Machine Learning

NRES 746

Fall 2018

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

Now we will run the same titanic analysis, but using a machine learning method- in this case, Random Forest. Just for kicks!

Let's set up the workspace with the functions and packages we need!

```
suppressMessages(suppressWarnings(library(party)))

source_github <- function(baseurl,scriptname) {
  # load package
   suppressMessages(suppressWarnings(require(RCurl)))

  # read script lines from website
  url <- sprintf("%s%s",baseurl,scriptname)
  script <- getURL(url, ssl.verifypeer = FALSE)

  script <- gsub("\r\n", "\n", script)     # get rid of carriage returns (not sure why this is necessar

  # parse lines and evaluate in the global environement
  eval(parse(text = script), envir= .GlobalEnv)
}

baseurl = "https://raw.githubusercontent.com/kevintshoemaker/Random-Forest-Functions/master/"
source_github(baseurl,"RF_Extensions.R")
```

First, we read in the data

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

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 encode your vector as a factor.

```
titanic$Survived <- as.factor(titanic$Survived)
```

Now let's define the predictors and response:

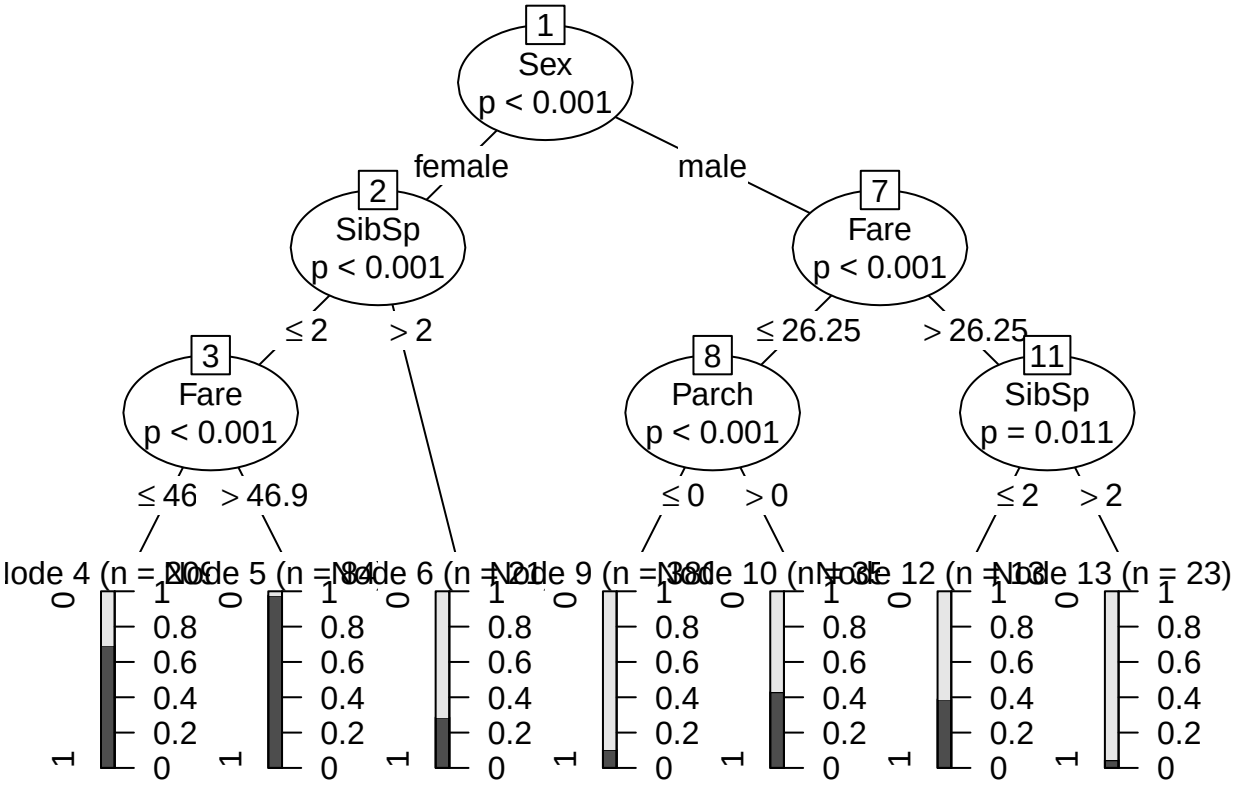
```
predictorNames <- c(  "Sex",       # nice readable names
                      "Age",
                      "Sibs/spouses",
                      "Parents/children",
                      "Fare"
)

pred.names=c(  "Sex",
               "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 conditional inference tree

This is also known as a CART analysis- single tree!

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

plot(TerrMamm.tr)
```



