

# R Notebook

## Exoplanet Classification Problem

For this project, we decided to perform classification on our data set. Classification is a way to predict a label, in our case categorical, based on the characteristics of the data. The

The objective of our project is to use machine learning classification models to determine if a given observation of a star should be classified as an exoplanet (a planet outside our solar system). The original data set comes from the Kepler Space Observatory (<https://www.kaggle.com/nasa/kepler-exoplanet-search-results>), and details 9,564 observations of potential exoplanets, along with 50 descriptive features ranging from identifiers to specific measurements. The column “koi\_disposition” labelled each of the potential exoplanets as either “CONFIRMED,” “FALSE POSITIVE,” or “CANDIDATE”. Those labeled “CANDIDATE” have not yet been determined to be exoplanets or not; the goal of our analysis will be to label them as “CONFIRMED” or “FALSE POSITIVE.”

NOTE: In this context, “false positive” does not indicate a false positive output from our model. Instead, it refers to the original observation, which was considered a candidate, to have been falsely identified as a candidate. A koi\_disposition of “FALSE POSITIVE” indicates that the candidate is not a planet; it is a negative result.

To solve this problem, we will carry out the following process:

1. Load, preprocess, and clean up data
2. Data visualization and exploratory data analysis
3. Creation and testing of candidate models:
  - 3.1) Models using non-scaled data:
    - 3.1.1) Decision Tree, Random Forest, and Support Vector Machine
    - 3.1.2) XGBoost
    - 3.1.3) Logistic Regression
  - 3.2) Models using scaled data:
    - 3.2.1) Neural Network: Original Variables
    - 3.2.2) Neural Network: PCA w/15 Variables
    - 3.2.3) Neural Network: PCA w/20 Variables
    - 3.2.4) K-Nearest Neighbours
    - 3.2.5) K-Means Clustering
4. Select best model
5. Use best model to make predictions

## 1. Data Loading, Pre-Processing and Clean Up

Load Libraries:

```

library(Matrix)      #extra Matrix functionality
library(rpart)       #Decision trees
library(rpart.plot)
library(randomForest)#random forest
library(class)       #KNN
library(e1071)       #misc. stats functionary
library(xgboost)     #XGBoost Algorithm
library(FNN)         #KNN
library(factoextra)  #PCA and clustering
library(ggplot2)     #extra plotting functionality
library(corrplot)    #extra plotting functionality
#visualization packages
library(dplyr)
library(reshape2)
library(tidyverse)
library(DiagrammeR)  #plotting for XGBoost
library(formulaic)   #automated formula creation
library(neuralnet)   #Neural Networks

```

The first step was to load the data, and convert our output variable, “koi\_disposition”, to a factor

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```

#read data
originalKepplerData = read.csv("cumulative.csv") #read data
factored_keppler_data = originalKepplerData
factored_keppler_data$koi_disposition = factor(originalKepplerData$koi_disposition) #factor character data
factored_keppler_data$koi_pdisposition = factor(originalKepplerData$koi_pdisposition)
head(factored_keppler_data)

```

	ro...	kepid	kepoi_na...	kepler_name	koi_disposition	koi_pdisposition	koi_score
	<int>	<int>	<chr>	<chr>	<fctr>	<fctr>	<dbl>
1	1	10797460	K00752.01	Kepler-227 b	CONFIRMED	CANDIDATE	1.000
2	2	10797460	K00752.02	Kepler-227 c	CONFIRMED	CANDIDATE	0.969
3	3	10811496	K00753.01		FALSE POSITIVE	FALSE POSITIVE	0.000
4	4	10848459	K00754.01		FALSE POSITIVE	FALSE POSITIVE	0.000
5	5	10854555	K00755.01	Kepler-664 b	CONFIRMED	CANDIDATE	1.000
6	6	10872983	K00756.01	Kepler-228 d	CONFIRMED	CANDIDATE	1.000

6 rows | 1-9 of 50 columns

Our next step was to conduct forms of dimensionality reduction on our 49 possible input variables. Dimensionality reduction is important for our large data set to reduce the computational requirements of models and reduce possible overfitting or bias from un-important features. First, we removed several entirely empty columns (with values of 0 or NA), unique row identifiers (observation numbers), as well as several which could only be filled once

the outcome of the observation was already known. For example, “kepler\_name” is the name given to a confirmed exoplanet, so it was removed from the data set. There were no unique outlying data points that had to be explored further.

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```

#remove all-NA columns:
remove_KOI_tech_factored = subset(factored_kepler_data, select = -c(koi_teq_err1)) #remove
ove
remove_KOI_tech_factored = subset(remove_KOI_tech_factored, select = -c(koi_teq_err2))
remove_NAs = na.exclude(remove_KOI_tech_factored) #remove any rows with NAs remaining

#Remove unique identifiers and rows that can only be known after the status of a planet
is known. They therefore are not useful inputs to determine the status of a candidate.
identifiers_removed = subset(
  remove_NAs,
  select = -c(
    rowid,
    kepid,
    kepoi_name,
    kepler_name,
    koi_pdisposition,
    koi_score
  )
)

#Also needs to remove flags, these can only be known after status is confirmed
identifiers_removed = subset(
  identifiers_removed,
  select = -c(
    koi_fpflag_ss,
    koi_fpflag_ec,
    koi_fpflag_co,
    koi_fpflag_nt,
    koi_tce_plnt_num,
    koi_tce_delivname
  )
)

#Now, we will separate in labeled and unlabeled data. The labeled data will be used to t
rain our model; once the best model is selected, we will use it to predict the labels of
the unlabeled dataset
candidates_final = identifiers_removed[identifiers_removed$koi_disposition ==
                                     "CANDIDATE",] #separate out just the candidates
labeled_final = identifiers_removed[identifiers_removed$koi_disposition !=
                                    "CANDIDATE",]
labeled_final = droplevels(labeled_final)
candidates_final = droplevels(candidates_final)

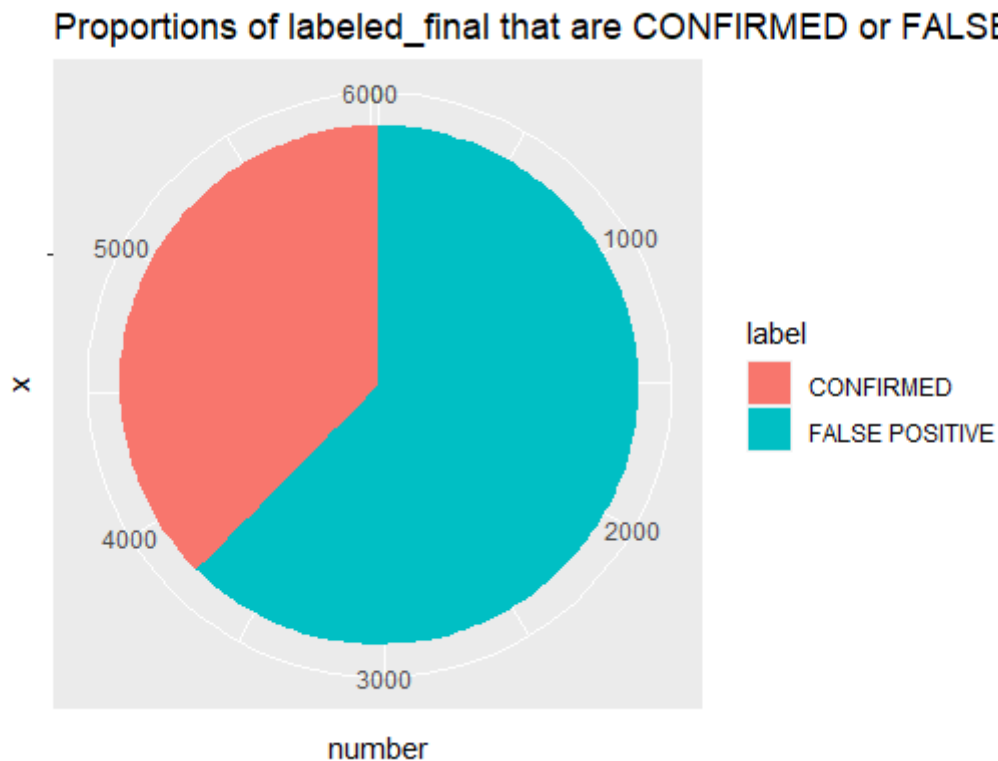
numFalse = sum(labeled_final$koi_disposition=="FALSE POSITIVE")
numConfirmed = sum(labeled_final$koi_disposition=="CONFIRMED")
##check
numFalse + numConfirmed == dim(labeled_final)[1]

```

```
[1] TRUE
```

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```
Proportions = data.frame(label = c("CONFIRMED","FALSE POSITIVE"), number = c(numConfirmed,numFalse))
bp = ggplot(Proportions,aes(x = "",y=number,fill=label))+geom_bar(width = 1,stat = "identity")
pie = bp+coord_polar("y", start = 0) + ggtitle("Proportions of labeled_final that are CONFIRMED or FALSE POSITIVE")
pie
```



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```
head(labeled_final)
```

koi_disposition <fctr>	koi_period <dbl>	koi_period_err1 <dbl>	koi_period_err2 <dbl>	koi_time0bk <dbl>	koi_time0b
1 CONFIRMED	9.488036	2.775e-05	-2.775e-05	170.5387	0.0
2 CONFIRMED	54.418383	2.479e-04	-2.479e-04	162.5138	0.0
3 FALSE POSITIVE	19.899140	1.494e-05	-1.494e-05	175.8503	0.0
4 FALSE POSITIVE	1.736952	2.630e-07	-2.630e-07	170.3076	0.0
5 CONFIRMED	2.525592	3.761e-06	-3.761e-06	171.5956	0.0
6 CONFIRMED	11.094321	2.036e-05	-2.036e-05	171.2012	0.0

6 rows | 1-7 of 36 columns

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```
head(candidates_final)
```

koi_disposition <fctr>	koi_period <dbl>	koi_period_err1 <dbl>	koi_period_err2 <dbl>	koi_time0bk <dbl>	koi_time0
38 CANDIDATE	4.959319	5.150e-07	-5.150e-07	172.2585	8
59 CANDIDATE	40.419504	1.139e-04	-1.139e-04	173.5647	2
63 CANDIDATE	7.240661	1.617e-05	-1.617e-05	137.7554	2
64 CANDIDATE	3.435916	4.729e-05	-4.729e-05	132.6624	1
73 CANDIDATE	1.626630	1.015e-06	-1.015e-06	169.8202	4
85 CANDIDATE	10.181584	6.188e-06	-6.188e-06	177.1419	4

6 rows | 1-7 of 36 columns

We are left with two datasets:

- candidates\_final, which has 1772 data points and 35 features, which will be what we use the best model on
- labeled\_final, which has 6031 data points and 35 features, which will be what we use to train and test candidate models, as well as build our final model.

## 2) Data Visualization and Exploratory Data Analysis

Select the variables to be used:

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```
#All variables have errors - for exploratory data analysis we will only be looking at the
#variables themselves, not their errors
variablesonly = labeled_final %>%
  select(koi_period, koi_time0bk, koi_impact, koi_duration, koi_depth, koi_prad, koi_te
q, koi_insol, koi_model_snr, koi_steff, koi_slogg, koi_srad, ra, dec, koi_kepmag)
```

Create a correlation heat map with only the variables (excluding the errors).

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```
cormat <- round(cor(variablesonly),2)
head(cormat)
```

```

      koi_period koi_time0bk koi_impact koi_duration koi_depth
koi_period      1.00      0.60      -0.03      0.33      -0.05
koi_time0bk      0.60      1.00      0.02      0.20      -0.05
koi_impact      -0.03      0.02      1.00      0.06      0.02
koi_duration      0.33      0.20      0.06      1.00      0.09
koi_depth      -0.05      -0.05      0.02      0.09      1.00
koi_prad      -0.01      -0.01      0.54      0.02      0.08

      koi_prad koi_teq koi_insol koi_model_snr koi_steff koi_slogg
koi_period   -0.01  -0.35   -0.02      -0.04      0.01   -0.04
koi_time0bk   -0.01  -0.28   -0.02      -0.04     -0.01    0.02
koi_impact     0.54   0.05   -0.01      0.03      0.08   -0.03
koi_duration   0.02  -0.19   -0.02      0.10      0.10   -0.13
koi_depth     0.08   0.06   -0.01      0.60      0.15   -0.03
koi_prad      1.00   0.12    0.05      0.05     -0.01   -0.17

      koi_srad   ra   dec koi_kepmag
koi_period    0.01 -0.05  0.02     -0.02
koi_time0bk   -0.01 -0.03  0.00      0.03
koi_impact     0.00  0.07 -0.03      0.02
koi_duration   0.02  0.04 -0.03     -0.10
koi_depth     -0.02  0.02 -0.01      0.00
koi_prad      0.19  0.03  0.00     -0.01

```

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```

melted_cormat <- melt(cormat)
head(melted_cormat)

```

	Var1 <fctr>	Var2 <fctr>	value <dbl>
1	koi_period	koi_period	1.00
2	koi_time0bk	koi_period	0.60
3	koi_impact	koi_period	-0.03
4	koi_duration	koi_period	0.33
5	koi_depth	koi_period	-0.05
6	koi_prad	koi_period	-0.01

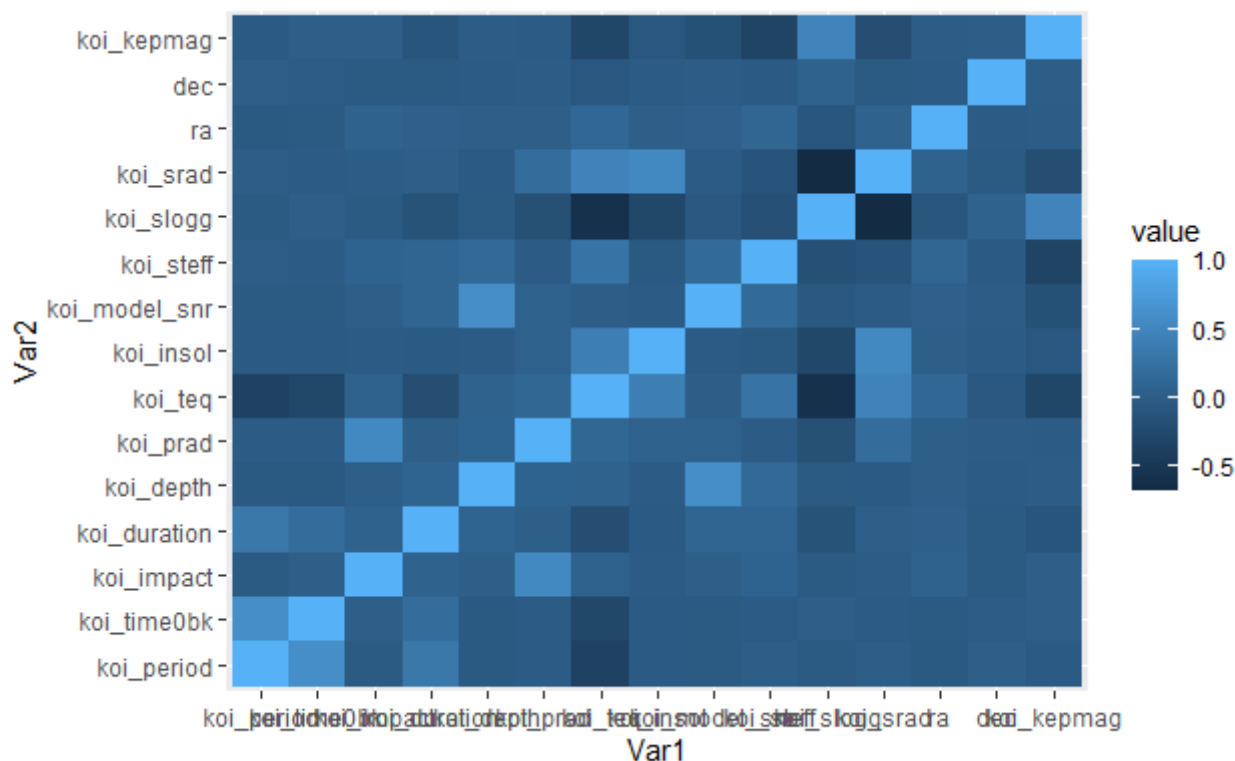
6 rows

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```

ggplot(data = melted_cormat, aes(x=Var1, y=Var2, fill=value)) +
  geom_tile()

```



Defining significant correlations as those greater than .4, there are a few; this will need to be dealt with in Logistic Regression, but should not affect other models.

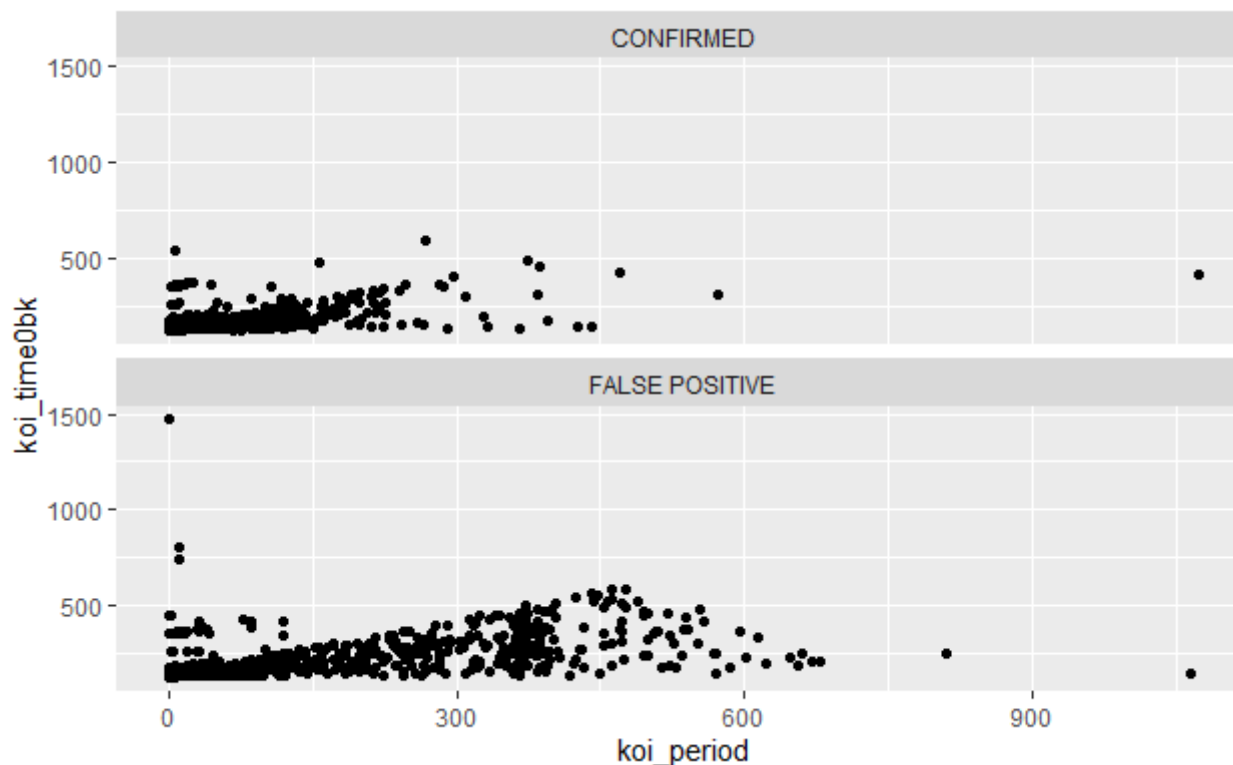
## Plots by FALSE POSITIVE and CONFIRMED

We will now observe the distribution of several variables across false positive and confirmed exoplanets. This will help determine where there is a clear pattern in certain variables.

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```
ggplot(data = labeled_final) +
  geom_point(mapping = aes(x = koi_period, y = koi_time0bk)) +
  facet_wrap(~ koi_disposition, nrow = 2)
```





