Machine Learning: Random Forest

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For those wishing to follow along with the R-based demo in class, click here for the companion R script for this lecture.

Machine Learning

Machine Learning may seem similar to statistics, but there are some important differences.

In statistics, we attempt to gain knowledge about a (statistical) population from a sample! We may also use our new understanding to make predictions and forecasts- but in statistics, prediction is often secondary to making inference about population parameters. The concept of the sampling distribution is central to statistics, as it allows us to account for uncertainty using p-values and confidence intervals. (OR, in Bayesian statistics, we use Bayes Rule to update our state of knowledge and account for uncertainty about population parameters)

In Machine Learning, we attempt to use available data to detect generalizable predictive patterns. In Machine Learning we often don't care as much about building our understanding of the system, we simply want to be able to make better predictions. Machine learning is generally not going to allow us to make inference about population parameters of interest using confidence bounds, p-values etc. However, the predictions we make using Machine Learning can be more accurate than the predictions we make using statistical models. And in many cases, machine learning can help to generate hypotheses that can be tested more rigorously using statistical inference.

In statistics, we as analysts have to do a lot of work conceiving of potential data-generating models (e.g., likelihood functions), fitting these models (e.g., MLE), testing goodness-of-fit, etc.

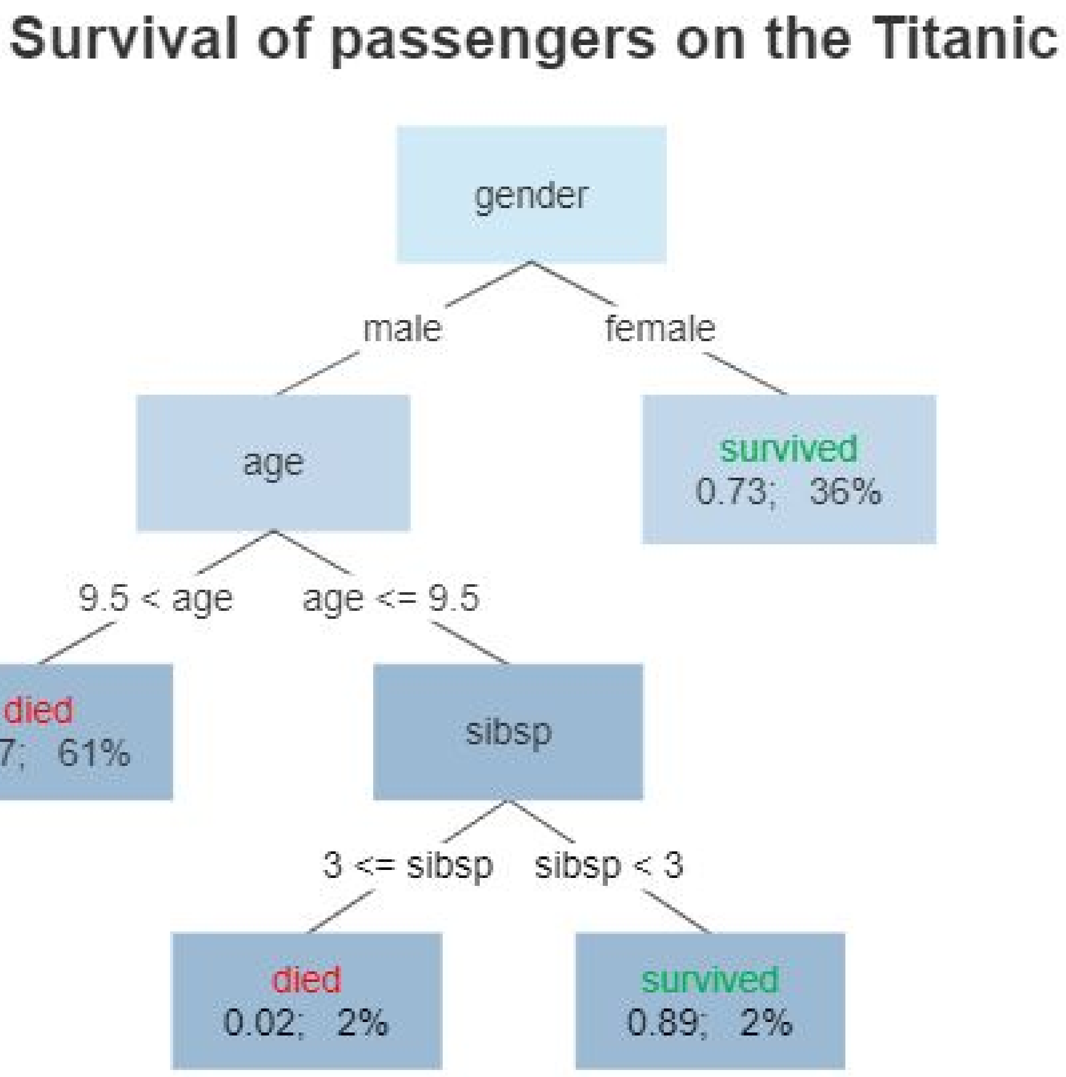
In Machine Learning, the analyst let's the computer do the heavy lifting. Machine Learning tends to impose fewer assumptions on the data than statistical models. For example, we don't need to assume that residuals follow a Normal distribution, or even that all relationships are linear! The computer algorithm tries to tease apart any signals that may be present in the data.

Decision trees

A decision tree is essentially a set of branching rules for determining an expected response from a set of predictor variables (features).

First, we use one of the features to divide our full data set such that the response variables are as similar as possible within the two resulting *branches* of the tree. For each of the resulting branches, we repeat this procedure, dividing the resulting branches again and again (recursively) until some endpoint rule is reached (e.g., 3 or fewer observations remaining in the branch). Each decision point in the tree is called a *node*. The final branches in the tree are called *leaves*.

Here is an example:



Random forest

Random Forest is one of the older and still most popular Machine Learning methods. It is relatively easy to understand, and tends to make very good predictions. A Random Forest consists of a large set of decision trees!

