# Problem Set 2

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Course: MACS30100 Perspectives on Computational Modeling (Winter 2020)

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### The Bayes Classifier

1.

#### a. Set seed

```
# Set seed
set.seed(110)
```

### b. Simulate a dataset

```
x_1 = runif(200, -1, 1)
x_2 = runif(200, -1, 1)
```

#### c. Calculate Y

```
ep = rnorm(200, 0, 0.25)

y = x_1 + x_1^2 + x_2 + x_2^2 + ep
```

### d. Calculate the probability of success

The log-odds is calculated by the following equation.

$$\log\left(\frac{Pr(success)}{1 - Pr(success)}\right) = X_1 + X_1^2 + X_2 + X_2^2 + \epsilon$$

By transforming the equation, the probability of success is:

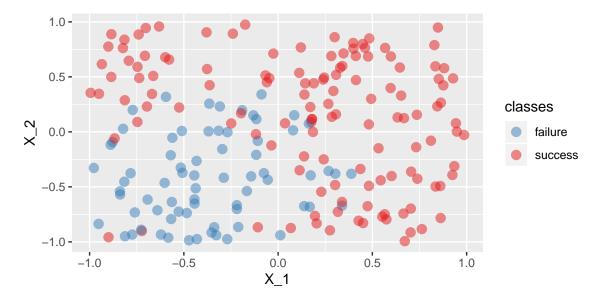
$$Pr(success) = \frac{e^{X_1 + X_1^2 + X_2 + X_2^2 + \epsilon}}{1 + e^{X_1 + X_1^2 + X_2 + X_2^2 + \epsilon}} = \frac{e^Y}{1 + e^Y}$$

```
pr \leftarrow exp(y) / (1 + exp(y))
```

### e. Plot each point from the dataset

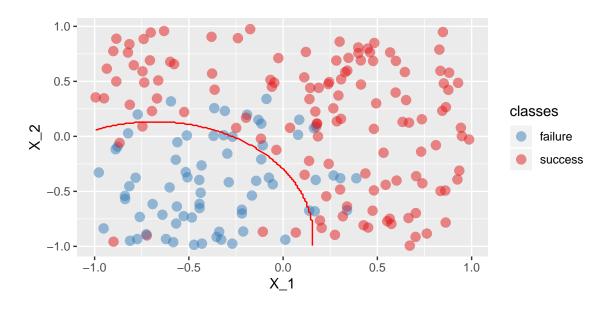
```
pr <= 0.5 ~0))
twoClassColor <- brewer.pal(3,'Set1')[1:2]
names(twoClassColor) <- c('success','failure')

df %>%
    ggplot(aes(x=X_1, y=X_2)) +
    geom_point(aes(color = cl), size = 3, alpha = .5) +
    scale_colour_manual(name = 'classes', values = twoClassColor)
```



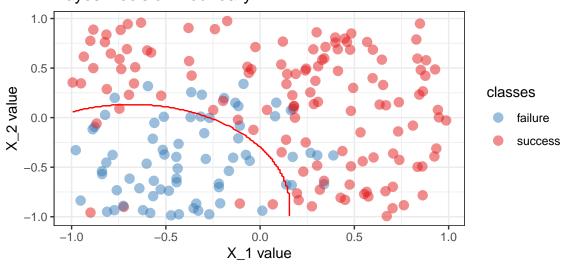
### f. Overlay with Bayes decision boundary

```
# Referring to http://www.cmap.polytechnique.fr/~lepennec/R/Learning/Learning.html
V <- 10
T < -4
TrControl <- trainControl(method = "repeatedcv",</pre>
                           number = V,
                           repeats = T)
df_model <- df %>%
 dplyr::select(X_1, X_2, cl)
nbp = 200
Pred1 <- seq(min(df_model$X_1), max(df_model$X_1), length = nbp)</pre>
Pred2 <- seq(min(df_model$X_2), max(df_model$X_2), length = nbp)</pre>
Grid <- expand.grid(X_1 = Pred1, X_2 = Pred2)</pre>
Model <- train(data=df_model, cl ~ ., method = "nb", trControl = TrControl,
               tuneGrid = data.frame(usekernel = c(FALSE), fL = c(0), adjust = c(1)))
Pred <- predict(Model, newdata = Grid)</pre>
df model %>%
  ggplot(aes(x=X_1, y=X_2)) +
  geom_point(aes(color = cl), size = 3, alpha = .5) +
  geom_contour(data = cbind(Grid, classes = Pred),
               aes(z = as.numeric(classes)),
               color = "red", breaks = c(1.5)) +
scale_colour_manual(name = 'classes', values = twoClassColor)
```