But remember that a single tree is not very robust- these are very liable to over-fitting! Random forest gets around this using random sampling in several creative ways!

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 tunings.

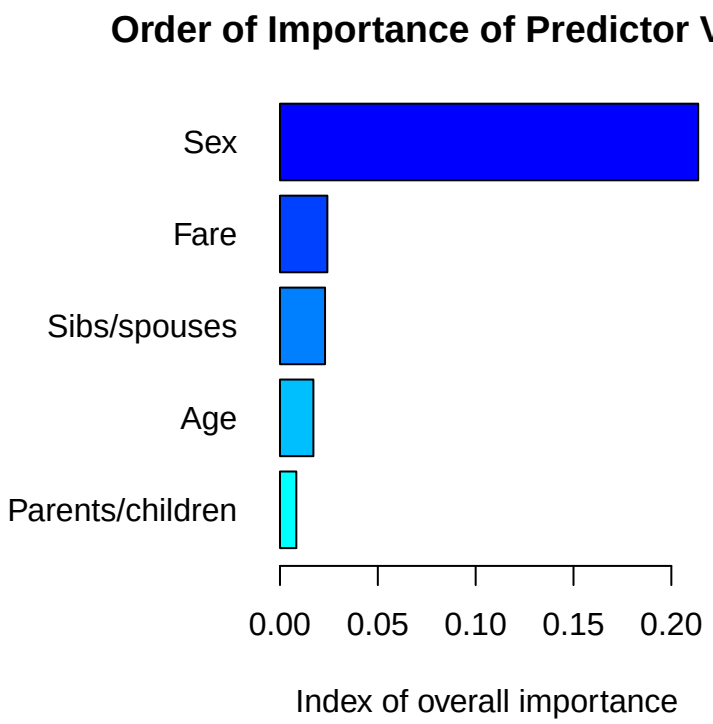
```
cforestControl <- cforest_unbiased(ntree=500,mtry=3)    # change back to 500!!
cforestControl@fraction <- 0.75
cforestControl@gtctrl@mincriterion <- 0.75
```

```
rf_model1 <- cforest(formula1, controls=cforestControl, data=titanic)
```

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
model1_importance<-varimp((rf_model1), conditional= FALSE)