The basic algorithm is as follows:

Build a large number of decision trees (e.g., 500) using the following algorithm:

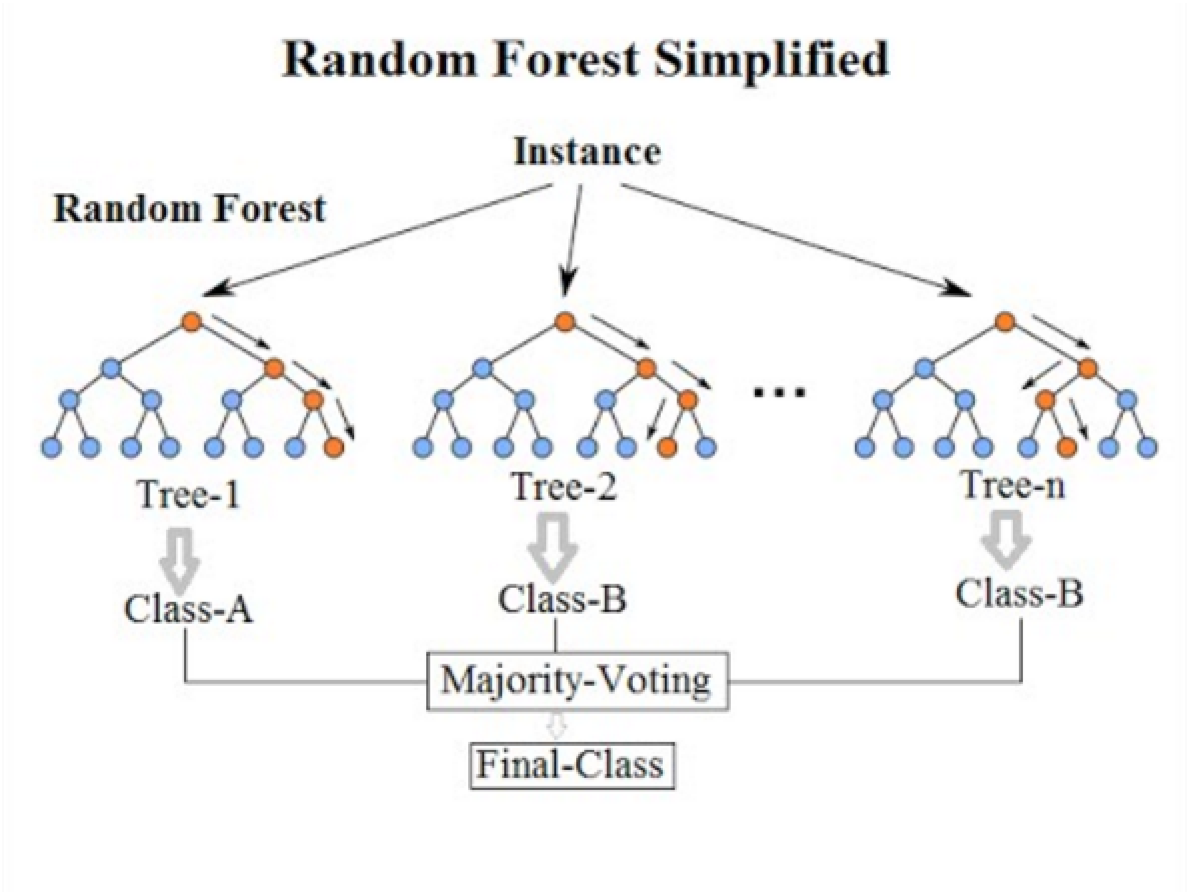
1. Draw a small bootstrap sample from the original dataset- generally much smaller than the original dataset.

2. Build a decision tree using this bootstrap sample. At each node of the decision tree, determine the optimal splitting rule using a restricted subset of the available predictor variables (randomly sampled

from the set of available features).

3. [for determining variable importance] Randomly shuffle each feature in turn and see how much the predictive power is reduced, using only ‘out of bag’ observations (data that were not used to build the tree) to assess predictive performance.

Once you have the full set of trees, you make predictions by using a weighted average (or majority-voting rule for categorical variables) of the predictions generated by all the trees based on all the component trees in the forest:



In Random Forest, each tree is meant to be somewhat independent from one another- in Machine Learning, each tree is a “weak learner”. All of the trees (the ‘committee’ so to speak) will generally be a much better and more robust, generalizable predictor than any single tree in the forest- or for that matter, any single tree you could generate. The use of bootstrapping and random sampling of features within the random forest algorithm ensures that each tree is a weak learner and is relatively independent from other trees in the forest. This way, the collection of semi-independent trees becomes a better predictor than any single tree could be!

Random forest is not only a good way of making predictions, it also helps us:

1. *Identify which features are most important for prediction*: By keeping track of which features tend to yield the biggest gains in prediction accuracy across all trees in the forest (generally we keep track of the ability to predict observations that were not used for fitting each tree- these are called ‘out of bag’ observations), we can easily generate robust indicators of variable importance.
2. *Identify non-linear relationships*. By plotting out our predicted response across a range of each predictor variable, we can see if any non-linear patterns emerge!
3. *Identify important interactions*. By comparing how predicted responses for one feature change across a range of another feature, we can assess the degree to which features interact to determine the expected response.

Example: the Titanic disaster

Let's evaluate which factors were related to surviving the Titanic disaster!

You can load the Titanic data example here. Alternatively you can use the 'titanic' package in R!

```
##########
# Titanic disaster example  (load data)

titanic <- read.csv("titanic.csv",header=T)
head(titanic)

# library(titanic)            # alternative: load titanic data from package
# titanic <- titanic_train
```

Let's first load a package that implements a fast/efficient version of random forest

While we're at it, let's load another package for running a single decision tree

```
library(ranger)    # fast implementation of random forest
library(party)     # good package for running decision tree analysis (and random forest- just slower)
```

When using categorical variables, we should make sure they are encoded as factors, not as numeric. Use class(data$Resp) to check the encoding, and use as.factor(data$Resp) to coerce your variable(s) to the 'factor' type.

```
class(titanic$Survived)
```

```
## [1] "integer"
```

```
titanic$Survived <- as.factor(titanic$Survived)    # code response variable as a factor variable (categ
titanic$Sex <- as.factor(titanic$Sex)

class(titanic$Survived)   # make sure it's a factor
```

```
## [1] "factor"
```

