Assignment 2

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Setup

```
# Load required libraries
library(ggplot2)
library(ggbiplot)
library(ROCR)
library(corrplot)
library(ISLR)
library(caret)
library(randomForest)
```

```
# Read data
ovarian.data <- na.omit(read.delim("ovarian.data", sep=",", header = FALSE))
features <- c("perimeter", "area", "smoothness", "symmetry", "concavity",
              paste("protein", seq(1, 25), sep=""))
names(ovarian.data) <- c("cell_id", "diagnosis", features)
# paste0(features,"_mean"), paste0(features,"_se"), paste0(features,"_worst"))

dim(ovarian.data)
head(ovarian.data)
```

Q1. Dimensionality Reduction

Q1.1

```
ovarian.pca <- prcomp(ovarian.data[,c(3:32)], center = TRUE,scale. = TRUE)
summary(ovarian.pca)
```

```
## Importance of components:
##                           PC1    PC2     PC3     PC4     PC5    PC6    PC7
## Standard deviation     3.5820 2.2873 1.62395 1.37410 1.24910 1.0844 0.8306
## Proportion of Variance 0.4277 0.1744 0.08791 0.06294 0.05201 0.0392 0.0230
## Cumulative Proportion  0.4277 0.6021 0.68997 0.75291 0.80492 0.8441 0.8671
##                            PC8     PC9    PC10    PC11   PC12   PC13   PC14
## Standard deviation     0.74686 0.67762 0.61684 0.60200 0.5771 0.5139 0.5021
## Proportion of Variance 0.01859 0.01531 0.01268 0.01208 0.0111 0.0088 0.0084
## Cumulative Proportion  0.88571 0.90101 0.91369 0.92578 0.9369 0.9457 0.9541
##                           PC15   PC16   PC17    PC18    PC19    PC20   PC21
## Standard deviation     0.45896 0.3989 0.3834 0.36254 0.32797 0.30949 0.3001
## Proportion of Variance 0.00702 0.0053 0.0049 0.00438 0.00359 0.00319 0.0030
## Cumulative Proportion  0.96110 0.9664 0.9713 0.97569 0.97928 0.98247 0.9855
##                           PC22    PC23    PC24   PC25    PC26    PC27    PC28
## Standard deviation     0.27191 0.26081 0.24722 0.2326 0.22154 0.20068 0.18042
## Proportion of Variance 0.00246 0.00227 0.00204 0.0018 0.00164 0.00134 0.00108
## Cumulative Proportion  0.98794 0.99020 0.99224 0.9940 0.99568 0.99702 0.99811
##                           PC29    PC30
## Standard deviation     0.17164 0.16532
## Proportion of Variance 0.00098 0.00091
## Cumulative Proportion  0.99909 1.00000
```

```r
str(ovarian.pca)
```

```
## List of 5
##  $ sdev    : num [1:30] 3.58 2.29 1.62 1.37 1.25 ...
##  $ rotation: num [1:30, 1:30] -0.22 -0.11 -0.229 -0.222 -0.137 ...
##   ..- attr(*, "dimnames")=List of 2
##   .. ..$ : chr [1:30] "perimeter" "area" "smoothness" "symmetry" ...
##   .. ..$ : chr [1:30] "PC1" "PC2" "PC3" "PC4" ...
##  $ center  : Named num [1:30] 14.1809 19.3922 92.1982 663.7854 0.0965 ...
##   ..- attr(*, "names")= chr [1:30] "perimeter" "area" "smoothness" "symmetry" ...
##  $ scale   : Named num [1:30] 3.5715 4.2746 24.1993 354.8356 0.0142 ...
##   ..- attr(*, "names")= chr [1:30] "perimeter" "area" "smoothness" "symmetry" ...
##  $ x       : num [1:625, 1:30] -4.476 0.448 1.916 1.874 -2.802 ...
##   ..- attr(*, "dimnames")=List of 2
##   .. ..$ : chr [1:625] "1" "2" "3" "4" ...
##   .. ..$ : chr [1:30] "PC1" "PC2" "PC3" "PC4" ...
##  - attr(*, "class")= chr "prcomp"
```