For koi\_period and koi\_time0bk, the distributions of the variables seem similar, with some outliers. That being said, FALSE POSITIVES can have significantly higher koi\_periods than CONFIRMEDs

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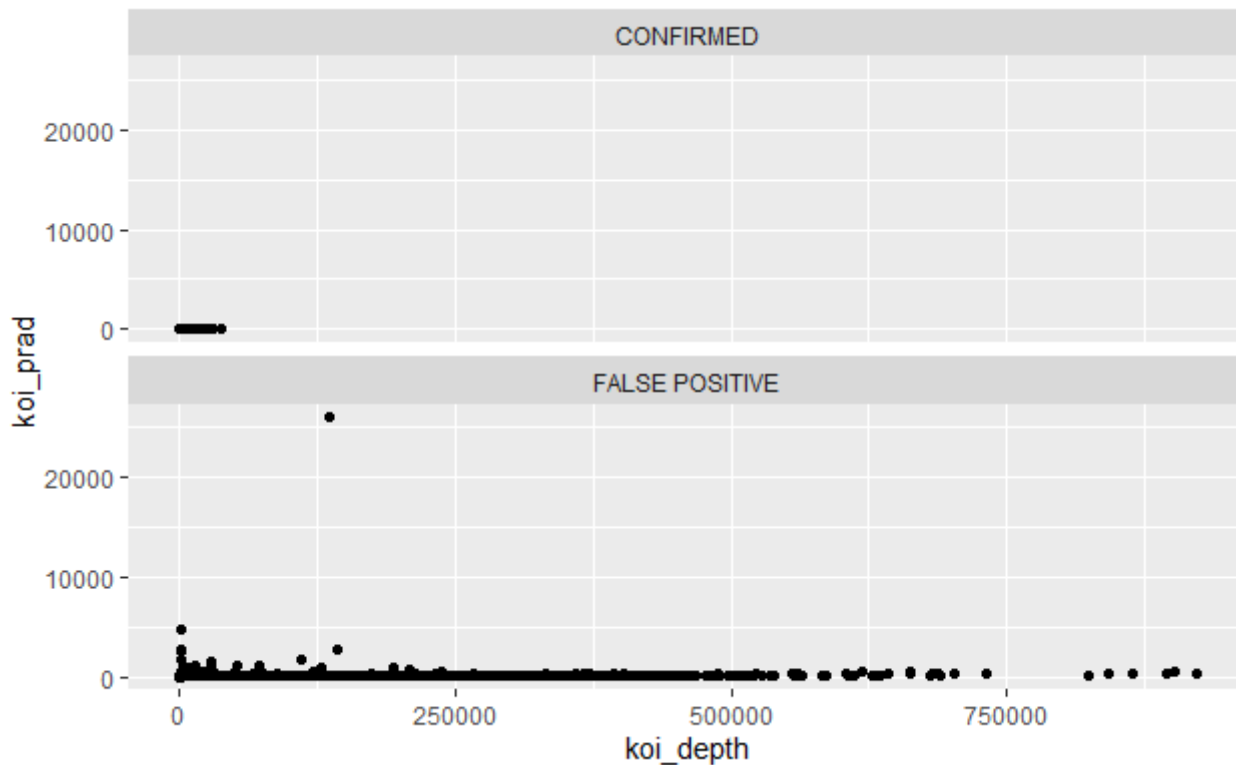
```
ggplot(data = labeled_final) +  
  geom_point(mapping = aes(x = koi_impact, y = koi_duration)) +  
  facet_wrap(~ koi_disposition, nrow = 2)
```



The plot of koi\_impact vs. koi\_duration shows clear differences between their distributions - CONFIRMEDs have a significantly small range for both variables, although those candidates that fall inside that range may be difficult to classify.

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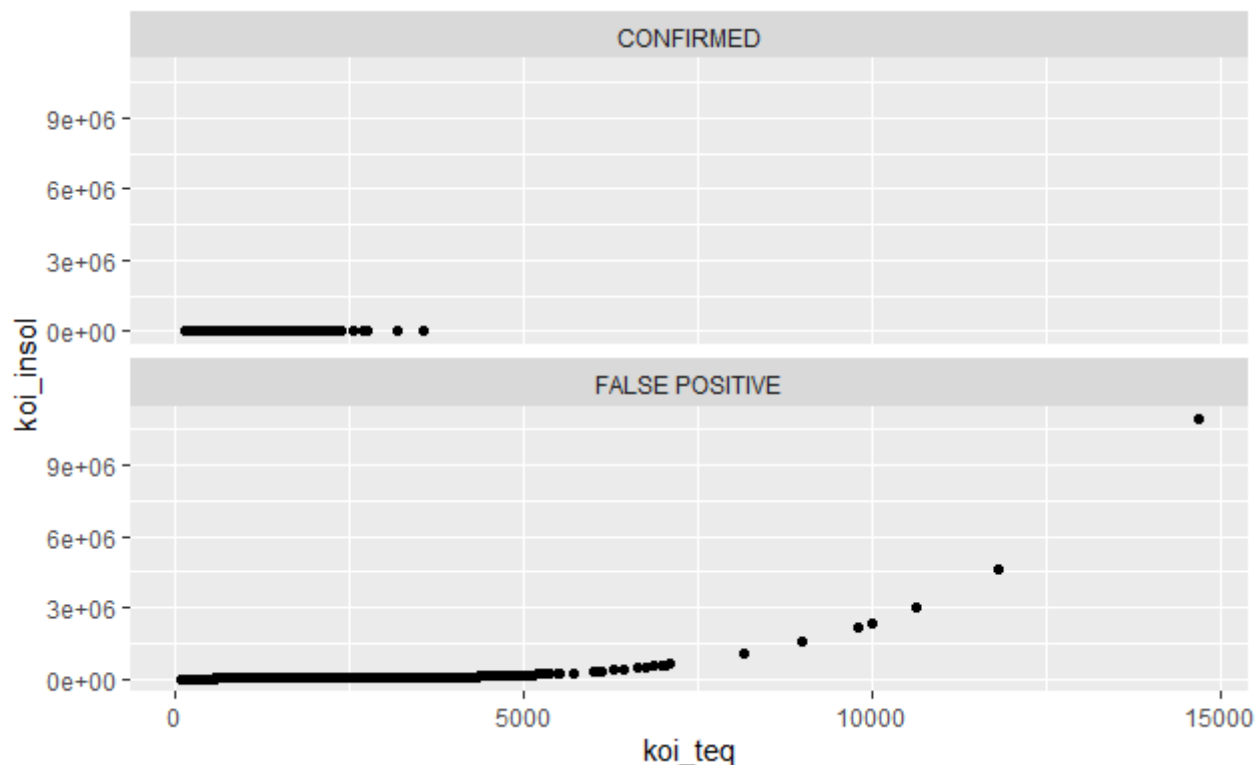
```
ggplot(data = labeled_final) +
  geom_point(mapping = aes(x = koi_depth, y = koi_prad)) +
  facet_wrap(~ koi_disposition, nrow = 2)
```



koi\_depth shows a clear difference: high koi\_depths almost always indicate FALSE POSITIVES

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```
ggplot(data = labeled_final) +
  geom_point(mapping = aes(x = koi_teq, y = koi_insol)) +
  facet_wrap(~ koi_disposition, nrow = 2)
```



koi\_teq has a significantly smaller range for CONFIRMED data points, and KOI\_insol stays closer to zero. If we look at

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```
summary(labeled_final$koi_insol)
```

Min.	1st Qu.	Median	Mean	3rd Qu.	Max.
0	36	219	8148	1332	10947555

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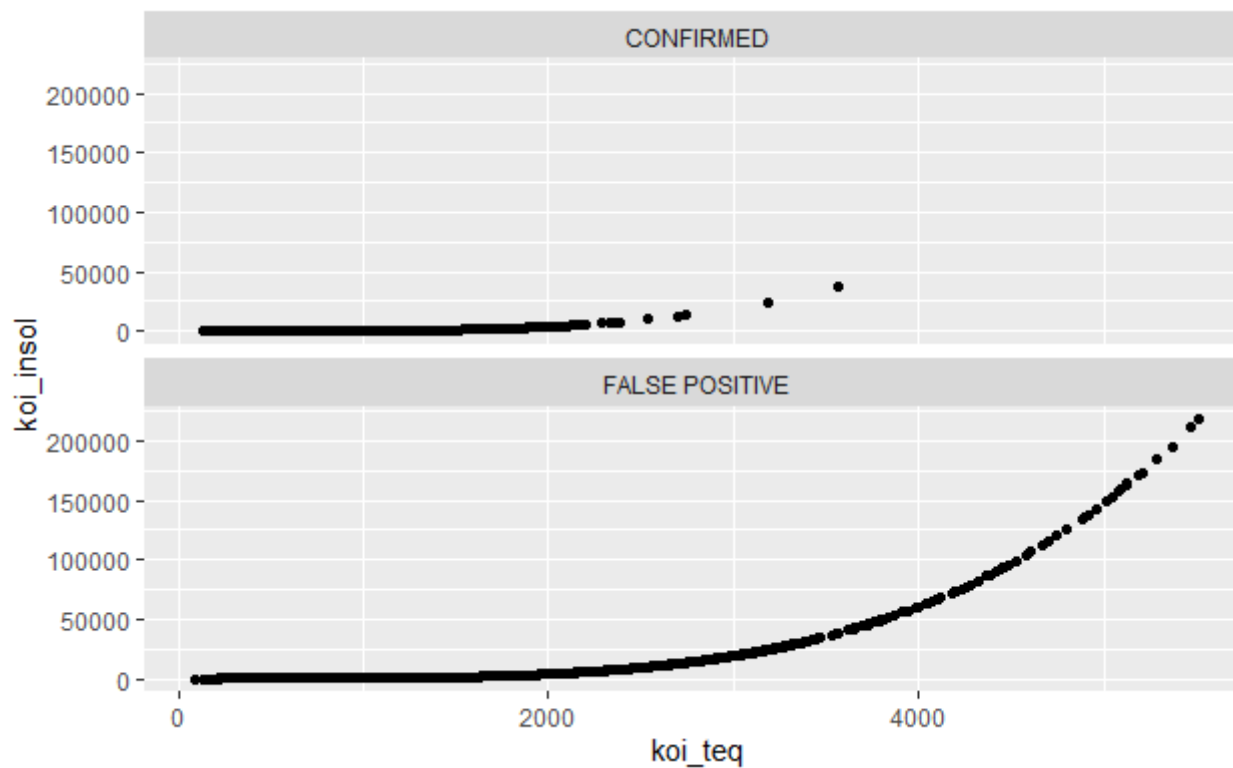
```
summary(labeled_final$koi_teq)
```

Min.	1st Qu.	Median	Mean	3rd Qu.	Max.
92	626	981	1192	1540	14667

This confirms that there are very large values for FALSE POSITIVES that are significantly outside the normal data range. It will be easy to classify these as FALSE POSITIVES. We can explore these graphs with a smaller range, to exclude the outliers:

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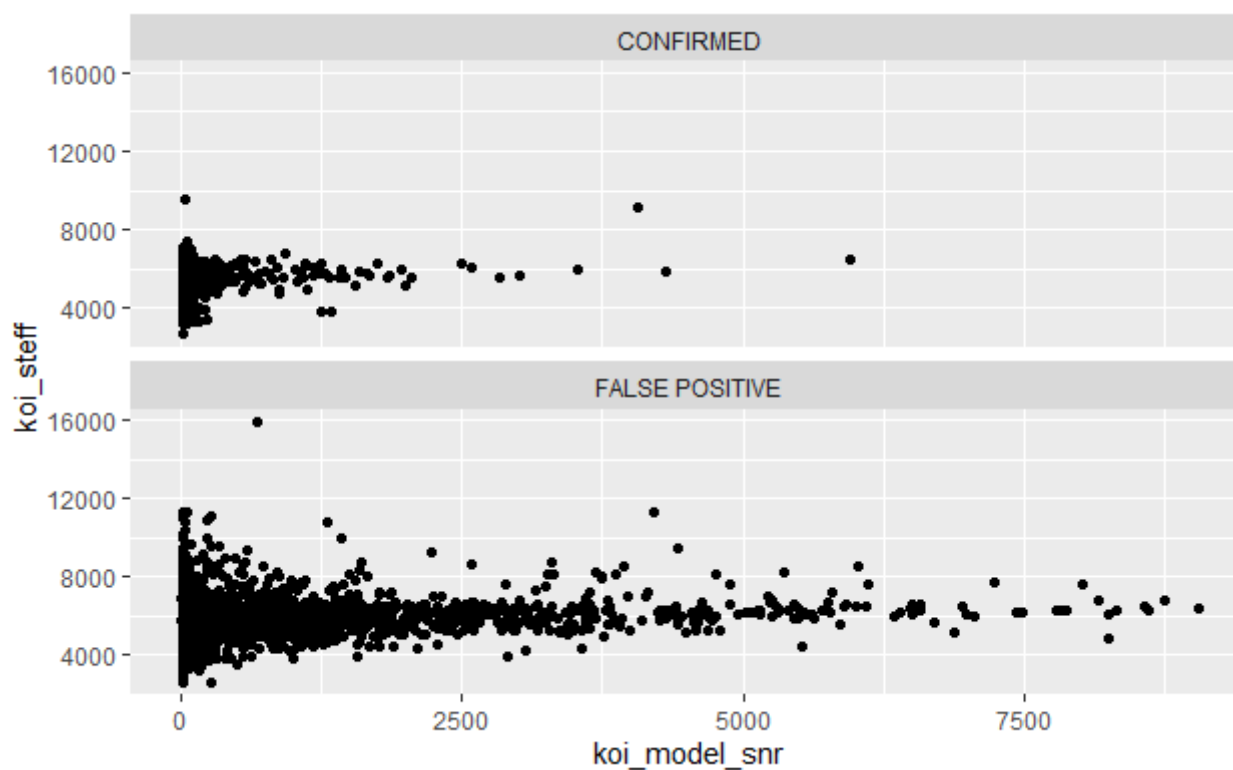
```
ggplot(data = labeled_final[labeled_final$koi_insol<250000,]) +
  geom_point(mapping = aes(x = koi_teq, y = koi_insol)) +
  facet_wrap(~ koi_disposition, nrow = 2)
```



This shows that for values of  $koi\_insol < 25000$  and  $koi\_teq < 3000$ , it becomes difficult to identify whether a given data point is FALSE POSITIVE or CONFIRMED.