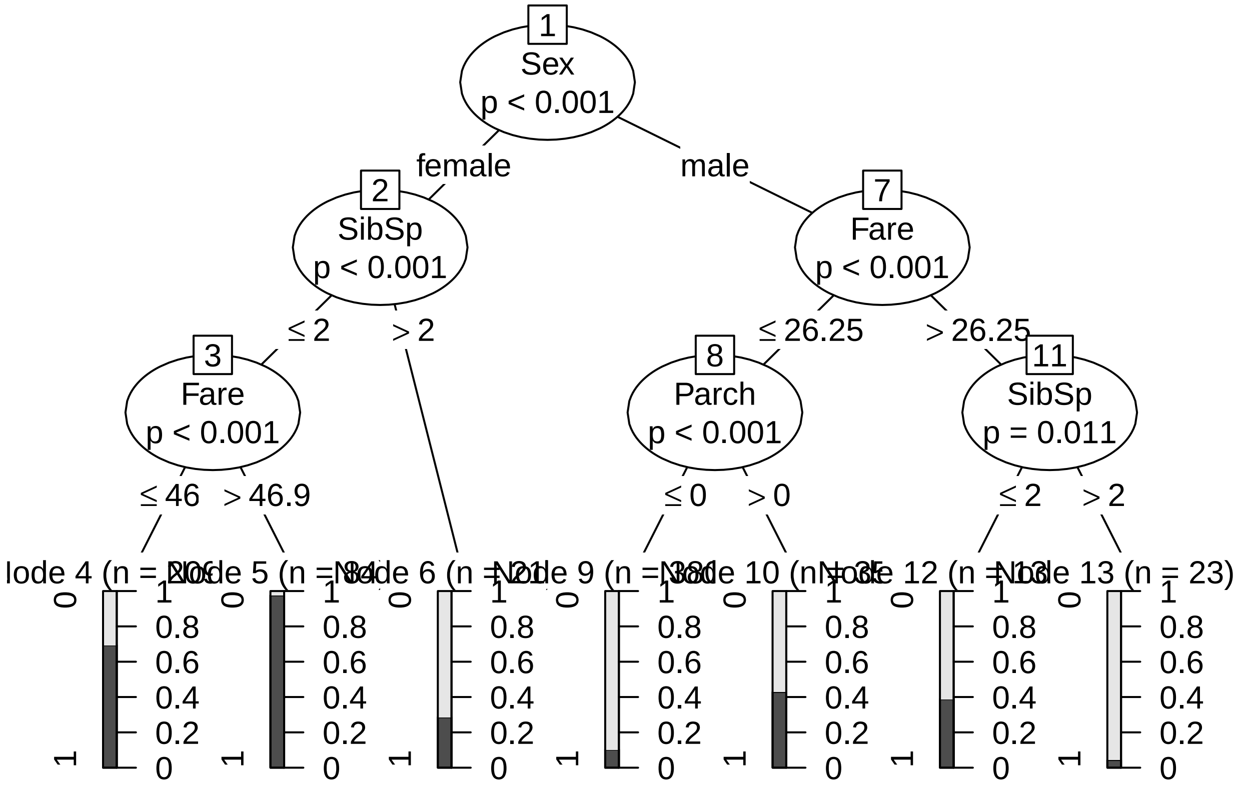
Now let's define the predictors and response:

```
predictorNames <- c(  "Sex",       # nice readable names
                      "Age",
                      "Sibs/spouses",
                      "Parents/children",
                      "Fare"
)

pred.names=c(  "Sex",      # the actual names from the data frame
               "Age",
               "SibSp",
               "Parch",
               "Fare"
)
# cbind(pred.names,predictorNames)

response="Survived"


formula1 <- as.formula(paste(response,"~",paste(pred.names,collapse="+")))    # formula for the RF mode
```

Run a decision tree

This is also known as a CART analysis (classification and regression tree) - a single tree, not a forest!

```
TerrMamm.tr <- ctree(formula=formula1, data=titanic, controls = ctree_control(mincriterion = 0.85,maxde

plot(TerrMamm.tr)
```



But remember that a single tree is not very robust- these are very likely to over-fit to the data! Random forest gets around this issue and is much more robust than CART analysis!

Like most machine learning algorithms, we can “tune” the algorithm in several different ways. If this were a “real” analysis, I would try several alternative parameter tunings.

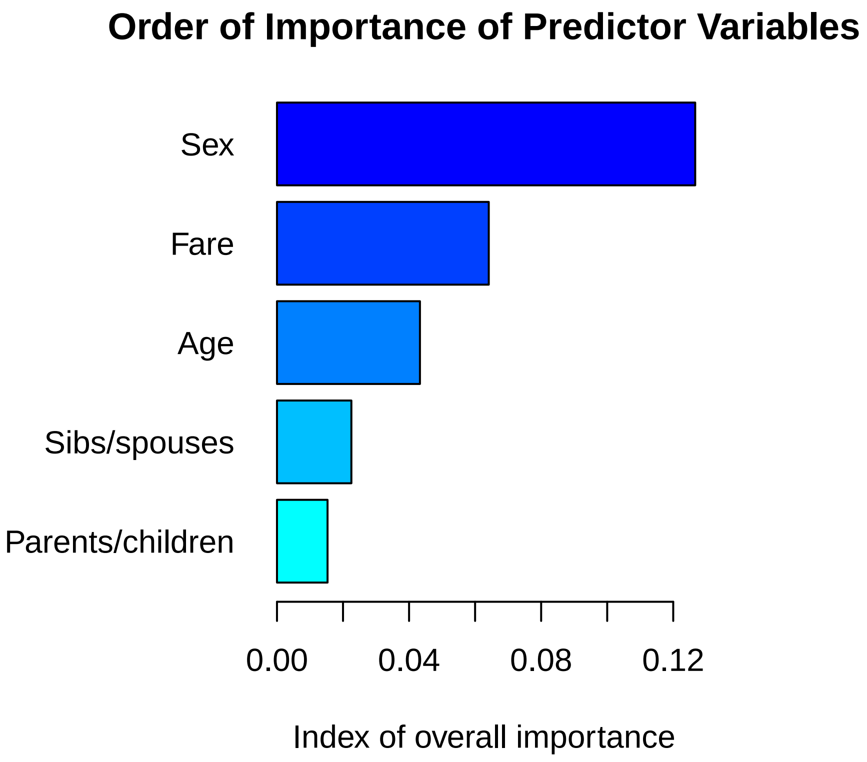
```
####### Run a random forest model!

titanic2 <- na.omit(titanic)    # remove missing data (ranger does not handle missing data- 'party' impl

thismod <- ranger(formula1, data=titanic2, probability=T,importance = 'permutation' )
```

Variable importance

One thing we can easily get from a RF analysis is an index of the relative importance of each predictor variable

```
    # get the importance values
varimp <- importance(thismod)
```