lengthndx <- length(model1_importance)
#par(mai=c(0.95,3.1,0.6,0.4))
par(mai=c(1.4,3.4,0.6,0.9))
col <- rainbow(lengthndx, start = 3/6, end = 4/6)
barplot(height=model1_importance[order(model1_importance,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(model1_importance),pred.names)][order(model1_importance,de
```

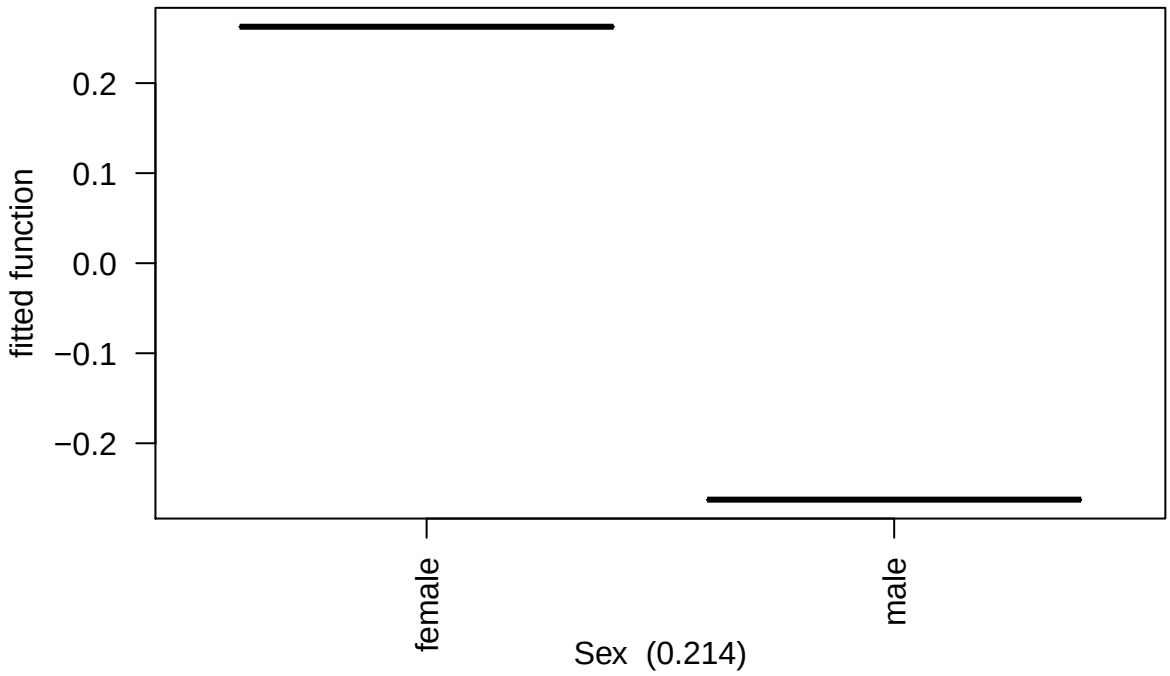


Univariate plots

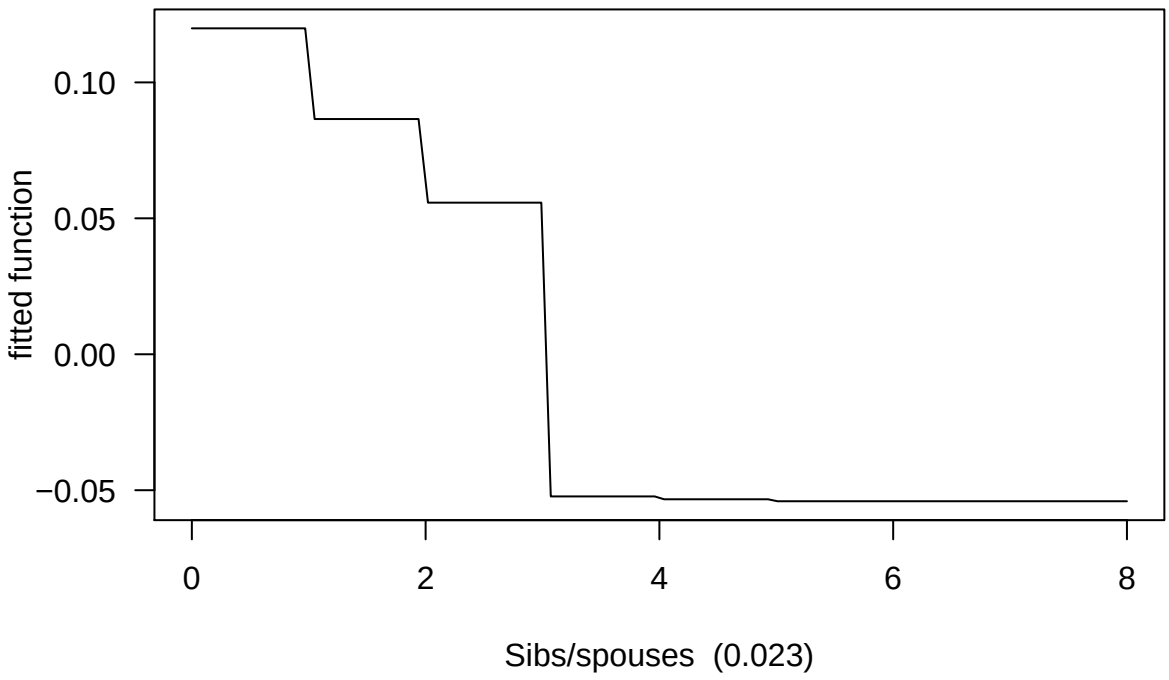
We can also generate univariate plots, also known as "partial dependence plots":

