Breast Cancer Project

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Introduction

Breast cancer is a type of cancer that starts in the breast. Breast cancer cells usually form a tumor that can often be seen on an x-ray or felt as a lump[1]. Breast tumors are either benign (non-cancerous) or malignant (cancerous). Since cancer is life threatening, it is crucial to predict if a breast tumor is benign or malignant with the highest possible accuracy levels.

Purpose

The purpose of this statistical analysis is to examine the ways in which malignant and benign tumors differ in their characteristics. The secondary purpose is to determine if an informative lower dimensional structure of the variables exists, and use that structure to train classification models to predict whether a lump is benign or malignant. Our goal is to select the classification model that yields the highest accuracy, but also to discuss the relative costs of False Positives versus False Negatives.

Scientific Questions

Are there statistically significant differences between mean vectors for benign tumors and malignant tumors? Can we use Principal Components Analysis (PCA) to reduce the dimensionality of the data and to identify/summarize crucial variables? Which classification model yields the highest accuracy for predicting if a tumor is benign or malignant?

Data Description

The data was collected from 699 patients of Dr. William H. Wolberg at the University of Wisconsin between January 1989 and November 1991. Samples arrived periodically as Dr. Wolberg reported his clinical cases. Measurements were derived from fine needle aspirations of human breast masses and analyses were performed on the masses. Each observation is described by the following nine features:

1: Clump Thickness
2: Cell Size Uniformity
3: Cell Shape Uniformity
4: Marginal Adhesion
5: Single Epithelial Cell Size

6: Bare Nuclei
7: Bland Chromatin
8: Normal Nucleoli
9: Mitosis

The fine needle aspirates for these nine features were graded 1 to 10 at the time of sample collection, with 1 being the closest to benign and 10 the closest to malignant. Each observation has one of two possible classes: benign or malignant. In the dataset, the benign class is labeled as 2 and the malignant class is labeled as 4. 458 (65.5%) of the observations were classified as benign and 241 (34.5%) of the observations were classified as malignant. The dataset used for this analysis is the Breast Cancer Wisconsin (Original) data set sourced from UCI's Machine Learning Repository[2].

Overview

Provide overview of conclusions of the data analysis, and a short road map for the remainder of the report.

Methods: Data Analysis

The data pre-processing and statistical analysis was performed using R version 4.0.2.

```r
library(tidyverse)

##### DATA CLEANING #####
# Read in data set.

# Read in the Breast Cancer data set.
bc.df <- read.table('Data/breast-cancer-wisconsin.data', sep=',')
# Add informative column names.
colnames(bc.df) = c('Id', 'Clump Thickness', 'Cell Size Uniformity',
                    'Cell Shape Uniformity', 'Marginal Adhesion',
                    'Single Epithelial Cell Size', 'Bare Nuclei',
                    'Bland Chromatin', 'Normal Nucleoli', 'Mitosis',
                    'Class')

# Calculate mean Bare Nuclei by Class.
mean.BareNuclei.2 <- bc.df %>%
  group_by(Class) %>%
  summarize(Mean = mean(as.numeric(`Bare Nuclei`),
                        na.rm=TRUE))%>%filter(Class == 2)
mean.BareNuclei.4 <- bc.df %>%
  group_by(Class) %>%
  summarize(Mean = mean(as.numeric(`Bare Nuclei`),
                        na.rm=TRUE))%>%filter(Class == 4)
```

```
# Impute missing Bare Nuclei data with the mean for each Class mean.
bc.df <- bc.df %>%
  mutate(`Bare Nuclei Revised` = ifelse(`Bare Nuclei` == "?" & Class == 2,
                                        round(mean.BareNuclei.2$Mean,2),
                                        ifelse(`Bare Nuclei` == "?" & Class =
= 4,
                                               round(mean.BareNuclei.4$Mean,2
), `Bare Nuclei`))) #%>%

# Convert Bare Nuclei Revised data to the int data type.
bc.df$`Bare Nuclei Revised` <- as.integer(bc.df$`Bare Nuclei Revised`)

# Convert Class to a factor variable.
bc.df$Class = as.factor(bc.df$Class)

##### SUMMARY STATISTICS #####
bc.df.mean <- dplyr::select(bc.df, -c("Id","Bare Nuclei")) %>% group_by(Class
) %>% summarise_all("mean")
#transpose from wide to long
bc.df.mean<-as.data.frame(t(dplyr::select(bc.df.mean,-"Class")))
colnames(bc.df.mean) <- c('Benign', 'Malignant')
bc.df.sd <- dplyr::select(bc.df, -c("Id","Bare Nuclei")) %>% group_by(Class)
%>% summarise_all("sd")
#transpose from wide to long
bc.df.sd<-as.data.frame(t(dplyr::select(bc.df.sd,-"Class")))
colnames(bc.df.sd) <- c('Benign', 'Malignant')

##### DATA SPLITTING #####
# Set a random seed for reproducibility.
set.seed(17)
# Count the number of observations in the data set.
num.obs <- dim(bc.df)[1]
# Set the proportion of observations to be in the training data set.
prop.train <- 0.7
# Set the number of observations to be in the training data set.
num.train <- round(num.obs*prop.train)
# set the indicies of the dataset to be in the training data set.
train.indices <- sample(1:num.obs, num.train, replace=FALSE)
# Subset the data into training and testing data sets.
train.bc.df <- bc.df[train.indices,]
test.bc.df <- bc.df[-train.indices,]

# Save the vector of the indicies of the independent variable columns.
X_col_indicies <- c(2, 3, 4, 5, 6, 8, 9, 10, 12)
```

Missing Data

Upon review of the dataset, missing values were identified in the Bare Nuclei feature for 16 observations. The missing values are denoted as “?” in the dataset. The missing Bare Nuclei values were imputed with the mean of the non-missing Bare Nuclei values from the corresponding class (benign or malignant). For example, if the missing Bare Nuclei was of the benign class, then that missing value was imputed with the mean of the Bare Nuclei values that were in the benign class. A new column, Bare Nuclei Revised, was added to the data set and this new column includes the imputed values.