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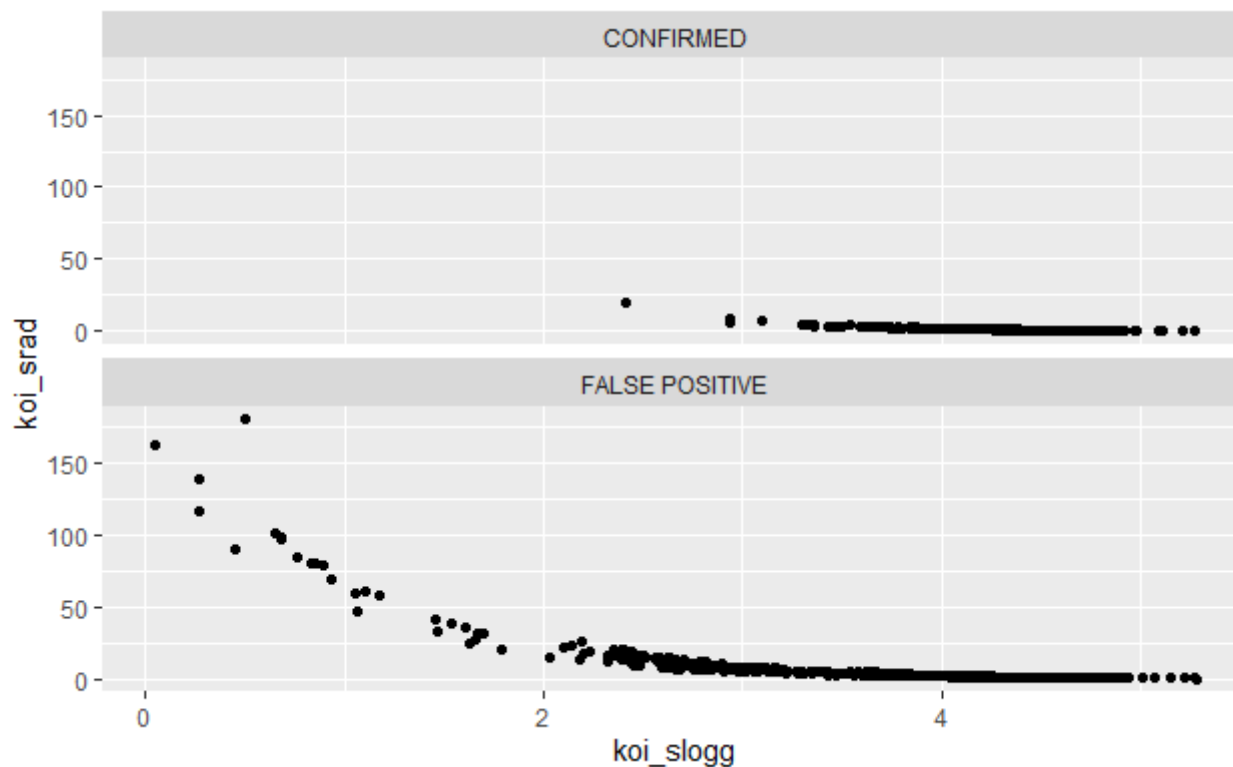
```
ggplot(data = labeled_final) +
  geom_point(mapping = aes(x = koi_model_snr, y = koi_steff)) +
  facet_wrap(~ koi_disposition, nrow = 2)
```



Once again, FALSE POSITIVES show significantly more variability on both axes than CONFIRMEDs

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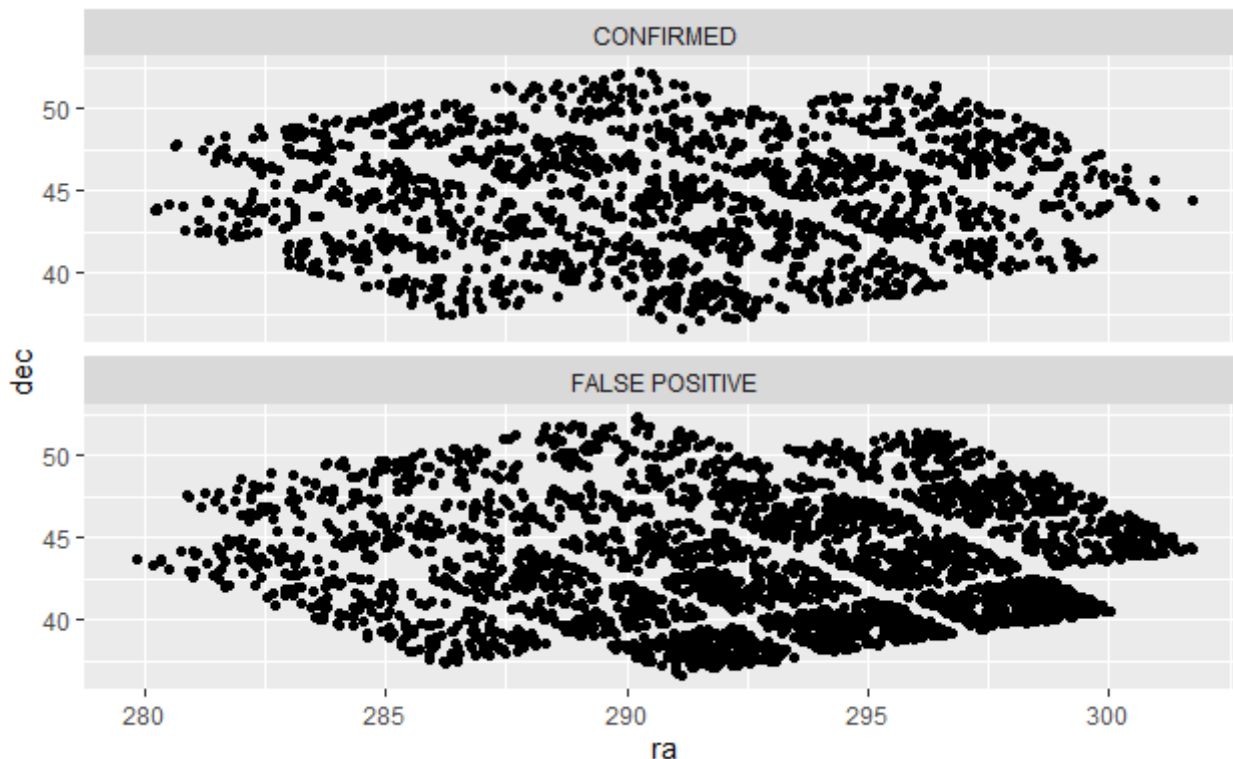
```
ggplot(data = labeled_final) +  
  geom_point(mapping = aes(x = koi_slogg, y = koi_srad)) +  
  facet_wrap(~ koi_disposition, nrow = 2)
```



FALSE POSITIVES can have significantly lower koi\_sloggs and higher koi\_srad than CONFIRMEDs

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```
ggplot(data = labeled_final) +  
  geom_point(mapping = aes(x = ra, y = dec)) +  
  facet_wrap(~ koi_disposition, nrow = 2)
```



Lastly, for ra and dec, there is no clear different in distribution for CONFIRMED or FALSE POSITIVE.

Overall, an easy way to determine FALSE POSITIVES tends to be to look for data points outside a given range. Inside that range, the determination of whether an observation is an exoplanet or not becomes more difficult.

### 3. Creation and testing of candidate models

To classify the data and determine which observations are, in fact, planets, our group first had to determine which model most accurately predicted our labeled data set. We first examined models that did not require scaling, these included: Decision Tree, Random Forest, XGBoost, Logistic Regression, and Support Vector Machines (SVM). Next, we examined models that required scaling, these included: KNN, Neural Network (with and without Principal Component Analysis), and K-means clustering. To choose the best model for our data set, our group decided to look at which model produced the lowest misclassification rate. However, it should be noted that in real-life application a number of other metrics should be considered as well. These include, but are not limited to, precision analysis (PR curves), recall, ROC-AUC, and F1 Scores.

When running the various models, our group incorporated K-fold cross-validation. The benefit of this approach is that it allows the model to become more generalized, helping with over-fitting concerns. In addition, we take the average result of five misclassification rates for each model, significantly lowering the chance that a given misclassification rate is produced only by chance due to a specific testing/training set. This allows us to be more confident that the model with the lowest misclassification rate truly is the best. Due to computational limits, we decided to use a K value of 5 as we believed that would be adequate for our purposes. Finally, when deciding the proportion of training and testing set, we decided to follow class standards with 80% training set and 20% testing set. Our specific data set is fairly large with ~6,031 rows; we believe having ~4,800 rows to train and ~1,200 rows to test is large enough for each purpose.

#### 3.1) Models using non-scaled data:

We first wanted to create a “baseline” model - that is, a model that predicts the average proportions of our training set every time. This will give a baseline misclassification rate that we are trying to beat.

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```
set.seed(123)
num_samples = dim(labeled_final)[1]
sampling.rate = 0.8
training = sample(1:num_samples, sampling.rate * num_samples, replace = FALSE)
trainingSet = subset(labeled_final[training,])
testing = setdiff(1:num_samples, training)
testingSet = subset(labeled_final[testing, ])
sizeTrainingSet = dim(trainingSet)[1]
sizeTestingSet = dim(testingSet)[1]
propC = sum(trainingSet[, 1] == "CONFIRMED") / sizeTrainingSet #the proportion of the training set that is confirmed
naivePredictions = sample(
  c("CONFIRMED", "FALSE POSITIVE"),
  sizeTestingSet,
  replace = TRUE,
  prob = c(propC, 1 - propC)
) #predict taking a random sample, with the same proportions as the training set

Errors = sum(testingSet$koi_disposition != naivePredictions)
ErrorRateNaive = Errors / sizeTestSet
paste("Naive Error Rate: ", round(ErrorRateNaive * 100, 2), "%", sep = "")
```

```
[1] "Naive Error Rate: 46.73%"
```

This “naive” method, which makes predictions based purely off proportions and chance, gives an error rate of 46.73%. This is the “number to beat” for the rest of our models.

### 3.1.1) Decision Tree, Random Forest, and SVM

The goal of a decision tree is to make splitting decisions on the data, in an effort to minimize the least squares, thus creating a tree-like structure. These models are useful as a starting point because they are easy to interpret as the plot can display which variables have the highest importance in the tree. Normalization and other data cleaning is also not required for this model. Adding more depth to the tree can reduce the fitting error to the data, but it can lead to overfitting the model. As a result, the complexity parameter, *cp*, must be tuned to ensure that the optimal depth-to-fit of the model is used. As the *cp* value decreases, so does the relative error in the model. We automatically prune our decision tree to select the *cp* where the change in error is less than 0.05; this is our first example of parameter tuning.

Random forest models are more accurate and robust but harder to interpret than a single tree. The model creates many decision trees with different randomized learning and testing sets, then the trees “vote” or “average” their results to determine the resultant random forest model. Though the model is not as interpretable as a single tree and it is more difficult to understand the significance of a single variable, it will result in lower misclassification rate. The number of trees in the forest is a parameter that needs to be tuned in this model. As the number of trees increases, the error decreases exponentially, reaching an asymptote of error.

SVM models are supervised learning models that use the data points to create a line to separate the data. This separation then decides the binary classification for each data point. While this model can be incredibly versatile and robust against outliers and inaccurate data, it may not be as accurate if there is much overlap between the data.

Helper Function:

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```
AllErrors = function(correctResults,
                      predictedResults,
                      sizeTestSet, numerical = 0) {
  isWrong = (correctResults != predictedResults)
  isRight = (correctResults == predictedResults)
  Errors = sum(correctResults != predictedResults)
  ErrorRate = Errors / sizeTestSet

  if (numerical == 0) {
    IsC = (predictedResults == 'CONFIRMED')
    IsF = (predictedResults == 'FALSE POSITIVE')
  }else{
    IsC = (predictedResults == 1)
    IsF = (predictedResults == 0)
  }

  FalsePositives = sum(isWrong & IsC)
  FalseNegatives = sum(isWrong & IsF)
  TruePositives = sum(isRight & IsC)
  TrueNegatives = sum(isRight & IsF)
  FP_Rate = (FalsePositives / (FalsePositives + TrueNegatives))#define FP rate as FP/(FP
+TN)
  FN_Rate = (FalseNegatives / (FalseNegatives + TruePositives))#define FN rate as FN/(FN
+TP)
  return(list(ErrorRate, FP_Rate, FN_Rate))
}
```

Code for decision tree, random forest, and SVM:

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```
NumFolds = 5
CreateErrorMatrix = function(numFolds) {
  return(rep(0, numFolds))
}

decTree_Error = CreateErrorMatrix(NumFolds)
decTree_FP = CreateErrorMatrix(NumFolds)
decTree_FN = CreateErrorMatrix(NumFolds)

RF_error = CreateErrorMatrix(NumFolds)
RF_error_FP = CreateErrorMatrix(NumFolds)
RF_error_FN = CreateErrorMatrix(NumFolds)
SVM_error = CreateErrorMatrix(NumFolds)
SVM_error_FP = CreateErrorMatrix(NumFolds)
SVM_error_FN = CreateErrorMatrix(NumFolds)
for (fold in 1:NumFolds) {
  #set up k-crossfold validation
  set.seed(fold)

  #split data into testing and training sets
  num_samples = dim(labeled_final)[1]
  sampling.rate = 0.8
  training = sample(1:num_samples, sampling.rate * num_samples, replace = FALSE)
  trainingSet = subset(labeled_final[training, ])
  testing = setdiff(1:num_samples, training)
  testingSet = subset(labeled_final[testing,])

  #Decision tree
  decTreeModel = rpart(koi_disposition ~ ., data = trainingSet)

  #Automatically select the stopping point where cp no longer improves error by 0.05
  errors = decTreeModel$cptable[, 3]
  decTreeChangeError = c(0, 0, 0, 0, 0, 0, 0, 0, 0, 0)
  for (i in 1:8) {
    decTreeChangeError[i] = errors[i + 1] - errors[i]
  }
  decTreeChangeError
  for (i in 1:9) {
    if (abs(decTreeChangeError[i]) < 0.05) {
      stopIndex = i
      break
    }
  }
  cps = decTreeModel$cptable[, 1]
  cpStop = cps[stopIndex]
```

```

prunedDecTreeModel = rpart::prune(decTreeModel, cp = cpStop) #Prune decision tree
decTreePredictions = predict(prunedDecTreeModel, testingSet, type = "class") #make pre
dictions
#Determine decision tree error
sizeTestSet = dim(testingSet)[1]
decTreeModel_errors = AllErrors(testingSet$koi_disposition,
                                decTreePredictions,
                                sizeTestSet)

decTree_Error[fold] = decTreeModel_errors[[1]]
decTree_FP[fold] = decTreeModel_errors[[2]]
decTree_FN[fold] = decTreeModel_errors[[3]]
#Random Forest
RandForestModel = randomForest(koi_disposition ~ ., data = trainingSet, ntrees = 200,
importance = TRUE)#visual inspection gives this as a good number for trees

predictedLabels = predict(RandForestModel, testingSet)

#Determine Random Forest Error
sizeTestSet = dim(testingSet)[1]
RF_Errors = AllErrors(testingSet$koi_disposition, predictedLabels, sizeTestSet)

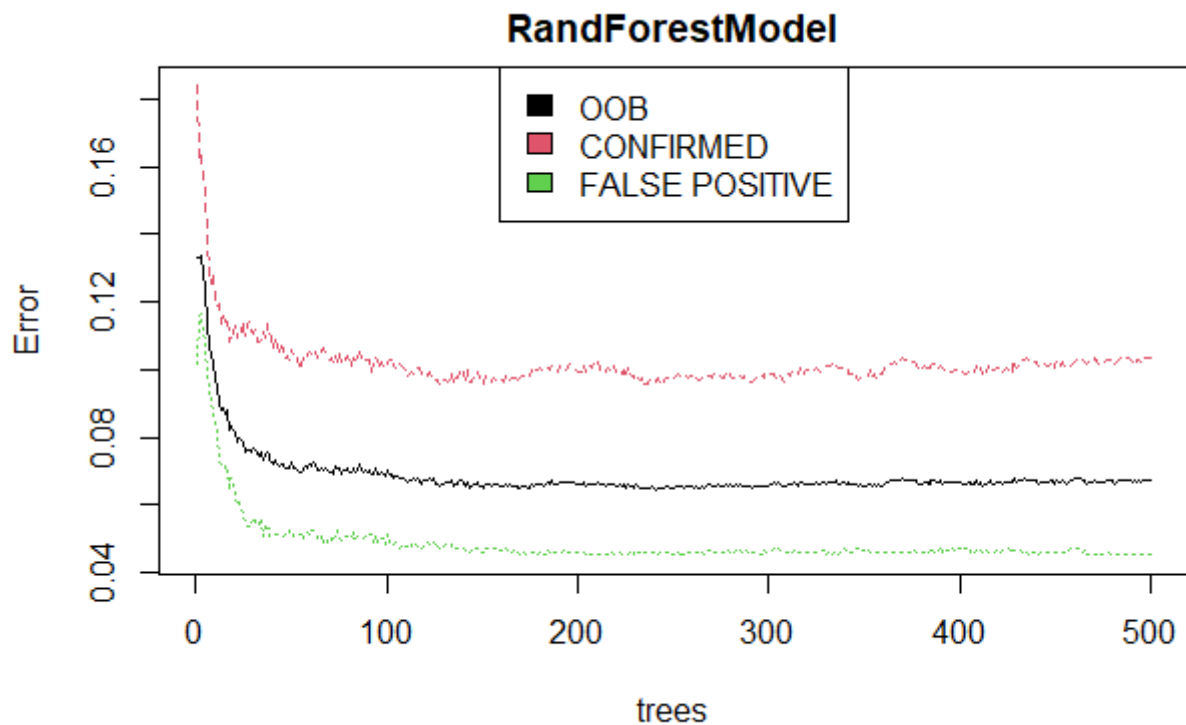
RF_error[fold] = RF_Errors[[1]]
RF_error_FP[fold] = RF_Errors[[2]]
RF_error_FN[fold] = RF_Errors[[3]]

#SVM Model
svmModel = svm(koi_disposition ~ ., data = trainingSet, kernel = "linear")
predictedlabelsSVM = predict(svmModel, testingSet)
#Determine SVM error
SVM_Errors = AllErrors(testingSet$koi_disposition,
                        predictedlabelsSVM,
                        sizeTestSet)

errorSVM = sum(predictedlabelsSVM != testingSet$koi_disposition)
misclassification_rateSVM = errorSVM / sizeTestSet
SVM_error[fold] = SVM_Errors[[1]]
SVM_error_FP[fold] = SVM_Errors[[2]]
SVM_error_FN[fold] = SVM_Errors[[3]]
}
#Show varimp plot and error plot of 1, example random forest

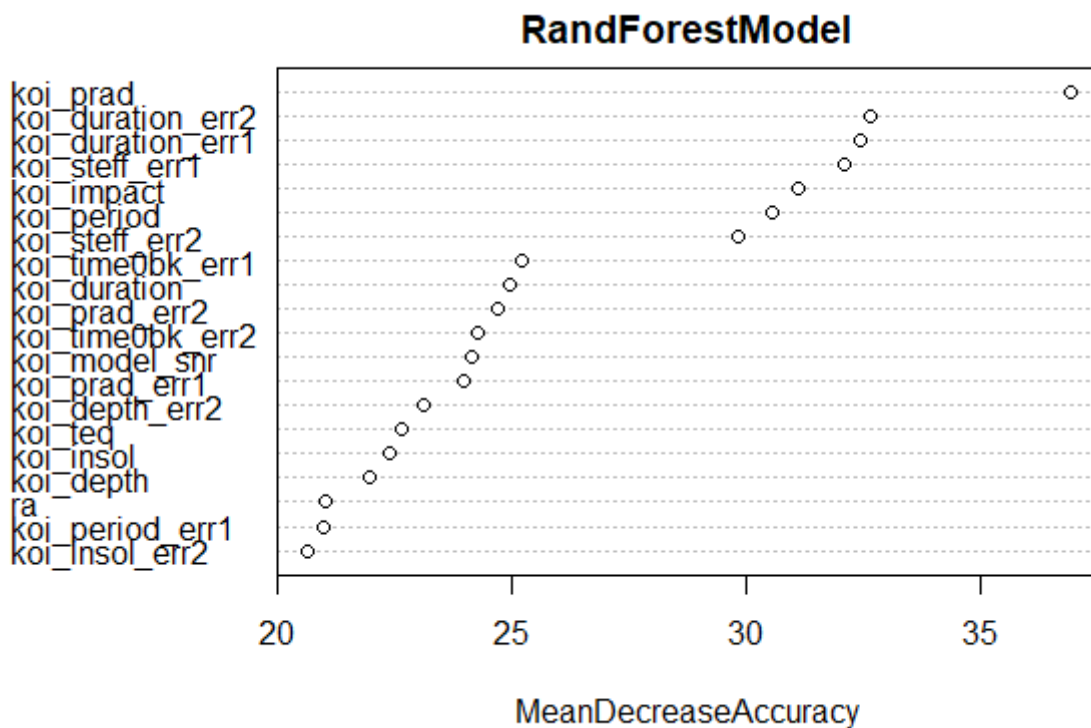
plot(RandForestModel) #the error stabilizes around 200 trees; this is why this is the nu
mber we chose to use
legend("top", colnames(RandForestModel$serr.rate), fill = 1:3)

```



Hide

```
varImpPlot(RandForestModel, type = 1, n.var = 20) #This shows that, for random forest, the most important variables are prad and the errors on duration. This shows that the importance of errors is actually quite high, which is not what would be intuitively expected. To better triage variable importance in models that cannot use all of the variables for computational reasons, (Neural Networks), we will therefore use PCA to reduce dimensionality
```



Hide

```
#Take average of errors from each fold to determine average error for each model
```

```
AvgErrorDT = mean(decTree_Error)
AvgFP_DT = mean(decTree_FP)
AvgFN_DT = mean(decTree_FN)
AvgErrorRF = mean(RF_error)
AvgFP_RF = mean(RF_error_FP)
AvgFN_RF = mean(RF_error_FN)
AvgErrorSVM = mean(SVM_error)
AvgFP_SVM = mean(SVM_error_FP)
AvgFN_SVM = mean(SVM_error_FN)
```

```
paste("DT Error: ", round(100 * AvgErrorDT, 2), "%", sep = "")
```

```
[1] "DT Error: 11.58%"
```

Hide

```
paste("RF Error: ", round(100 * AvgErrorRF, 2), "%", sep = "")
```

```
[1] "RF Error: 6.66%"
```

Hide

```
paste("SVM Error: ", round(100 * AvgErrorSVM, 2), "%", sep = "")
```

```
[1] "SVM Error: 8.7%"
```

All three models give low misclassification rates <12%, but Random Forest gives the best misclassification rate at only 6.74%.

