## **Exploratory Data Mining via Search Strategies Lab #3**

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#### **Outline**

This script will go over Decision Trees and generalizations in R.

Resources:

Basic intro to Decision Trees: http://www.statmethods.net/advstats/cart.html Full list of data mining packages in R:

http://cran.r-project.org/web/views/MachineLearning.html Two packages will be used and their caret equivalents:

- rpart (tree accomplishes very similar thing):http: //cran.r-project.org/web/packages/rpart/vignettes/longintro.pdf
- party:

http://cran.r-project.org/web/packages/party/vignettes/party.pdf

In caret, method =

- "rpart" tuning = cp (complexity parameter)
- ▶ "rpart2" tuning = maxdepth
- "rpartCost" tuning = cp and cost
- "ctree" tuning = mincriterion (p value thresholds)
- ▶ "ctree2" tuning = maxdepth

### Lets load the main packages

```
library(caret)
library(rpart)
library(pROC)
library(randomForest)
library(gbm)
library(ISLR)
library(party)
library(MASS) # for boston data
data(Boston)
```

# Regression

## Regression (continous outcome)

Use rpart first with the Boston data use regression first – predicting median value of homes

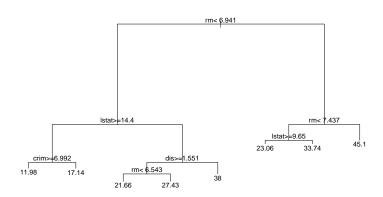
```
#str(Boston)
# lets get a baseline with linear regression
lm.Boston <- lm(medv ~., data=Boston)
#summary(lm.Boston)</pre>
```

We do pretty well with linear regression R-squared of .74

### **CART**

How about if we just blindly apply Decision Trees

```
rpart.Boston <- rpart(medv ~., data=Boston)
#summary(rpart.Boston)
plot(rpart.Boston); text(rpart.Boston)</pre>
```



### **CART Continued**

```
pred1 <- predict(rpart.Boston)</pre>
cor(pred1,Boston$medv)**2
## [1] 0.8075721
Doing really well – Rsquared = 0.81
# this can be hard to interpret, so I like to look at a different output
rpart.Boston
## n = 506
##
## node), split, n, deviance, yval
##
         * denotes terminal node
##
##
    1) root 506 42716.3000 22.53281
##
      2) rm< 6.941 430 17317.3200 19.93372
        4) lstat>=14.4 175 3373.2510 14.95600
##
          8) crim>=6.99237 74 1085.9050 11.97838 *
##
          9) crim< 6.99237 101 1150.5370 17.13762 *
##
        5) lstat< 14.4 255 6632.2170 23.34980
##
         10) dis>=1.5511 248 3658.3930 22.93629
##
           20) rm< 6.543 193 1589.8140 21.65648 *
##
##
           21) rm>=6.543 55 643.1691 27.42727 *
##
         11) dis< 1.5511 7 1429.0200 38.00000 *
      3) rm>=6.941 76 6059.4190 37.23816
##
                                                  4□ → 4□ → 4 □ → 1 □ → 9 Q (~)
        6) mm / 7 /27 /6 1000 6100 20 1120/
```

### **Lasso Regression**

##

## [1,] 0.7403028

What if we tried regularized (penalized) regression instead? Note: for glmnet, both the x's and y have to be in separate matrices - and all class = numeric - don't worry about response, doesn't have to be factor for logistic —— just specify "binomial" v.B <- Boston\$medv x.B <- sapply(Boston[,-14],as.numeric)</pre> # alpha =1 for lasso, 0 for ridge library(glmnet) cv <- cv.glmnet(x.B,y.B,alpha=1)</pre> lasso.reg <- glmnet(x.B,y.B,alpha=1,family="gaussian",lambda=cv\$lambda.min) lasso.resp <- predict(lasso.reg,newx=x.B)</pre> cor(y.B,lasso.resp)\*\*2

Taking into account cross-validation, we do worse compared to linear regression with no tuning.