Summary Statistics: Mean

Table 1 shown to the right, shows the mean value for each feature by class (benign or malignant). For the benign class, each of the means fall between 1 and 3. For the malignant class, each of the means fall between 5 and 8 with the exception of Mitosis. The Mitosis mean for the malignant class is 2.59 which is far below the means for the other features in the malignant class.

```r
knitr::kable(bc.df.mean, align = 'c',
             caption =  'Mean Summary Statistics', digits = 2)
```

Mean Summary Statistics

	Benign	Malignant
Clump Thickness	2.96	7.20
Cell Size Uniformity	1.33	6.57
Cell Shape Uniformity	1.44	6.56
Marginal Adhesion	1.36	5.55
Single Epithelial Cell Size	2.12	5.30
Bland Chromatin	2.10	5.98
Normal Nucleoli	1.29	5.86
Mitosis	1.06	2.59
Bare Nuclei Revised	2.40	4.70

Summary Statistics: Standard Deviation

Table 2 shown to the right, shows the standard deviation value for each feature by class (benign or malignant). For the benign class, each of the standard deviations fall between 0 and 2. For the malignant class, each of the standard deviations fall between 2 and 4. This indicates that there is more variability in the malignant class when compared to the benign class.

```r
knitr::kable(bc.df.sd, align = 'c',
             caption =  'Standard Deviation Summary Statistics', digits = 3)
```

Standard Deviation Summary Statistics

	Benign	Malignant
Clump Thickness	1.674	2.429

Cell Size Uniformity	0.908	2.720
Cell Shape Uniformity	0.998	2.562
Marginal Adhesion	0.997	3.210
Single Epithelial Cell Size	0.917	2.452
Bland Chromatin	1.080	2.274
Normal Nucleoli	1.059	3.351
Mitosis	0.502	2.558
Bare Nuclei Revised	1.204	2.646

Data Pre-Processing

After imputing the missing Bare Nuclei values, the Bare Nuclei Revised variable was converted to an integer and the Class variable was converted to a factor with levels 2 and 4. Then the observed data was randomly split into a testing and training dataset. 70% (n = 489) of the observations were assigned to the testing dataset and 30% (n = 210) of the observations were assigned to the training dataset.

Methods: Statistical Models

Let us define the p observed features in a data vector, X, such that $X = (X_1, \dots, X_p)^T$ where

X_1: Clump Thickness in {1,2,3,4,5,6,7,8,9,10}
X_2: Cell Size Uniformity in {1,2,3,4,5,6,7,8,9,10}
X_3: Cell Shape Uniformity in {1,2,3,4,5,6,7,8,9,10}
X_4: Marginal Adhesion in {1,2,3,4,5,6,7,8,9,10}
X_5: Single Epithelial Cell Size in {1,2,3,4,5,6,7,8,9,10}
X_6: Bland Chromatin in {1,2,3,4,5,6,7,8,9,10}
X_7: Normal Nucleoli in {1,2,3,4,5,6,7,8,9,10}
X_8: Mitosis in {1,2,3,4,5,6,7,8,9,10}
X_9: Bare Nuclei Revised in {1,2,3,4,5,6,7,8,9,10}

Hotelling's T^2 Two-Sample Test

Add mathematical models and methods here

Principal Components Analysis (PCA)

The main goal of PCA is to identify linear combinations of X of the form $Y_i = a_i^T X$, where $i = 1,2, \dots, q$,that explains most of the variability in X. Usually, $q < p$. a_i^T is a vector of length p which represents the PC loadings and tells us how the original features are weighted to get the PCs. Y_i represents the new variables and are ordered according to their importance. For instance, Y_1 is designed to capture the most variability in the original features by any linear combination. Y_2 then captures the most of the remaining variability while being uncorrelated to Y_1, and so on. We hope that the first few Y_i's capture most of the variability in X. If we are able to capture most of the variability in X with a few Y_i's , then we have achieved dimensionality reduction by condensing a sufficient portion of the information present in the original set of features via linear combinations while losing as little information as possible.

We used the prcomp function from the stats package in R to conduct the PCA. The PCA was run using the training dataset with the center and scale arguments set equal to true to standardize the dataset. The results and interpretation of the PC loadings will be discussed in the results section.

Classification

Scientific Question #2: Which classification model yields the highest accuracy for predicting if a tumor is benign or malignant, provided there are statistically significant differences in the measurements taken from benign and malignant masses?

After establishing there are statistically significant differences between benign and malignant masses in the measured variable and if there was a lower dimensional representation of the data containing sufficient information, we proceeded to build predictive models using the caret package. The tested models include K-Nearest Neighbors (KNN), Linear Discriminant Analysis (LDA), Quadratic Discriminant Analysis (QDA), Classification Trees, and Support Vector Machines (SVM) with a Radial Basis Kernel. The performance of these models were examined using 5-fold Cross Validation repeated 20 times, for 100 total resamples from the training data set. This process was repeated for data transformed based on the results from the Principal Components Analysis. The distribution of accuracies and Cohen's κ were evaluated to select a model for evaluation on the withheld testing data set.

The following hyperparameters were evaluated for each model on both the raw training data and a subset of the PCA scores of the training data.

KNN: k in {1,3,5,7,9}
LDA: None
QDA: None
Classification Tree: cp in {0.05,0.1,0.15, … ,0.5}
SVM: C in {0.25,0.5,1,2,4} and sigma in {0.125,0.25,0.5,1,2,4,8}

After choosing the model(s) with the best results from the cross-validation, the model(s) were tested on the testing data set and the Accuracy, Apparent Error Rate (APER), sensitivity, and specificity were examined, as well as the costs of False Positives and False Negatives.