```
##### Make univariate plots of the relationships- plot one relationship at a time
```

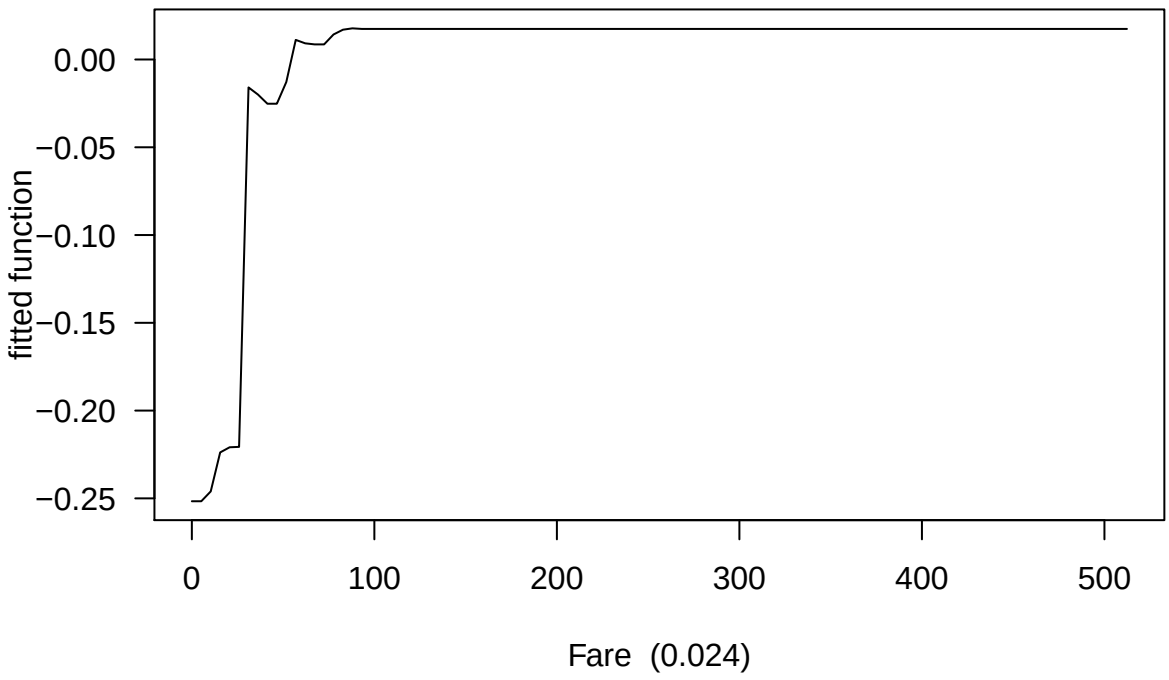
```
RF_UnivariatePlots(object=rf_model1, varimp=model1_importance, data=titanic,  #
                   predictors=pred.names[1], labels=predictorNames[1], allpredictors=pred.names,plot.lay
```



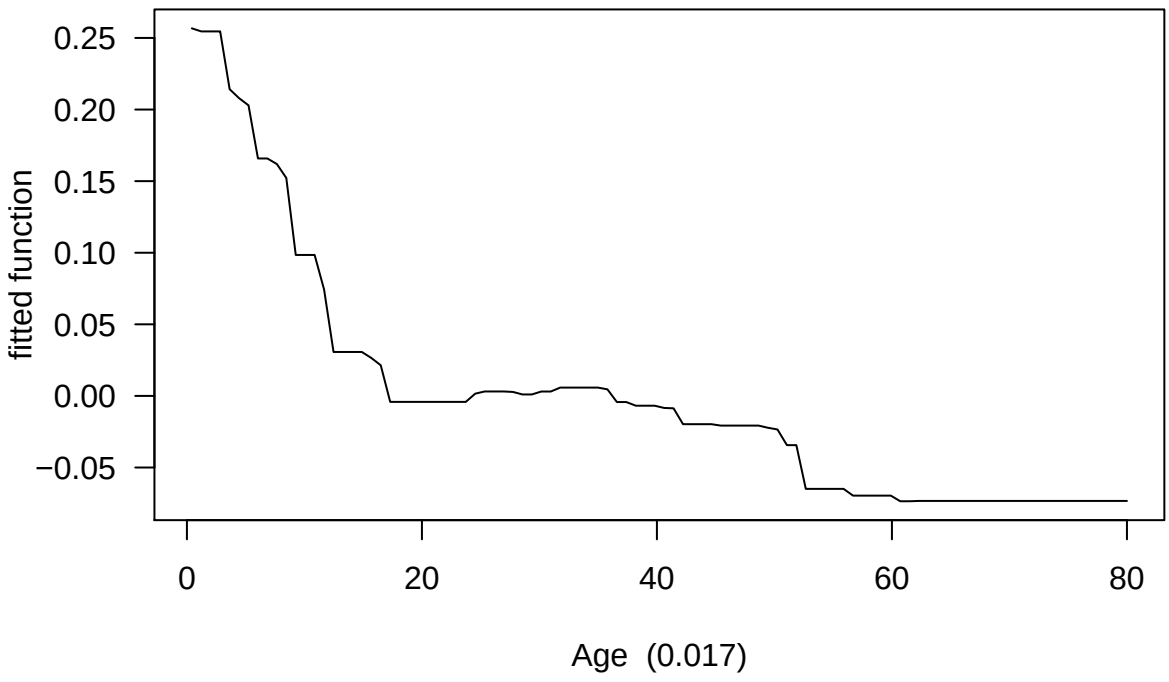

