## Statistics 452: Statistical Learning and Prediction

Chapter 8, Part 2: Bagging and Random Forests

Brad McNeney

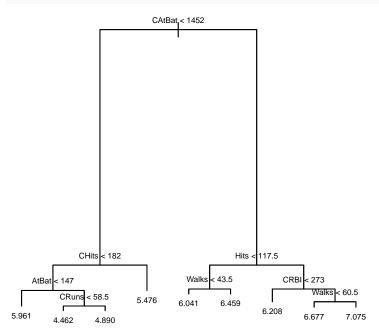
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#### Example: The Hitters Data Set

Example tree grown, but not pruned.

```
library(ISLR)
data(Hitters)
library(dplyr)
Hitters <- mutate(Hitters, 1Salary = log(Salary)) %>%
    select(-Salary) %>%
    na.omit()
library(tree)
t1 <- tree(1Salary ~ ., data=Hitters)</pre>
```

## plot(t1) text(t1,cex=.5)



#### Bootstrapping

▶ A bootstrap sample from *n* observations is obtained by drawing *n* observations, with replacement, from the sample

```
set.seed(543)
n < -6
x <- round(rnorm(n),1)
sort(x)
## [1] -1.0 -0.2 0.2 0.4 0.8 1.4
sort(sample(x,size=n,replace=TRUE)) # bootstrap sample 1,
## [1] -0.2 0.4 0.4 0.8 0.8 0.8
sort(sample(x,size=n,replace=TRUE)) # bootstrap sample 2
## [1] -1.0 -0.2 0.2 0.2 0.2 0.2
sort(sample(x,size=n,replace=TRUE)) # bootstrap sample 3
## [1] -0.2 -0.2 -0.2 0.2 0.4 0.8
```

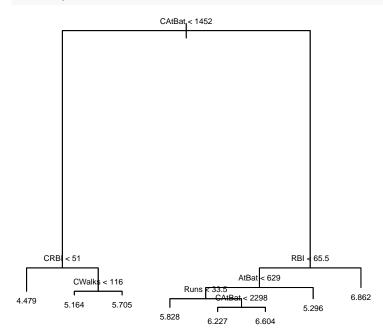
#### **Empirical Distribution**

- The data-generating process in our example is a normal distribution.
- ► The empirical distribution of our sample is the distribution under which each sampled value is equally likely.
- Resampling amounts to sampling from the empirical distribution.
- ▶ If empirical close to data-generating distribution, resampled samples are like new samples from the data-generating distribution.

## Example: Tree from a Bootstrap Sample

```
# Use sample_n() from dplyr
n <- nrow(Hitters)
bHitters <- sample_n(Hitters,size=n,replace=TRUE)
t1b <- tree(lSalary ~ .,data=bHitters)</pre>
```

```
plot(t1b)
text(t1b,cex=.5)
```



## Bootstrap Aggregation (Bagging)

- For a general statistical learning method that provides an estimate,  $\hat{f}(x)$  of the model f(x), we can aggregate over estimates fit to bootstrap samples.
- ▶ If  $\hat{f}^b(x)$  is the fitted model from the bth bootstrap sample, the aggregate estimator is

$$\hat{f}_{avg}(x) = \frac{1}{B} \sum_{b=1}^{B} \hat{f}^b(x),$$

where B is the number of bootstrap samples.

- Bagging has been found to be useful for improving predictions from decision trees.
  - ▶ Grow each tree "deep" and don't prune.
  - Average predictions over trees.

#### Bias-Variance Tradeoff

- ▶ The deeply-grown trees have high variance, but low bias.
- Averaging many deep trees is an attempt to reduce the variance.
- ► However, if trees are highly correlated (e.g., similar first few splits) then averaging does not reduce variance.
  - ▶ Return to this point when we discuss random forests.

## Bagging for Classification

- ▶ When the outcome *Y* is categorical, one approach to the aggregate prediction of category is the "majority vote":
  - Record the predicted class from each tree (each bootstrap sample) and take the most common prediction as the aggregate prediction.

# Estimating Test Error with Out-of-Bag (OOB) Observations

- ► On average about 2/3 are and 1/3 of observations are not resampled
  - ▶ See small bootstrap samples of size 6 above.
- ► Those not resampled are called out-of-bag (OOB)
- ▶ Regression trees: The OOB prediction for the *i*th observation is the average of its predicted values from trees grown on boostrap samples that did not include *i*.
  - ► The OOB MSE is the average squared error between observed values and their OOB predictions.
- ▶ Classification trees: The OOB prediction for the *i*th observation is the majority vote from trees grown on bootstrap samples that did not include *i*.
  - ► The OOB classification error is the proportion of misclassified OOB predictions.
- ▶ OOB errors are valid because the predictions use only trees not fit to the corresponding observation.

## Variable Importance

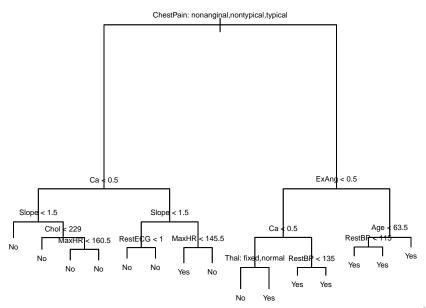
- ▶ There isn't one tree to interpret now.
- ▶ Need an overall measure of the importance of a variable.
- ► For a single tree, a variable's importance can be measured by the amount that the node homogeneity (RSS for regression, Gini for classification) is decreased by splitting on the variable.
  - ► Homogeneity of tree including variable minus homogeneity if variable was not available to split on.