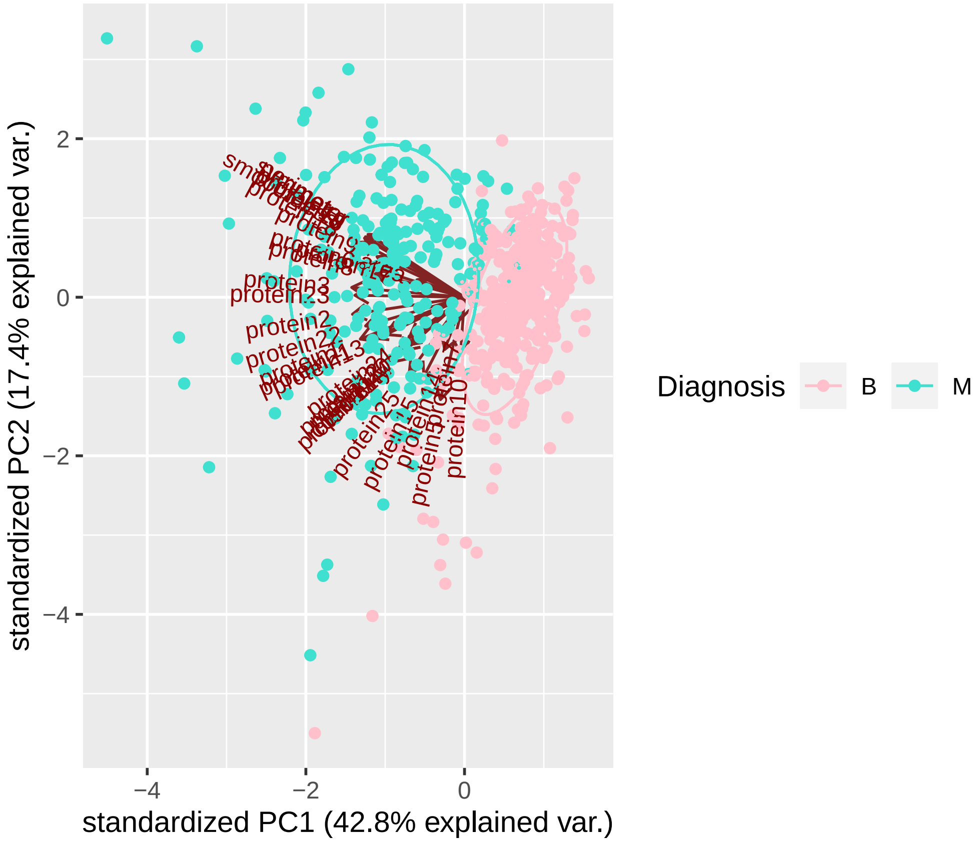
About 42.77% of the variation in the data is associated with PC1.

Q1.2 To represent 90% of the variance in the data by dimensionality reduction, you would need about 9 PCs.