```
RF_UnivariatePlots(object=rf_model1, varimp=model1_importance, data=titanic,  #
                   predictors=pred.names[3], labels=predictorNames[3], allpredictors=pred.names,plot.lay
```




```
RF_UnivariatePlots(object=rf_model1, varimp=model1_importance, data=titanic,  #
                   predictors=pred.names[5], labels=predictorNames[5], allpredictors=pred.names,plot.la
```




```
RF_UnivariatePlots(object=rf_model1, varimp=model1_importance, data=titanic,  #
                   predictors=pred.names[2], labels=predictorNames[2], allpredictors=pred.names,plot.la
```



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

```
# NOTE: this one can take a very long time   ...
rf_findint <- RF_FindInteractions(object=rf_model1,data=titanic,predictors=pred.names)
```

```
## 1  2  3  4
```

```
rf_findint$interactions1
```

```
##       Sex    Age  SibSp  Parch   Fare
## Sex     0 4.1779 6.2339 8.1656 1.1435
## Age     0 0.0000 3.3493 2.0526 0.7259
## SibSp   0 0.0000 0.0000 0.1488 1.5800
## Parch   0 0.0000 0.0000 0.0000 1.1472
## Fare    0 0.0000 0.0000 0.0000 0.0000
```

```
rf_findint$rank.list1
```

Interactions

```
### plot interaction strength

lengthndx <- min(9,nrow(rf_findint$rank.list1))
par(mai=c(0.95,3.1,0.6,0.4))
barplot(height=(rf_findint$rank.list1[c(1:min(9,nrow(rf_findint$rank.list1))),5][c(lengthndx:1)]),
        horiz=T,las=1,main=paste(response, sep=""),
```

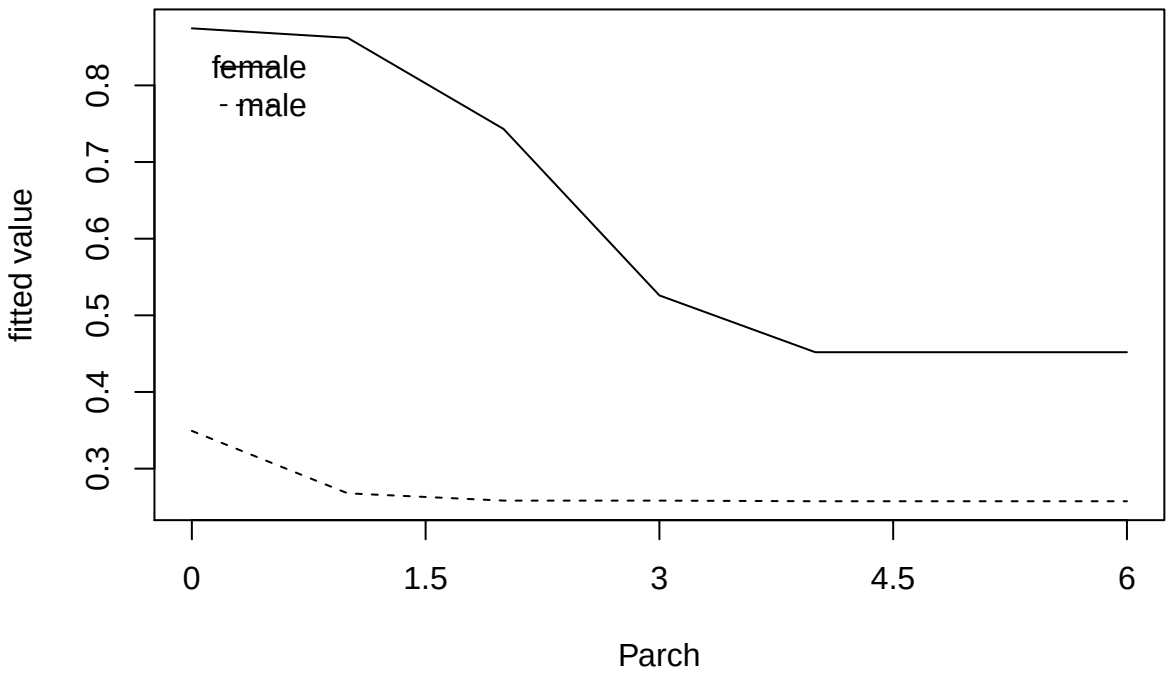
```
        xlab="Index of interaction strength",col=brewer.pal(lengthndx,"Blues"),
        names.arg=paste("",predictorNames[match(rf_findint$rank.list1[,2][c(lengthndx:1)],pred.names)],
```