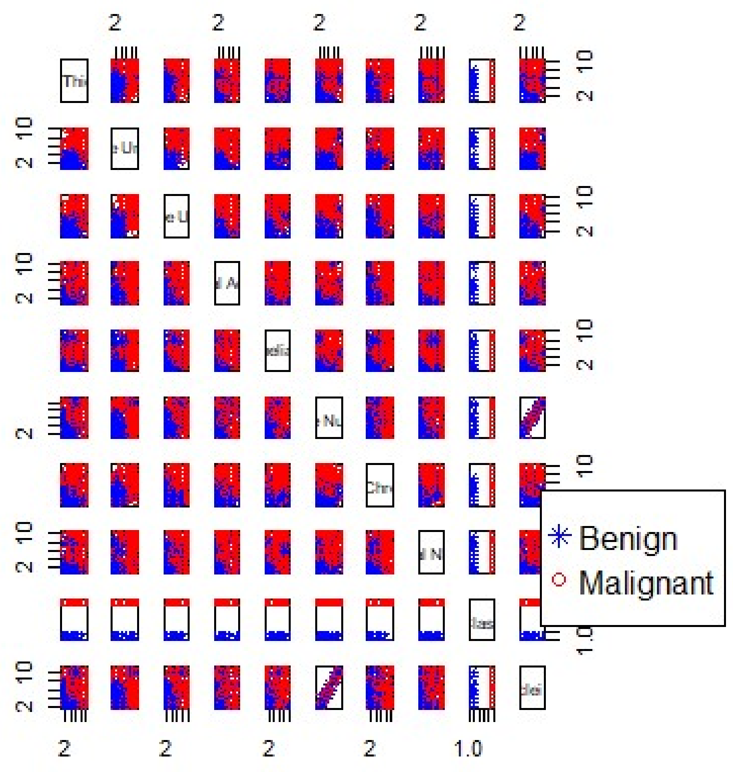
Methods: Results

Hotelling's T2 Two Sample Test Results

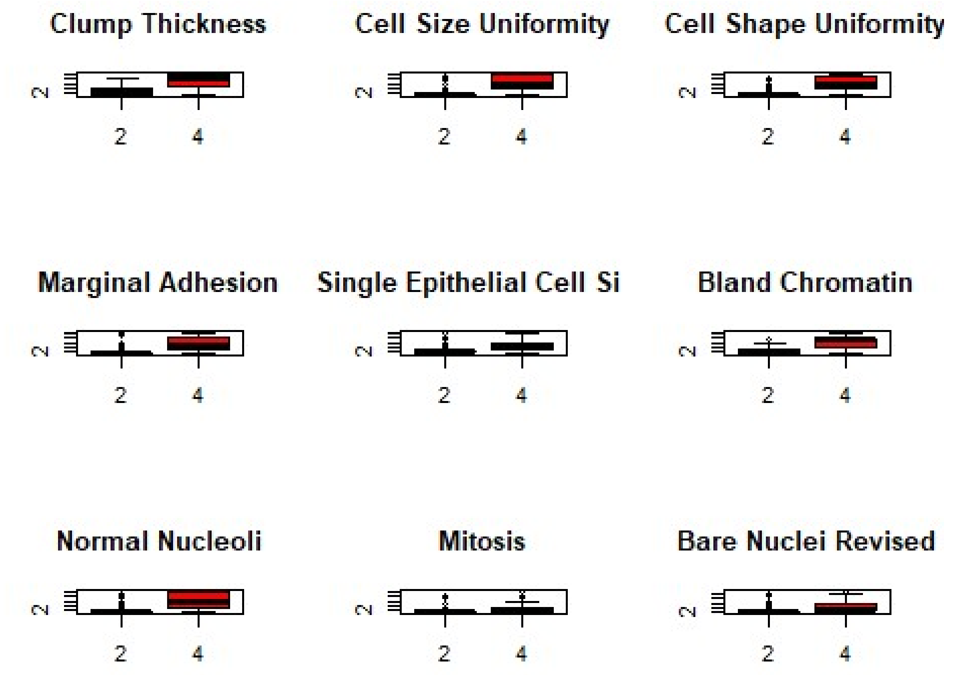
Scientific Question #1: Are there statistically significant differences between mean vectors for benign tumors and malignant tumors?

Add results here

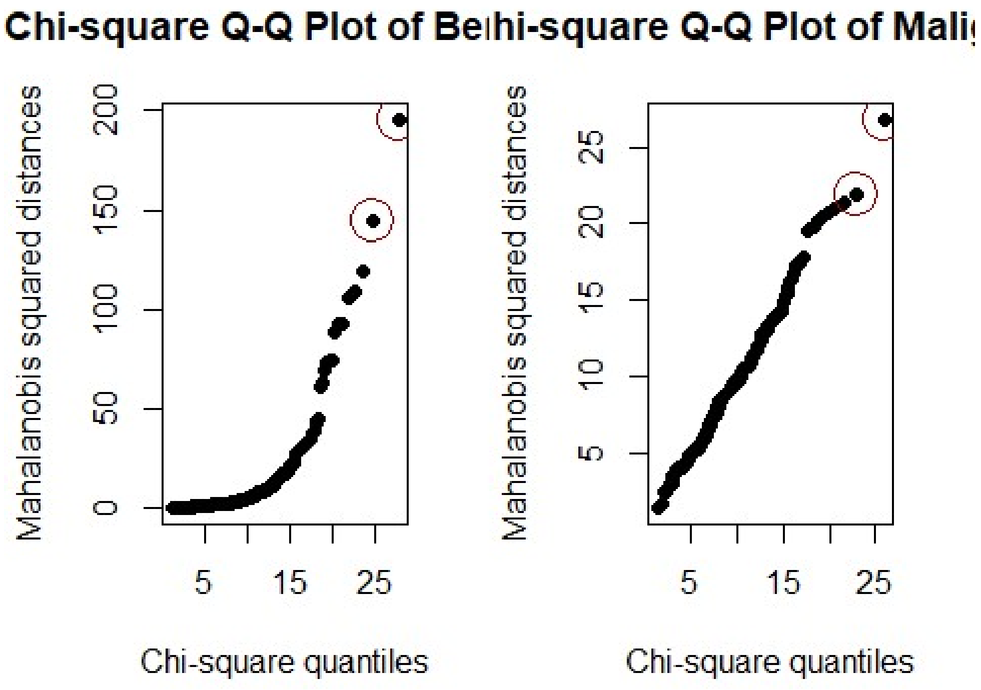
```
# pair plot
pairs(bc.df[,-c(1,10)],
      col = c(4, 2)[as.numeric(bc.df$Class)],   # Change color by group
      pch = c(8, 1)[as.numeric(bc.df$Class)],   # Change points by group
      main = "Pair Plot of Benign and Malignant for All Variables", oma=c(2,2
,2,16))
par(xpd = TRUE)
legend("bottomright", col=c(4, 2),pch = c(8, 1),
       legend = c("Benign", "Malignant"))
```



```
# boxplot
par(mfrow=c(3,3))
for(col_index in X_col_indicies){
  boxplot(bc.df[,col_index] ~ Class, data = bc.df, col=c(4,2),
          xlab='', ylab = '', main=names(bc.df)[col_index])
}
```



```r
library(ICSNP)

# Seperate the 2 classes into dataframes for mean vector comparison.
X = as.matrix(bc.df[bc.df$Class == "2", X_col_indicies]) # class 2
Y = as.matrix(bc.df[bc.df$Class == "4", X_col_indicies]) # class 4

#normality check
################## chisquare.plot ##############
chisquare.plot <- function(x, mark, title) {
  # x = A nxp data matrix, mark: number of extreme points to mark,
  # p = number of variables, n = sample size
  p <- ncol(x)
  n <- nrow(x)
  # xbar and s
  xbar <- colMeans(x)
  s <- cov(x)
  # Mahalanobis dist, sorted
  x.cen <- scale(x, center = T, scale = F)
  d2 <- diag(x.cen %*% solve(s) %*% t(x.cen))
  sortd <- sort(d2)
  # chi-sq quantiles
  qchi <- qchisq((1:n - 0.5)/n, df = p)
  # plot, mark points with heighest distance
  plot(qchi, sortd, pch = 19, xlab = "Chi-square quantiles",
       ylab = "Mahalanobis squared distances",
       main = title)
  points(qchi[(n - mark + 1):n], sortd[(n - mark + 1):n], cex = 3, col = "#99
0000")
}
###########################################
par(mfrow=c(1,2))
chisquare.plot(X,2, "Chi-square Q-Q Plot of Benign")
chisquare.plot(Y,2, "Chi-square Q-Q Plot of Malignant")
```



```
## Two-sample Hotelling's T2 test
HotellingsT2(X,Y)

##
##  Hotelling's two sample T2-test
##
## data:  X and Y
## T.2 = 312.56, df1 = 9, df2 = 689, p-value < 2.2e-16
## alternative hypothesis: true location difference is not equal to c(0,0,0,0
,0,0,0,0,0)

## Bonferroni intervals
alpha = 0.05 # old significance level
p = 2 # number of intervals/variables
# mean vectors
xbar = colMeans(X)
ybar = colMeans(Y)
difference = xbar - ybar
# covariances of each group
S.x = cov(X)
```

```
S.y = cov(Y)
# bc.df statistics summary
stats = round(cbind(xbar, ybar, sqrt(diag(S.x)), sqrt(diag(S.y))),3)
colnames(stats) = c('Benign Mean', 'Malignant Mean', 'Benign Sd', 'Malignant
Sd')
stats
```

```
##                              Benign Mean Malignant Mean Benign Sd Malignant
Sd
## Clump Thickness                    2.956          7.195     1.674          2.
429
## Cell Size Uniformity               1.325          6.573     0.908          2.
720
## Cell Shape Uniformity              1.443          6.560     0.998          2.
562
## Marginal Adhesion                  1.365          5.548     0.997          3.
210
## Single Epithelial Cell Size        2.120          5.299     0.917          2.
452
## Bland Chromatin                    2.100          5.979     1.080          2.
274
## Normal Nucleoli                    1.290          5.863     1.059          3.
351
## Mitosis                            1.063          2.589     0.502          2.
558
## Bare Nuclei Revised                2.402          4.701     1.204          2.
646
```

```
# sample sizes
m = nrow(X)
n = nrow(Y)
# pooled covariance matrix
S.pool = ((m-1)*S.x + (n-1)*S.y) / (m + n - 2)
# critical value
crit = qt(alpha/(2*p), df = m+n-2, lower.tail = F)
# Bonferroni intervals
half.width = crit*sqrt(diag(S.pool)*(1/m + 1/n))
lower = difference - half.width
upper = difference + half.width
int.bonf = cbind(lower, upper)
int.bonf
```