#### **CART Plots**

So the plot for rpart didn'tcome out that well. Good news, there are better options for plotting.

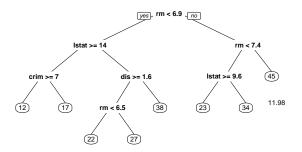
http://blog.revolutionanalytics.com/2013/06/plotting-classification-and-regression-trees-with-plotrpart.html Let's load some new packages:

```
library(rattle)
library(rpart.plot)
library(RColorBrewer)
library(partykit)
```

Note: rattle is package that uses a GUI (think SPSS) for data mining applications check out book: http:

//www.amazon.com/Data-Mining-Rattle-Excavating-Knowledge/dp/1441998896 Anyways, lets try some new, prettier plots:

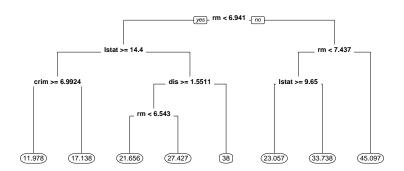
```
# prp(); from rpart.plot
prp(rpart.Boston);text(rpart.Boston)
```



### **CART Plotting Continued**

Note, prp() offers many additional capabilities for tweaking the plot For instance:

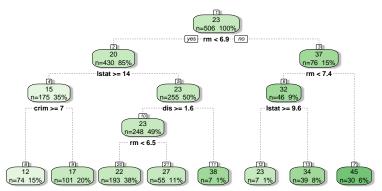
```
# ?prp
prp(rpart.Boston,varlen=10,digits=5,fallen.leaves=T)
```



### **CART Plotting Continued**

#### Probably my favorite, fancyRpartPlot()

```
#fancyRpartPlot(); from rattle
fancyRpartPlot(rpart.Boston)
```



Rattle 2016-Aug-12 10:13:47 RJacobucci

#### **Conditional Inference Trees**

So what about with conditional inference trees?

What if we want a smaller tree? This can be accomplished a number of ways. We can prespecify the maxdepth, the minimum number of people per node, as well as making more restrictive splitting criterion.

Example of prespecifying the depth with ctree()

```
ctree.Boston <- ctree(medv ~., data=Boston)
#plot(ctree.Boston) # too big of a tree
pred2 <- predict(ctree.Boston)
cor(pred2,Boston$medv)**2</pre>
```

## [1] 0.8746338

We do better than rpart, Rsquared = 0.87

#### **Conditional Inference Trees Continued**

Biggest difference between ctree() and rpart() is that ctree() does not demonstrate bias with respect to the number of response options, and supposedly had less of a propensity to overfit than rpart().

Note: the models are not optimizing based on Rsquared, most likely MSE

So what do we think now? Are we happy with results? Remember, decision trees are generally quite robust, so it may not be necessary to check assumptions. – See Table  $10.1\ \text{ESL}$ 

But what about generalizability?

Although not as serious as with SVM for instance, Decision Trees have a propensity to overfit, meaning the tree structure won't generalize well

So let's try just creating a simple Training and Test datasets

```
train = sample(dim(Boston)[1], dim(Boston)[1]/2) # half of sample
Boston.train = Boston[train, ]
Boston.test = Boston[-train, ]
```

### **Linear Regression with CV**

```
lm.train <- lm(medv ~., data=Boston.train)
pred.lmTest <- predict(lm.train,Boston.test)
cor(pred.lmTest,Boston.test$medv)**2</pre>
```

```
## [1] 0.7068753
```

Note: we are taking our Im object trained on the train dataset, and using these fixed coefficients to predict values on the test dataset.

In SEM, this is referred to as a tight replication strategy No difference in using a test dataset – both Rsq are 0.74

How about with rpart?