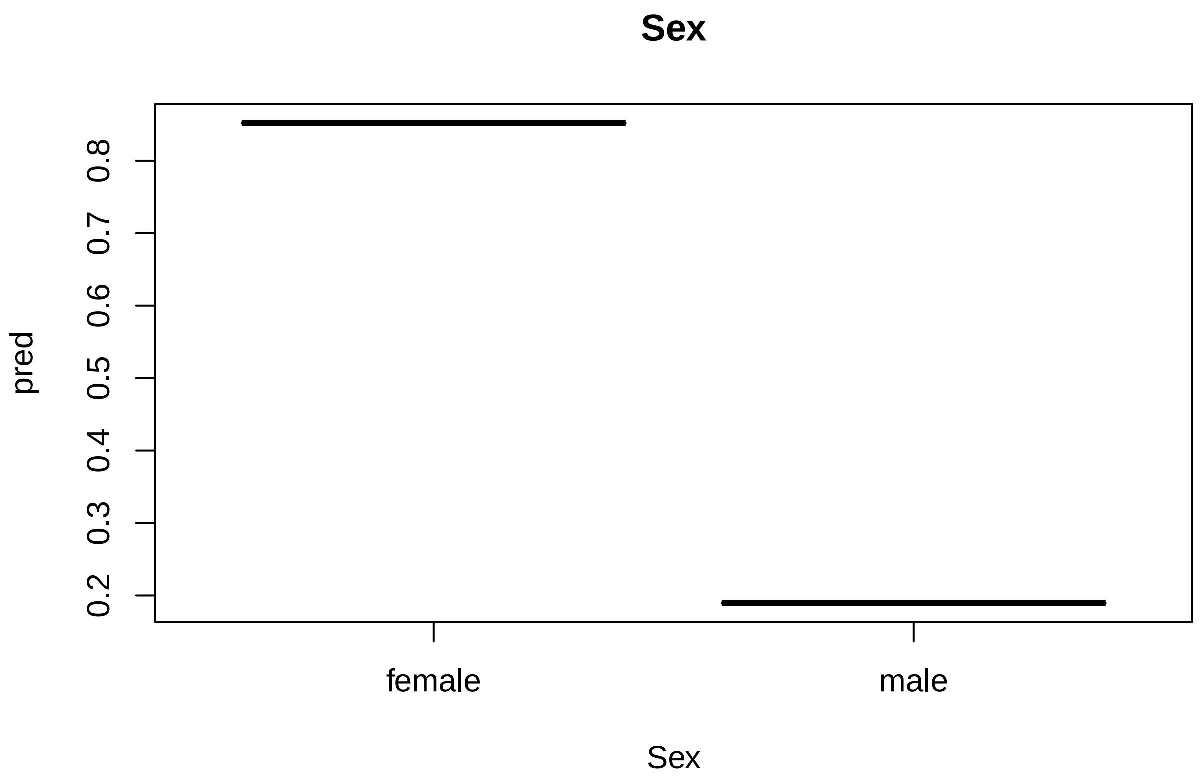
```r
lengthndx <- length(varimp)
#par(mai=c(0.95,3.1,0.6,0.4))
par(mai=c(1.2,3.4,0.6,0.9))
col <- rainbow(lengthndx, start = 3/6, end = 4/6)
barplot(height=varimp[order(varimp,decreasing = FALSE)],
        horiz=T,las=1,main="Order of Importance of Predictor Variables",
        xlab="Index of overall importance",col=col,
        names.arg=predictorNames[match(names(varimp),pred.names)][order(varimp,decreasing = FALSE)])
```

