segmenting the predictor space into a number of simple regions. In order to make a prediction for a given observation, we typically use the mean or the mode of the training observations in the region to which it belongs. Since the set of splitting rules used to segment the predictor space can be summarized in a tree, these types of approaches are known as decision tree methods.

In addition to basic decision trees, we will also introduce random forests and boosting in this module. Each of these approaches involves producing multiple trees which are then combined to yield a single consensus prediction. We will see that combining a large number of trees can often result in dramatic improvements in prediction accuracy, at the expense of some loss in interpretation.

2. SIMPLE CLASSIFICATION TREES

Decision trees can be applied to both regression and classification problems. However, this module will focus on the slightly simpler classification tree. See ISL for more detail on regression trees. To illustrate the process of building a classification tree, we will consider the case where we have a binary outcome with two predictor variables X1 and X2. However, the method can be applied to any number of predictor variables.

Roughly speaking, there are two steps to building the tree.

1. We divide the set of possible values for X1 and X2 into J distinct and non-overlapping regions, R1, R2,...,RJ .
2. For every observation that falls into a given region, we make the same prediction, which is 1 if more than 50% of the outcome values for the training observations in that region are equal to 1, and 0 otherwise.

But how do we construct the regions R1,...,RJ ? In theory, the regions could have any shape. However, we choose to divide the predictor space into boxes for simplicity and for ease of interpretation of the resulting predictive model. This means that the groups will be described by partitions of X1 and X2. The goal is to find boxes that minimize the number of incorrect predictions.

Unfortunately, it is computationally infeasible to consider every possible partition of our predictor variables (it might be feasible for two variables, but quickly gets too complicated if we add more). For

this reason, we take a top-down, greedy approach that is known as recursive binary splitting. The recursive binary splitting approach is top-down because it begins at the top of the tree (at which point all observations belong to a single region) and then successively splits the predictor space; each split is indicated via two new branches further down on the tree. It is greedy because at each step of the tree-building process, the best split is made at that particular step, rather than looking ahead and picking a split that will lead to a better tree in some future step.

So, we consider X1 and X2 and all possible "cuts" of each variable. If our variables were age and gender, gender would have one cutpoint, and age would have a number of cutpoints equal to the number of ages in the dataset. Then we pick the variable and cutpoint such that the resulting tree of two branches has the lowest number of incorrect predictions.

Next, we repeat the process, looking for the best predictor and cutpoint in order to split the data further so as to minimize the number of incorrect predictions in each of the resulting regions. However, this time, we split one of the two previously identified regions to get 3 regions. The process continues until a stopping criterion is reached; for instance, we may continue until no region contains more than five observations.

The process described above may produce good predictions on the training set, but is likely to overfit the data, leading to poor test set performance. We can "prune" the tree to prevent this issue. See ISL for further details on pruning.

We'll illustrate in R this with a dataset where observations are passengers on the Titanic. The dataset contains variables that give some information about each passenger such as class, gender, age and whether they survived the shipwreck. First, we'll load relevant dataset and packages. We'll also create a test and training dataset.

