# Homework 2

PSTAT 131/231, Winter 2019

## Due on Sunday February 10, 2019 at 11:59 pm

## Spam detection with spambase dataset

Following packages are needed below:

```
library(tidyverse)
library(plyr)
library(class)
library(maptree)
library(ROCR)
library(randomForest)
library(kableExtra)
library(stargazer)
```

Data Info: The Data Set was obtained by the UCI Machine Learning database. From the website,

The "spam" concept is diverse: advertisements for products/web sites, make money fast schemes, chain letters, pornography...

Our collection of spam e-mails came from our postmaster and individuals who had filed spam. Our collection of non-spam e-mails came from filed work and personal e-mails, and hence the word 'george' and the area code '650' are indicators of non-spam. These are useful when constructing a personalized spam filter. One would either have to blind such non-spam indicators or get a very wide collection of non-spam to generate a general purpose spam filter.

Dataset spambase.tab can be read with the following code. Next, standardize each numerical attribute in the dataset. Each standardized column should have zero mean and unit variance.

```
spam <- read_table2("spambase.tab", guess_max=2000)
spam <- spam %>%
    mutate(y = factor(y, levels=c(0,1), labels=c("good", "spam"))) %>% # label as factors
    mutate_at(.vars=vars(-y), .funs=scale) # scale others
```

Attribute Information: The last column of 'spambase.tab' denotes whether the e-mail was considered spam (1) or not (0), i.e. unsolicited commercial e-mail. Most of the attributes indicate whether a particular word or character was frequently occurring in the e-mail. The run-length attributes (55-57) measure the length of sequences of consecutive capital letters. For the statistical measures of each attribute, see the end of this file. Here are the definitions of the attributes:

- 48 continuous real [0,100] attributes of type word\_freq\_WORD = percentage of words in the e-mail that match WORD, i.e. 100 \* (number of times the WORD appears in the e-mail) / total number of words in e-mail. A WORD in this case is any string of alphanumeric characters bounded by non-alphanumeric characters or end-of-string.
- 6 continuous real [0,100] attributes of type char\_freq\_CHAR = percentage of characters in the e-mail that match CHAR, i.e. 100 \* (number of CHAR occurrences) / total characters in e-mail

- 1 continuous real [1,...] attribute of type capital\_run\_length\_average = average length of uninterrupted sequences of capital letters
- 1 continuous integer [1,...] attribute of type capital\_run\_length\_longest = length of longest uninterrupted sequence of capital letters
- 1 continuous integer [1,...] attribute of type capital\_run\_length\_total = sum of length of uninterrupted sequences of capital letters = total number of capital letters in the e-mail
- 1 nominal {0,1} class attribute of type spam = denotes whether the e-mail was considered spam (1) or not (0), i.e. unsolicited commercial e-mail.

Classification Task: We will build models to classify emails into good vs. spam.

In this dataset, we will apply several classification methods and compare their training error rates and test error rates. We define a new function, named <code>calc\_error\_rate()</code>, that will calculate misclassification error rate. Any error in this homework (unless specified otherwise) imply misclassification error.

```
calc_error_rate <- function(predicted.value, true.value){
  return(mean(true.value!=predicted.value))
}</pre>
```

Throughout this homework, we will calculate the error rates to measure and compare classification performance. To keep track of error rates of all methods, we will create a matrix called **records**:

```
records = matrix(NA, nrow=3, ncol=2)
colnames(records) <- c("train.error", "test.error")
rownames(records) <- c("knn", "tree", "logistic")</pre>
```

Training/test sets: Split randomly the data set in a train and a test set:

```
set.seed(1)
test.indices = sample(1:nrow(spam), 1000)
spam.train=spam[-test.indices,]
spam.test=spam[test.indices,]
```

10-fold cross-validation: Using spam.train data, 10-fold cross validation will be performed throughout this homework. In order to ensure data partitioning is consistent, define folds which contain fold assignment for each observation in spam.train.