Q1.3

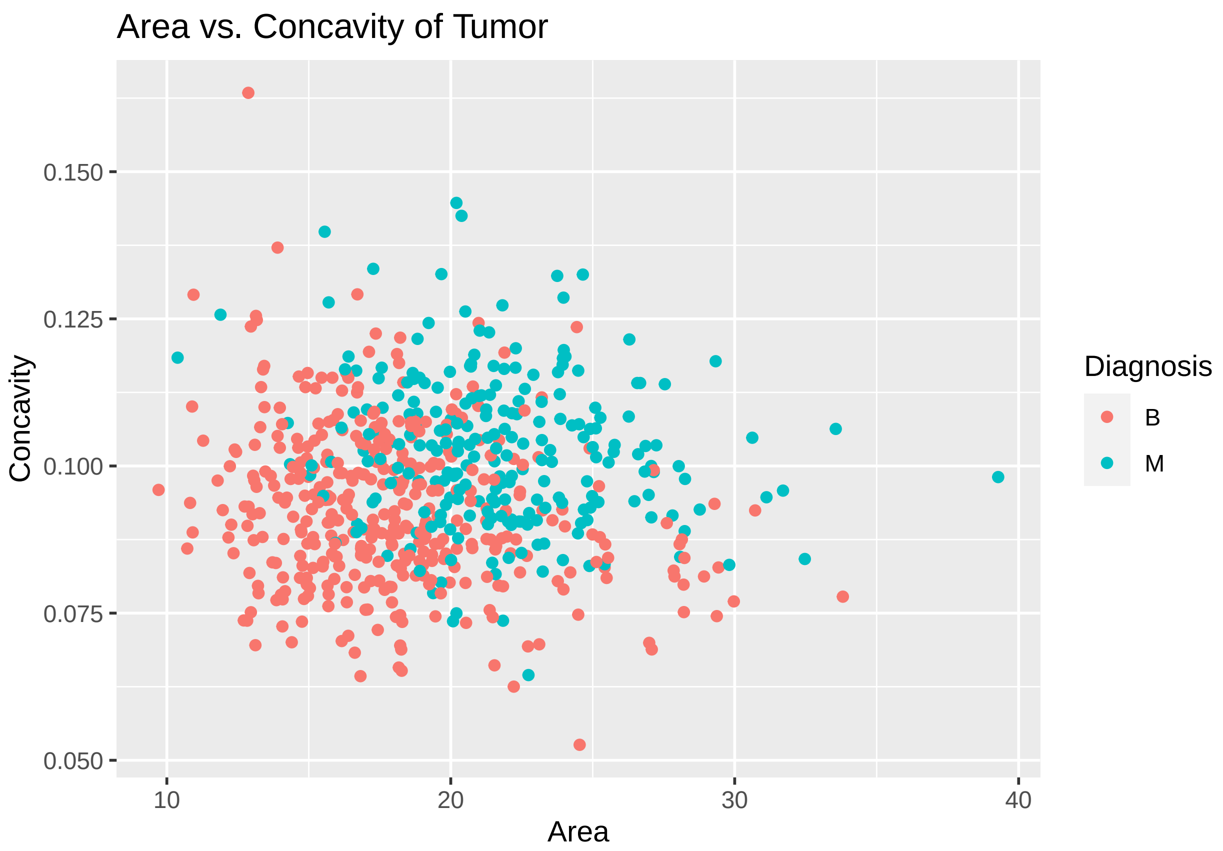
```r
diagnosis <- ovarian.data[,2]

ggbiplot(ovarian.pca, choices=c(1,2), ellipse=TRUE, groups=diagnosis) +
  scale_color_manual(name="Diagnosis", values=c("pink", "turquoise")) +
  scale_shape_manual(name="Variety", values=c(2)) +
  geom_point(aes(colour=diagnosis), size = 0.01) +
  theme(legend.direction ="horizontal",legend.position = "right")
```



Q1.4

```
q1.4_plot <- ggplot(ovarian.data, aes(x = area, y = concavity)) +
  geom_point(aes(color = diagnosis)) +
  labs(title = "Area vs. Concavity of Tumor",
       x = "Area",
       y = "Concavity",
       color = "Diagnosis")
q1.4_plot
```



Q1.5 The first plot using the first two important PCs has two distinct groups, while in the second one they are a lot more mixed. This is because the first two PCs have the highest proportion of the variation in the dataset, so they will have the most difference between them.

Q1.6

Q2. Clustering

Q2.1

```r
# Scaling the data
ovarian.scaled <- scale(ovarian.data[,c(3:32)])

# Set seed to get reproducible results


# Performing kmeans
km.out <- kmeans(ovarian.scaled, centers = 2, iter.max = 1, nstart = 20)
km.out$cluster <- ifelse(km.out$cluster == 1, "M", "B")
table(ovarian.data$diagnosis, km.out$cluster)
```

```
##
##         B   M
##     B 371  14
##     M  35 205
```

```r
mean(ovarian.data$diagnosis == km.out$cluster)
```

```
## [1] 0.9216
```

There is a good amount of concordance between the identified clusters and the true labels of the cell. The model had an accuracy of 92.16%.