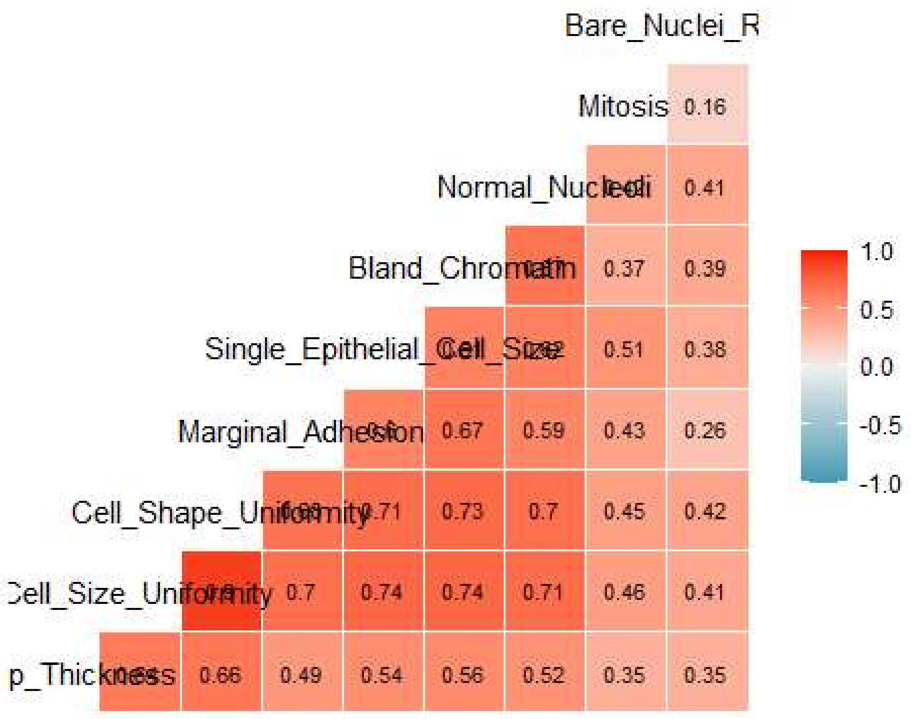
```
##                                 lower     upper
## Clump Thickness             -4.590312 -3.887066
## Cell Size Uniformity        -5.561346 -4.933228
## Cell Shape Uniformity       -5.422027 -4.811842
## Marginal Adhesion           -4.549452 -3.816726
## Single Epithelial Cell Size -3.468066 -2.889270
## Bland Chromatin             -4.164017 -3.593616
## Normal Nucleoli             -4.956102 -4.189253
## Mitosis                           -1.803867 -1.247919
## Bare Nuclei Revised               -2.627205 -1.971791
```

Principal Components Analysis (PCA) Results

Scientific Question #2: Can we use PCA to reduce the dimensionality of the data and to identify/summarize crucial variables?

The results of the PCA importance of components are displayed below in Table 3. The output shows that 70.7% of the total variation in the training data can be explained by PC1 and PC2. We typically retain PCs that explain between 70% and 95% of the total variation.

```
##### PCA (Principle Components Analysis #####
# Scientific Question 2
# Can we use PCA to reduce the dimensionality of the data and
# to identify/summarize crucial variables?
library(knitr)

library(GGally)

# Split the training and testing data sets into independent
# variables and dependent variables.
train.bc.df.class <- train.bc.df$Class
train.bc.df.X <- select(train.bc.df, -c("Id","Bare Nuclei","Class"))
test.bc.df.class <- test.bc.df$Class
test.bc.df.X <- select(test.bc.df, -c("Id","Bare Nuclei","Class"))

# Plot a correlation matrix.
ggcorr(train.bc.df.X, label=TRUE, label_size=3, label_round=2)
```