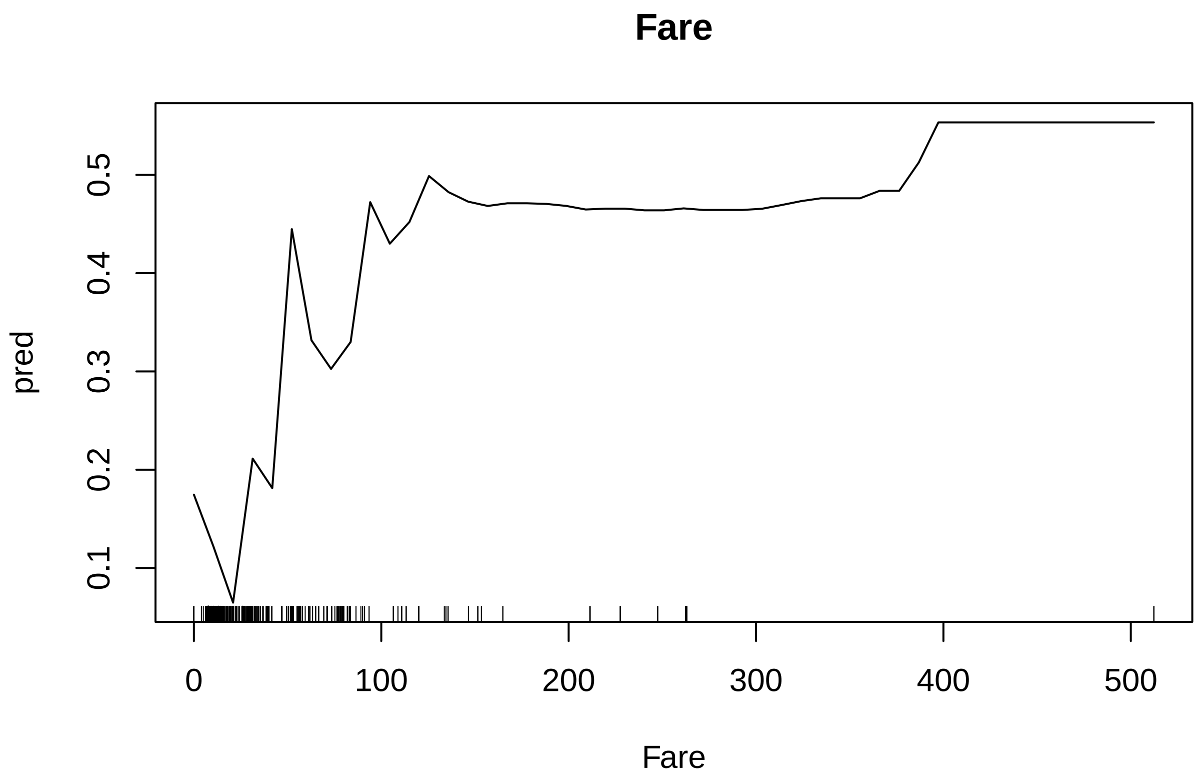


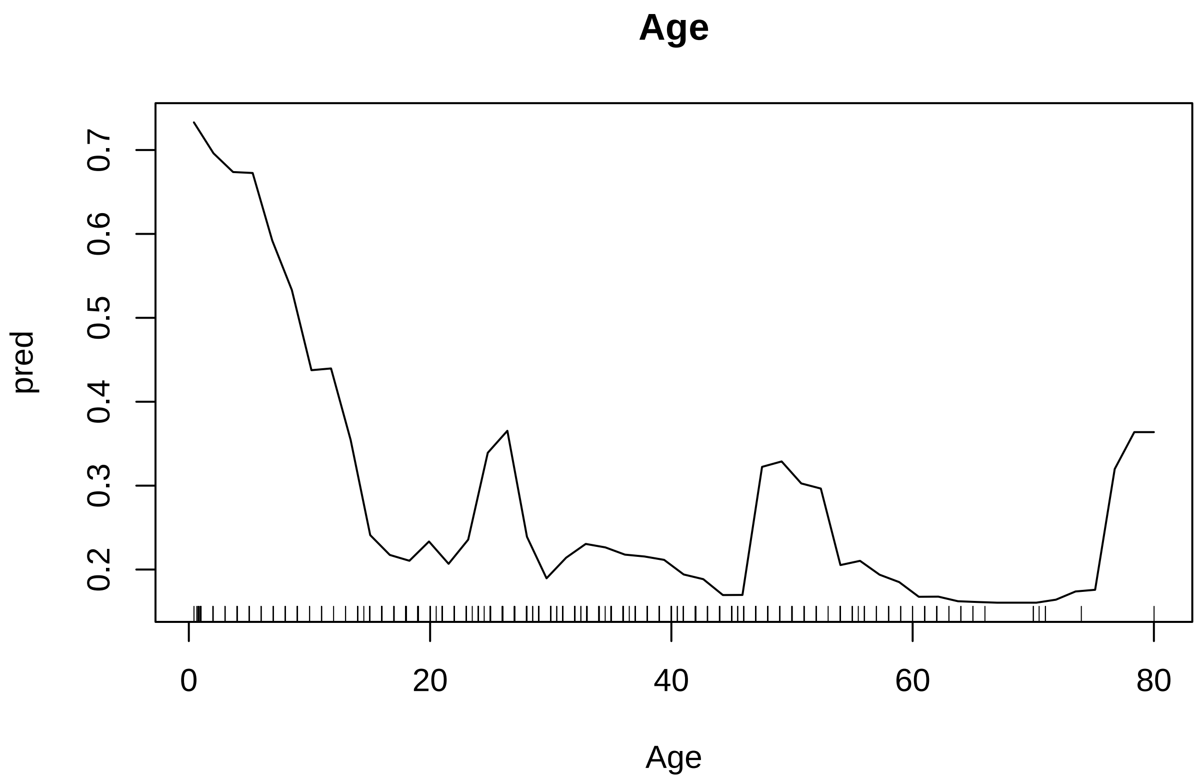
Univariate predictions

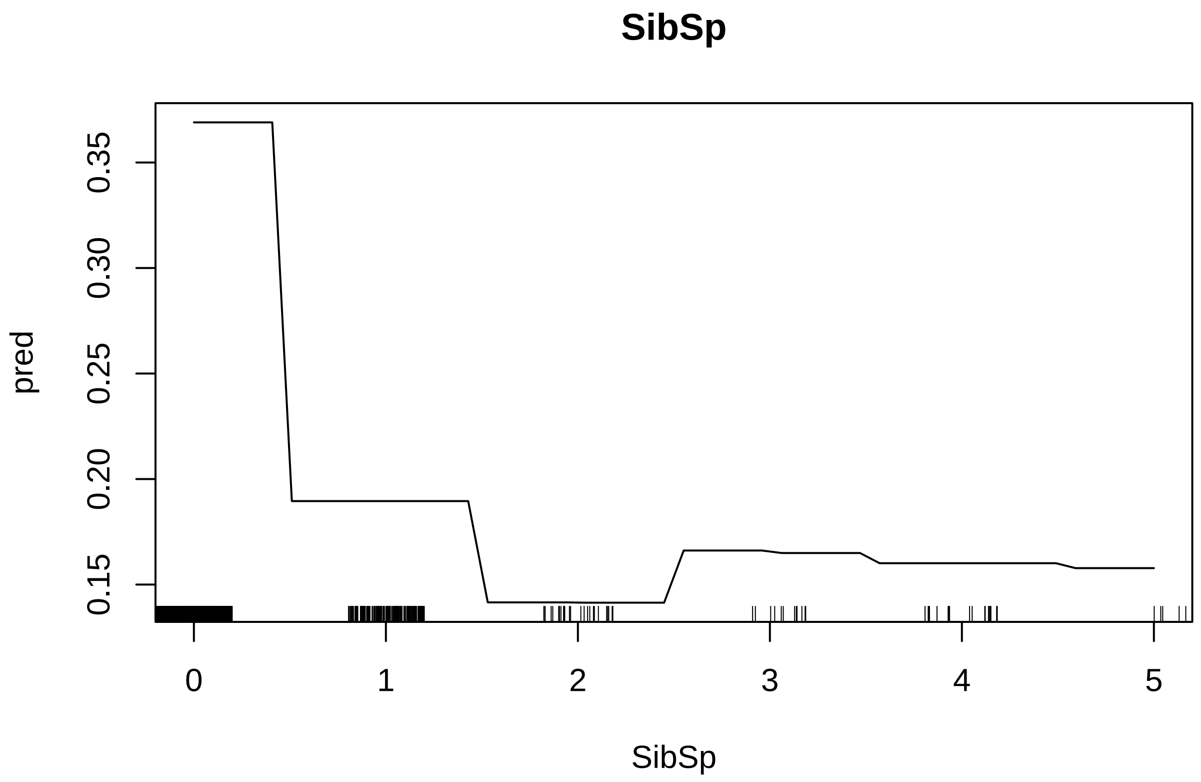
We can also generate univariate predictive plots, also known as "partial dependence plots". Note the use of the 'predict' function!