#### **CART CV**

```
rpart.train <- rpart(medv ~., data=Boston.train)
pred.rpartTest <- predict(rpart.train,Boston.test)
cor(pred.rpartTest,Boston.test$medv)**2</pre>
```

## [1] 0.7299716

Not as good – drops from 0.81 to 0.76 – still better than Im()

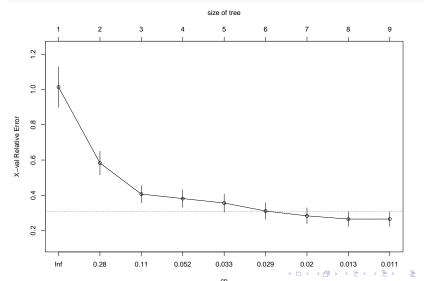
But with rpart, it is common to prune trees back. What if we try this, is there less of a drop in  $\mathbb{R}^2$ ?

Note: rpart automatically does internal CV, varying the complexity paramter (cp). If you use the tree package instead, you will have to use cv.tree()

### **CART Pruning**

With plotcp() we are going to choose the error within 1 SE of the lowest cross-validated error. This will be used to prune

plotcp(rpart.train)



### **CART Pruning Continued**

## 7 0.013260

## 8 0.012100

## 9 0.010000

```
printcp(rpart.train)
##
## Regression tree:
## rpart(formula = medv ~ ., data = Boston.train)
##
## Variables actually used in tree construction:
  [1] age crim lstat rm
                             tax
##
## Root node error: 24098/253 = 95.251
##
## n = 253
##
          CP nsplit rel error xerror xstd
##
## 1 0.491102
                 0 1.00000 1.01420 0.115293
## 2 0.160787
                 1 0.50890 0.58289 0.066792
## 3 0.072844
                 2 0.34811 0.40677 0.049227
## 4 0.036758
                 3 0.27527 0.38152 0.049815
## 5 0.029632
                     0.23851 0.35634 0.051564
## 6 0.029057
                 5
                     0.20888 0.31094 0.046913
```

6

0.17982 0.28364 0.045076

0.16656 0.26523 0.041999

0.15446 0.26539 0.041833

## **Rpart Error Explained**

rel error – The error on the whole sample (lower the better) xerror – Error on the cross-validation folds xstd – variability in error across CV folds

## **CART Pruning Continued**

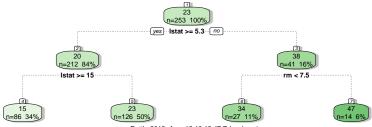
```
# rsq.rpart(rpart.train) ## another way to get cp plots
prune.Bos <- prune(rpart.train,0.053)

pred.prune <- predict(prune.Bos,Boston.test)
cor(pred.prune,Boston.test$medv)</pre>
```

## [1] 0.7734145

Plot Pruned Tree

```
#plot(prune.Bos); text(prune.Bos)
fancyRpartPlot(prune.Bos)
```



#### **CTree CV**

```
ctree.train <- ctree(medv ~., data=Boston.train)
#plot(ctree.train) # huge tree
pred.ctreeTest <- predict(ctree.train,Boston.test)
cor(pred.ctreeTest,Boston.test$medv)**2</pre>
```

## [1] 0.6470982

It is worth noting how much more of an effect there was for using a test dataset with the tree methods as compared to lm(), this is pretty typical, and much more important with more "flexible" methods such as random forests, gbm, svm etc...

# Classification

#### Classification

#### Two Biggest Things To Remember:

- 1. Make sure functions outcome variable is categorical; as.factor(outcome)
- 2. Using predict() changes. Variable across packages

As a baseline, we will use logistic regression.

```
library(ISLR)
data(Default)
#head(Default)
str(Default)
```

```
## 'data.frame': 10000 obs. of 4 variables:
## $ default: Factor w/ 2 levels "No","Yes": 1 1 1 1 1 1 1 1 1 1 1 1 1 ...
## $ student: Factor w/ 2 levels "No","Yes": 1 2 1 1 1 2 1 2 1 1 ...
## $ balance: num 730 817 1074 529 786 ...
## $ income : num 44362 12106 31767 35704 38463 ...
```