## K-Nearest Neighbor Method

1. (Selecting number of neighbors) Use 10-fold cross validation to select the best number of neighbors best.kfold out of six values of k in kvec = c(1, seq(10, 50, length.out=5)). Use the folds defined above and use the following do.chunk definition in your code. Again put set.seed(1) before your code. What value of k leads to the smallest estimated test error?

```
grouped_means = aggregate(error.folds[, 1:2], list(error.folds$neighbors), mean)
colnames(grouped_means) = c("neighbors", "train.error", "val.error")
best.kfold = grouped_means$neighbors[which.min(grouped_means$val.error)]
```

2. (Training and Test Errors) Now that the best number of neighbors has been determined, compute the training error using spam.train and test error using spam.test or the k = best.kfold. Use the function calc\_error\_rate() to get the errors from the predicted class labels. Fill in the first row of records with the train and test error from the knn fit.

```
knn_train_pred = knn(train = spam.train[1:(ncol(spam.train)-1)], test = spam.train[1:57],
    cl = spam.train$y, k = best.kfold)
knn_test_pred = knn(train = spam.train[1:57], test = spam.test[1:57],
```

```
cl = spam.train$y, k = best.kfold)

# calculate the training and test error and input values in records matrix for KNN
records[1] = calc_error_rate(knn_train_pred, spam.train$y)
records[1,2] = calc_error_rate(knn_test_pred, spam.test$y)
```

#### Decision Tree Method

3. (Controlling Decision Tree Construction) Function tree.control specifies options for tree construction: set minsize equal to 5 (the minimum number of observations in each leaf) and mindev equal to 1e-5. See the help for tree.control for more information. The output of tree.control should be passed into tree function in the control argument. Construct a decision tree using training set spam.train, call the resulting tree spamtree. summary(spamtree) gives some basic information about the tree. How many leaf nodes are there? How many of the training observations are misclassified?

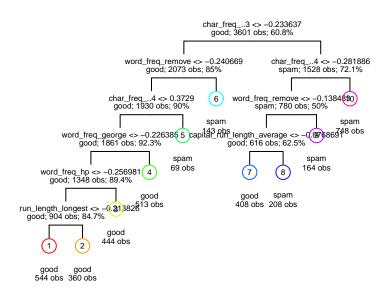
```
control = tree.control(minsize=5,mindev = 1e-5,
                       nobs=nrow(spam.train))
spamtree = tree(y~.,data = spam.train, control = control)
summary(spamtree)
##
## Classification tree:
## tree(formula = y ~ ., data = spam.train, control = control)
## Variables actually used in tree construction:
   [1] "char_freq_..3"
                                      "word freq remove"
##
   [3] "char_freq_..4"
                                      "word_freq_george"
##
   [5] "word_freq_hp"
                                      "capital_run_length_longest"
##
   [7] "word_freq_receive"
                                      "word_freq_free"
##
   [9] "word_freq_direct"
                                      "capital_run_length_average"
## [11] "word_freq_re"
                                      "word_freq_you"
## [13] "capital run length total"
                                      "word freq credit"
## [15] "word_freq_our"
                                      "word_freq_your"
## [17] "word_freq_will"
                                      "char_freq_..1"
## [19] "word_freq_meeting"
                                      "word_freq_1999"
## [21] "word_freq_make"
                                      "word_freq_hpl"
## [23] "char_freq_."
                                      "word_freq_over"
## [25] "word_freq_font"
                                      "word_freq_report"
## [27] "word_freq_money"
                                      "word_freq_address"
## [29] "word_freq_all"
                                      "word_freq_000"
## [31] "word_freq_data"
                                      "word_freq_project"
## [33] "word_freq_people"
                                      "word_freq_email"
## [35] "word_freq_415"
                                      "word freq edu"
## [37] "word_freq_technology"
                                      "word freq mail"
## [39] "word_freq_business"
                                      "char_freq_..2"
## [41] "word_freq_order"
                                      "char_freq_..5"
## Number of terminal nodes: 184
## Residual mean deviance: 0.04748 = 162.2 / 3417
## Misclassification error rate: 0.01333 = 48 / 3601
```

There are 184 leaf nodes. 48 of the total 3601 training observations were misclassified resulting in a misc

4. (Decision Tree Pruning) We can prune a tree using the prune.tree function. Pruning iteratively removes the leaves that have the least effect on the overall misclassification. Prune the tree until there are only 10 leaf

nodes so that we can easily visualize the tree. Use draw.tree function from the maptree package to visualize the pruned tree. Set nodeinfo=TRUE.

```
pruned_spamtree = prune.tree(tree = spamtree, best = 10)
draw.tree(tree = pruned_spamtree, size = 2, cex = .5, nodeinfo=TRUE)
```