## 3.1.2) XGBoost

XGBoost stands for “extreme gradient boosting” and is an open-source tree learning algorithm similar to random forests that is also widely used in industry. This model seeks to minimize an objective function representing model complexity and loss (error), using a gradient descent algorithm to minimize loss when adding new models. This is known as tree boosting; random forest models differ because they use a tree bagging algorithm, possibly leading to different model accuracies.

XGBoost outputs a probability between 0 and 1, rather than a binary classification. For this reason, it is necessary to determine the “threshold” where a value stops being a FALSE POSITIVE, and start being a CONFIRMED. Questioning the classification threshold which is built into our models can help us develop more accurate models. For example, arbitrarily assuming that the threshold for classifying based on our XGBoost model was exactly 0.5 could have resulted in a higher misclassification rate if we were to consider all possible thresholds. As a result, we

conducted threshold analysis on all our models that output probabilities by looping through all classification thresholds at 0.1 increments, plotted them against their respective misclassification rates, and took the minimum as the optimal. The first model that we have done this for is XGBoost.

[Hide](#)

```
xgb.set.config(verbosity = 0)
```

```
[1] TRUE
```

[Hide](#)

```

threshold = 0.1
XGBoost_error_thresholds = rep(0, 10)
XGBoost_FP_thresholds = rep(0,10)
XGBoost_FN_thresholds = rep(0,10)
index = 1

while (threshold < 1) {
  #loop that reruns the algorithm with increments of 0.1 in the threshold
  XGB_error = CreateErrorMatrix(NumFolds)
  XGB_FNs = CreateErrorMatrix(NumFolds)
  XGB_FPs = CreateErrorMatrix(NumFolds)
  for (fold in 1:NumFolds) {
    #k cross-fold validation
    set.seed(fold)

    num_samples = dim(labeled_final)[1]

    #create testing and training set
    sampling.rate = 0.8
    training = sample(1:num_samples, sampling.rate * num_samples, replace = FALSE)
    trainingSet = subset(labeled_final[training,])
    testing = setdiff(1:num_samples, training)
    testingSet = subset(labeled_final[testing, ])

    #XGBoost model
    xgTrain = data.matrix(trainingSet)
    xgTrain[, 1] = ifelse(xgTrain[, 1] == 2, 1, 0)

    xgBoostModel = xgboost(
      data = xgTrain[, 2:36],
      label = xgTrain[, 1],
      max.depth = 6,
      eta = .22,
      nrounds = 100,
      verbose = 0,
      objective = "binary:logistic",
      eval_metric="error"
    )
    xgTest = data.matrix(testingSet)
    xgTest[, 1] = ifelse(xgTest[, 1] == 2, 1, 0)

    #make predictions
    BoostPredictions = predict(xgBoostModel, data.matrix(testingSet)[, 2:36])

    BoostPredictionsRounded = ifelse(BoostPredictions > threshold, 1, 0) #convert probab
ilities to ouputs of 1 or 0 based on whether they are greater than the threshold - this
is where parameter tuning occurs.

```

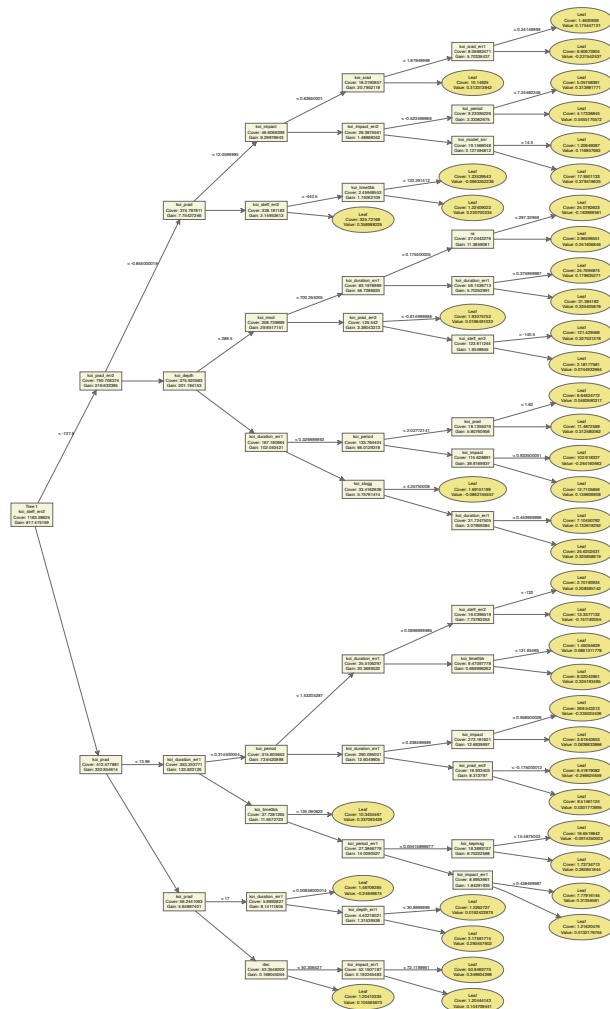
```

BoostErrors = AllErrors(xgTest[, 1], BoostPredictionsRounded, dim(xgTest)[1], 1)
XGB_error[fold] = BoostErrors[[1]]
XGB_FPs = BoostErrors[[2]]
XGB_FNs = BoostErrors[[3]]

}
XGBoost_error_thresholds[index] = mean(XGB_error) #average the error from all folds
XGBoost_FP_thresholds[index] = mean(XGB_FPs)
XGBoost_FN_thresholds[index] = mean(XGB_FNs)

index = index + 1
threshold = threshold + .1
}
xgbPlot = xgb.plot.tree(model = xgBoostModel,
                        trees = 1,
                        render = TRUE)
xgbPlot #plot an example tree

```



Hide

```
#Determine correct threshold value
XGBoost_error_thresholds#shows the average error at each threshold
```

```
[1] 0.07854184 0.06611433 0.06197183 0.06081193 0.06081193 0.06362883
[7] 0.06545153 0.06992543 0.07887324 0.62220381
```

Hide

```
order(XGBoost_error_thresholds) #Lowest error is threshold = .4
```

```
[1] 4 5 3 6 7 2 8 1 9 10
```

Hide

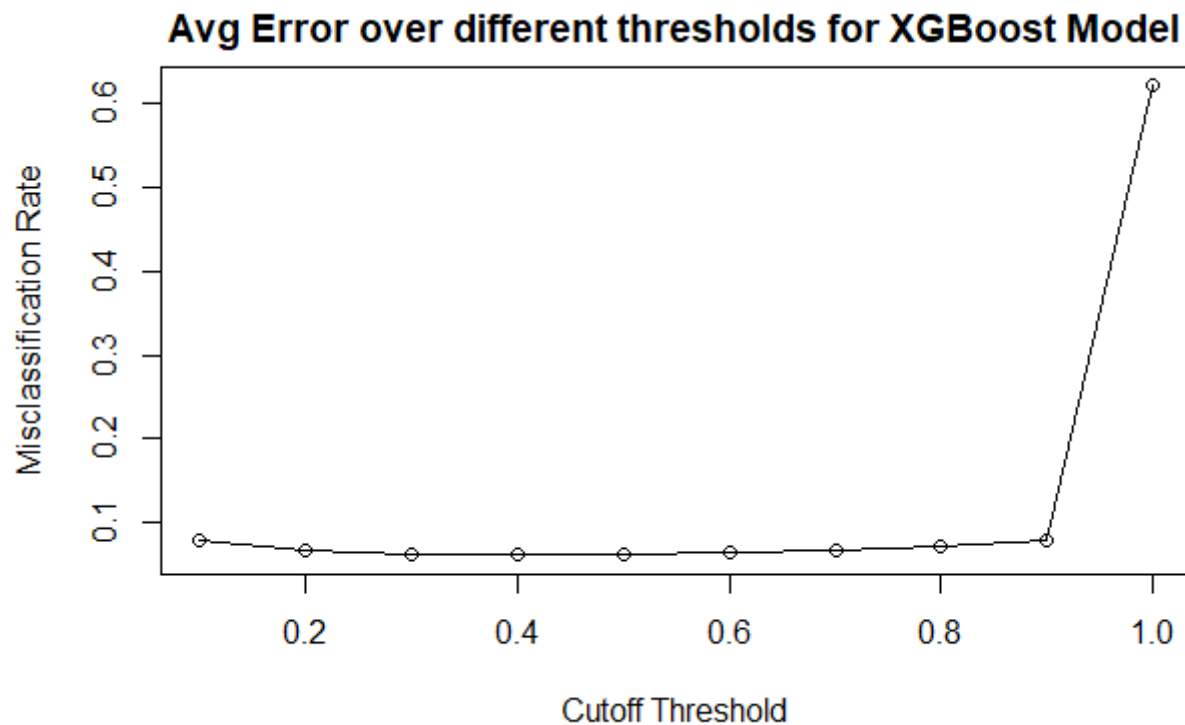
```
AvgErrorXGB = XGBoost_error_thresholds[(order(XGBoost_error_thresholds)[1])] #chose the
  threshold with the lowest error as the one we use
AvgFP_XGB = XGBoost_FP_thresholds[(order(XGBoost_error_thresholds)[1])]
AvgFN_XGB = XGBoost_FN_thresholds[(order(XGBoost_error_thresholds)[1])]
paste("XGBoost Error: ", round(AvgErrorXGB*100,2), "%", sep = "")
```

```
[1] "XGBoost Error: 6.08%"
```

Hide

```
#plot the error thresholds
plot(
  x = 1:10 / 10,
  y = XGBoost_error_thresholds,
  main = "Avg Error over different thresholds for XGBoost Model",
  xlab = "Cutoff Threshold",
  ylab = "Misclassification Rate"
)
lines(x = 1:10 / 10, y = XGBoost_error_thresholds)
```





XGBoost gives an error rate of 6.08%. This is significantly better than any model run so far. The threshold analysis graph above shows that the best misclassification rate for XGBoost is at the threshold = .4.

### 3.1.5) Logistic Regression

Logistic regression models is a supervised classification algorithm that builds a regression model to predict the classification by assigning data entries to binary values, based on the Sigmoid function. When performing logistic regression, it is important to consider the problems that arise from multicollinearity which can cause unstable estimates and inaccuracy. For this reason, we decided to first remove all major multicollinearity from the model.

[Hide](#)

```
#Check for multicollinearity
corrFrame = data.frame(cor(labeled_final[, 2:36]))
corrplot(cor(labeled_final[, 2:36])) #many multicollinear variables. Definine collinearity as correlation >.4
```



```
GLM_Data = data.frame(labeled_final$koi_disposition)

#all err2s are collinear with err1s. Removing err1s
variable_counter = 2
variable.names = colnames(labeled_final)
for (i in 2:length(labeled_final)) {
  variable.names[i]
  error1 = grepl("_err1", variable.names[i], fixed = TRUE)
  if (error1 == FALSE) {
    GLM_Data[, variable_counter] = labeled_final[, i]
    variable_counter = variable_counter + 1
  } else{
    variable.names[i] = NA
  }
}

variable.names = na.omit(variable.names)
colnames(GLM_Data) = variable.names
GLM_Data
```

koi_disposition <fctr>	koi_period <dbl>	koi_period_err2 <dbl>	koi_time0bk <dbl>	koi_time0bk_err2 <dbl>	koi_impact <dbl>
CONFIRMED	9.4880356	-2.775e-05	170.5387	-2.16e-03	0.146
CONFIRMED	54.4183827	-2.479e-04	162.5138	-3.52e-03	0.586

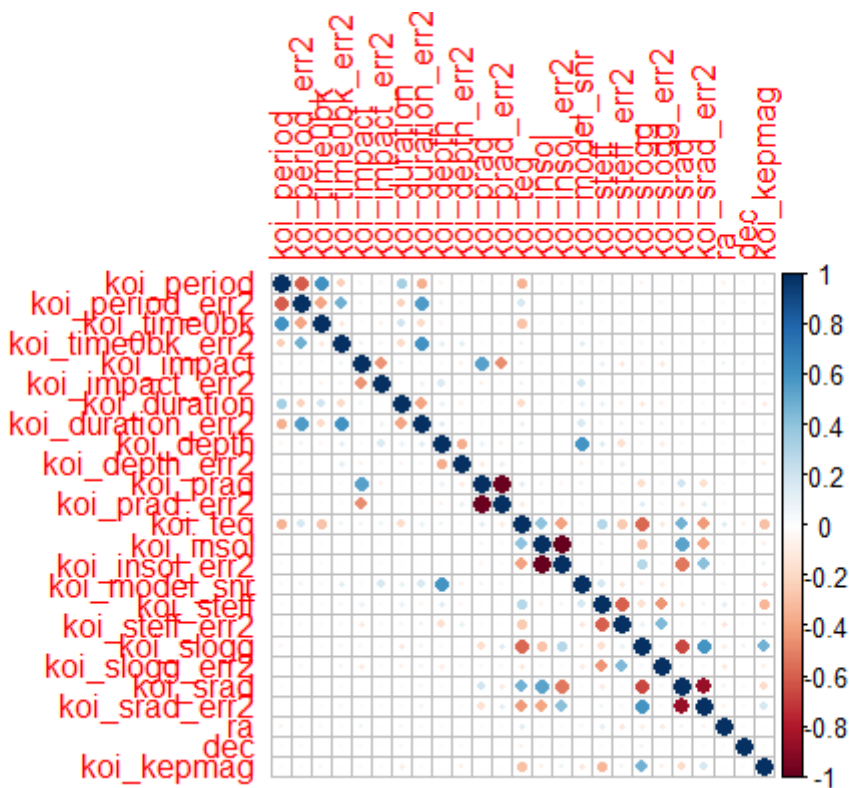
koi_disposition <fctr>	koi_period <dbl>	koi_period_err2 <dbl>	koi_time0bk <dbl>	koi_time0bk_err2 <dbl>	koi_impact <dbl>
FALSE POSITIVE	19.8991399	-1.494e-05	175.8503	-5.81e-04	0.969
FALSE POSITIVE	1.7369525	-2.630e-07	170.3076	-1.15e-04	1.276
CONFIRMED	2.5255918	-3.761e-06	171.5956	-1.13e-03	0.701
CONFIRMED	11.0943205	-2.036e-05	171.2012	-1.41e-03	0.538
CONFIRMED	4.1344351	-1.046e-05	172.9794	-1.90e-03	0.762
CONFIRMED	2.5665890	-1.781e-05	179.5544	-4.61e-03	0.755
FALSE POSITIVE	7.3617896	-2.128e-05	132.2505	-2.53e-03	1.169
CONFIRMED	16.0686467	-1.088e-05	173.6219	-5.17e-04	0.052

1-10 of 6,031 rows | 1-6 of 26 columns

Previous123456...100Next

Hide

```
corrFrame2 = data.frame(cor(GLM_Data[, 2:dim(GLM_Data)[2]]))
corrplot(cor(GLM_Data[, 2:dim(GLM_Data)[2]])) #Many correlated variables remain
```