My favorite function in R is str(), as it gives the class of each variable and other summary characteristics. Most important thing to note is that the "default" variable is already coded as a factor variable, meaning that R now knows it is categorical, and will change the cost function (thus estimator) accordingly. This is really important because rpart, random Forest and other packages do not automatically detect whether it is a regression or classification problem. If you don't change the outcome variable to its proper class, you could get a suboptimal answer (use the wrong estimator i.e. regression instead of logistic regression)

## Logistic Regression Now let's do logistic regression ( D ) ( D ) ( D ) ( D )

#### **ROC Curves**

good intro to using ROC:

https://ccrma.stanford.edu/workshops/mir2009/references/ROCintro.pdf These plots are a balanace of sensitivity and specificity. Ideally the curve gets as close as possible to the upper left corner.

To get this plot, we need to get our predictions from our logistic model.

```
glm.probs=predict(lr.out,type="response")
#glm.pred00=ifelse(glm.probs>0.5,1,0)

rocCurve <- roc(Default$default,glm.probs)
pROC::auc(rocCurve)</pre>
```

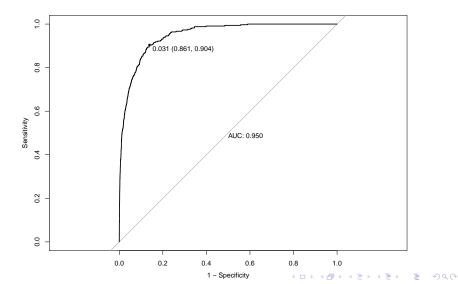
## Area under the curve: 0.9496

```
pROC::ci(rocCurve)
```

## 95% CI: 0.9402-0.959 (DeLong)

### Plot ROC Curve

```
# quartz()
plot(rocCurve, legacy.axes = TRUE,print.thres=T,print.auc=T)
```



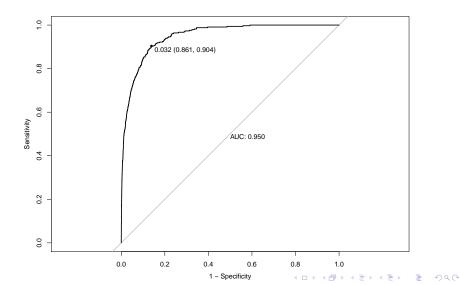
### **Lasso Logistic Regression**

How about lasso logistic regression?

```
library(glmnet)
yy = as.numeric(Default$default)
xx = sapply(Default[,2:4],as.numeric)
lasso.out <- cv.glmnet(xx,yy,family="binomial",alpha=1,nfolds=10) #alpha=1 ==
# find best lambda
11 <- lasso.out$lambda.min
lasso.probs <- predict(lasso.out,newx=xx,s=l1,type="response")</pre>
Results from lasso using CV
rocCurve.lasso <- roc(Default$default,lasso.probs)</pre>
pROC::auc(rocCurve.lasso)
## Area under the curve: 0.9495
pROC::ci(rocCurve.lasso)
## 95% CI: 0.9401-0.959 (DeLong)
```

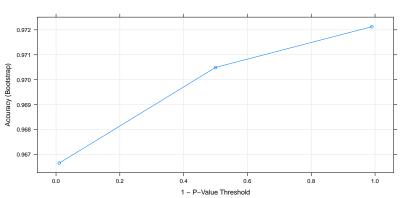
### **Plot ROC**

```
# quartz()
plot(rocCurve.lasso, legacy.axes = TRUE,print.thres=T,print.auc=T)
```

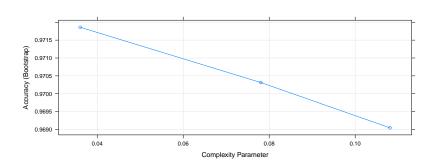


### **Using Decision Trees for Classification**

Instead of demonstrating how to use <code>rpart()</code> or <code>ctree()</code>, I prefer to use the train() from caret. This makes it much easier to test out multiple different methods, as well as automatically vary the tuning parameters such as depth, complexity etc.. <code>train()</code> for <code>ctree</code>



## train() for rpart



## train() Continued

In train() and through trainControl() you can see that it automatically varies different tuning parameters (see caret documentation for the different options for each method), while defaulting to bootstrap estimation to test out each. This is a great way to prevent overfitting.