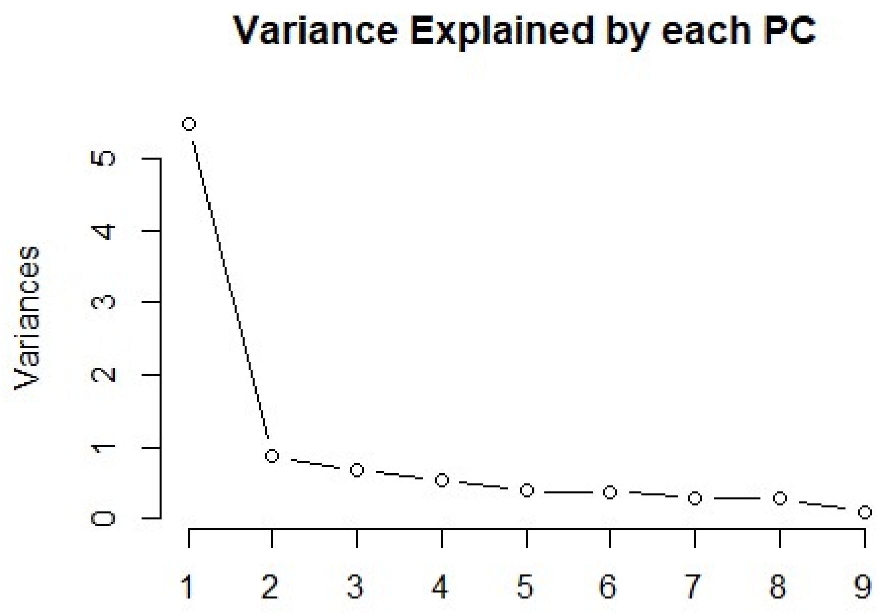
```
# Shows that Cell Shape Uniformity and Cell Size Uniformity are highly correl
ated (0.90).
cor(train.bc.df.X)

##                             Clump Thickness Cell Size Uniformity
## Clump Thickness                   1.0000000            0.6429847
## Cell Size Uniformity              0.6429847            1.0000000
## Cell Shape Uniformity             0.6631989            0.9049778
## Marginal Adhesion                 0.4912901            0.6986296
## Single Epithelial Cell Size       0.5421161            0.7391602
## Bland Chromatin                   0.5577657            0.7431113
## Normal Nucleoli                   0.5235813            0.7106115
## Mitosis                           0.3544657            0.4570546
## Bare Nuclei Revised               0.3544358            0.4080672
##                             Cell Shape Uniformity Marginal Adhesion
## Clump Thickness                         0.6631989         0.4912901
## Cell Size Uniformity                    0.9049778         0.6986296
## Cell Shape Uniformity                   1.0000000         0.6841941
## Marginal Adhesion                       0.6841941         1.0000000
## Single Epithelial Cell Size             0.7061165         0.5979035
## Bland Chromatin                         0.7288692         0.6722778
## Normal Nucleoli                         0.6992053         0.5905170
## Mitosis                                 0.4466957         0.4325498
## Bare Nuclei Revised                     0.4203279         0.2554196
##                             Single Epithelial Cell Size Bland Chromatin
## Clump Thickness                               0.5421161       0.5577657
## Cell Size Uniformity                          0.7391602       0.7431113
## Cell Shape Uniformity                              0.7061165       0.7288692
## Marginal Adhesion                                  0.5979035       0.6722778
## Single Epithelial Cell Size                        1.0000000       0.6104333
## Bland Chromatin                                    0.6104333       1.0000000
## Normal Nucleoli                                    0.6169662       0.6729169
## Mitosis                                            0.5081960       0.3678463
## Bare Nuclei Revised                                0.3767608       0.3948828
##                               Normal Nucleoli   Mitosis Bare Nuclei Revised
## Clump Thickness                     0.5235813 0.3544657           0.3544358
## Cell Size Uniformity                0.7106115 0.4570546           0.4080672
## Cell Shape Uniformity               0.6992053 0.4466957           0.4203279
## Marginal Adhesion                   0.5905170 0.4325498           0.2554196
## Single Epithelial Cell Size         0.6169662 0.5081960           0.3767608
## Bland Chromatin                     0.6729169 0.3678463           0.3948828
## Normal Nucleoli                     1.0000000 0.4185491           0.4142987
## Mitosis                             0.4185491 1.0000000           0.1649736
## Bare Nuclei Revised                 0.4142987 0.1649736           1.0000000

# Standardize the variables.
train.bc.df.X.std <- scale(train.bc.df.X, center=TRUE, scale=TRUE)

# Perform PCA.
data.pca <- prcomp(train.bc.df.X.std)

# Extract the importance of each component.

# standard deviation
st.dev <- data.pca$sdev
# variance
var <- st.dev^2
# total variance
TV <- sum(var)
#proportion of variance explained
prop <- var/TV
#cumulative proportion of variance explained
pve <- cumsum(var)/TV
#combine in a table
tab <- rbind(st.dev, prop, pve)
rownames(tab) <- c("Standard deviation", "Proportion of variance",
                   "Cumulative proportion")
colnames(tab) <- paste0("PC",1:9)
knitr::kable(tab, align = 'c',
             caption = 'PCA Importance of Components', digits = 3)
```

PCA Importance of Components

	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	PC9
Standard deviation	2.343	0.935	0.822	0.729	0.620	0.616	0.538	0.530	0.304
Proportion of variance	0.610	0.097	0.075	0.059	0.043	0.042	0.032	0.031	0.010
Cumulative proportion	0.610	0.707	0.782	0.841	0.884	0.926	0.958	0.990	1.000

The scree plot depicted in Figure 1 on the right displays the amount of variance explained for each PC. The scree plot shows a bend at PC2 which indicates that we should retain at least PC1 and PC2. Based on the cumulative proportion of variance explained and inspection of the scree plot, we will retain PC1 and PC2 for further analysis.

```r
# Make a Scree Plot to help determine how many PCs to retain.
screeplot(data.pca, type = "line", main = "Variance Explained by each PC")
```



The loadings of the first two PCs are shown below in Table 4.

```r
# The elbow in the graph is at PC2.
# PC 1 and 2 explain 74% of the variability
# Display the loadings for PC1 and PC2 for review.
```

```r
#round(data.pca$rotation[, 1:2], 3)
knitr::kable(data.pca$rotation[, 1:2], align = 'c',
             caption = 'Loadings of the First Two PCs', digits = 3)
```

Loadings of the First Two PCs

	PC1	PC2
Clump Thickness	0.315	0.095
Cell Size Uniformity	0.393	-0.008
Cell Shape Uniformity	0.390	0.021
Marginal Adhesion	0.337	-0.218
Single Epithelial Cell Size	0.351	-0.105
Bland Chromatin	0.357	0.066
Normal Nucleoli	0.349	0.066
Mitosis	0.246	-0.570
Bare Nuclei Revised	0.218	0.773