Q2.2

```r
accuracies <- numeric(10)

# Repeat kmeans 10 times
for(i in 1:10){
  km.out <- kmeans(ovarian.scaled, centers = 2, iter.max = 10, nstart = 20)
  km.out$cluster <- ifelse(km.out$cluster == 1, "M", "B")
  accuracies[i] <- mean(ovarian.data$diagnosis == km.out$cluster)
}

mean(accuracies)
```

```
## [1] 0.58432
```

The values change from run to run because the results of the kmeans algorithm is dependent on the initializtion of the centers, which is different each time.

Q2.3

```r
# Transform pca results to dataframe
pca.data <- as.data.frame(ovarian.pca$x[,1:5])

# Perform kmeans analysis
km.out <- kmeans(pca.data, centers = 2, nstart = 20)
km.out$cluster <- ifelse(km.out$cluster == 1, "M", "B")
table(ovarian.data$diagnosis, km.out$cluster)
```

```
##
##       B   M
##   B  16 369
##   M 205  35
```

```r
mean(ovarian.data$diagnosis == km.out$cluster)
```

```
## [1] 0.0816
```

```r
# Perform kmeans analysis 10 times
accuracies.pca <- numeric(10)

for(i in 1:10){
  km.out <- kmeans(pca.data, centers = 2, nstart = 20)
  km.out$cluster <- ifelse(km.out$cluster == 1, "M", "B")
  accuracies.pca[i] <- mean(ovarian.data$diagnosis == km.out$cluster)
}

mean(accuracies.pca)
```

```
## [1] 0.41632
```

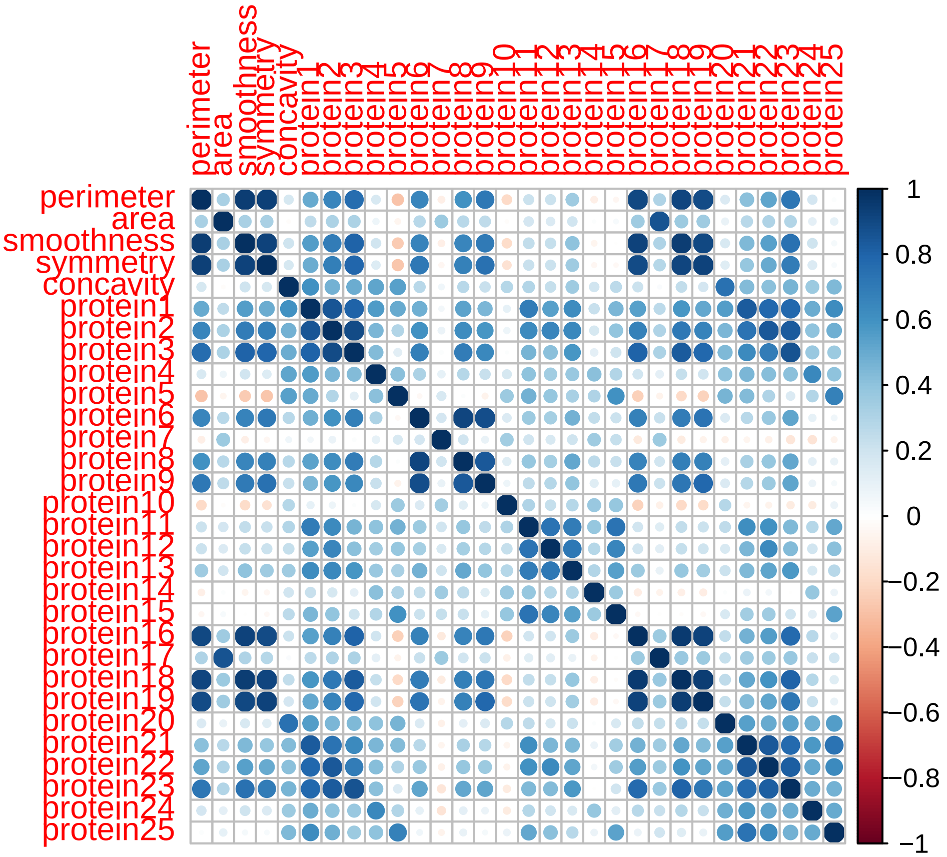
Q2.4 The results from 2.3 were very slightly worse than 2.2. The highest average from 2.2 was 0.9216, while the highest from 2.3 was 0.9184. This is because the entire data set is used in 2.2 and most of the variance in the data is covered.