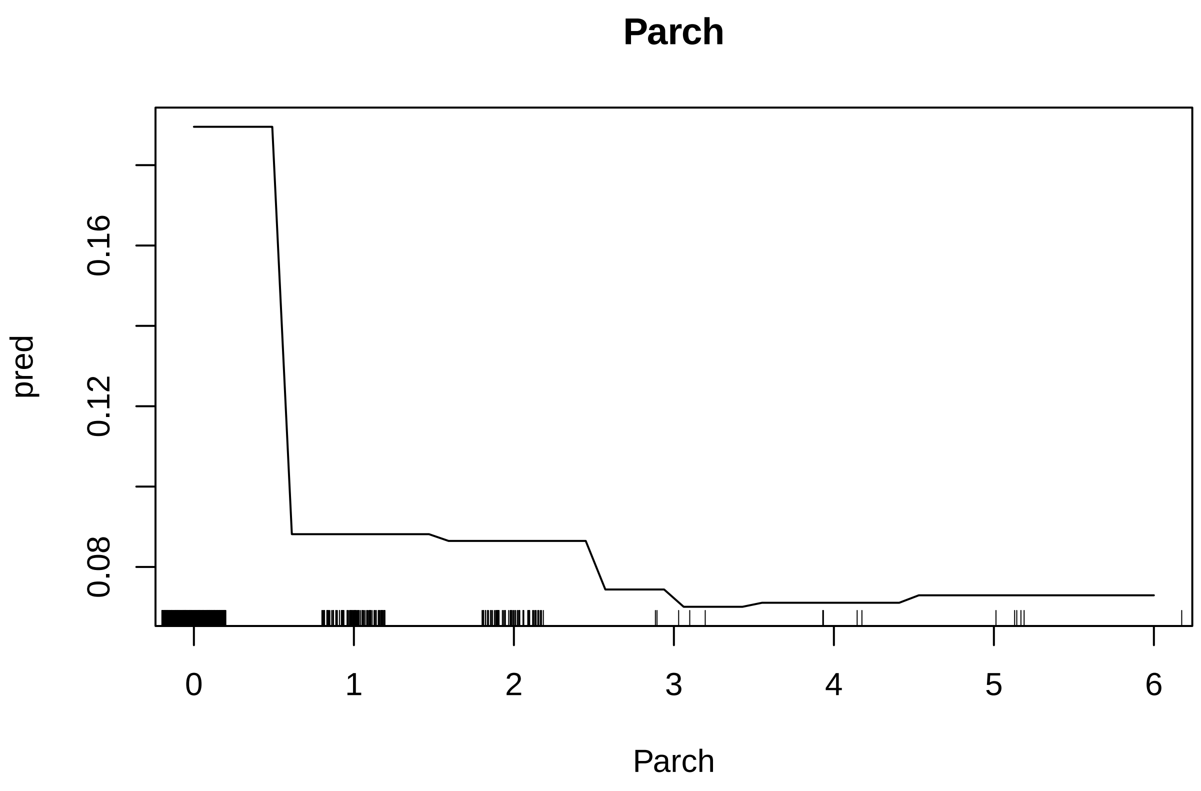
```r
##### Make univariate plots of the relationships- plot one relationship at a time
varstoplot <- names(sort(varimp,decreasing = T))   # plot in order of decreasing importance
par(mai=c(1,1,.8,.1))
p=1
for(p in 1:length(pred.names)){            # loop through all predictor variables
  thisvar <- varstoplot[p]

  if(is.factor(titanic2[[thisvar]])){                    # make 'newdata' that spans the range of the p
    nd <- data.frame(x=as.factor(levels(titanic2[[thisvar]])))
  }else{
    nd <- data.frame(x=seq(min(titanic2[[thisvar]]),max(titanic2[[thisvar]]),length=50))
  }
  names(nd) <- thisvar

  othervars <- setdiff(pred.names,thisvar)    # set other variables at their mean value (or for factors
  temp <- sapply(othervars,function(t){ if(is.factor(titanic2[[t]])){ nd[[t]] <<- titanic2[[t]][1]}else
  #nd

  pred = predict(thismod,data=nd,type="response")$predictions[,2]     # use 'predict' function to make p

  plot(pred~nd[,1],type="l",xlab=thisvar,main=thisvar)         # plot the predictions
  if(!is.factor(nd[,1])) rug(jitter(titanic2[[thisvar]]))   # with 'rug' for quantitative vars

}
```




Fare
pred
0.1
0.2
0.3
0.4
0.5
0
100
200
300
400
500
Fare


Age
pred
0.2
0.3
0.4
0.5
0.6
0.7
0
20
40
60
80
Age


SibSp
pred
0.15
0.20
0.25
0.30
0.35
0
1
2
3
4
5
SibSp



Interactions

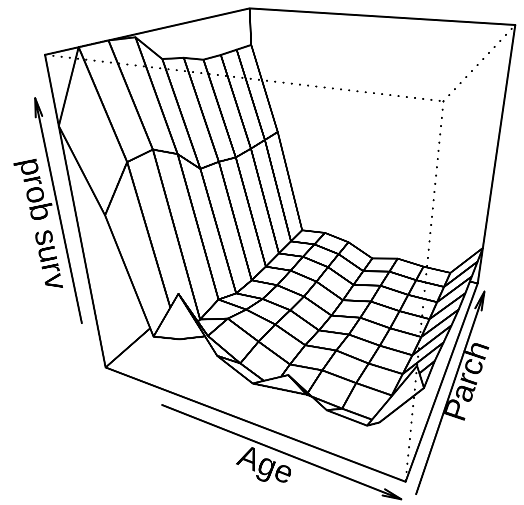
Finally, we can find and plot the most important interactions!

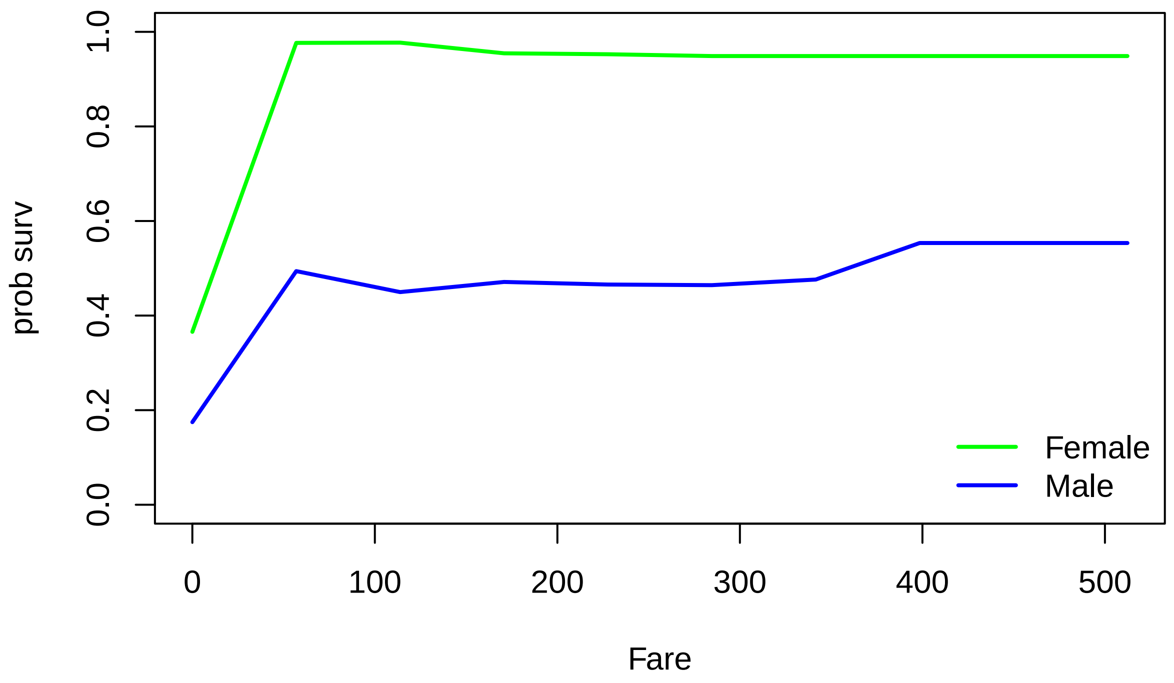
In the following code block we assess the strength of all possible two-way interactions, by measuring the difference between the RF predictions across each 2-D parameter space and a fully additive model. Don't worry if this doesn't make sense- see me another time if you'd like me to explain the code in more detail!