### g. Title and axis labels & h. Colored Background

# **Bayes Decision Boundary**



## Exploring Simulated Differences between LDA and QDA

### 2. In case Bayes decision boundary is linear

### a. Repeat simulation 1,000 times

```
train_lda2 = c()
test_1da2 = c()
train_qda2 = c()
test_qda2 = c()
for (i in 1:1000) {
  # i data generation
  x_1 = runif(1000, -1, 1)
  x_2 = runif(1000, -1, 1)
  ep = rnorm(1000, 0, 0.25)
  y = case\_when(x_1 + x_2 + ep >= 0 \sim TRUE,
                 x_1 + x_2 + ep < 0 \sim FALSE
  df2 \leftarrow data.frame(x_1, x_2, y)
  # ii split
  split <- initial_split(df2, prop = .7)</pre>
  train <- training(split)</pre>
  test <- testing(split)</pre>
  # iii training
  1da2 \leftarrow MASS::1da(y \sim x_1 + x_2, data = train)
  qda2 \leftarrow MASS::qda(y \sim x_1 + x_2, data = train)
  # iv error
  train_lda2 = c(train_lda2, sum(predict(lda2, train)$class != train$y) / 700)
  test_lda2 = c(test_lda2, sum(predict(lda2, test)$class != test$y) / 300)
  train_qda2 = c(train_qda2, sum(predict(qda2, train)$class != train$y) / 700)
  test_qda2 = c(test_qda2, sum(predict(qda2, test)$class != test$y) / 300)
}
```

### b. Summarize the results

```
df2_result <- data.frame(train_lda2, test_lda2, train_qda2, test_qda2)
df2_result <- df2_result %>%
  gather(dset, error)
df2_result %>%
  group_by(dset) %>%
  summarise(mean = mean(error), sd = sd(error))
```

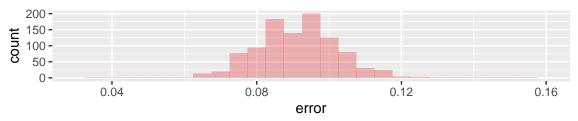
| mean      | $\operatorname{sd}$                 |
|-----------|-------------------------------------|
| 0.0934167 | 0.0168609                           |
| 0.0938367 | 0.0169069                           |
| 0.0911400 | 0.0109330                           |
| 0.0909057 | 0.0110357                           |
|           | 0.0934167<br>0.0938367<br>0.0911400 |

```
lda_p1 <- df2_result %>%
    ggplot(aes(x=error)) +
    scale_colour_manual(name = 'classes', values = twoClassColor) +
```

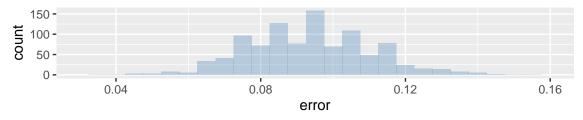
## Warning: Removed 2 rows containing missing values (geom\_bar).

## Warning: Removed 2 rows containing missing values (geom\_bar).

### LDA Train Data Error Rate



### LDA Test Data Error Rate

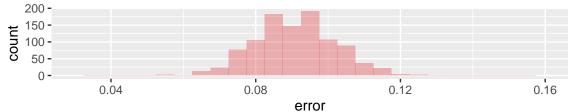


```
alpha = 0.3, binwidth = 0.005) +
scale_x_continuous(limits = c(0.03,0.16)) +
ggtitle("QDA Test Data Error Rate")
grid.arrange(qda_p1, qda_p2, nrow = 2)
```

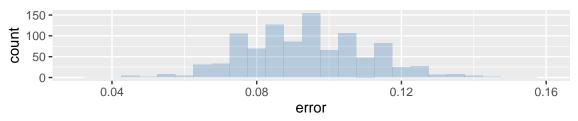
## Warning: Removed 2 rows containing missing values (geom\_bar).

## Warning: Removed 2 rows containing missing values (geom\_bar).

# **QDA Train Data Error Rate**



### QDA Test Data Error Rate



### 3. In case Bayes decision boundary is non-linear

```
train_lda2 = c()
test_1da2 = c()
train_qda2 = c()
test_qda2 = c()
for (i in 1:1000) {
  \# i data generation
  x_1 = runif(1000, -1, 1)
  x_2 = runif(1000, -1, 1)
  ep = rnorm(1000, 0, 0.25)
  y = case\_when(x_1 + x_1^2 + x_2 + x_2^2 + ep >= 0 ~ TRUE,
                 x_1 + x_1^2 + x_2 + x_2^2 + ep < 0 \sim FALSE
  df2 \leftarrow data.frame(x_1, x_2, y)
  # ii split
  split <- initial_split(df2, prop = .7)</pre>
  train <- training(split)</pre>
  test <- testing(split)</pre>
  # iii training
  1da2 \leftarrow MASS::1da(y \sim x_1 + x_2, data = train)
  qda2 \leftarrow MASS::qda(y \sim x_1 + x_2, data = train)
```

```
# iv error
train_lda2 = c(train_lda2, sum(predict(lda2, train)$class != train$y) / 700)
test_lda2 = c(test_lda2, sum(predict(lda2, test)$class != test$y) / 300)
train_qda2 = c(train_qda2, sum(predict(qda2, train)$class != train$y) / 700)
test_qda2 = c(test_qda2, sum(predict(qda2, test)$class != test$y) / 300)
}
```