Hence the first PC can be constructed as follows: $Y_1 = 0.306X_1 + 0.380X_2 + 0.377X_3 + 0.334X_4 + 0.337X_5 + 0.347X_6 + 0.332X_7 + 0.235X_8 + 0.330X_9$

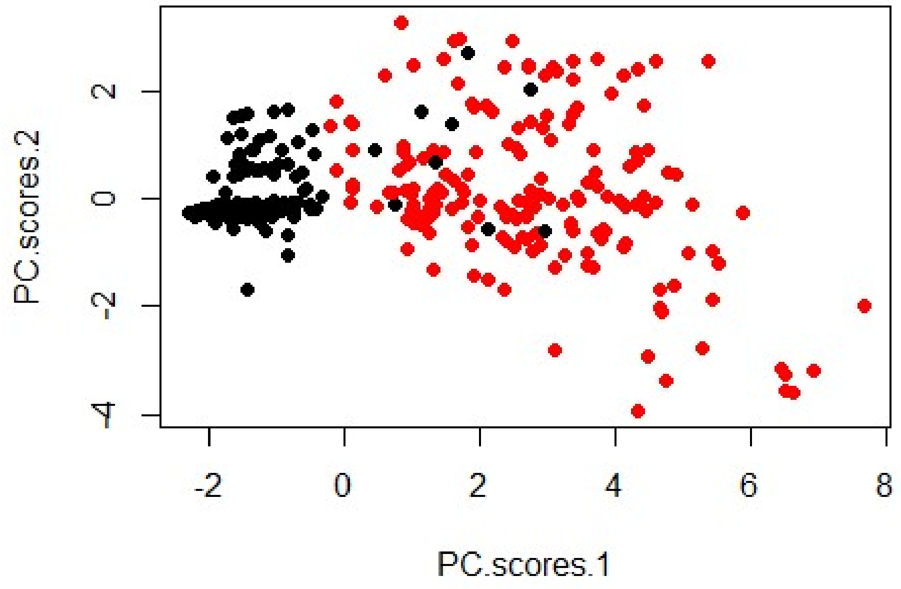
We can interpret the first PC as a roughly equally weighted sum of the nine features.

Hence the second PC can be constructed as follows: $Y_2 = 0.164X_1 + 0.058X_2 + 0.087X_3 + 0.039X_4 - 0.217X_5 + 0.201X_6 - 0.003X_7 - 0.889X_8 + 0.288X_9$

We can interpret the second PC as a contrast between Mitosis and Single Epithelial Cell Size with Clump Thickness, Bland Chromatin, and Bare Nuclei Revised. The PC2 loadings for the other four features (Cell Size Uniformity, Cell Shape Uniformity, Marginal Adhesion, and Normal Nucleoli) are close to zero and are not important in PC2. Although several features are important for PC2, the second PC is strongly weighted by Mitosis.

Y_1 and Y_2 represent the PC scores which are computed by multiplying the standardized training dataset by their respective PC loadings. The PC scores are then used as the predictors in the classification models. Figure 2 displays a scatter plot of PC1 scores and PC2 scores colored by class (black represents benign and red represents malignant).

```r
# PC1 is roughly equally weighted.
# PC2 is essentially the effect of Mitosis.
PC1 <- data.pca$rotation[, 1]
PC2 <- data.pca$rotation[, 2]
PC.scores.1 <- train.bc.df.X.std %*% PC1
PC.scores.2 <- train.bc.df.X.std %*% PC2
# Plot PC score 1 vs PC score 2 colored by class.
plot(PC.scores.1,PC.scores.2, pch=19, col=train.bc.df.class)
```



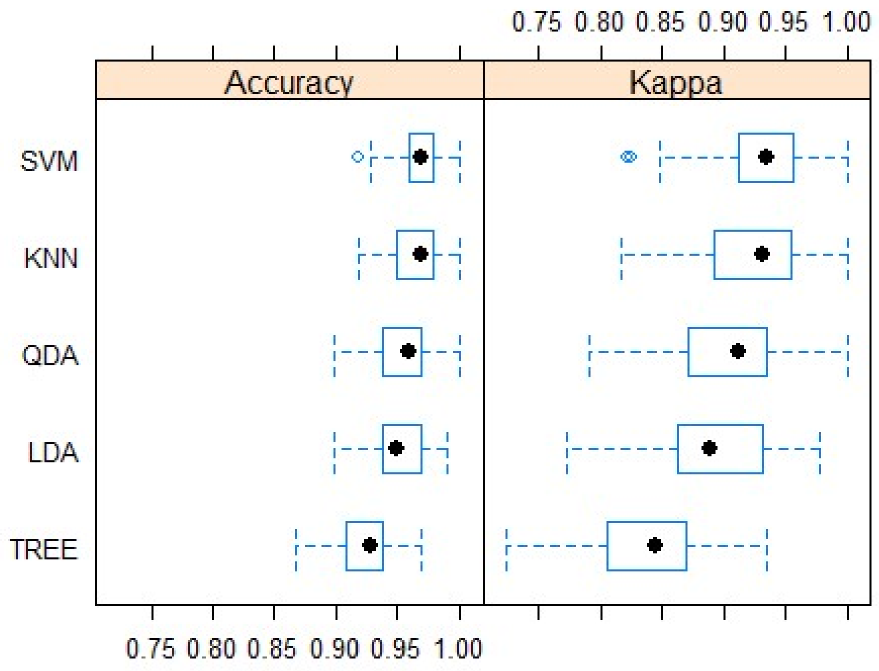
Classification

Scientific Question #3: Which classification model yields the highest accuracy for predicting if a tumor is benign or malignant?