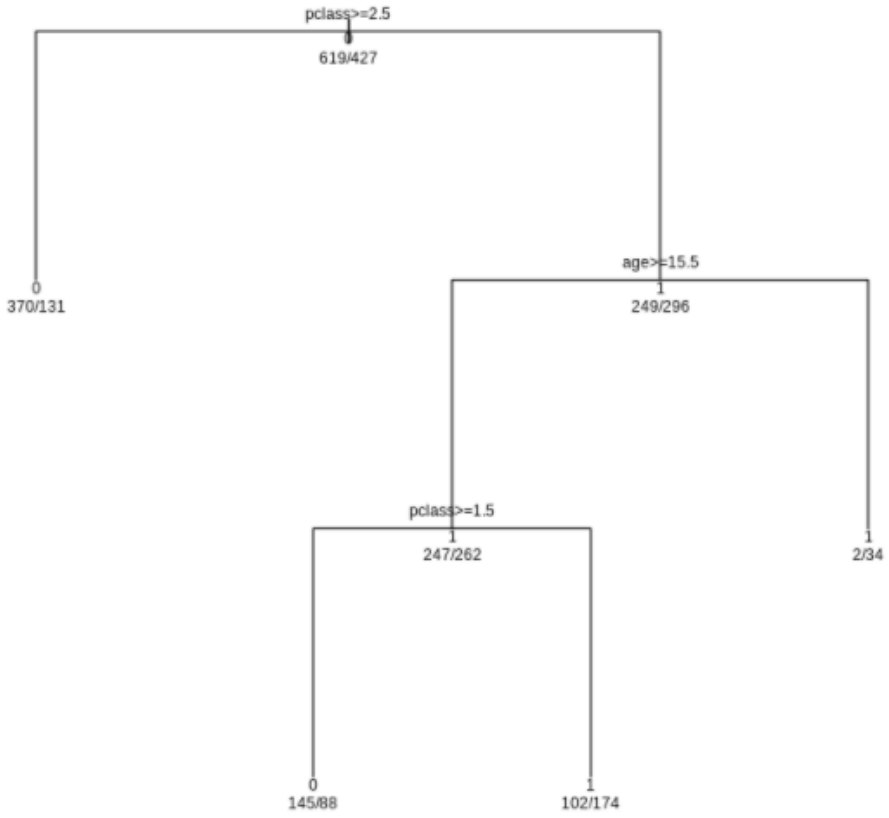
```
# Load required packages
# For the tree functions
require(rpart)
require(party)
# For Random Forest
require(randomForest)
# For Boosting
require(gbm)

# Read the data and remove observations with missing data
Titanic <- read.csv("Titanic.csv", header = TRUE)
# remove obs with missing data, and select a few predictors
Titanic <-
na.omit(Titanic[,c("survived","pclass","sex","age","sibsp")])
attach(Titanic)
names(Titanic)
dim(Titanic)

# for reproducibility
set.seed(1234)

# create train and test sets (~40% for training, ~60% for testing)
Titanic$randu <- runif(nrow(Titanic),0,1)
Titanic.train <- Titanic[Titanic$randu < .4,]
Titanic.test <- Titanic[Titanic$randu >= .4,]
```

Now we use the function rpart to create a simple tree using only the age and class variables. This automatically performs the recursive binary splitting process for us. Below, we see that it makes the correct prediction about 65% of the time in the test dataset. CP=0.05 is the pruning parameter. Typically we'd use cross validation to select the optimal pruning parameter, but we're keeping it simple here and just picking one. We find an error rate of around 35%

```
# Simple classification tree using rpart on training data
simp.tree <- rpart(as.factor(survived) ~ pclass + age, data =
Titanic.train, method="class", cp=.05)
# Fit model to test data and calculate MSE, which is just %
incorrect predictions
Titanic.test$pred<-predict(simp.tree, Titanic.test, type = c(
"class"))
Titanic.test$pred<-ifelse(Titanic.test$pred=="1", 1, 0)
mean((Titanic.test$pred-Titanic.test$survived)^2)
```

Next, we can fit the model to the full dataset and generate a picture of the actual tree. For the condition at each node, TRUE goes to the left, and FALSE to the right. The 0 or 1 at the bottom of the node is the prediction for that node, and the number below that is Survive=0/Survive=1.

```
# plot model on full dataset
simp.tree.full <- rpart(as.factor(survived) ~ pclass + age, data =
Titanic, method="class", cp=.05)
plot(simp.tree.full, uniform = TRUE) # plot tree
text(simp.tree.full, use.n = TRUE, all = TRUE, cex = 0.6, main =
"Titanic") # add labels to tree
```



3. RANDOM FORESTS

Random forests is a technique that uses multiple trees. A typical procedure uses the following steps:

1. Choose a bootstrap sample of the observations and start to grow a tree.
2. At each node of the tree, choose a random sample of the predictors to make the next decision. Do not prune the trees.
3. Repeat this process many times to grow a forest of trees.
4. In order to determine the classification of a new observation, have each tree make a classification and use a majority vote for the final prediction.