In examining both plots, it seems as both methods do comparably well, while also they both have different tuning parameters (X-axis). Based on these plots, I would increase the number of values for the tuning parameters, as the accuracy did not reach a maximum necessarily outside of the tails. (tuneLength = 3 is default)

### using a confusion matrix

```
train.class <- predict(train.rpart,Default,type="raw")</pre>
confusionMatrix(train.class,Default$default)
## Confusion Matrix and Statistics
##
       Reference
##
## Prediction No Yes
##
         No 9639 243
                28 90
##
         Yes
##
##
                  Accuracy : 0.9729
                    95% CI: (0.9695, 0.976)
##
      No Information Rate: 0.9667
##
      P-Value [Acc > NIR] : 0.0002082
##
##
##
                     Kappa: 0.3885
##
    Monemar's Test P-Value : < 2.2e-16
##
##
               Sensitivity: 0.9971
##
               Specificity: 0.2703
            Pos Pred Value: 0.9754
##
##
            Neg Pred Value: 0.7627
##
                Prevalence: 0.9667
##
            Detection Rate: 0.9639
      Detection Prevalence: 0.9882
##
```

4 D > 4 B > 4 B > 4 B > 9 Q P

## Confusion matrix terminology

$$\mathsf{Accuracy} - \mathsf{TP} + \mathsf{TN}/\mathsf{\ total}$$

Specificity - TN/ Actual Negative

Sensitivity - TP/ Actual Positive

https://en.wikipedia.org/wiki/Confusion\_matrix

## table()

The typical way of getting a table of classification results:

```
table(train.class,Default$default)
```

```
## ## train.class No Yes ## No 9639 243 ## Yes 28 90
```

I use confusionMatrix() because I am lazy and don't want to calculate all of the other statistics

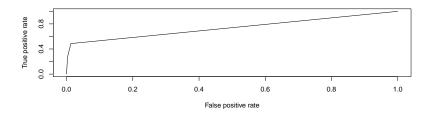
## Changing the cutoff for class assignment

This uses the optimal cutoff from the pROC plot

```
train.prob <- predict(train.rpart,Default,type="prob")[,2]</pre>
train.class2 <- ifelse(train.prob > .031,1,0)
confusionMatrix(as.numeric(Default$default)-1,train.class2,positive="1")
## Confusion Matrix and Statistics
##
##
            Reference
## Prediction
##
           0 9541 126
            1 171 162
##
##
##
                  Accuracy: 0.9703
##
                    95% CI: (0.9668, 0.9735)
##
       No Information Rate: 0.9712
##
       P-Value [Acc > NIR] : 0.71715
##
##
                    Kappa : 0.5065
    Mcnemar's Test P-Value: 0.01068
##
##
##
               Sensitivity: 0.5625
               Specificity: 0.9824
##
            Pos Pred Value: 0.4865
##
            Neg Pred Value: 0.9870
##
               Prevalence: 0.0288
##
                                                ◆□▶ ◆□▶ ◆三▶ ◆三 ◆○○○
```

## **Another Way to Get Optimal Threshold**

```
library(ROCR)
pred <- prediction(train.prob,as.numeric(Default$default)-1)
perf <- performance(pred,"tpr","fpr")
#str(perf)
plot(perf)</pre>
```



# **Boosting and Random Forests**

## **Boosting and RF Setup**

For this, we will use the **caret** package as an interface to both the **gbm** and **randomForest** packages.

Because gbm and random forests take much longer to run, we could set up parallelization through caret and other packages. http://topepo.github.io/caret/parallel.html

In my experience, unless your dataset is huge, parallelization with random forests tends to take longer than setting up only serial computation.

In caret, randomForest has two implementations, method="rf" and method="parRF" with parRF being the parallel version. The only tuning parameter for both is mtry.

Note, that using the train() will take longer, as it is using different tuning parameters and by default using bootstrap sampling to prevent overfitting.