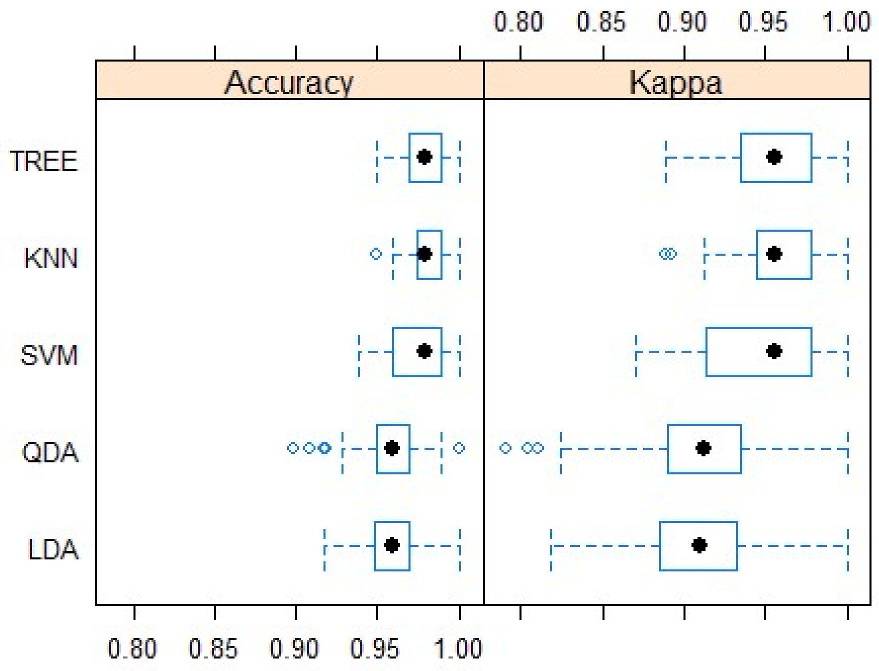
```
# Create a dataframe only holding the X variables and the Class, starting wit
ht he X variables.
train.df = train.bc.df.X
test.df = test.bc.df.X
# Re-attach the Class to the independent variables of the training and testin
g dataframes.
train.df$Class <- train.bc.df.class
test.df$Class <- test.bc.df.class
# This is essential to get rpart to run on this data.
colnames(train.df) <- make.names(colnames(train.df))
colnames(test.df) <- make.names(colnames(train.df))

# Set the number of principal components to keep.
num.keep <- 2

# Re-fit prcomp() so it knows to center and scale input data.
pca.fit <- prcomp(train.bc.df.X, center=TRUE, scale=TRUE)

# Create a new dataframe to hold the prcomp() transformed training data.
train.pca <- as.data.frame(pca.fit$x[, 1:num.keep])
# Create a new dataframe to hold the prcomp() transformed testing data.
```

```r
test.pca <- as.data.frame(predict(pca.fit, test.bc.df.X)[, 1:num.keep])

# Re-attach the Class to the PCA-trainsformed training and testing dataframes
.
train.pca$Class <- train.bc.df.class
test.pca$Class <- test.bc.df.class

library(caret)

# We will be using 5-fold cross-validation, repeating the process 20 times.
TrControl <- trainControl(method = "repeatedcv",
                          number = 5,
                          repeats = 20)

# Fit a KNN classifier by selecting the model with the best number of neighbo
rs
# by performing 5-fold cross-validation tuning the k parameter using the odd
numbers
# from 1 up to 9.
knn.model <- train(Class ~ ., data = train.df,
                   method = "knn",
                   trControl = TrControl,
                   tuneGrid = expand.grid(k = seq(1, 9, by=2)))

# Perform 5-fold cross-validation using a LDA classifier.
lda.model <- train(Class ~ ., data = , train.df,
                   method = "lda",
                   trControl = TrControl)

# Perform 5-fold cross-validation using a QDA classifier.
qda.model <- train(Class ~ ., data = , train.df,
                   method = "qda",
                   trControl = TrControl)

# Fit a tree classifier by selecting the model with the best complexity param
eter (cp)
# by performing 5-fold cross-validation tuning the cp parameter using 0.001,
0.01,
# and 0.1
tree.model <- train(Class ~ ., data = train.df,
                    method = "rpart",
                    trControl = TrControl,
                    tuneGrid = expand.grid(cp = seq(0.05, 0.5, by=0.05)))

# Fit a SVM classifier with a radial kernel by selecting the model tuning the
C and
# sigma parameters by performing 5-fold cross-validation tuning
# the C parameter from 0.25 to 4, doubling each time, and the sigma parameter
from
# 0.125 to 8, doubling each time
```

```
svm.model <- train(Class ~ ., data = train.df,
                   method = "svmRadial",
                   trControl = TrControl,
                   tuneGrid = expand.grid(C = 2^c(-2:2),
                                          sigma = 2^(-3:3)))

# Summarize the Accuracy and Cohen's Kappa for each model in the 5-fold CV.
resamp <- resamples(list(KNN = knn.model, LDA = lda.model, QDA = qda.model,
                         TREE = tree.model, SVM = svm.model))

# Display the summary of the model performances.
summary(resamp)

##
## Call:
## summary.resamples(object = resamp)
##
## Models: KNN, LDA, QDA, TREE, SVM
## Number of resamples: 100
##
## Accuracy
##           Min.   1st Qu.    Median      Mean   3rd Qu.      Max. NA's
## KNN  0.9175258 0.9489796 0.9690722 0.9644172 0.9795918 1.0000000    0
## LDA  0.8979592 0.9387755 0.9489796 0.9494887 0.9690722 0.9897959    0
## QDA  0.8979592 0.9387755 0.9591837 0.9562424 0.9693878 1.0000000    0
## TREE 0.8673469 0.9081633 0.9285714 0.9256701 0.9387755 0.9693878    0
## SVM  0.9183673 0.9591837 0.9693878 0.9703471 0.9795918 1.0000000    0
##
## Kappa
##           Min.   1st Qu.    Median      Mean   3rd Qu.      Max. NA's
## KNN  0.8166352 0.8919722 0.9322842 0.9227766 0.9549839 1.0000000    0
## LDA  0.7719870 0.8640604 0.8885593 0.8889319 0.9321615 0.9779180    0
## QDA  0.7910448 0.8715596 0.9122257 0.9072393 0.9345794 1.0000000    0
## TREE 0.7234043 0.8046217 0.8444382 0.8409821 0.8699690 0.9345794    0
## SVM  0.8222222 0.9122257 0.9345794 0.9360928 0.9561129 1.0000000    0

# Make a boxplot of the model Accuracies and Cohen's Kappas.
bwplot(resamp)
```



```
# Fit a KNN classifier by selecting the model with the best number of neighbo
rs
# by performing 5-fold cross-validation tuning the k parameter using the odd
numbers
# from 1 up to 9.
knn.model.pca <- train(Class ~ ., data = train.pca,
                       method = "knn",
                       trControl = TrControl,
                       tuneGrid = expand.grid(k = seq(1, 9, by=2)))

# Perform 5-fold cross-validation using a LDA classifier.
lda.model.pca <- train(Class ~ ., data = , train.pca,
                       method = "lda",
                       trControl = TrControl)

# Perform 5-fold cross-validation using a QDA classifier.
qda.model.pca <- train(Class ~ ., data = , train.pca,
                       method = "qda",
                       trControl = TrControl)

# Fit a tree classifier by selecting the model with the best complexity param
eter (cp)
# by performing 5-fold cross-validation tuning the cp parameter using 0.001,
0.01,
# and 0.1
tree.model.pca <- train(Class ~ ., data = train.pca,
                        method = "rpart",
                        trControl = TrControl,
                        tuneGrid = expand.grid(cp = seq(0.05, 0.5, by=0.05)))