Q3. Classification

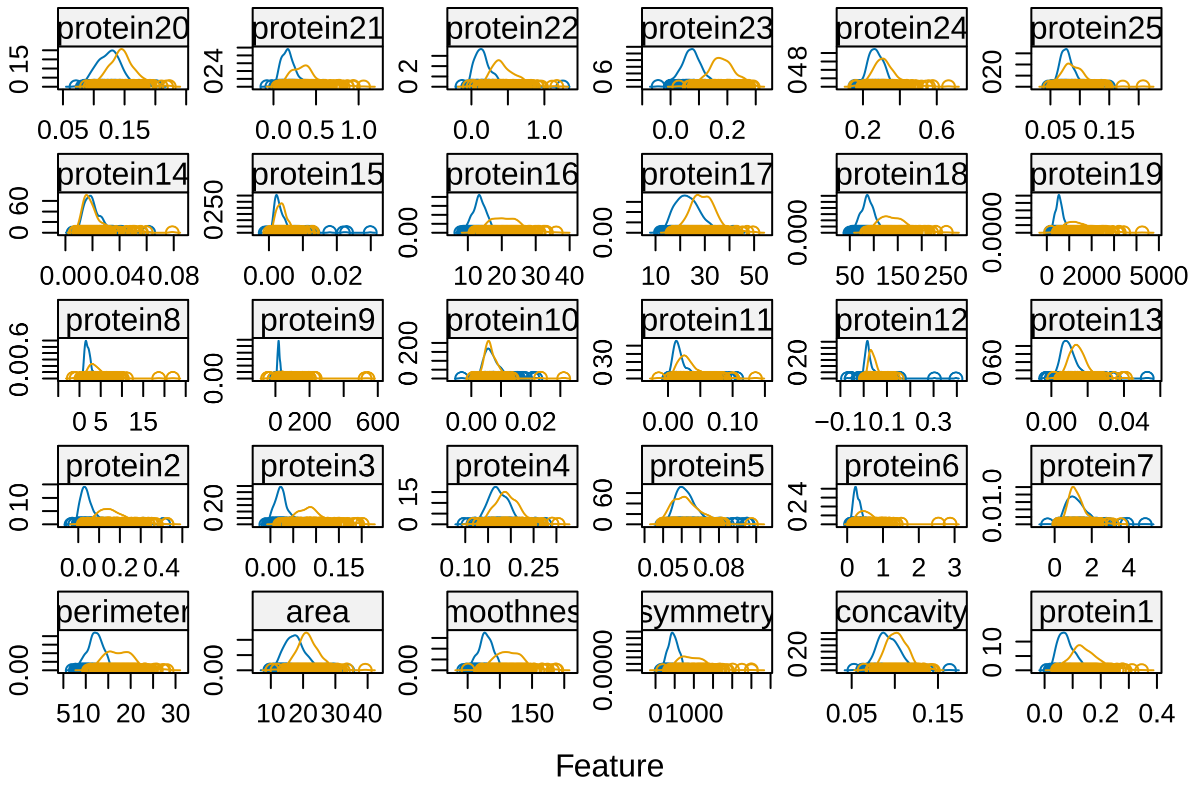
```
# Divide dataset into training and testing sets
ovarian.data.train <- ovarian.data[sample(nrow(ovarian.data))[1:(nrow(ovarian.data)/2)],]
ovarian.data.test <- ovarian.data[sample(nrow(ovarian.data))[(nrow(ovarian.data)/2):(nrow(ovarian.data)
```