To let train() pick the values of mtry, just set tuneLength to however many different values you want it to try. Default is 3.

#### **Run Random Forest**

```
#library(snowfall); #sfInit(parallel=T, cpus=4)
cont <- trainControl(allowParallel=TRUE,method="cv")</pre>
train.rf1 <- train(medv ~ ., data=Boston.train,method="rf",</pre>
                   trControl=cont,
                   importance=T,tuneLength=3)
train.rf1
## Random Forest
##
## 253 samples
##
   13 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 228, 228, 227, 228, 229, 227, ...
## Resampling results across tuning parameters:
##
     mtry RMSE Rsquared
##
     2 4.059928 0.8485182
##
     7 3.782779 0.8589950
##
##
     13 3.902765 0.8463466
##
## RMSE was used to select the optimal model using the smallest value.
## The finel welve wand for the model was mtmr - 7
```

#### Performance on a holdout

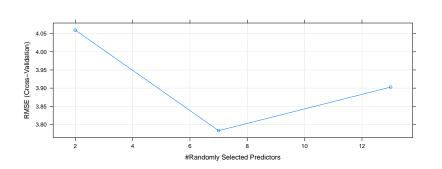
```
# see how we do on hold out sample
# automatically chooses best model for prediction
pred.test1 <- predict(train.rf1,Boston.test)
cor(pred.test1,Boston.test$medv)**2</pre>
```

## [1] 0.8818734

Best practice is to only do this with one model. I.e. choose between best random forest and boosting models, take this one model and check performance on test dataset and report.

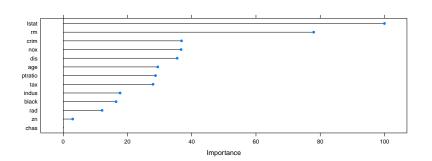
## **Plot Performance**

#### plot(train.rf1)



# Variable Importance

```
#rf <- train.rf1$finalModel
imp <-varImp(train.rf1)
plot(imp)</pre>
```



#### **Cforest**

cforest is implemented as method="cforest" with the only tuning parameter being mtry

```
train.cf1 <- train(medv ~., data=Boston.train,method="cforest")
#train.cf1

#plot(train.cf1)

#varImp(train.cf1)

# see how we do on hold out sample
pred.test2 <- predict(train.cf1,Boston.test)
cor(pred.test2,Boston.test$medv)**2</pre>
```

```
## [1] 0.7976894
```

#### Classification

For classification, a couple other things to use paired with train()

```
# set up data
data(Carseats)
#attach(Carseats)
#hist(Carseats$Sales)
High=ifelse(Carseats$Sales<=8,"No","Yes")
Carseats=data.frame(Carseats, High)
Carseats$Sales <- NULL
Carseats$ShelveLoc <- as.numeric(Carseats$ShelveLoc)

train2 = sample(dim(Carseats)[1], dim(Carseats)[1]/2) # half of sample
Carseats.train = Carseats[train2, ]
Carseats.test = Carseats[-train2, ]</pre>
```

### Now run random forests

```
train.rf2 <- train(as.factor(High) ~ .,</pre>
                   data=Carseats.train,method="rf",trControl=cont)
#train.rf2
rf.probs=predict(train.rf2,newdata=Carseats.test,type="prob")[,2]
rocCurve22 <- roc(Carseats.test$High,rf.probs)</pre>
#auc(rocCurve22):#
rf.class=predict(train.rf2,newdata=Carseats.train)
confusionMatrix(Carseats.train$High,rf.class)
## Confusion Matrix and Statistics
##
##
             Reference
## Prediction No Yes
##
          No 115
          Yes 0 85
##
##
                  Accuracy: 1
##
##
                    95% CI: (0.9817, 1)
       No Information Rate: 0.575
##
##
       P-Value [Acc > NIR] : < 2.2e-16
##
##
                     Kappa: 1
##
    Mcnemar's Test P-Value : NA
##
##
               Sensitivity: 1.000
                                                  4 D > 4 A > 4 B > 4 B > B 9 9 9
```