# Fit a SVM classifier with a radial kernel by selecting the model tuning the
C and
# sigma parameters by performing 5-fold cross-validation tuning
# the C parameter from 0.25 to 4, doubling each time, and the sigma parameter
from
# 0.125 to 8, doubling each time
svm.model.pca <- train(Class ~ ., data = train.pca,
                       method = "svmRadial",
                       trControl = TrControl,
                       tuneGrid = expand.grid(C = 2^c(-2:2),
                                              sigma = 2^(-3:3)))

# Summarize the Accuracy and Cohen's Kappa for each model in the 5-fold CV.
resamp.pca <- resamples(list(KNN = knn.model.pca, LDA = lda.model.pca, QDA =
qda.model.pca,
                         TREE = tree.model.pca, SVM = svm.model.pca))

# Display the summary of the model performances.
summary(resamp.pca)

##
## Call:
## summary.resamples(object = resamp.pca)
##
## Models: KNN, LDA, QDA, TREE, SVM
## Number of resamples: 100
##
## Accuracy
##           Min.   1st Qu.    Median      Mean   3rd Qu. Max. NA's
## KNN  0.9489796 0.9768830 0.9795918 0.9805702 0.9897959    1    0
## LDA  0.9175258 0.9484536 0.9589733 0.9565443 0.9693878    1    0
## QDA  0.8979592 0.9489796 0.9591837 0.9574679 0.9693878    1    0
## TREE 0.9489796 0.9693878 0.9795918 0.9806785 0.9897959    1    0
## SVM  0.9387755 0.9591837 0.9793814 0.9754576 0.9897959    1    0
##
## Kappa
##           Min.   1st Qu.    Median      Mean   3rd Qu. Max. NA's
## KNN  0.8881789 0.9503115 0.9561129 0.9583259 0.9779180    1    0
## LDA  0.8175896 0.8852459 0.9093813 0.9045515 0.9320388    1    0
## QDA  0.7910448 0.8895899 0.9127698 0.9088872 0.9342782    1    0
## TREE 0.8881789 0.9345794 0.9561129 0.9585903 0.9779180    1    0
## SVM  0.8699690 0.9133127 0.9555556 0.9472229 0.9777880    1    0

bwplot(resamp.pca)
```



```
library(klaR)

# Get predictions for the test set from the tree model.
tree.preds <- predict(tree.model.pca, test.pca)
# Make a confusion matrix for the tree model.
tree.emat <- errormatrix(test.pca$Class, tree.preds,
                         relative = TRUE)
# Display the confusion matrix for the tree model.
round(tree.emat, 3)

##         predicted
## true         2     4 -SUM-
##   2     0.938 0.062 0.062
##   4     0.015 0.985 0.015
##   -SUM- 0.100 0.900 0.048

# Get predictions for the test set from the knn model.
knn.preds <- predict(knn.model.pca, test.pca)
# Make a confusion matrix for the knn model.
knn.emat <- errormatrix(test.pca$Class, knn.preds,
                        relative = TRUE)
# Display the confusion matrix for the knn model.
round(knn.emat, 3)

##         predicted
## true         2     4 -SUM-
##   2     0.938 0.062 0.062
##   4     0.015 0.985 0.015
##   -SUM- 0.100 0.900 0.048

# Calculate the accuracy for the tree model.
tree.accuracy <- sum(tree.preds == test.pca$Class) / length(tree.preds)
# Calculate the APER for the tree model.
tree.aper <- sum(tree.preds != test.pca$Class) / length(tree.preds)
# Calculate the sensistivity for the tree model.
tree.true.pos <- test.pca[test.pca$Class == 4, 'Class']
tree.true.pos.preds <- tree.preds[test.pca$Class == 4]
tree.sensitivity <- sum(tree.true.pos == tree.true.pos.preds) / length(tree.t
rue.pos)
# Calculate the specificity for the tree model.
tree.true.neg <- test.pca[test.pca$Class == 2, 'Class']
tree.true.neg.preds <- tree.preds[test.pca$Class == 2]
tree.specificity <- sum(tree.true.neg == tree.true.neg.preds) / length(tree.t
rue.neg)

print(paste('Tree Model Accuracy: ', round(100*tree.accuracy, 5), '%', sep=''
))

## [1] "Tree Model Accuracy: 95.2381%"

print(paste('Tree Model APER: ', round(100*tree.aper, 5), '%', sep=''))

## [1] "Tree Model APER: 4.7619%"

print(paste('Tree Model Sensitivity: ', round(100*tree.sensitivity, 5), '%',
sep=''))

## [1] "Tree Model Sensitivity: 98.48485%"

print(paste('Tree Model Specificity: ', round(100*tree.specificity, 5), '%',
sep=''))

## [1] "Tree Model Specificity: 93.75%"

# Calculate the accuracy for the knn model.
knn.accuracy <- sum(knn.preds == test.pca$Class) / length(knn.preds)
# Calculate the APER for the knn model.
knn.aper <- sum(knn.preds != test.pca$Class) / length(knn.preds)
# Calculate the sensistivity for the knn model.
knn.true.pos <- test.pca[test.pca$Class == 4, 'Class']
knn.true.pos.preds <- knn.preds[test.pca$Class == 4]
knn.sensitivity <- sum(knn.true.pos == knn.true.pos.preds) / length(knn.true.
pos)
# Calculate the specificity for the knn model.
knn.true.neg <- test.pca[test.pca$Class == 2, 'Class']
knn.true.neg.preds <- knn.preds[test.pca$Class == 2]
knn.specificity <- sum(knn.true.neg == knn.true.neg.preds) / length(knn.true.
neg)
```

```r
print(paste('K-NN Model Accuracy: ', round(100*knn.accuracy, 5), '%', sep='')
)

## [1] "K-NN Model Accuracy: 95.2381%"

print(paste('K-NN Model APER: ', round(100*knn.aper, 5), '%', sep=''))

## [1] "K-NN Model APER: 4.7619%"

print(paste('K-NN Model Sensitivity: ', round(100*knn.sensitivity, 5), '%', s
ep=''))

## [1] "K-NN Model Sensitivity: 98.48485%"

print(paste('K-NN Model Specificity: ', round(100*knn.specificity, 5), '%', s
ep=''))

## [1] "K-NN Model Specificity: 93.75%"

# Set the proportion of tree predictions equal to knn predictions.
proportion.equal <- sum(tree.preds == knn.preds) / length(tree.preds)

print(paste('Percent of Tree Model Predictions equal to K-NN Model Prediction
s: ',
            round(100*proportion.equal, 5), '%', sep=''))

## [1] "Percent of Tree Model Predictions equal to K-NN Model Predictions: 10
0%"
```

Conclusions