This method produces surprisingly good out-of-sample fits, particularly with highly nonlinear data. One defect of random forests is that they are a bit of a black box—they don't offer simple summaries of relationships in the data. As we have seen earlier, a single tree can offer some insight about how predictors interact. But a forest of a thousand trees cannot be easily interpreted. However, random forests can determine which variables are "important" in predictions in the sense of contributing the biggest improvements in prediction accuracy.

We'll illustrate this below using the titanic dataset again. R fits a random forest using a single command. We'll calculate the error rate again, this time using the confusion matrix. We find an overall error rate of 22.5%.

```
#### Random Forests #####
# It is important to set seed to for replicating results as there's a
lot of randomization that happens in Random Forests
set.seed(1234)

#Fit the training data
# nodesize is minimum size of terminal nodes
# mtry is number of variables randomly sampled as candidates at each
split
# ntree is the number of bootstrap samples
model.rf <- randomForest(as.factor(survived) ~ pclass + sex + age +
sibsp, data = Titanic.train, mtry = 4, nodesize = 30, ntree = 500)
#predict outcomes on the test data
pred.rf <- predict(model.rf, newdata = Titanic.test)
#compare actual and predicted outcomes
conf.rf <- table(pred.rf, Titanic.test$survived)
conf.rf
#calculate the error rate
(conf.rf[1,2]+conf.rf[2,1])/sum(conf.rf)
#total decrease in node impurities from splitting on the variable,
averaged over all trees
importance(model.rf)
```

4. BOOSTING

Boosting involves repeated estimation where misclassified observations are given increasing weight in each repetition. The final estimate is then a vote or an average estimate across the repeated estimates.

First, an initial tree is fit. Given that model, we fit a decision tree to the residuals. That is, we fit a tree using R= (1= misclassified positive, -1=misclassified negative), rather than the outcome Y , as the response. We then add this new decision tree into the fitted function in order to update the residuals. This process is repeated B times.

Boosting has three tuning parameters:

1. The number of trees B. Unlike bagging and random forests, boosting can overfit if B is too large, although this overfitting tends to occur slowly if at all. We use cross-validation to select B.
2. The shrinkage parameter λ, a small positive number. This controls the rate at which boosting learns. Typical values are 0.01 or 0.001, and the right choice can depend on the problem. Very small λ can require using a very large value of B in order to achieve good performance.
3. The number d of splits in each tree or the "interaction depth", controls the interaction order of the boosted model, since d splits can involve at most d variables. Typically, 1 or 2 is a good choice, and we can compare using the test error rate.

Below, we find an error rate of 20.9% implementing a boosting model on the titanic dataset in R.

```
### Boosting #####
model.boost <- gbm(survived ~ pclass + sex + age + sibsp,
                   data = Titanic.train,
                   distribution = "bernoulli",
                   n.trees = 10000,
                   shrinkage = 0.001,
                   interaction.depth = 1)

pred.boost <- predict(model.boost, newdata = Titanic.test, type
="response", n.trees=1000)
pred.boost <- ifelse(pred.boost >=0.5 , 1, 0)
conf.boost <- table(pred.boost, Titanic.test$survived)
conf.boost
(conf.boost[1,2]+conf.boost[2,1])/sum(conf.boost)
```

5. BIBLIOGRAPHY/FURTHER READING

1. Varian, Hal R. 2014. "Big Data: New Tricks for Econometrics." Journal of Economic Perspectives, 28(2): 3-28.
2. Gareth James, Daniela Witten, Trevor Hastie, and Robert Tibshirani (2013). An Introduction to Statistical Learning, Volume 112. Springer