### **Confusion Matrix on Test Data**

```
#auc(rocCurve4);#ci(rocCurve4);#plot(rocCurve4)
rf.classTest=predict(train.rf2,Carseats.test)
confusionMatrix(Carseats.test$High,rf.classTest)
## Confusion Matrix and Statistics
##
##
            Reference
## Prediction No Yes
         No 98 23
##
         Yes 28 51
##
##
##
                  Accuracy: 0.745
##
                    95% CI: (0.6787, 0.8039)
##
       No Information Rate: 0.63
##
       P-Value [Acc > NIR] : 0.0003656
##
##
                    Kappa: 0.4605
##
    Mcnemar's Test P-Value: 0.5754030
##
               Sensitivity: 0.7778
##
##
               Specificity: 0.6892
            Pos Pred Value: 0.8099
##
##
            Neg Pred Value: 0.6456
##
               Prevalence: 0.6300
            Detection Rate: 0.4900
##
                                                 ◆□▶ ◆□▶ ◆□▶ ◆□▶ □ ◆○○○
```

## cforest for binary

automatically knows it is binary, unlike randomForest

```
train.cf2 <- train(High ~ .,
            data=Carseats.train,method="cforest",trControl=cont)
#train.cf2
cf.probs=predict(train.cf2)
rocCurve33 <- roc(Carseats.train$High,as.numeric(cf.probs));#auc(rocCurve33)</pre>
#plot(rocCurve33.add=T.col=3)
cf.class=predict(train.cf2$finalModel)
confusionMatrix(Carseats.train$High,cf.class) # no errors
## Confusion Matrix and Statistics
##
            Reference
##
## Prediction No Yes
##
         No 110
         Yes 8 77
##
##
##
                  Accuracy: 0.935
##
                    95% CI: (0.8914, 0.9649)
      No Information Rate: 0.59
##
##
       P-Value [Acc > NIR] : <2e-16
##
##
                     Kappa : 0.8664
   Mcnemar's Test P-Value: 0.5791
                                                ◆□▶◆問▶◆団▶◆団▶ ■ 釣@@
##
```

#### **CForest on Test Data**

```
cf.classTest=predict(train.cf2,newdata=Carseats.test)
cf.probs2=predict(train.cf2,newdata=Carseats.test,type="prob")[,2]
rocCurve333 <- roc(Carseats.test$High,as.numeric(cf.probs2));#auc(rocCurve33)
#plot(rocCurve333,add=T,col=3)</pre>
```

### **CForest Test Confusion Matrix**

```
confusionMatrix(Carseats.test$High,cf.classTest)
```

```
## Confusion Matrix and Statistics
##
##
           Reference
## Prediction No Yes
         No 96 25
##
         Yes 28 51
##
##
##
                  Accuracy: 0.735
##
                    95% CI: (0.6681, 0.7948)
##
      No Information Rate: 0.62
##
      P-Value [Acc > NIR] : 0.0003995
##
##
                     Kappa : 0.4419
##
   Mcnemar's Test P-Value: 0.7835305
##
##
               Sensitivity: 0.7742
               Specificity: 0.6711
##
##
            Pos Pred Value: 0.7934
##
            Neg Pred Value: 0.6456
                Prevalence: 0.6200
##
##
            Detection Rate: 0.4800
     Detection Prevalence: 0.6050
##
##
         Balanced Accuracy: 0.7226
```

# **Boosting**

```
packages: "gbm" and "ada" – both can be accessed through caret Example tuning parameters for "gbm: http://topepo.github.io/caret/training.html
For this, I am going to use method="ada" which is one of the forms of boosting. Currently, problem with method="gbm"
Basic set up to compare results to RF:
```

# **Compare ROC Curves**

```
plot(rocCurve22,col=c(1)) # color black is rf
plot(rocCurve333,add=T,col=c(2)) # color red is cforest
plot(rocCurve3,add=T,col=c(3)) # color green is gbm
```