Q3.1

```
# Plot correlation between pairs of variables
correlations <- cor(ovarian.data[,3:32])
corrplot(correlations, method="circle")
```



```
# Plot density distribution of each variable, separated by diagnosis
x <- ovarian.data[,3:32]
y <- as.factor(ovarian.data[,2])
scales <- list(x=list(relation="free"), y=list(relation="free"))
featurePlot(x=x, y=y, plot="density", scales=scales)
```



```r
# Change diagnosis column to factors
ovarian.data.train$diagnosis <- as.factor(ovarian.data.train$diagnosis)

# Logistic regression training model
training.model <- glm(diagnosis ~. -cell_id, data = ovarian.data.train, family = binomial)

# Predicting on testing model
probabilities <- predict(training.model, ovarian.data.test, type = "response")
predicted.diagnosis <- ifelse(probabilities > 0.5, "M", "B")
prediction <- as.factor(predicted.diagnosis)
actual <- as.factor(ovarian.data.test$diagnosis)

# Confusion matrix
table(prediction, actual)
```

```
##             actual
## prediction   B   M
##            B 172   2
##            M  12 127
```

```r
# To calculate accuracy, precision, recall
accuracy <-mean(prediction == actual)
precision <- posPredValue(prediction, actual, positive='M', negative = 'B')
recall <- sensitivity(prediction, actual, positive="M")
accuracy
```

```
## [1] 0.9552716
```

```
precision
```

```
## [1] 0.9136691
```

```
recall
```

```
## [1] 0.9844961
```

Q3.2

```
# Logistic regression training model using top 5 PCs
pca.training.model <- glm(diagnosis ~ perimeter + area + smoothness + symmetry
                          + concavity, data = ovarian.data.train, family = binomial)

# Predicting on testing set
pca.probabilities <- predict(pca.training.model, ovarian.data.test, type = "response")
pca.predicted.diagnosis <- ifelse(pca.probabilities > 0.5, "M", "B")
pca.prediction <- as.factor(pca.predicted.diagnosis)

# Confusion matrix
table(pca.prediction, actual)
```

```
##                actual
## pca.prediction   B   M
##              B 175  16
##              M   9 113
```

```
# To calculate accuracy, precision, recall
pca.accuracy <-mean(pca.prediction == actual)
pca.precision <- posPredValue(pca.prediction, actual, positive='M', negative = 'B')
pca.recall <- sensitivity(pca.prediction, actual, positive="M")
pca.accuracy
```

```
## [1] 0.9201278
```

```
pca.precision
```

```
## [1] 0.9262295
```

```
pca.recall
```