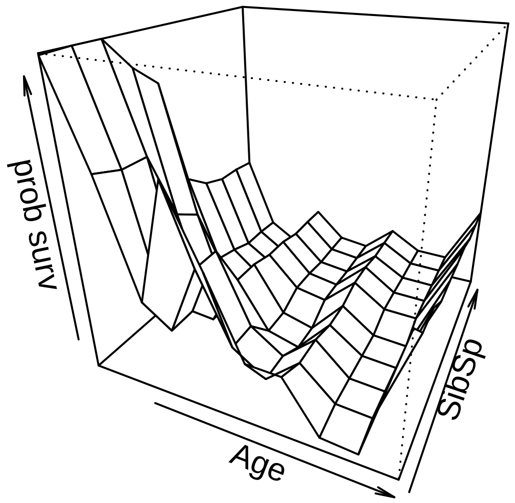
```
allcomb <- as.data.frame(t(combn(pred.names,2)))     # all bivariate combinations of the predictor varia
names(allcomb) <- c("var1","var2")

allcomb$int1 <- NA     # for storing relative interaction intensity
allcomb$int2 <- NA

p=1
for(p in 1:nrow(allcomb)){      # loop through all bivariate combinations
  var1 = allcomb$var1[p]
  var2 = allcomb$var2[p]

  if(!is.factor(titanic2[[var1]])){         # break each variable into bins for making predictions
    all1= seq(min(titanic2[[var1]]),max(titanic2[[var1]]),length=10)
  }else{
    all1=as.factor(levels(titanic2[[var1]]))
  }
  if(!is.factor(titanic2[[var2]])){
    all2 = seq(min(titanic2[[var2]]),max(titanic2[[var2]]),length=10)
  }else{
    all2=as.factor(levels(titanic2[[var2]]))
  }

  nd <- expand.grid(all1,all2)     # make 'newdata' data frame for making predictions across the 2-D pa

  names(nd) <- c(var1,var2)

  othervars <- setdiff(pred.names,c(var1,var2))      # set all other vars at their mean value (or use f
  temp <- sapply(othervars,function(t){ if(is.factor(titanic2[[t]])){ nd[[t]] <<- titanic2[[t]][1]}else

  pred = predict(thismod,data=nd,type="response")$predictions[,2]   # make predictions using 'predict()

  additive_model <- lm(pred~nd[[var1]]+nd[[var2]])     # fit a fully additive model from RF predictions

  pred_add = predict(additive_model)    # generate predictions using the additive model (for comparison

  allcomb$int1[p] <- sqrt(mean((pred-pred_add)^2))   # metric of interaction strength (dif between RF a

  maximp <- mean(varimp[c(var1,var2)])    # for weighted interaction importance

  allcomb$int2[p] <- allcomb$int1[p]/maximp   # weighted measure that includes overall importance and i

}

allcomb <- allcomb[order(allcomb$int1,decreasing = T),]
allcomb
```

Next, we visualize our top interactions!

```
### visualize interactions
ints.torun <- 1:3
int=2
for(int in 1:length(ints.torun)){
  thisint <- ints.torun[int]
  var1 = allcomb$var1[thisint]
  var2 = allcomb$var2[thisint]

  if(!is.factor(titanic2[[var1]])){
    all1= seq(min(titanic2[[var1]]),max(titanic2[[var1]]),length=10)
  }else{
    all1=as.factor(levels(titanic2[[var1]]))
  }
  if(!is.factor(titanic2[[var2]])){
    all2 = seq(min(titanic2[[var2]]),max(titanic2[[var2]]),length=10)
  }else{
    all2=as.factor(levels(titanic2[[var2]]))
  }

  nd <- expand.grid(all1,all2)
  names(nd) <- c(var1,var2)

  othervars <- setdiff(pred.names,c(var1,var2))
  temp <- sapply(othervars,function(t)if(is.factor(titanic2[[t]])){ nd[[t]] <<- titanic2[[t]][1]}else{ 

  pred = predict(thismod,data=nd,type="response")$predictions[,2]
  predmat = matrix(pred,nrow=length(all1),ncol=length(all2))

  if(!is.factor(titanic2[[var1]])){
    persp(all1,all2,predmat,theta=25,phi=25,xlab=var1,ylab=var2,zlab="prob surv")
  }else{
    plot(predmat[1,]~all2,xlab=var2,ylab="prob surv",type="l",ylim=c(0,1),col="green",lwd=2)
    lines(all2,predmat[2,],col="blue",lwd=2)
    legend("bottomright",bty="n",lty=c(1,1),col=c("green","blue"),lwd=c(2,2),legend=c("Female","Male"))
  }

}
```




prob surv
0.0
0.2
0.4
0.6
0.8
1.0
0
100
200
300
400
500
Fare
Female
Male



Model performance

Finally, let's bring this home by looking at model performance!

```
####################################
#################### CROSS VALIDATION CODE

n.folds = 10       # set the number of "folds"
foldVector = rep(c(1:n.folds),times=floor(length(titanic2$Survived)/9))[1:length(titanic2$Survived)]
```