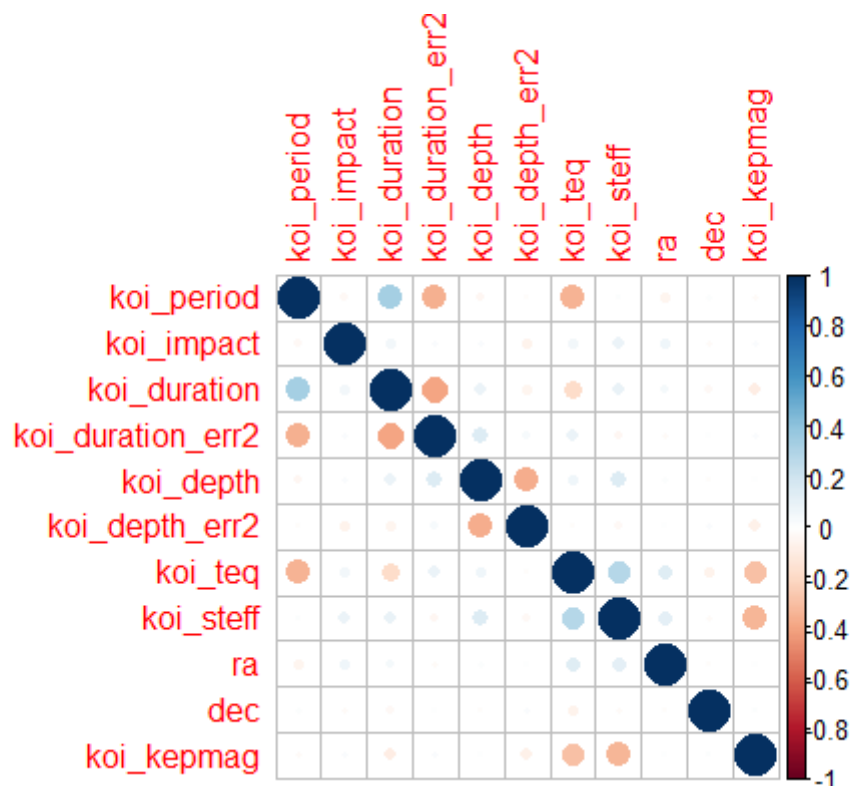


Hide

```

#KOI_period is collinear with koi_time0b
GLM_Data = subset(GLM_Data, select = -c(koi_time0bk))
#koi_period_err is collinear with koi_time0bk error
GLM_Data = subset(GLM_Data, select = -c(koi_time0bk_err2))
#Koi_period is collinear with koi_period_err2
GLM_Data = subset(GLM_Data, select = -c(koi_period_err2))
#koi_impact is collinear with koi_impact_err2
GLM_Data = subset(GLM_Data, select = -c(koi_impact_err2))
#koi_depth is collinear with koi_model_snr
GLM_Data = subset(GLM_Data, select = -c(koi_model_snr))
#koi impact is collinear with koi_prad and koi_prad_err
GLM_Data = subset(GLM_Data, select = -c(koi_prad, koi_prad_err2))
#koi_teq is collinear with KOI_insol, Koi_insol_err, koi_slogg, koi_srada, and koi_srada_e
rr
GLM_Data = subset(GLM_Data,
                  select = -c(koi_insol, koi_insol_err2, koi_slogg, koi_srada, koi_srada_e
rr2))
#koi_steff is collinear with koi_steff_err2 and koi_slogg_err2
GLM_Data = subset(GLM_Data, select = -c(koi_slogg_err2, koi_steff_err2))
corrplot(cor(GLM_Data[, 2:dim(GLM_Data)[2]]))

```


[Hide](#)

```
#All major multicollinearity has now been removed
```

Similarly to XGBoost, the cutoff threshold for prediction must be tuned. Our group decided to run multiple tests ranging from 0.1 to 1 to determine that the ideal threshold value of 0.5 should be used as that corresponded with the lowest average error.

Hide

```

threshold = 0.1
GLM_error = CreateErrorMatrix(NumFolds)
GLM_error_thresholds = rep(0, 10)
GLM_FP_thresholds = rep(0, 10)
GLM_FN_thresholds = rep(0, 10)
index = 1
while (threshold < 1) {
  #loop for threshold analysis
  GLM_error = CreateErrorMatrix(NumFolds)
  GLM_FP = CreateErrorMatrix(NumFolds)
  GLM_FN = CreateErrorMatrix(NumFolds)
  for (fold in 1:5) {
    #K-cross fold validation

    #training/testing set
    set.seed(fold)
    num_samples = dim(GLM_Data)[1]
    sampling.rate = 0.8
    training = sample(1:num_samples, sampling.rate * num_samples, replace = FALSE)
    trainingSet = subset(GLM_Data[training,])
    testing = setdiff(1:num_samples, training)
    testingSet = subset(GLM_Data[testing, ])
    defaultW = getOption("warn")
    options(warn = -1)
    #set up model
    LogisticReg = glm(koi_disposition ~ .,
                      data = trainingSet,
                      family = binomial(logit))

    options(warn = defaultW)
    predictions = predict(LogisticReg, testingSet, type = "response")
    predictedLabels = rep(0, sizeTestSet)
    predictedLabels = ifelse(predictions > threshold, 'FALSE POSITIVE', 'CONFIRMED') #th
is parameter is tuned

    GLMErrors = AllErrors(testingSet$koi_disposition, predictedLabels, sizeTestSet, 0)
    #determine error
    # error = sum(predictedLabels != testingSet$koi_disposition)
    #misclassificationRateLR = error / sizeTestSet
    #GLM_error[fold] = misclassificationRateLR
    GLM_error[fold] = GLMErrors[[1]]
    GLM_FP[fold] = GLMErrors[[2]]
    GLM_FN[fold] = GLMErrors[[3]]

  }

  GLM_error_thresholds[index] = mean(GLM_error)
  GLM_FP_thresholds[index] = mean(GLM_FP)
  GLM_FN_thresholds[index] = mean(GLM_FN)
  index = index + 1
  threshold = threshold + .1
}

```

```
}
order(GLM_error_thresholds) #Lowest error is threshold = .5
```

```
[1] 5 4 6 3 7 2 8 9 1 10
```

Hide

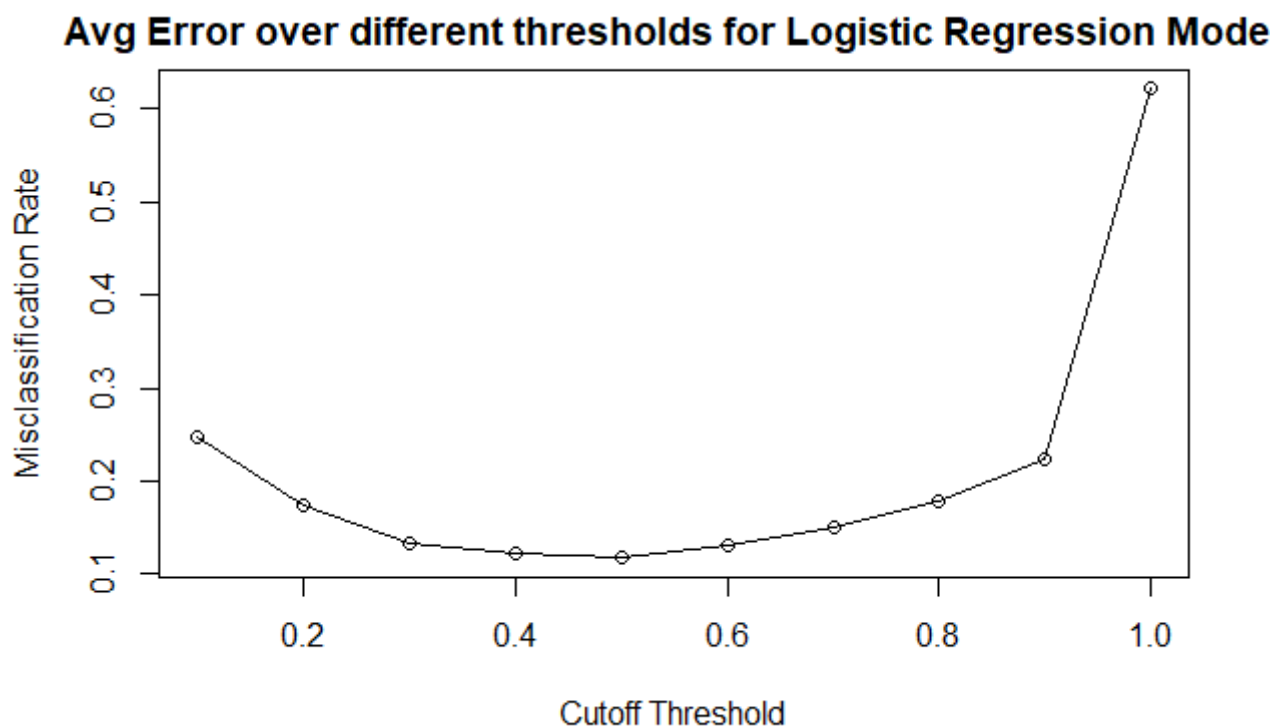
```
AvgErrorGLM = GLM_error_thresholds[order(GLM_error_thresholds)[1]]
AvgFP_GLM = GLM_FP_thresholds[order(GLM_error_thresholds)[1]]
AvgFN_GLM = GLM_FN_thresholds[order(GLM_error_thresholds)[1]]

paste("Logistic Regression Error: ", round(AvgErrorGLM*100,2), "%", sep="")
```

```
[1] "Logistic Regression Error: 11.73%"
```

Hide

```
plot(
  x = 1:10 / 10,
  y = GLM_error_thresholds,
  main = "Avg Error over different thresholds for Logistic Regression Model",
  xlab = "Cutoff Threshold",
  ylab = "Misclassification Rate"
)
lines(x = 1:10 / 10, y = GLM_error_thresholds)
```



Logistic Regression has an error rate of 11.7%, making it the worst model yet. Its error is best when threshold = .5.

## 3.2) Models using scaled data:

The models below all require normalization of the data to be effective. This is an important step as all features need to be in the same scale. If not, the features with larger scales would dominate the model causing it to be inaccurate. To do this, we used the “scale” function to normalize all the dependent variables. We also changed the independent variable, `koi_disposition`, to be binary

### 3.2.2) Neural Network: Original Variables

The Neural Network model is built through functions, “neurons” that are then organized into layers. It is an advanced model that is ideally suited for complex problems as it requires significant computational resources. In addition, it is quite difficult to understand afterwards given the complexity of the math within the model. Our group was able to see the significant use of computational resources as our computer was unable to run the model. For this reason, the group did not use K-fold cross-validation in order to lower the computational power required to run the model, but in real-life application K-fold cross-validation should still be done.

When choosing the number of neurons and hidden layers it is important to find the right balance between accuracy and over-fitting. Our group manually adjusted the number of neurons and hidden layers, testing variations such as 4&2, 5&1, 6, 3&1, etc, until we found that two neurons and one hidden layer allowed the model to converge. The next step in the model was to choose the threshold value for classification. This was similar to choosing the threshold as we did in Logistic Regression. The ideal threshold of 0.5 was found by plotting the average error for each threshold ranging from 0.1 to 1 as that corresponded with the lowest misclassification rate.

[Hide](#)

```
#Create testing and training set
set.seed(123)
scaled_data = data.frame(scale(labeled_final[, 2:36])) #normalize data
scaled_data$koi_disposition = ifelse(labeled_final$koi_disposition == "CONFIRMED", 1, 0)
num_samples = dim(scaled_data)[1]
sampling.rate = 0.8
training = sample(1:num_samples, sampling.rate * num_samples, replace = FALSE)
trainingSet.norm = subset(scaled_data[training,])
testing = setdiff(1:num_samples, training)
testingSet.norm = subset(scaled_data[testing, ])
sizeTestSet = dim(testingSet.norm)[1]

#set up variables for neural network. Since 36 variables put too much computational strain,
dimensionality reduction needed to take place. We chose to take only the features, not their errors, to reduce dimensionality.

koiDP.name = "koi_disposition"
numCols = dim(testingSet.norm)[2]
variable.names = colnames(testingSet.norm)[1:numCols - 1]
variable.names
```



```

[1] "koi_period"      "koi_period_err1"  "koi_period_err2"
[4] "koi_time0bk"     "koi_time0bk_err1" "koi_time0bk_err2"
[7] "koi_impact"      "koi_impact_err1"  "koi_impact_err2"
[10] "koi_duration"    "koi_duration_err1" "koi_duration_err2"
[13] "koi_depth"       "koi_depth_err1"   "koi_depth_err2"
[16] "koi_prad"        "koi_prad_err1"    "koi_prad_err2"
[19] "koi_teq"         "koi_insol"        "koi_insol_err1"
[22] "koi_insol_err2"  "koi_model_snr"    "koi_steff"
[25] "koi_steff_err1"  "koi_steff_err2"   "koi_slogg"
[28] "koi_slogg_err1"  "koi_slogg_err2"   "koi_srad"
[31] "koi_srad_err1"   "koi_srad_err2"    "ra"
[34] "dec"             "koi_kepmag"

```

Hide

```

for (i in 1:length(variable.names)) {
  error = grepl("_err", variable.names[i], fixed = TRUE)
  if (error) {
    variable.names[i] = NA
  }
}

variable.names = na.omit(variable.names)
variable.names = variable.names[1:15]
#use formulaic library to create formula
nn.form <-
  create.formula(outcome.name = koiDP.name,
                 input.names = variable.names)
nn.form #15 variables

```

```

$formula
koi_disposition ~ koi_period + koi_time0bk + koi_impact + koi_duration +
  koi_depth + koi_prad + koi_teq + koi_insol + koi_model_snr +
  koi_steff + koi_slogg + koi_srad + ra + dec + koi_kepmag
<environment: 0x00000155aac47e00>

$inclusion.table

```

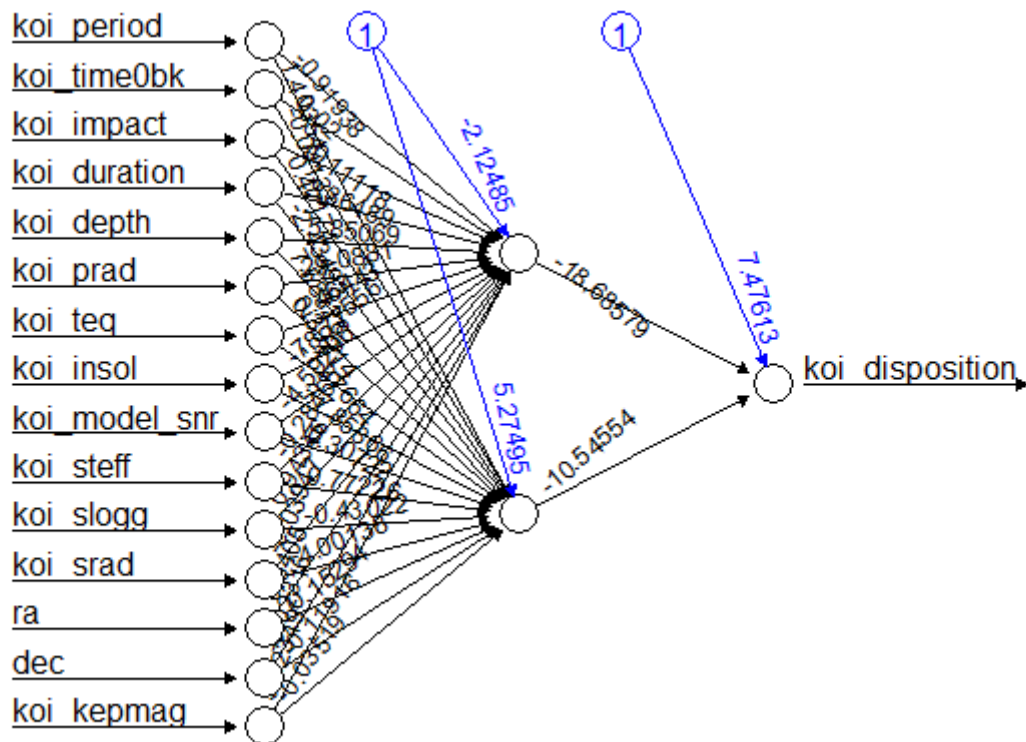
0 rows

```
$interactions.table
```

0 rows

Hide

```
#Fit neural network
nnModel1 = neuralnet(
  nn.form,
  data = trainingSet.norm,
  hidden = 2,
  linear.output = FALSE,
  act.fct = "logistic",
)
plot(nnModel1)
```


[Hide](#)

```
#Predict
predictedLabels = compute(nnModel1, testingSet.norm[, variable.names])

#tune threshold parameter
threshold = .1
NNErrors = CreateErrorMatrix(10)
NN_FPs = CreateErrorMatrix(10)
NN_FNs = CreateErrorMatrix(10)
index = 1
while (threshold <= 1) {
  results = data.frame(actual = testingSet.norm$koi_disposition,
                        prediction = predictedLabels$net.result)
  results$roundedPrediction = ifelse(results$prediction > threshold, 1, 0)
  #error = sum(results$actual != results$roundedPrediction)
  Errors = AllErrors(results$actual, results$roundedPrediction, sizeTestSet, 1)
  NNErrors[index] = Errors[[1]]
  NN_FPs[index] = Errors[[2]]
  NN_FNs[index] = Errors[[3]]
  threshold = threshold + .1
  index = index + 1
}

order(NNErrors) #lowest misclass rate is at threshold = .5
```

```
[1] 5 4 6 3 7 2 8 1 9 10
```

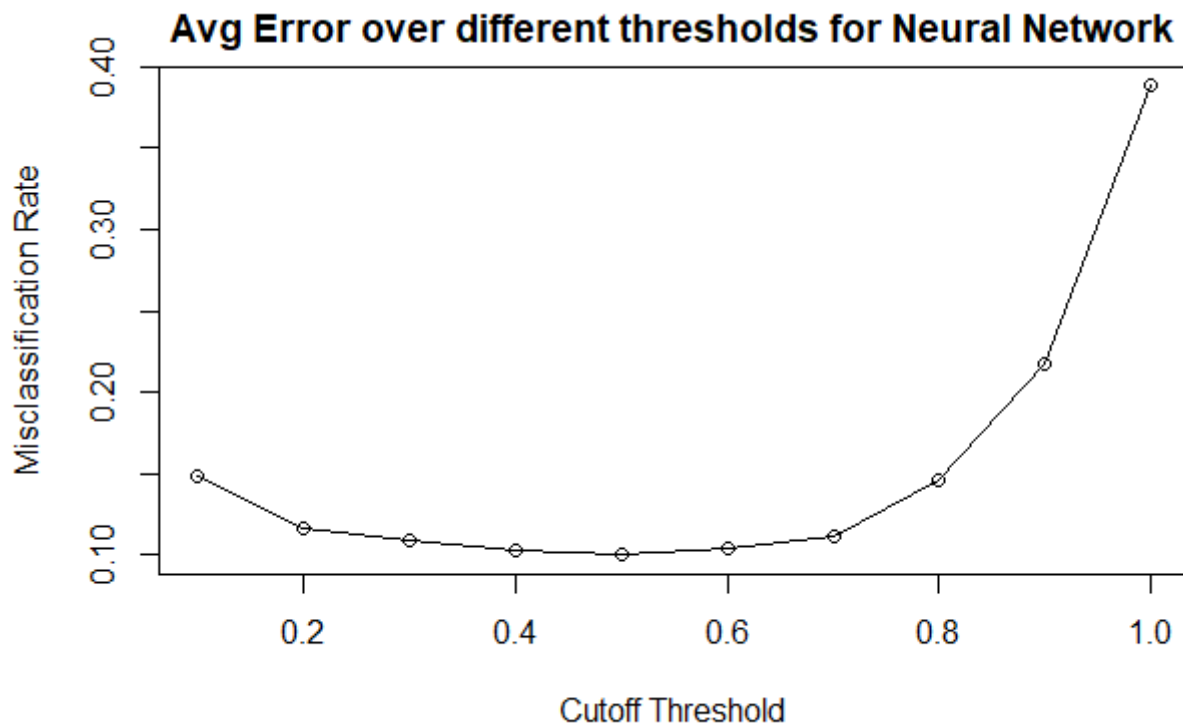
Hide

```
NeuralNetMisClassRate = NNErrors[order(NNErrors)[1]]
AvgFP_NN = NN_FPs[order(NNErrors)[1]]
AvgFN_NN = NN_FNs[order(NNErrors)[1]]
paste("Neural Net Misclassification Rate: ", round(100*NeuralNetMisClassRate, 2), "%", sep=
"")
```

```
[1] "Neural Net Misclassification Rate: 10.02%"
```

Hide

```
plot(
  x = 1:10 / 10,
  y = NNErrors,
  main = "Avg Error over different thresholds for Neural Network",
  xlab = "Cutoff Threshold",
  ylab = "Misclassification Rate"
)
lines(x = 1:10 / 10, y = NNErrors)
```



In this run, NN had an error rate of 0.1002486, with an optimal cutoff threshold of .5. We will revisit the NN below, to look at ways to use PCA to capture variation while reducing necessary computational resources.