5. In this problem we will use cross validation to prune the tree. Fortunately, the tree package provides an easy to use function to do the cross validation for us with the cv.tree function. Use the same fold partitioning you used in the KNN problem (refer to cv.tree help page for detail about rand argument). Also be sure to set method=misclass. Plot the misclassification as function of tree size. Determine the optimal tree size that minimizes misclassification. Important: if there are multiple tree sizes that have the same minimum estimated misclassification, you should choose the smallest tree. This reflects the idea that we want to choose the simplest model that explains the data well ("Occam's razor"). Show the optimal tree size best.size.cv in the plot.

```
# need to use do_chunk() to do this
cv = cv.tree(spamtree, FUN = prune.misclass, K = 10, rand = folds)
best.cv = min(cv$size[which(cv$dev == min(cv$dev, na.rm = TRUE))])
cv$size
                                         70
    [1] 184 153 148 134 116 108
                                     76
                                             65
                                                 62 46
                                                         37
                                                              30
                                                                  28
                                                                      20
                                 96
## [18]
         17
            13 11
                      8
                          7
                              6
                                  3
                                      2
                                          1
best.cv
## [1] 37
```

size\_df = as\_data\_frame(cv\$size)
dev\_df = as\_data\_frame(cv\$dev)
tree = c(size = size\_df, dev = dev\_df)

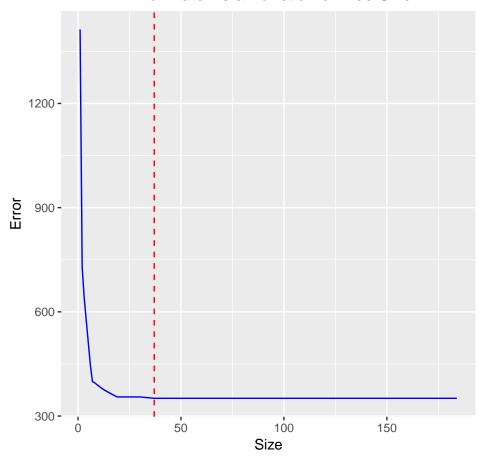
The best size for the tree is 37 leaf nodes

tree\_df = as\_data\_frame(tree)

```
tree_size_plot = ggplot(data = tree_df, aes(x = size.value, y = dev.value)) +
    geom_line(color = "blue") +
    xlab("Size") +
    ylab("Error") +
    ggtitle("Error Rate As a Function of Tree Size") +
    theme(plot.title = element_text(hjust = 0.5)) +
    geom_vline(aes(xintercept=best.cv), linetype='dashed', color = "red")

tree_size_plot
```

### Error Rate As a Function of Tree Size



#### 6. (Training and Test Errors)

We previous pruned the tree to a small tree so that it could be easily visualized. Now, prune the original tree to size best.size.cv and call the new tree spamtree.pruned. Calculate the training error and test error when spamtree.pruned is used for prediction. Use function calc\_error\_rate() to compute misclassification error. Also, fill in the second row of the matrix records with the training error rate and test error rate.

```
records[2,1] = calc_error_rate(pruned.predict.train, spam.train$y)
records[2,2] = calc_error_rate(pruned.predict.test, spam.test$y)
```

## Logistic regression

##

##

good 574

26

spam

55

345

7. In a binary classification problem, let p represent the probability of class label "1"", which implies 1-p represents probability of class label "0". The *logistic function* (also called the "inverse logit") is the cumulative distribution function of logistic distribution, which maps a real number z to the open interval (0,1):

$$p(z) = \frac{e^z}{1 + e^z}. (1)$$

a. Show that indeed the inverse of a logistic function is the *logit* function:

$$z(p) = \ln\left(\frac{p}{1-p}\right). \tag{2}$$

- b. The logit function is a commonly used *link function* for a generalized linear model of binary data. One reason for this is that implies interpretable coefficients. Assume that  $z = \beta_0 + \beta_1 x_1$ , and p = logistic(z). How does the odds of the outcome change if you increase  $x_1$  by two? Assume  $\beta_1$  is negative: what value does p approach as  $x_1 \to \infty$ ? What value does p approach as  $x_1 \to -\infty$ ?
- 8. Use logistic regression to perform classification. Logistic regression specifically estimates the probability that an observation as a particular class label. We can define a probability threshold for assigning class labels based on the probabilities returned by the glm fit.

```
# run linear regression of the y column on all other columns in spam.train
glm.fits=glm(y~., data=spam.train, family =binomial)
## Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred
glm.probs.train = predict(glm.fits, spam.train, type="response")
glm.probs.test = predict(glm.fits, spam.test, type="response")
spam.trainY = spam.train$y
glm.pred.train = rep("good",3601)
glm.pred.train[glm.probs.train > .5] = "spam"
table(glm.pred.train, spam.trainY)
##
                 spam.trainY
  glm.pred.train good spam
##
             good 2087 154
##
##
             spam 101 1259
spam.testY = spam.test$y
glm.pred.test=rep("good",1000)
glm.pred.test[glm.probs.test > .5]="spam"
table(glm.pred.test, spam.testY)
##
                spam.testY
## glm.pred.test good spam
```

Table 1: Training and Test Error for Different Modeling Approaches

	train.error	test.error
knn	0.0805	0.099
tree	0.0555	0.076
logistic	0.0708	0.081

```
# calculate the training and test error and input values in records matrix for logistic regression
records[3,1] = calc_error_rate(glm.pred.train, spam.trainY)
records[3,2] = calc_error_rate(glm.pred.test, spam.testY)
```

The tree method has the lowest test error (7.6%) of all of the methods, followed by logistic (8.1%) and then KNN (9.9%)

In this problem, we will simply use the "majority rule". If the probability is larger than  $50\$  class as a

## Receiver Operating Characteristic curve

9. (ROC curve) We will construct ROC curves based on the predictions of the *test* data from the model defined in **spamtree.pruned** and the logistic regression model above. Plot the ROC for the test data for both the decision tree and the logistic regression on the same plot. Compute the area under the curve for both models (AUC). Which classification method seems to perform the best by this metric?

**Hints**: In order to construct the ROC curves one needs to use the vector of predicted probabilities for the test data. The usage of the function predict() may be different from model to model.

- For trees the matrix of predicted probabilities (for Good and Spam) will be provided by using
- For logistic regression one needs to predict type response

```
pruned.predict.test = predict(spamtree.pruned, spam.test, type = "vector")
pred.tree <- prediction(pruned.predict.test[,2], spam.testY)</pre>
perf.tree <- performance(pred.tree, "tpr", "fpr")</pre>
logistic.probs.test = predict(glm.fits, spam.test, type="response")
pred.logistic = prediction(logistic.probs.test, spam.testY)
perf.logistic <- performance(pred.logistic, "tpr", "fpr")</pre>
perf.tree@x.name = perf.logistic@x.name= "False Positive Rate"
perf.tree@y.name = perf.logistic@y.name= "True Positive Rate"
# plot the two ROC curves on the same plot
plot(perf.tree, type = "1", col = "red")
par(new=TRUE)
plot(perf.logistic, type="l", col = "blue")
legend(0.8, 0.2, legend=c("Tree", "Logistic"), col=c("red", "blue"), lty=1:2, cex=1.5)
title("ROC", cex = 1.5)
# Calculate AUC
auc.tree = performance(pred.tree, "auc")@y.values
auc.logistic = performance(pred.logistic, "auc")@y.values
```

auc.tree
auc.logistic

Based on the AUC metric, the logistic method seems to perform better than the tree method because it has an AUC = 0.975 versus 0.967.

10. In the SPAM example, take "positive" to mean "spam". If you are the designer of a spam filter, are you more concerned about the potential for false positive rates that are too large or true positive rates that are too small? Argue your case.

You would prefer to include SPAM in your mailbox and have recipients self-sort a few emails rather than automatically filtering out good messages. As a result, you are very concerned with a high false positive rate because that would cause an important message to be sent to spam which could cause the recipient to miss the message. It is less concerning to have a small true positive rate because then the individual will just have to do more sorting but they will never miss an important message.