Then, we do the cross validation, looping through each fold of the data, leaving out each fold in turn for model training.

```
counter = 1
CV_df <- data.frame(
  CVprediction = numeric(nrow(titanic2)),      # make a data frame for storage
  realprediction = 0,
  realdata = 0
)
i=1
for(i in 1:n.folds){
  fit_ndx <- which(foldVector!=i)
  validate_ndx <- which(foldVector==i)
  model <- ranger(formula1, data = titanic2[fit_ndx,],probability=T,importance = 'permutation')
  CV_df$CVprediction[validate_ndx]  <- predict(model,data=titanic2[validate_ndx,],type="response")$predi
  CV_df$realprediction[validate_ndx]  <-  predict(thismod,data=titanic2[validate_ndx,],type="response")$
  CV_df$realdata[validate_ndx] <- titanic2$Survived[validate_ndx]
}

fact=TRUE
if(fact){
  CV_df$realdata=CV_df$realdata-1
}

CV_RMSE = sqrt(mean((CV_df$realdata - CV_df$CVprediction)^2))       # root mean squared error for holdo
real_RMSE = sqrt(mean((CV_df$realdata - CV_df$realprediction)^2))  # root mean squared error for residu

# print RMSE statistics

cat("The RMSE for the model under cross-validation is: ", CV_RMSE, "\n")
```

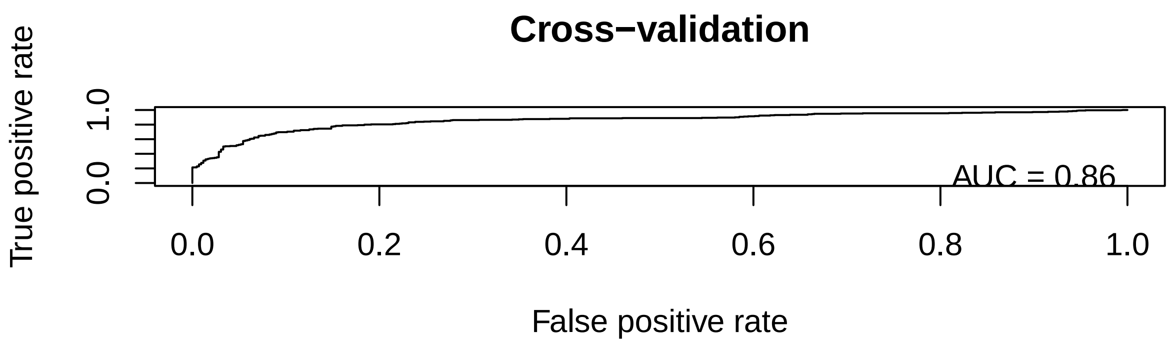
```
## The RMSE for the model under cross-validation is:  0.3701149
```

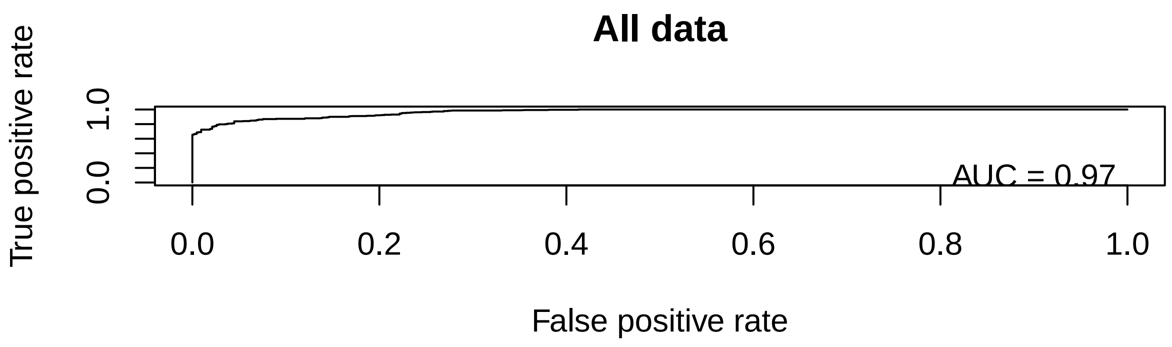
```
cat("The RMSE for the model using all data for training is: ", real_RMSE, "\n")
```

```
## The RMSE for the model using all data for training is:  0.2819101
```

Let's plot out the ROC curves!

```
library(ROCR)
library(rms)

par(mfrow=c(2,1))
pred <- prediction(CV_df$CVprediction,CV_df$realdata)     # for holdout samples in cross-validation
perf <- performance(pred,"tpr","fpr")
auc <- performance(pred,"auc")
plot(perf, main="Cross-validation")
text(.9,.1,paste("AUC = ",round(auc@y.values[[1]],2),sep=""))

pred <- prediction(CV_df$realprediction,CV_df$realdata)     # for final model
perf <- performance(pred,"tpr","fpr")
auc <- performance(pred,"auc")
plot(perf, main="All data")
text(.9,.1,paste("AUC = ",round(auc@y.values[[1]],2),sep=""))
```





Finally, we can use a pseudo-R-squared metric as an alternative metric of performance

```
CV_df$CVprediction[which(CV_df$CVprediction==1)] <- 0.9999       # ensure that all predictions are not
CV_df$CVprediction[which(CV_df$CVprediction==0)] <- 0.0001
CV_df$realprediction[which(CV_df$realprediction==1)] <- 0.9999
CV_df$realprediction[which(CV_df$realprediction==0)] <- 0.0001

fit_deviance_CV <- mean(-2*(dbinom(CV_df$realdata,1,CV_df$CVprediction,log=T)-dbinom(CV_df$realdata,1,C
fit_deviance_real <- mean(-2*(dbinom(CV_df$realdata,1,CV_df$realprediction,log=T)-dbinom(CV_df$realdata
null_deviance <- mean(-2*(dbinom(CV_df$realdata,1,mean(CV_df$realdata),log=T)-dbinom(CV_df$realdata,1,C
deviance_explained_CV <- (null_deviance-fit_deviance_CV)/null_deviance   # based on holdout samples
deviance_explained_real <- (null_deviance-fit_deviance_real)/null_deviance   # based on full model...

# print RMSE statistics

cat("The McFadden R2 for the model under cross-validation is: ", deviance_explained_CV, "\n")
```

```
## The McFadden R2 for the model under cross-validation is:  0.3531686
```

```
cat("The McFadden R2 for the model using all data for training is: ", deviance_explained_real, "\n")
```

```
## The McFadden R2 for the model using all data for training is:  0.5882819
```

— End of demo—