```
## Warning in brewer.pal(lengthndx, "Blues"): minimal value for n is 3, returning requested palette wit
```

Now let's visualize the interactions:

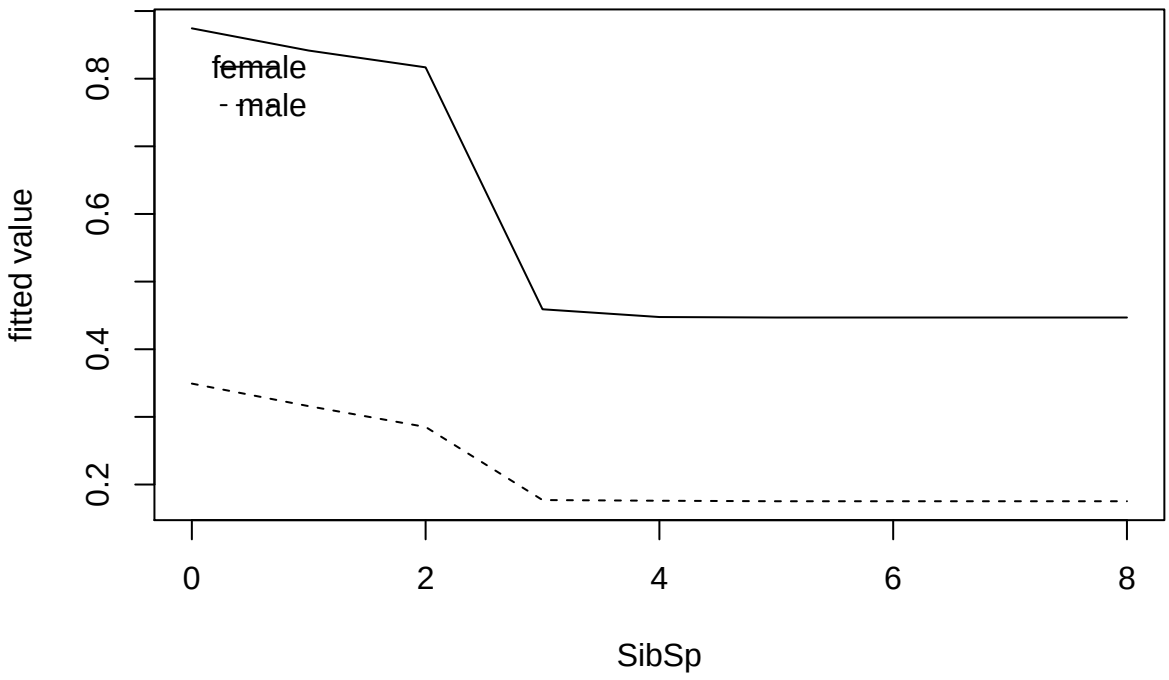
```
rf_findint$rank.list1
fam="binomial"

RF_InteractionPlots(x=1,y=4,object=rf_model1,data=titanic,predictors=pred.names,family=fam)
```

```
## maximum value =  0.87
```



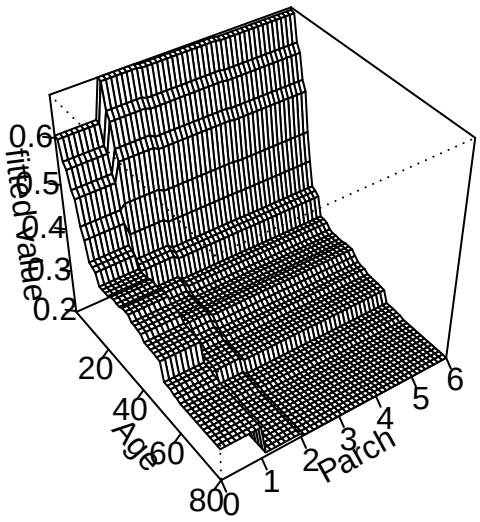

```
RF_InteractionPlots(x=1,y=3,object=rf_model1,data=titanic,predictors=pred.names,family=fam)
```

```
## maximum value =  0.87
```




```
RF_InteractionPlots(x=2,y=4,object=rf_model1,data=titanic,predictors=pred.names,family=fam)
```