# Problems below for 231 students only

11. A multivariate normal distribution has density

$$f(x) = \frac{1}{(2\pi)^{p/2} |\Sigma|^{1/2}} exp\left(-\frac{1}{2}(x - \mu_k)^T \Sigma^{-1}(x - \mu)\right)$$

In quadratic discriminant analysis with two groups we use Bayes rule to calculate the probability that Y has class label "1":

$$Pr(Y = 1 \mid X = x) = \frac{f_1(x)\pi_1}{\pi_1 f_1(x) + \pi_2 f_2(x)}$$

where  $\pi_2 = 1 - \pi_1$  is the prior probability of being in group 2. Suppose we classify  $\hat{Y} = k$  whenever  $Pr(Y = k \mid X = x) > \tau$  for some probability threshold  $\tau$  and that  $f_k$  is a multivariate normal density with covariance  $\Sigma_k$  and mean  $\mu_k$ . Note that for a vector x of length p and a  $p \times p$  symmetric matrix A,  $x^TAx$  is the vector quadratic form (the multivariate analog of  $x^2$ ). Show that the decision boundary is indeed quadratic by showing that  $\hat{Y} = 1$  if

$$\delta_1(x) - \delta_2(x) > M(\tau)$$

where

$$\hat{\delta}_k(x) = -\frac{1}{2}(x - \mu_k)^T \Sigma_k^{-1}(x - \mu_k) - \frac{1}{2}\log|\Sigma_k| + \log \pi_k$$

and  $M(\tau)$  is some function of the probability threshold  $\tau$ . What is the decision threshold, M(1/2), corresponding to a probability threshold of 1/2?

$$P(Y = 1|X = x) = \frac{\pi_1 f_1(x)}{\pi_1 f_1(x) + \pi_2 f_2(x)} > \tau$$

$$\pi_1 f_1(x) > \tau \left( \pi f_1(x) + \pi_2 f_2(x) \right)$$

$$\pi_1 f_1(x) (1 - \tau) > \pi_2 f_2(x) \tau$$

$$\begin{split} \frac{\pi_1 f_1(x)(1-\tau)}{\pi_2 f_2(x)} > \tau \\ \frac{\pi_1 f_1(x)}{\pi_2 f_2(x)} > \frac{\tau}{1-\tau} \\ \frac{\frac{\pi_1 f_1(x)}{(2\pi)^{p/2} |\Sigma_1|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_1)^T \Sigma_1^{-1}(x-\mu_1)\right)}{(2\pi)^{p/2} |\Sigma_2|^{1/2}} \exp\left(-\frac{1}{2}(x-\mu_2)^T \Sigma_2^{-1}(x-\mu_2)\right)} > \frac{\tau}{1-\tau} \\ -\frac{1}{2}(x-\mu_1)^T \Sigma_1^{-1}(x-\mu_1) - \frac{1}{2} \log |\Sigma_1| + \log \pi_1 - (-\frac{1}{2}(x-\mu_2)^T \Sigma_2^{-1}(x-\mu_2) - \frac{1}{2} \log |\Sigma_2| + \log \pi_2) > \log\left(\frac{\tau}{1-\tau}\right) \\ \delta_1(x) - \delta_2(x) > \log\left(\frac{\tau}{1-\tau}\right) \\ Thus, M(\tau) = \log\left(\frac{\tau}{1-\tau}\right) \\ For, \tau = \frac{1}{2} \\ \delta_1(x) - \delta_2(x) > \log\left(\frac{1}{2}\right) \\ \delta_1(x) - \delta_2(x) > \log(1) \\ \delta_1(x) - \delta_2(x) > 0 \end{split}$$

Thus the decision boundary for M(1/2) = 0.

#### Algae Classification

Questions 12-13 relate to algaeBloom dataset. Get the dataset algaeBloom.txt from the homework archive file, and read it with the following code:

In homework 1 and homework 2, we investigated basic exploratory data analysis for the algaeBloom dataset. One of the explaining variables is a1, which is a numerical attribute. In homework 2, we conducted linear regression for variable a1 using other 8 chemical variables and 3 categorical variables. Here, after standardization, we will transform a1 into a categorical variable with 2 levels: high and low, and conduct classification predictions using those 11 variables (i.e. do not include a2, a3,..., a7).