## Neural Network: PCA w/15 Variables

Principal Component Analysis allows us to reduce dimensionality while capturing as much of the underlying variation in the data as possible. The first application of PCA we found was for Neural Networks, which are very computationally difficult. We decided to first use a PCA with 15 variables, the same number of variables as our original neural network. This would mean the same computational strain, but with features that are guaranteed to capture as much variation as possible with that number of variables.

[Hide](#)

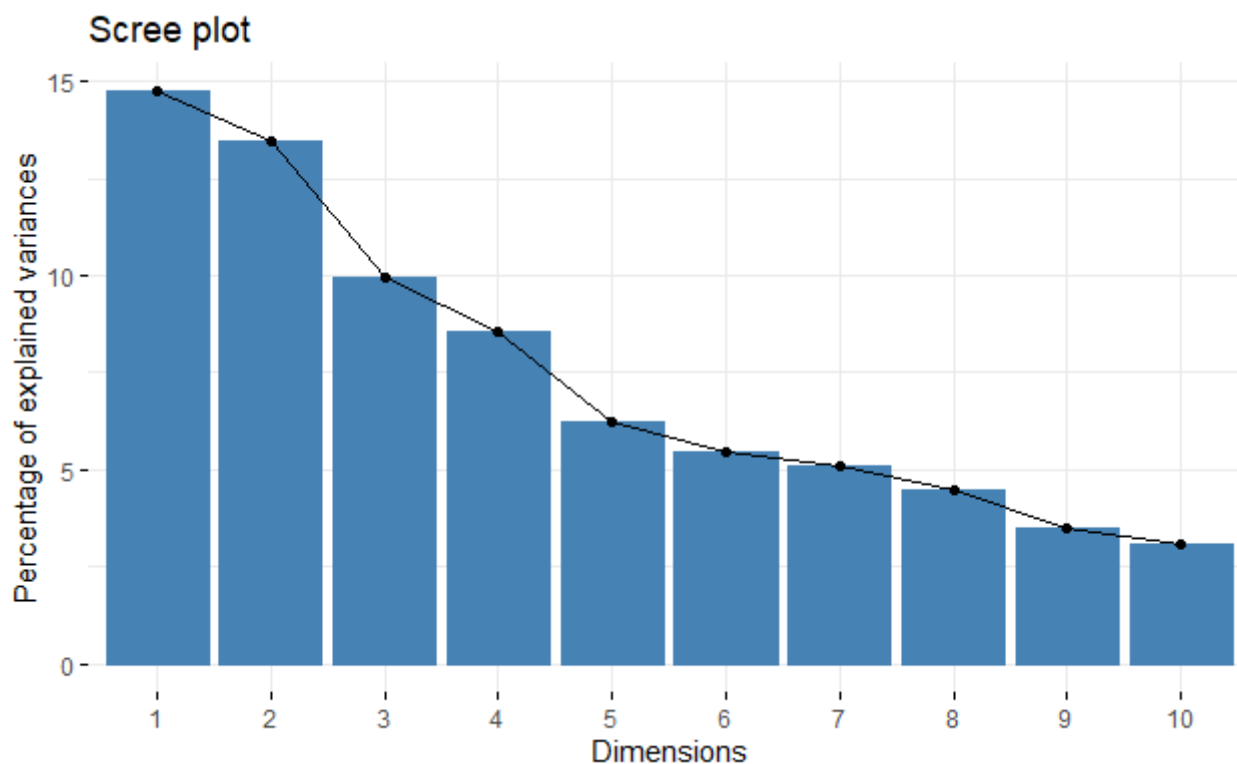
```
res.pca.exoplanets = prcomp(identifiers_removed[2:36], center = TRUE, scale = TRUE) #perform PCA
summary(res.pca.exoplanets)
```

## Importance of components:

	PC1	PC2	PC3	PC4	PC5	PC6
Standard deviation	2.2712	2.1730	1.86778	1.72894	1.47639	1.37931
Proportion of Variance	0.1474	0.1349	0.09967	0.08541	0.06228	0.05436
Cumulative Proportion	0.1474	0.2823	0.38196	0.46737	0.52965	0.58400
	PC7	PC8	PC9	PC10	PC11	PC12
Standard deviation	1.33622	1.25447	1.10767	1.04188	1.01171	0.98148
Proportion of Variance	0.05101	0.04496	0.03506	0.03101	0.02924	0.02752
Cumulative Proportion	0.63502	0.67998	0.71503	0.74605	0.77529	0.80282
	PC13	PC14	PC15	PC16	PC17	PC18
Standard deviation	0.95840	0.93448	0.88263	0.78194	0.77439	0.75012
Proportion of Variance	0.02624	0.02495	0.02226	0.01747	0.01713	0.01608
Cumulative Proportion	0.82906	0.85401	0.87627	0.89374	0.91087	0.92695
	PC19	PC20	PC21	PC22	PC23	PC24
Standard deviation	0.67294	0.63205	0.58189	0.55938	0.54423	0.48547
Proportion of Variance	0.01294	0.01141	0.00967	0.00894	0.00846	0.00673
Cumulative Proportion	0.93989	0.95130	0.96097	0.96991	0.97838	0.98511
	PC25	PC26	PC27	PC28	PC29	PC30
Standard deviation	0.44729	0.37145	0.31152	0.23244	0.12420	0.10799
Proportion of Variance	0.00572	0.00394	0.00277	0.00154	0.00044	0.00033
Cumulative Proportion	0.99083	0.99477	0.99754	0.99909	0.99953	0.99986
	PC31	PC32	PC33	PC34	PC35	
Standard deviation	0.07019	2.036e-15	5.773e-16	5.354e-16	3.988e-16	
Proportion of Variance	0.00014	0.000e+00	0.000e+00	0.000e+00	0.000e+00	
Cumulative Proportion	1.00000	1.000e+00	1.000e+00	1.000e+00	1.000e+00	

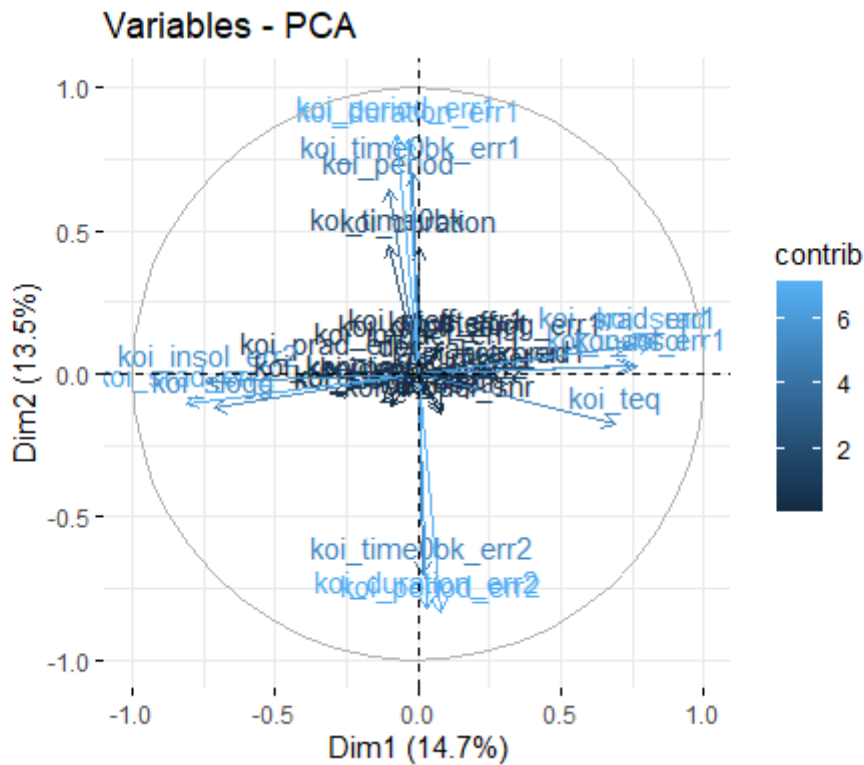
Hide

fviz\_eig(res.pca.exoplanets)



Hide

```
fviz_pca_var(res.pca.exoplanets, col.var = "contrib")
```



Hide

```
PoV <-
  res.pca.exoplanets$sdev ^ 2 / sum(res.pca.exoplanets$sdev ^ 2) #get proportions of variance
numPcas = 15
sum(PoV[1:numPcas]) #This gives us 88% explanation of variance. This is the number of variable in the original neural network, so we are using this to get a better NN with the same number of variables
```

```
[1] 0.876268
```

Hide

```
newDataSet = data.frame(res.pca.exoplanets$x[, 1:numPcas])
newDataSet$label = identifiers_removed$koi_disposition

candidates_PCA = newDataSet[identifiers_removed$koi_disposition ==
  "CANDIDATE", ] #separate out just the candidates
labeled_PCA = newDataSet[identifiers_removed$koi_disposition !=
  "CANDIDATE", ]
labeled_PCA = droplevels(labeled_PCA)
candidates_PCA = droplevels(candidates_PCA)
```

While our PCA does not show any one dimension to account for an overwhelming amount of variance, it does clearly indicate that a significant portion of variance can be explained using significantly fewer than 36 principal components.

### Rerunning Neural Network Model

[Hide](#)

```
set.seed(123)
NN_labeled_PCA = labeled_PCA[, 1:numPcas]
NN_labeled_PCA$koi_disposition = ifelse(labeled_PCA$label == "CONFIRMED", 1, 0)
summary(scaled_data)
```

koi_period	koi_period_err1	koi_period_err2	koi_time0bk
Min. : -0.4049	Min. : -0.1768	Min. : -26.7574	Min. : -0.64352
1st Qu.: -0.3844	1st Qu.: -0.1762	1st Qu.: 0.1590	1st Qu.: -0.43439
Median : -0.3277	Median : -0.1736	Median : 0.1736	Median : -0.37877
Mean : 0.0000	Mean : 0.0000	Mean : 0.0000	Mean : 0.00000
3rd Qu.: -0.1552	3rd Qu.: -0.1590	3rd Qu.: 0.1762	3rd Qu.: 0.07978
Max. : 11.9778	Max. : 26.7574	Max. : 0.1768	Max. : 23.11291
koi_time0bk_err1	koi_time0bk_err2	koi_impact	
Min. : -0.36586	Min. : -31.75989	Min. : -0.84878	
1st Qu.: -0.32745	1st Qu.: 0.00669	1st Qu.: -0.52855	
Median : -0.22068	Median : 0.22068	Median : -0.03305	
Mean : 0.00000	Mean : 0.00000	Mean : 0.00000	
3rd Qu.: -0.00669	3rd Qu.: 0.32745	3rd Qu.: 0.37679	
Max. : 31.75989	Max. : 0.36586	Max. : 32.39182	
koi_impact_err1	koi_impact_err2	koi_duration	koi_duration_err1
Min. : -0.2207	Min. : -37.0338	Min. : -0.79008	Min. : -0.46838
1st Qu.: -0.2173	1st Qu.: -0.3289	1st Qu.: -0.45677	1st Qu.: -0.40374
Median : -0.2034	Median : 0.2248	Median : -0.26098	Median : -0.28282
Mean : 0.0000	Mean : 0.0000	Mean : 0.00000	Mean : 0.00000
3rd Qu.: -0.1824	3rd Qu.: 0.4915	3rd Qu.: 0.07348	3rd Qu.: -0.02716
Max. : 8.2794	Max. : 0.5591	Max. : 19.80016	Max. : 16.23186
koi_duration_err2	koi_depth	koi_depth_err1	
Min. : -16.23186	Min. : -0.3491	Min. : -0.25725	
1st Qu.: 0.02716	1st Qu.: -0.3471	1st Qu.: -0.22666	
Median : 0.28282	Median : -0.3432	Median : -0.19211	
Mean : 0.00000	Mean : 0.0000	Mean : 0.00000	
3rd Qu.: 0.40374	3rd Qu.: -0.3030	3rd Qu.: -0.09117	
Max. : 0.46838	Max. : 9.5013	Max. : 49.18710	
koi_depth_err2	koi_prad	koi_prad_err1	
Min. : -49.18710	Min. : -0.09248	Min. : -0.06598	
1st Qu.: 0.09117	1st Qu.: -0.08857	1st Qu.: -0.06405	
Median : 0.19211	Median : -0.08497	Median : -0.06156	
Mean : 0.00000	Mean : 0.00000	Mean : 0.00000	
3rd Qu.: 0.22666	3rd Qu.: -0.01473	3rd Qu.: -0.02127	
Max. : 0.25725	Max. : 73.22898	Max. : 75.98152	
koi_prad_err2	koi_teq	koi_insol	
Min. : -76.00748	Min. : -1.2681	Min. : -0.04894	
1st Qu.: 0.03814	1st Qu.: -0.6527	1st Qu.: -0.04872	
Median : 0.05676	Median : -0.2437	Median : -0.04762	
Mean : 0.00000	Mean : 0.0000	Mean : 0.00000	
3rd Qu.: 0.05834	3rd Qu.: 0.4011	3rd Qu.: -0.04094	
Max. : 0.05933	Max. : 15.5272	Max. : 65.69789	
koi_insol_err1	koi_insol_err2	koi_model_snr	
Min. : -0.06739	Min. : -68.06196	Min. : -0.3877	
1st Qu.: -0.06706	1st Qu.: 0.04559	1st Qu.: -0.3714	
Median : -0.06516	Median : 0.05053	Median : -0.3514	
Mean : 0.00000	Mean : 0.00000	Mean : 0.0000	
3rd Qu.: -0.05080	3rd Qu.: 0.05123	3rd Qu.: -0.2215	
Max. : 69.45869	Max. : 0.05136	Max. : 9.1486	
koi_steff	koi_steff_err1	koi_steff_err2	koi_slogg
Min. : -3.71885	Min. : -3.0066	Min. : -20.71031	Min. : -9.8852
1st Qu.: -0.48298	1st Qu.: -0.8168	1st Qu.: -0.45354	1st Qu.: -0.2227



```

Median : 0.06731   Median : 0.2676   Median : 0.03832   Median : 0.2918
Mean    : 0.00000   Mean    : 0.0000   Mean    : 0.00000   Mean    : 0.0000
3rd Qu.: 0.49193   3rd Qu.: 0.6430   3rd Qu.: 0.65961   3rd Qu.: 0.5374
Max.    :12.43001   Max.    :11.0913   Max.    : 2.09635   Max.    : 2.2474
koi_slogg_err1   koi_slogg_err2   koi_srad         koi_srad_err1
Min.    :-0.9095   Min.    :-9.1764   Min.    :-0.28040   Min.    :-0.35977
1st Qu.: -0.5830   1st Qu.: -0.8374   1st Qu.: -0.15546   1st Qu.: -0.22791
Median : -0.3753   Median : 0.1305   Median : -0.12554   Median : -0.10044
Mean    : 0.0000   Mean    : 0.0000   Mean    : 0.00000   Mean    : 0.00000
3rd Qu.: 0.2109   3rd Qu.: 0.6666   3rd Qu.: -0.06386   3rd Qu.: 0.00834
Max.    :10.0123   Max.    : 1.9621   Max.    :31.37715   Max.    :36.00187
koi_srad_err2    ra          dec          koi_kepmag
Min.    :-56.21894   Min.    :-2.58287   Min.    :-2.0123   Min.    :-5.4016
1st Qu.: 0.07577   1st Qu.: -0.69660   1st Qu.: -0.8514   1st Qu.: -0.5886
Median : 0.14915   Median : 0.04099   Median : -0.0363   Median : 0.1868
Mean    : 0.00000   Mean    : 0.00000   Mean    : 0.0000   Mean    : 0.0000
3rd Qu.: 0.17252   3rd Qu.: 0.80352   3rd Qu.: 0.8106   3rd Qu.: 0.7616
Max.    : 0.21002   Max.    : 2.00621   Max.    : 2.3631   Max.    : 3.5325
koi_disposition
Min.    :0.0000
1st Qu.:0.0000
Median :0.0000
Mean    :0.3761
3rd Qu.:1.0000
Max.    :1.0000

```

Hide

```
head(scaled_data)
```

	koi_period <dbl>	koi_period_err1 <dbl>	koi_period_err2 <dbl>	koi_time0bk <dbl>	koi_time0bk_err1 <dbl>	koi_time0bk_err2 <dbl>
1	-0.2987063	-0.1712251	0.1712251	0.23459560	-0.2443950	0.2443950
2	0.2208034	-0.1269747	0.1269747	0.09358276	-0.1676082	0.1676082
3	-0.1783273	-0.1738000	0.1738000	0.32792873	-0.3335467	0.3335467
4	-0.3883287	-0.1767501	0.1767501	0.23053324	-0.3598575	0.3598575
5	-0.3792100	-0.1760470	0.1760470	0.25316557	-0.3025497	0.3025497
6	-0.2801336	-0.1727105	0.1727105	0.24623540	-0.2867407	0.2867407