```
## maximum value =  0.69
```



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(titanic$Survived)/9))[1:length(titanic$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(titanic)),      # make a data frame for storage
  realprediction = 0,
  realdata = 0
)

for(i in 1:n.folds){
  fit_ndx <- which(foldVector!=i)
  validate_ndx <- which(foldVector==i)
  model <- cforest(formula1, data = titanic[fit_ndx,], controls=cforestControl)
  predict_CV  <- predict(model,newdata=titanic[validate_ndx,],type="prob")
  predict_real  <-  predict(rf_model1,newdata=titanic[validate_ndx,],type="prob")
```

```
  REAL <- titanic$Survived[validate_ndx]
  for(j in 1:length(which(foldVector==i))){
    CV_df$CVprediction[counter] <- as.numeric(predict_CV[[j]][,2])
    CV_df$realprediction[counter] <- as.numeric(predict_real[[j]][,2])
    CV_df$realdata[counter] <- REAL[j]
    counter = counter + 1
  }
}

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")
```

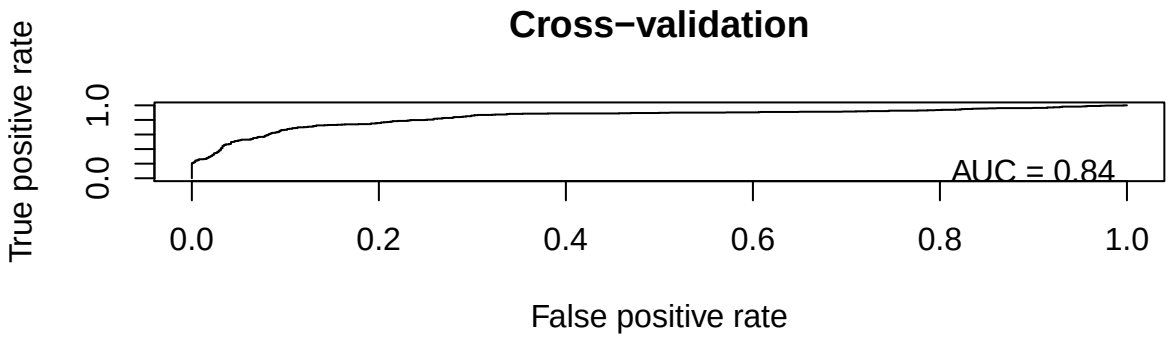
```
## The RMSE for the model under cross-validation is:  0.3748958
```

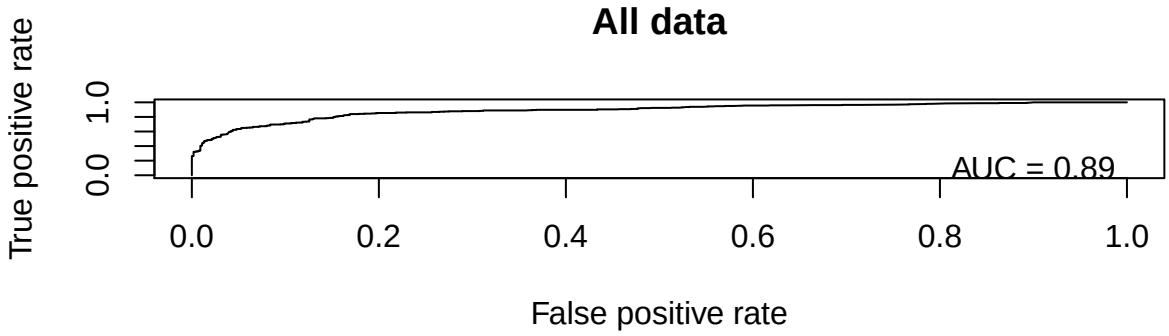
```
cat("The RMSE for the model using all data for training is: ", real_RMSE, "\n")
```

```
## The RMSE for the model using all data for training is:  0.3540952
```

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 the same pseudo-R-squared metric we learned above 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:  0.3349298
```

```
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:  0.3939271
```

[–this is the final regular lecture–]