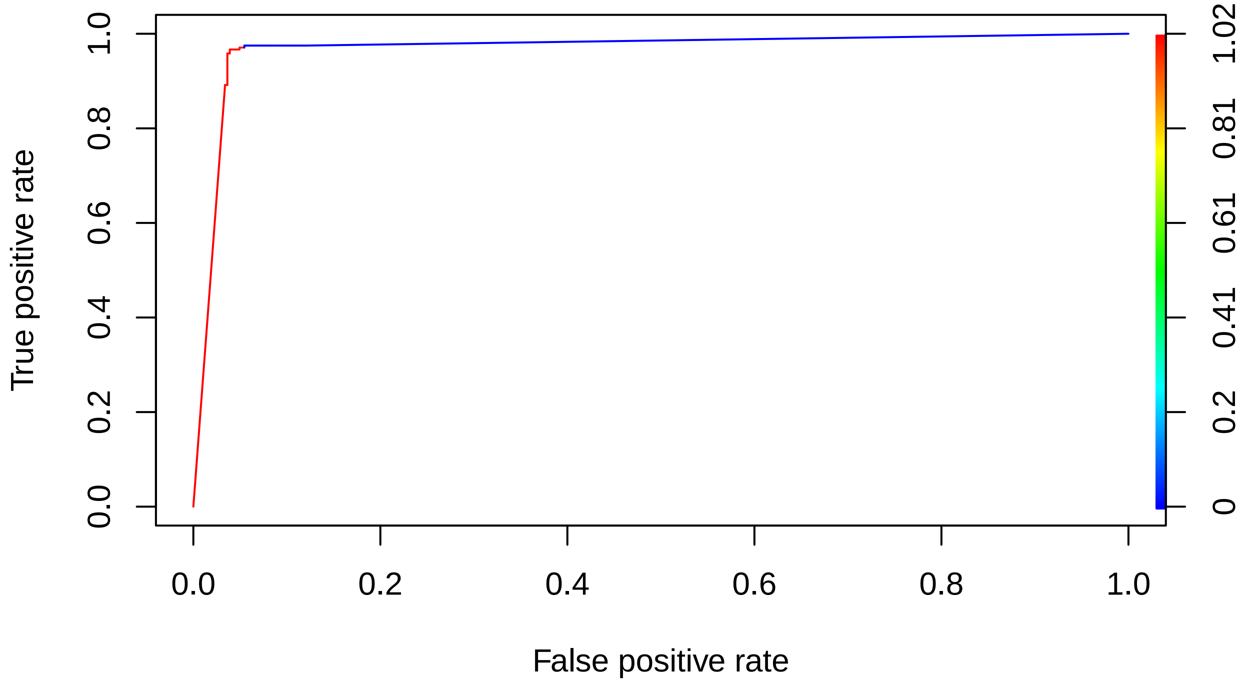
```
## [1] 0.875969
```

Q3.3

Q3.4

Q3.5

```
pred.prob <- predict(training.model, ovarian.data, type="response")
predict <- prediction(pred.prob, ovarian.data$diagnosis, label.ordering=c("B","M"))
perform <- performance(predict,"tpr","fpr")
plot(perform,colorize=TRUE)
```



Given the above ROC curve, we can tell that there is very little overlap of the two classes. The curve is very close to the top left corner which indicates that the model does a good job at classifying the data into categories and that the model has very good separability.

The ROC curve provides a more comprehensive view of a model's performance by showing how sensitivity and specificity change with different classification thresholds, which can in turn be used to select an optimal cut-off value for the diagnostic test. It can also help with understanding of the separability of the classes through graphical visualization.

Q3.6

```
set.seed(123)

# Split into training (70%) and testing (30%)
chunk <- sample(nrow(ovarian.data), 0.7 * nrow(ovarian.data))
rf.training <- ovarian.data[chunk, ]
rf.testing <- ovarian.data[-chunk, ]

# Random forest model
rf.training$diagnosis <- as.factor(rf.training$diagnosis)
ovarian.rf <- randomForest(diagnosis ~.-cell_id, rf.training)
```

```
# Predicting on train set
pred.train <- predict(ovarian.rf, rf.training, type = "class")

# Checking classification accuracy
table(pred.train, rf.training$diagnosis)
```

```
##
## pred.train   B   M
##          B 273   0
##          M   0 164
```

```
# Predicting on Validation set
pred.test <- predict(ovarian.rf, rf.testing, type = "class")

# Checking classification accuracy
mean(pred.test == rf.testing$diagnosis)
```

```
## [1] 0.962766
```

```
table(pred.test, rf.testing$diagnosis)
```

```
##
## pred.test   B   M
##         B 109   4
##         M   3  72
```

```
# Repeat with top 5 PCs

# Random forest model
pca.rf <- randomForest(diagnosis ~ perimeter + area + smoothness + symmetry
                          + concavity, rf.training)

# Predicting on Validation set
pca.pred.test <- predict(pca.rf, rf.testing, type = "class")

# Checking classification accuracy
mean(pca.pred.test == rf.testing$diagnosis)
```

```
## [1] 0.9308511
```

```
table(pca.pred.test, rf.testing$diagnosis)
```

```
##
## pca.pred.test   B   M
##             B 107   8
##             M   5  68
```

Contributions

All members contributed to coding and reviewing each other's work. Some written questions were worked on together, and the remaining ones divided among group members. The final assigment was reviewed by each group member before submitting.