6 rows | 1-7 of 36 columns

Hide

```

num_samples = dim(scaled_data)[1]
sampling.rate = 0.8

#create training/testing sets
training = sample(1:num_samples, sampling.rate * num_samples, replace = FALSE)
trainingSet.norm.PCA = subset(NN_labeled_PCA[training,])
testing = setdiff(1:num_samples, training)
testingSet.norm.PCA = subset(NN_labeled_PCA[testing, ])
sizeTestSet = dim(testingSet.norm)[1]
label.name = "label"
variable.names = rep(0, numPcas)
numCols = dim(testingSet.norm.PCA)[2]
variable.names = colnames(testingSet.norm.PCA)[1:numCols - 1]
variable.names

```

```

[1] "PC1"  "PC2"  "PC3"  "PC4"  "PC5"  "PC6"  "PC7"  "PC8"  "PC9"  "PC10"
[11] "PC11" "PC12" "PC13" "PC14" "PC15"

```

Hide

```

nn.form <-
  create.formula(outcome.name = koiDP.name,
                 input.names = variable.names)
nn.form

```

```

$formula
koi_disposition ~ PC1 + PC2 + PC3 + PC4 + PC5 + PC6 + PC7 + PC8 +
  PC9 + PC10 + PC11 + PC12 + PC13 + PC14 + PC15
<environment: 0x00000155ad9863e8>

$inclusion.table

```

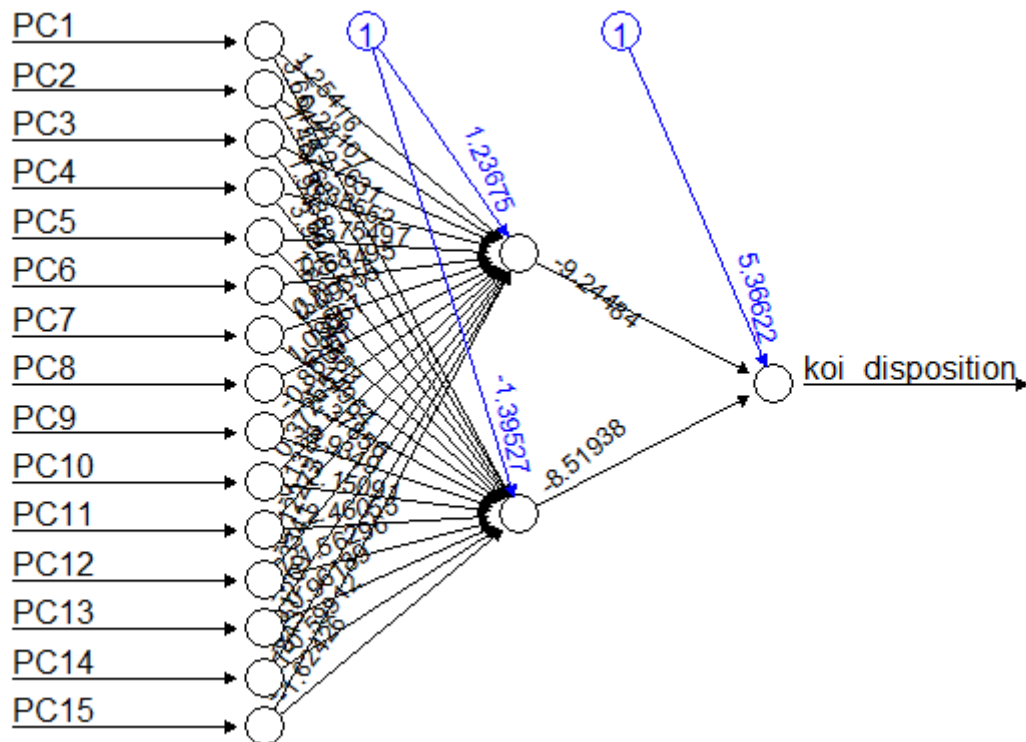
0 rows

```
$interactions.table
```

0 rows

Hide

```
#rerun neural network
nnModel2 = neuralnet(
  nn.form,
  data = trainingSet.norm.PCA,
  hidden = 2,
  linear.output = FALSE,
  act.fct = "logistic"
)
plot(nnModel2)
```


[Hide](#)

```
#Find results
predictedLabels = compute(nnModel2, testingSet.norm.PCA[, variable.names])

#Tune threshold
threshold = .1
NNErrors = rep(0, 10)
NN_FNs = rep(0,10)
NN_FPs = rep(0,10)
index = 1
while (threshold <= 1) {
  results = data.frame(actual = testingSet.norm.PCA$koi_disposition,
                        prediction = predictedLabels$net.result)
  results$roundedPrediction = ifelse(results$prediction > threshold, 1, 0)
  error = sum(results$actual != results$roundedPrediction)
  Errors = AllErrors(results$actual,results$roundedPrediction,sizeTestSet,1)
  NNErrors[index] = Errors[[1]]
  NN_FPs[index] = Errors[[2]]
  NN_FNs[index] = Errors[[3]]

  threshold = threshold + .1
  index = index + 1
}
order(NNErrors) #lowest misclassification rate is at threshold = .4
```

```
[1] 4 6 5 3 7 2 8 1 9 10
```

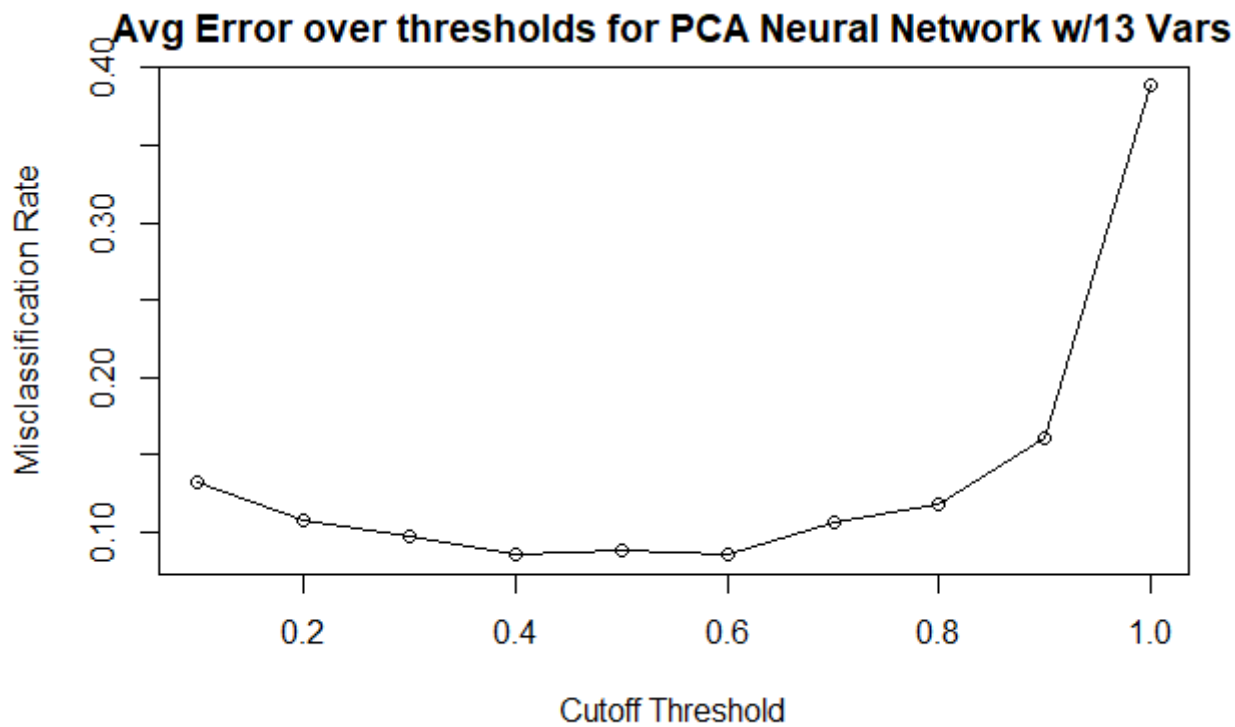
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```
PCA_15_v_NeuralNetMisClassRate = NNErrors[order(NNErrors)[1]]
Avg_FP_PCA15NN = NN_FPs[order(NNErrors)[1]]
Avg_FN_PCA15NN = NN_FNs[order(NNErrors)[1]]
paste("Neural Net (PCA, 15 var) Misclassification Rate: ",round(100*PCA_15_v_NeuralNetMi
sClassRate,2),"%",sep="")
```

```
[1] "Neural Net (PCA, 15 var) Misclassification Rate: 8.53%"
```

Hide

```
plot(
  x = 1:10 / 10,
  y = NNErrors,
  main = "Avg Error over thresholds for PCA Neural Network w/13 Vars",
  xlab = "Cutoff Threshold",
  ylab = "Misclassification Rate"
)
lines(x = 1:10 / 10, y = NNErrors)
```



We get a better misclassification rate from the PCA version of NN using 13 variables of 8.53%, which is 1.49% less than our last Neural Network, and an optimal cutoff threshold of .5.

### 3.2.3) Neural Network: PCA w/20 Variables

Lastly (for NNs), we decided to see how many variables could capture 95% of variation. We found that 20 variables was sufficient; this means that 16 of our 36 variables, or 44.44% represent only 5% of variation.

[Hide](#)

```
#Last Neural Network, PCA, with 95% of variation explained
numVars = (dim((labeled_final))[2])
for (i in 1:(numVars)) {
  if (sum(PoV[1:i]) >= .95) {
    numPcas = i
    break
  }
}

sum(PoV[1:numPcas])
```

```
[1] 0.9513002
```

[Hide](#)

```
newDataSet = data.frame(res.pca.exoplanets$x[, 1:numPcas])

newDataSet$label = identifiers_removed$koi_disposition

candidates_PCA = newDataSet[identifiers_removed$koi_disposition ==
                             "CANDIDATE",] #separate out just the candidates
labeled_PCA = newDataSet[identifiers_removed$koi_disposition !=
                          "CANDIDATE",]
labeled_PCA = droplevels(labeled_PCA)
candidates_PCA = droplevels(candidates_PCA)
```

Hide

```
set.seed(123)
NN_labeled_PCA = labeled_PCA[, 1:numPcas]
NN_labeled_PCA$koi_disposition = ifelse(labeled_PCA$label == "CONFIRMED", 1, 0)
head(scaled_data)
```

	koi_period <dbl>	koi_period_err1 <dbl>	koi_period_err2 <dbl>	koi_time0bk <dbl>	koi_time0bk_err1 <dbl>	koi_time0bk_err2 <dbl>
1	-0.2987063	-0.1712251	0.1712251	0.23459560	-0.2443950	0.2443950
2	0.2208034	-0.1269747	0.1269747	0.09358276	-0.1676082	0.1676082
3	-0.1783273	-0.1738000	0.1738000	0.32792873	-0.3335467	0.3335467
4	-0.3883287	-0.1767501	0.1767501	0.23053324	-0.3598575	0.3598575
5	-0.3792100	-0.1760470	0.1760470	0.25316557	-0.3025497	0.3025497
6	-0.2801336	-0.1727105	0.1727105	0.24623540	-0.2867407	0.2867407

6 rows | 1-7 of 36 columns

Hide

```
#testing and training sets
num_samples = dim(scaled_data)[1]
sampling.rate = 0.8
training = sample(1:num_samples, sampling.rate * num_samples, replace = FALSE)
trainingSet.norm.PCA = subset(NN_labeled_PCA[training,])
testing = setdiff(1:num_samples, training)
testingSet.norm.PCA = subset(NN_labeled_PCA[testing, ])
sizeTestSet = dim(testingSet.norm)[1]
label.name = "label"
variable.names = rep(0, numPcas)

numCols = dim(testingSet.norm.PCA)[2]
variable.names = colnames(testingSet.norm.PCA)[1:numCols - 1]

nn.form <-
  create.formula(outcome.name = koiDP.name,
                 input.names = variable.names)
nn.form
```

```
$formula
koi_disposition ~ PC1 + PC2 + PC3 + PC4 + PC5 + PC6 + PC7 + PC8 +
  PC9 + PC10 + PC11 + PC12 + PC13 + PC14 + PC15 + PC16 + PC17 +
  PC18 + PC19 + PC20
<environment: 0x00000155bfa33960>

$inclusion.table
```

0 rows

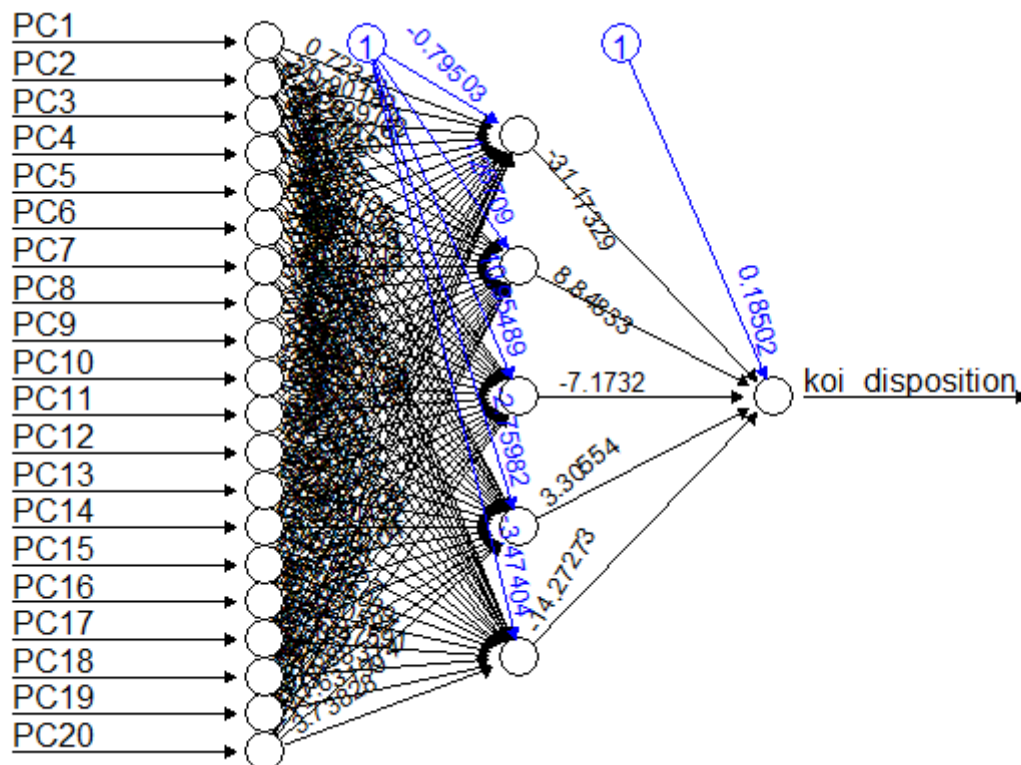
```
$interactions.table
```

0 rows

Hide

```
library(neuralnet)
nnModel3 = neuralnet( #parameters tuned manually to ensure this stays computationally tr
actable
  nn.form,
  data = trainingSet.norm.PCA,
  hidden = c(5),
  linear.output = FALSE,
  act.fct = "logistic",
  stepmax=17000,
  threshold = 0.1
)

plot(nnModel3)
```



Hide

```
#Make prediction
predictedLabels = compute(nnModel3, testingSet.norm.PCA[, variable.names])

index = 1
threshold = .1
NNErrors = rep(0, 10)
NN_FPs = rep(0,10)
NN_FNs = rep(0,10)
while (threshold <= 1) { #tune threshold parameter
  results = data.frame(actual = testingSet.norm.PCA$koi_disposition,
                        prediction = predictedLabels$net.result)
  results$roundedPrediction = ifelse(results$prediction > threshold, 1, 0)
  error = sum(results$actual != results$roundedPrediction)
  Errors = AllErrors(results$actual, results$roundedPrediction, sizeTestSet, 1)
  NNErrors[index] = Errors[[1]]
  NN_FPs[index] = Errors[[2]]
  NN_FNs[index] = Errors[[3]]
  threshold = threshold + .1
  index = index + 1
}
NNErrors #lowest error is with threshold = .6
```

```
[1] 0.09196355 0.07705054 0.07456504 0.07125104 0.06876553 0.06628003
[7] 0.07539354 0.08367854 0.09444905 0.38856669
```

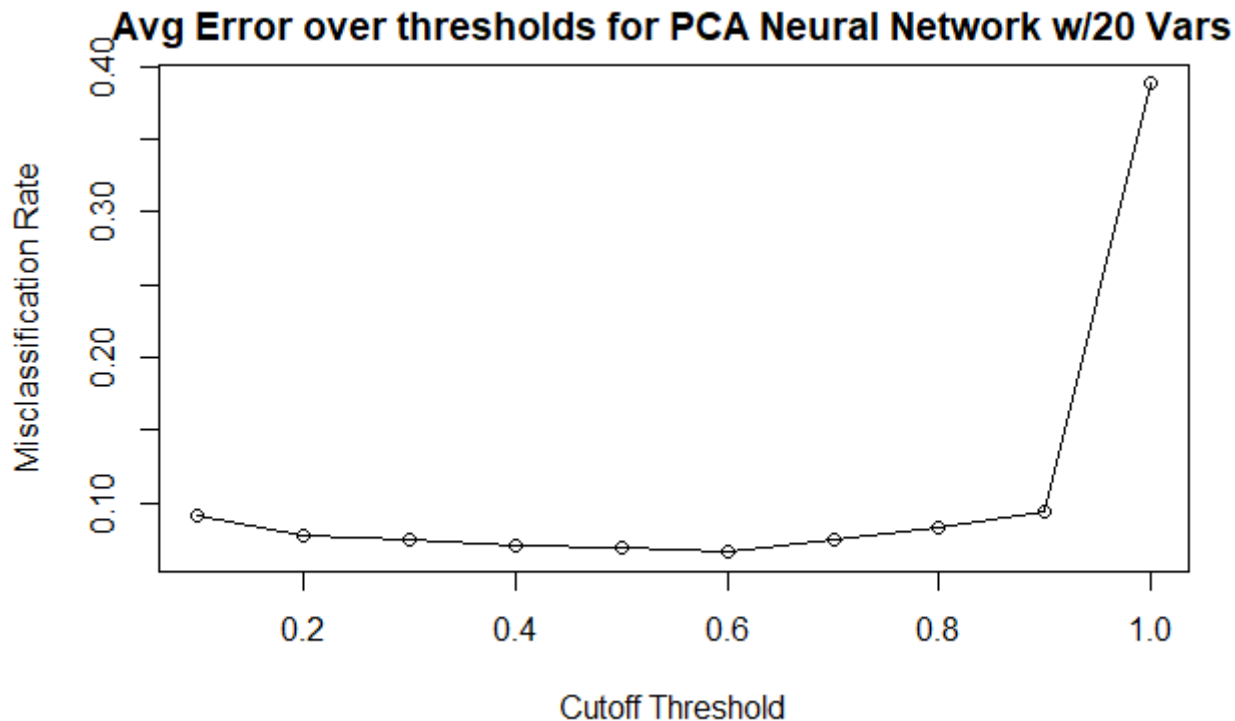
Hide