12. (Variable Standardization and Discretization) Improve the normality of the the numerical attributes by taking the log of all chemical variables. *After* log transformation, impute missing values using the median method from homework 1. Note: do not take the log transform of a1 since it is not a chemical variable. Transform the variable a1 into a categorical variable with two levels: high if a1 is greater than 0.5, and low if a1 is smaller than or equal to 0.5.

```
algae_log = algae

# start by performing log transform on chemical columns in algae
algae_log[,4:11] <- log(algae[,4:11])

# use the median of values in each chemical column to impute any missing values in that col.
algae_log_med <- algae_log %>%
    mutate_at(.vars = c('mxPH','mn02','Cl','N03','NH4',
    'oP04','P04','Chla'), .funs = funs(ifelse(is.na(.), median(., na.rm = TRUE), .)))

# need to create categorical variables for "high" or "low" depending on if the value of al is above or below
#algae_log_med$

algae_log_final = algae_log_med %>%
```

mutate(a1 = as.character(ifelse(a1 > 0.5, "high", "low")))

#### 13. Linear and Quadratic Discriminant Analysis

a. In LDA we assume that  $\Sigma_1 = \Sigma_2$ . Use LDA to predict whether a1 is high or low using the MASS::lda() function. The CV argument in the MASS::lda function uses Leave-one-out cross validation LOOCV) when estimating the fitted values to avoid overfitting. Set the CV argument to true. Plot an ROC curve for the fitted values.

#### library(MASS)

```
##
## Attaching package: 'MASS'

## The following object is masked from 'package:dplyr':
##
## select

algae.lda.fit = lda(a1 ~ ., algae_log_final, CV = TRUE)

algae.lda.pred = prediction(algae.lda.fit[["posterior"]][,2], algae_log_final$a1)
algae.lda.perf = performance(algae.lda.pred, measure="tpr", x.measure="fpr")
```

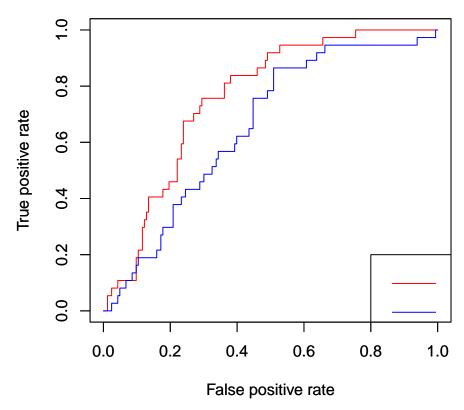
b. Quadratic discriminant analysis is strictly more flexible than LDA because it is not required that  $\Sigma_1 = \Sigma_2$ . In this sense, LDA can be considered a special case of QDA with the covariances constrained to be the same. Use a quadratic discriminant model to predict the a1 using the function MASS::qda. Again setting CV=TRUE and plot the ROC on the same plot as the LDA ROC. Compute the area under the ROC (AUC) for each model. To get the predicted class probabilities look at the value of posterior in the 1da and qda objects. Which model has better performance? Briefly explain, in terms of the bias-variance tradeoff, why you believe the better model outperforms the worse model?

```
algae.qda.fit = qda(a1 ~ ., algae_log_final, CV = TRUE)

algae.qda.pred = prediction(algae.qda.fit[["posterior"]][,2], algae_log_final$a1)
algae.qda.perf = performance(algae.qda.pred, measure="tpr", x.measure="fpr")

# plot the two ROC curves on the same plot
plot(algae.lda.perf, type = "l", col = "red")
par(new=TRUE)
plot(algae.qda.perf, type="l", col = "blue")
legend(0.8, 0.2, legend=c("LDA", "QDA"), col=c("red", "blue"), lty=1, cex=1.5)
title("ROC for LDA and QDA of Algae Data", cex = 1.5)
```

## **ROC for LDA and QDA of Algae Data**



```
# Calculate AUC
auc.lda = performance(algae.lda.pred, "auc")@y.values
auc.qda = performance(algae.qda.pred, "auc")@y.values

## [[1]]
## [1] 0.7590781

auc.qda
```

## [[1]] ## [1] 0.6559443

Based on the AUC analysis, the LDA outperforms QDA with AUC of 0.759 and 0.656 respectively. QDA allows for more flexible modeling of the data set because it assumes quadratic decision boundary rather than a linear boudary. While this reduces bias, it also increases the variance. Additionally in this case, the predictors for both the high and low algae groups have similar correlations, so we don't need the flexibility that QDA offers for situations with different correlations among predictors. As a result, the added variance with QDA analysis comes at a cost with a decrease in true positive rate and an increase in the false positive rate for the QDA case in the figure above. Thus, LDA makes more sense to use in this situation.