#### Example: Heart Data

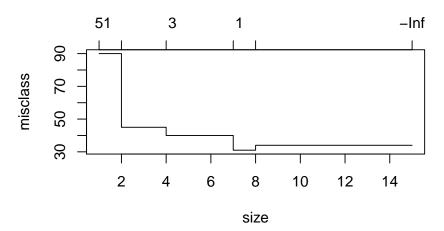
```
uu <- url("http://www-bcf.usc.edu/~gareth/ISL/Heart.csv")
Heart <- read.csv(uu,row.names=1)
Heart <- na.omit(Heart)
dim(Heart) # Train on 2/3, test on 1/3

## [1] 297 14

set.seed(1)
train <- sample(1:nrow(Heart),size=2*nrow(Heart)/3,replace=FALSE)
t1 <- tree(AHD ~ ., data=Heart,subset=train)</pre>
```



cv.t1 <- cv.tree(t1,FUN=prune.misclass) # use class'n err for CV
plot(cv.t1) # Suggest size 7</pre>

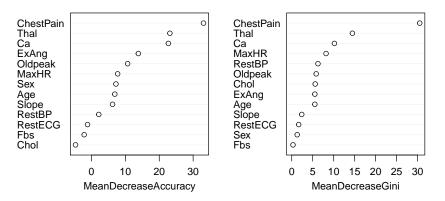


```
t1.best <- prune.tree(t1,best=7)</pre>
summary(t1.best)
##
## Classification tree:
## snip.tree(tree = t1, nodes = c(13L, 7L, 10L, 11L, 4L))
## Variables actually used in tree construction:
## [1] "ChestPain" "Ca"
                              "Slope"
                                           "ExAng"
                                                        "Thal"
## Number of terminal nodes: 7
## Residual mean deviance: 0.6276 = 119.9 / 191
## Misclassification error rate: 0.101 = 20 / 198
hpred <- predict(t1.best,newdata=Heart[-train,],type="class")
tt <- table(hpred, Heart[-train,]$AHD)</pre>
t.t.
##
## hpred No Yes
    No 42 15
##
## Yes 10 32
sum(tt[row(tt) != col(tt)])/sum(tt)
## [1] 0.2525253
```

#### Bagging on Heart Data

```
##
## Call:
   randomForest(formula = AHD ~ ., data = Heart, mtry = 13, importance = TRUE,
##
                 Type of random forest: classification
##
                       Number of trees: 500
## No. of variables tried at each split: 13
##
##
           OOB estimate of error rate: 15.66%
## Confusion matrix:
      No Yes class.error
##
## No 95 13 0.1203704
## Yes 18 72 0.2000000
```

#### bag.heart



► See help("importance") for a definition of accuracy.

## Classification Error for Bagged Trees

```
bag.hpred <- predict(bag.heart,newdata=Heart[-train,],type="class")</pre>
tt <- table(bag.hpred, Heart[-train,]$AHD)</pre>
tt
##
## bag.hpred No Yes
##
         No 47 17
         Yes 5 30
##
sum(tt[row(tt) != col(tt)])/sum(tt)
## [1] 0.222222
```

#### Random Forests

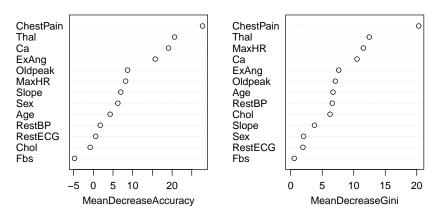
- Bootstrap datasets may yield correlated trees.
  - ► E.G., if we have one or two strong predictors, all trees might share the first few splits.
- Random forests avoid this by restricing the predictors to a random subset.
  - ▶ New subset at each split.
  - ▶ Subset size? Text: "... typically we choose  $m \approx \sqrt{p}$ ".

#### Random Forests on Heart Data

```
rf.heart <- randomForest(AHD ~ ., data=Heart, subset=train,
                          mtry=sqrt(13),importance=TRUE) #m<p for RF
rf.heart
##
## Call:
   randomForest(formula = AHD ~ ., data = Heart, mtry = sqrt(13),
                                                                        importa
##
                  Type of random forest: classification
                        Number of trees: 500
##
## No. of variables tried at each split: 4
##
           00B estimate of error rate: 13.64%
##
## Confusion matrix:
      No Yes class.error
##
## No 95 13 0.1203704
## Yes 14 76 0.1555556
```

```
rf.hpred <- predict(rf.heart,newdata=Heart[-train,],type="class")</pre>
tt <- table(rf.hpred,Heart[-train,]$AHD)</pre>
tt
##
## rf.hpred No Yes
        No 48 17
##
##
       Yes 4 30
sum(tt[row(tt) != col(tt)])/sum(tt)
## [1] 0.2121212
```

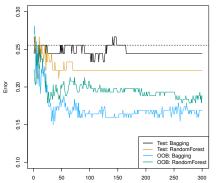
#### rf.heart



Chest pain still most important, but not by such a wide margin.

#### Number of Trees

- Bagging and random forests are not very sensitive to the number of trees B.
- ► Can try different values and make sure *B* large enough that error has stabilized.



► Text, Fig. 8.8. Not sure what Test error is based on, but assume it is from a hold-out validation sample. OOB error is lower than test error; maybe trees are based on more data (no hold-out)?