```

PCA_20_v_NeuralNetMisClassRate = NNErrors[order(NNErrors)[1]]
Avg_FP_PCA20NN = NN_FPs[order(NNErrors)[1]]
Avg_FN_PCA20NN = NN_FNs[order(NNErrors)[1]]
plot(
  x = 1:10 / 10,
  y = NNErrors,
  main = "Avg Error over thresholds for PCA Neural Network w/20 Vars",
  xlab = "Cutoff Threshold",
  ylab = "Misclassification Rate"
)
lines(x = 1:10 / 10, y = NNErrors)

```



As expected, this version has the lowest misclassification rate of 6.63%, which is 1.91% lower than the 13 variable PCA NN, and 3.4% lower than the original neural network. As you can see, however, we are reaching a point of diminishing returns; adding ~15% more variation only decreased the error rate by 1.91%

### 3.2.4) K-Nearest Neighbours

kNN works by computing the euclidean distances of the test features to training data points, known as "neighbours". This model requires pre-processing because the distances from each data point must be in the same scale, therefore we first normalized the training and testing features. This model has an input parameter,  $k$ , which represents the number of neighbours considered. Both too-small and too-large values of  $k$  can be detrimental. To tune this parameter, we tested several values of  $k$  in a loop, selecting the  $k$  which resulted in the lowest misclassification rate.

[Hide](#)

```

numKs = 10
k_errors = rep(0, numKs)
k_FPs = rep(0, numKs)
k_FNs = rep(0, numKs)
for (ki in 1:numKs) {
  #tune k parameter
  avgErrors_fold = CreateErrorMatrix(NumFolds)
  avgFP_fold = CreateErrorMatrix(NumFolds)
  avgFN_fold = CreateErrorMatrix(NumFolds)
  for (fold in 1:NumFolds) {
    #k-fold cross validation
    set.seed(fold)
    #make normalized training and testing sets
    scaled_data = data.frame(scale(labeled_final[, 2:36]))
    scaled_data$koi_disposition = ifelse(labeled_final$koi_disposition == "CONFIRMED", 1
, 0)
    summary(scaled_data)
    head(scaled_data)
    num_samples = dim(scaled_data)[1]
    sampling.rate = 0.8
    training = sample(1:num_samples, sampling.rate * num_samples, replace = FALSE)
    trainingSet.norm = subset(scaled_data[training,])
    testing = setdiff(1:num_samples, training)
    testingSet.norm = subset(scaled_data[testing, ])
    sizeTestSet = dim(testingSet.norm)[1]

    trainingfeatures = subset(trainingSet.norm, select = c(-koi_disposition))
    traininglabels = trainingSet.norm$koi_disposition
    testingfeatures = subset(testingSet.norm, select = c(-koi_disposition))
    testinglabels = testingSet.norm$koi_disposition

    #fit model and predict
    predictedLabels = knn(trainingfeatures, testingfeatures, traininglabels, k =
      ki)

    #determine error
    error = sum(predictedLabels != testingSet.norm$koi_disposition)
    Errors = AllErrors(testingSet.norm$koi_disposition,
      predictedLabels,
      sizeTestSet,
      1)

    misclassification_rate = error / sizeTestSet
    avgErrors_fold[fold] = Errors[[1]]
    avgFP_fold[fold] = Errors[[2]]
    avgFN_fold[fold] = Errors[[3]]

  }

  k_errors[ki] = mean(avgErrors_fold)
  k_FPs[ki] = mean(avgFP_fold)
  k_FNs[ki] = mean(avgFN_fold)

```

```
}
print(order(k_errors))
```

```
[1] 4 6 8 7 10 5 9 3 2 1
```

Hide

```
#The lowest average error (this run) is from the model with k = 4.
AvgError_best_knn = k_errors[order(k_errors)[1]]
AvgFP_knn = k_FPs[order(k_errors)[1]]
AvgFN_knn = k_FNs[order(k_errors)[1]]
```

KNN produces an error of 9.08%, with an optimal k-value of 4

## 3.2.5) K-Means Clustering

Clustering is an unsupervised model which uses randomly generated centroids and assigns every point to a centroid based on euclidean distance. The model then iterates to find the centroid locations which minimize the distances to the data points in the clusters. Since this model also requires calculation of euclidean distance, the normalized data set was also used here.

Since our data set was labelled, the supervised models will likely yield a better misclassification rate than k-Means clustering. We include clustering in case the algorithm found unforeseen relationships in the unlabelled data features.

Hide

```
#scale full data set.
set.seed(123)
scaled_data = data.frame(scale(labeled_final[, 2:36]))
scaled_data$koi_disposition = ifelse(labeled_final$koi_disposition == "CONFIRMED", 2, 1)
num_samples = dim(scaled_data)[1]
features = subset(scaled_data, select = c(-koi_disposition))
#fit the model
kclustering = kmeans(features, centers = 2, nstart = 25)#we used two clusters, one for C
ONFIRMED, and one for FALSE POSITIVE. We will then attempt to match clusters to classifi
cations; there are two potential configurations (1 = confirmed and 2 = confirmed); which
ever one results in a misclassification rate of less than 50% will be the accepted confi
guration.
#visualize the clusters
fviz_cluster(kclustering, data = features)
```

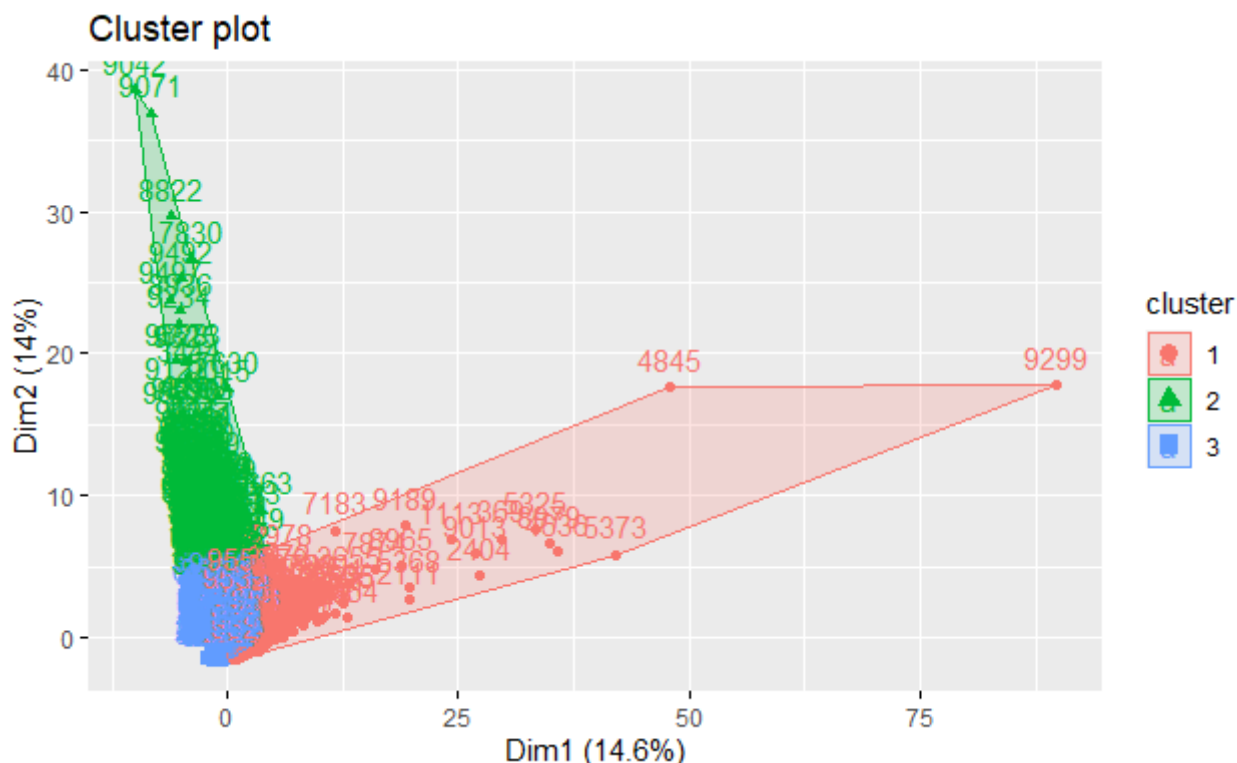


1	2
275	5756

Unsurprisingly, clustering has the largest error, of 41.83%; given this is an unsupervised method and our data has labels. Clustering seems to have put nearly all values in category “2,” which has resulted in a misclassification rate that is roughly the same as the proportions of CONFIRMED and FALSE POSITIVES in the original data set. The fact that clustering is almost only predicting one value can be seen in its terrible false negative rate of 99.56%. One hypothesis for why this might be is because there are certain values that are different enough from the rest of the data set that they are not clearly negative or positive results, and these are being clustered together. To test this, I will try again with 3 centers.

Hide

```
#scale full data set.
set.seed(123)
scaled_data = data.frame(scale(labeled_final[, 2:36]))
scaled_data$koi_disposition = ifelse(labeled_final$koi_disposition == "CONFIRMED", 2, 1)
num_samples = dim(scaled_data)[1]
features = subset(scaled_data, select = c(-koi_disposition))
#fit the model
kclustering = kmeans(features, centers = 3, nstart = 25)#we used two clusters, one for C
ONFIRMED, and one for FALSE POSITIVE. We will then attempt to match clusters to classifi
cations; there are two potential configurations (1 = confirmed and 2 = confirmed); which
ever one results in a misclassification rate of less than 50% will be the accepted confi
guration.
#visualize the clusters
fviz_cluster(kclustering, data = features)
```



```
summary(factor(kclustering$cluster))
```

```
  1    2    3
1126 245 4660
```

With three clusters, we are still getting category 2 with very few values, but have more robust categories 1 and 3. I will therefore labeled category 2 “inconclusive” and get a misclassification rate using categories 1 and 3.

Hide

```
scaled_data$koi_disposition = ifelse(labeled_final$koi_disposition == "CONFIRMED", 3, 1)
error = sum(scaled_data$koi_disposition != kclustering$cluster)
misclassification_rate = error / dim(scaled_data)[1]
isWrong = (scaled_data$koi_disposition != kclustering$cluster)
isRight = (scaled_data$koi_disposition == kclustering$cluster)
IsC = (kclustering$cluster == 3)
IsF = (kclustering$cluster == 1)
FalsePositives = sum(isWrong & IsC)
FalseNegatives = sum(isWrong & IsF)
TruePositives = sum(isRight & IsC)
TrueNegatives = sum(isRight & IsF)
Clustering_FP_2_Rate = (FalsePositives / (FalsePositives + TrueNegatives))#define FP rate as FP/(FP+TN)
Clustering_FN_2_Rate = (FalseNegatives / (FalseNegatives + TruePositives))#define FN rate as FN/(FN+TP)

AvgErrorClustering_2 = misclassification_rate
if (AvgErrorClustering_2 > .5) {
  AvgErrorClustering_2 = 1 - AvgErrorClustering_2#since clustering does not know which cluster is CONFIRMED and which is FALSE POSITIVE, they can be flipped
  Clustering_FP_2_Rate = 1 - Clustering_FP_2_Rate
  Clustering_FN_2_Rate = 1 - Clustering_FN_2_Rate
}

paste("Clustering 2 Error Rate: ", round(AvgErrorClustering_2*100,2), "%", sep = "")
```

```
[1] "Clustering 2 Error Rate: 45.18%"
```

This produces an error rate barely better than that of the naive model, but with more sensible false positive/false negative rates of 69.2% and 1.77%. Although this is not better than any of our other models, it illustrates an interesting application of unsupervised learning to find categories that might not be immediately apparent in the labeled data.

## 4) Select Best Model

Hide

```
error_output = data.frame(  
  "Model" = c(  
    "Decision Tree",  
    "GLM",  
    "Random Forest",  
    "SVM",  
    "Neural Net",  
    "KNN",  
    "Clustering",  
    "PCA 15 Var NN",  
    "PCA 20 Var NN",  
    "XGBoost"  
  ),  
  "Misclassification Rate" = c(  
    AvgErrorDT,  
    AvgErrorGLM,  
    AvgErrorRF,  
    AvgErrorSVM,  
    NeuralNetMisClassRate,  
    AvgError_best_knn,  
    AvgErrorClustering_2,  
    PCA_15_v_NeuralNetMisClassRate,  
    PCA_20_v_NeuralNetMisClassRate,  
    AvgErrorXGB  
  ), "False Positive Rate" = c(  
    AvgFP_DT,  
    AvgFP_GLM,  
    AvgFP_RF,  
    AvgFP_SVM,  
    AvgFP_NN,  
    AvgFP_knn,  
    Clustering_FP_2_Rate,  
    Avg_FP_PCA15NN,  
    Avg_FP_PCA20NN,  
    AvgFP_XGB  
  ), "False Negative Rate" = c(  
    AvgFN_DT,  
    AvgFN_GLM,  
    AvgFN_RF,  
    AvgFN_SVM,  
    AvgFN_NN,  
    AvgFN_knn,  
    Clustering_FN_2_Rate,  
    Avg_FN_PCA15NN,  
    Avg_FN_PCA20NN,  
    AvgFN_XGB  
  )  
)  
print(error_output)
```

Model <chr>	Misclassification.Rate <dbl>	False.Positive.Rate <dbl>	False.Negative.Rate <dbl>
Decision Tree	0.11582436	0.12863903	0.09471457
GLM	0.11731566	0.10041469	0.14515929
Random Forest	0.06661143	0.04633321	0.10000657
SVM	0.08699254	0.08095670	0.09689713
Neural Net	0.10024855	0.10840108	0.08742004
KNN	0.09080365	0.07241510	0.12097613
Clustering	0.45183220	0.69200227	0.01769912
PCA 15 Var NN	0.08533554	0.08807588	0.08102345
PCA 20 Var NN	0.06628003	0.05149051	0.08955224
XGBoost	0.06081193	0.10307018	0.04660453

1-10 of 10 rows

All models beat the naive misclassification rate of 46.73%, with all except clustering beating it by a significant margin. XGBoost has the lowest misclassification rate; although it has a slightly higher False Positive rate than some other model, it still has the best overall accuracy. We will remake this model using the full dataset.

## #5 Make predictions

Remake the XGBoost model using the full dataset:

[Hide](#)

```
xgData = data.matrix(labeled_final)
xgData[, 1] = ifelse(xgData[, 1] == 2, 1, 0)

xgBoostModelFinal = xgboost(
  data = xgData[, 2:36],
  label = xgData[, 1],
  max.depth = 6,
  eta = .22,
  nrounds = 100,
  verbose = 0,
  objective = "binary:logistic",
  eval_metric="error"
)
xgPredict = data.matrix(candidates_final)
xgPredict[, 1] = ifelse(xgPredict[, 1] == 2, 1, 0)
```

Predict labels of candidates dataset, and write it to file

[Hide](#)



```
#make predictions
BoostPredictions = predict(xgBoostModelFinal, data.matrix(candidates_final)[, 2:36])
BoostPredictionsRounded = ifelse(BoostPredictions > .4, 1, 0)
predictedLabels = ifelse(BoostPredictionsRounded == 1, "FALSE POSITIVE", "CONFIRMED")
candidates_final$koi_disposition = predictedLabels
head(candidates_final)
```

koi_disposition <chr>	koi_period <dbl>	koi_period_err1 <dbl>	koi_period_err2 <dbl>	koi_time0bk <dbl>	koi_time0
38 CONFIRMED	4.959319	5.150e-07	-5.150e-07	172.2585	8
59 FALSE POSITIVE	40.419504	1.139e-04	-1.139e-04	173.5647	2
63 FALSE POSITIVE	7.240661	1.617e-05	-1.617e-05	137.7554	2
64 FALSE POSITIVE	3.435916	4.729e-05	-4.729e-05	132.6624	1
73 FALSE POSITIVE	1.626630	1.015e-06	-1.015e-06	169.8202	4
85 FALSE POSITIVE	10.181584	6.188e-06	-6.188e-06	177.1419	4

6 rows | 1-7 of 36 columns

Hide

```
write.csv(candidates_final, "labeledCandidates.csv")

numConfirmed = sum(candidates_final[,1]=="CONFIRMED")
numFalse = sum(candidates_final[,1]=="FALSE POSITIVE")
Proportions = data.frame(label = c("CONFIRMED","FALSE POSITIVE"), number = c(numConfirmed, numFalse))
bp = ggplot(Proportions, aes(x = "", y=number, fill=label))+geom_bar(width = 1, stat = "identity")
pie = bp+coord_polar("y", start = 0) + ggtitle("Proportions of final predictions that are CONFIRMED or FALSE POSITIVE")
```

As shown in the pie above, our final model is predicting more non-planets than confirmed planets. Given that our XGBoost model has a higher False Positive than False Negative rate, it is likely that some of these CONFIRMEDs are in fact incorrect, meaning that there are likely slightly more FALSEs and slightly fewer CONFIRMED than predicted.

In conclusion, this model can be used to identify new planets in the future. Given more computational resources, the candidate models for neural networks would likely be able to be parameter tuned more, and run with more input variables. Given our limited computational power, however, we believe this to be a strong model for predicting whether a given stellar observation is an exoplanet.