#### b. Summarize the results

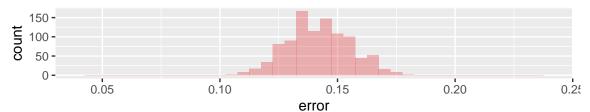
```
df2_result <- data.frame(train_lda2, test_lda2, train_qda2, test_qda2)
df2_result <- df2_result %>%
  gather(dset, error)
df2_result %>%
  group_by(dset) %>%
  summarise(mean = mean(error), sd = sd(error))
```

| dset          | mean      | $\overline{\mathrm{sd}}$ |
|---------------|-----------|--------------------------|
| test_lda2     | 0.1427233 | 0.0199135                |
| $test\_qda2$  | 0.1067600 | 0.0171807                |
| $train\_lda2$ | 0.1420243 | 0.0133372                |
| $train\_qda2$ | 0.1051986 | 0.0110349                |

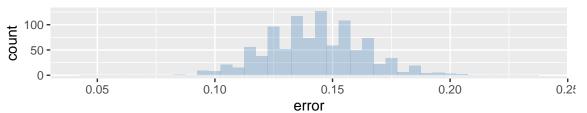
```
lda_p1 <- df2_result %>%
  ggplot(aes(x=error)) +
  scale_colour_manual(name = 'classes', values = twoClassColor) +
  geom_histogram(data=subset(df2_result, dset == 'train_lda2'),
                 fill = brewer.pal(3, 'Set1')[1],
                 alpha = 0.3, binwidth = 0.005) +
  scale_x_continuous(limits = c(0.04,0.24)) +
  ggtitle("LDA Train Data Error Rate")
lda p2 <- df2 result %>%
  ggplot(aes(x=error)) +
  scale_colour_manual(name = 'classes', values = twoClassColor) +
  geom_histogram(data=subset(df2_result, dset == 'test_lda2'),
                 fill = brewer.pal(3, 'Set1')[2],
                 alpha = 0.3, binwidth = 0.005) +
  scale_x_continuous(limits = c(0.04,0.24)) +
  ggtitle("LDA Test Data Error Rate")
grid.arrange(lda_p1, lda_p2, nrow = 2)
```

- ## Warning: Removed 2 rows containing missing values (geom\_bar).
- ## Warning: Removed 2 rows containing missing values (geom\_bar).

### LDA Train Data Error Rate



## LDA Test Data Error Rate

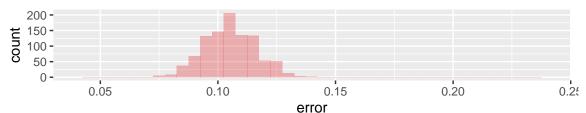


```
qda_p1 <- df2_result %>%
  ggplot(aes(x=error)) +
  scale_colour_manual(name = 'classes', values = twoClassColor) +
  geom_histogram(data=subset(df2_result, dset == 'train_qda2'),
                 fill = brewer.pal(3, 'Set1')[1],
                 alpha = 0.3, binwidth = 0.005) +
  scale_x_continuous(limits = c(0.04, 0.24)) +
  ggtitle("QDA Train Data Error Rate")
qda_p2 <- df2_result %>%
  ggplot(aes(x=error)) +
  scale_colour_manual(name = 'classes', values = twoClassColor) +
  geom_histogram(data=subset(df2_result, dset == 'test_qda2'),
                 fill = brewer.pal(3, 'Set1')[2],
                 alpha = 0.3, binwidth = 0.005) +
  scale x continuous(limits = c(0.04, 0.24)) +
  ggtitle("QDA Test Data Error Rate")
grid.arrange(qda_p1, qda_p2, nrow = 2)
```

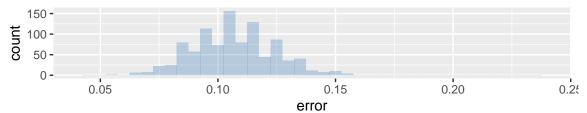
## Warning: Removed 2 rows containing missing values (geom\_bar).

## Warning: Removed 2 rows containing missing values (geom\_bar).

### **QDA Train Data Error Rate**



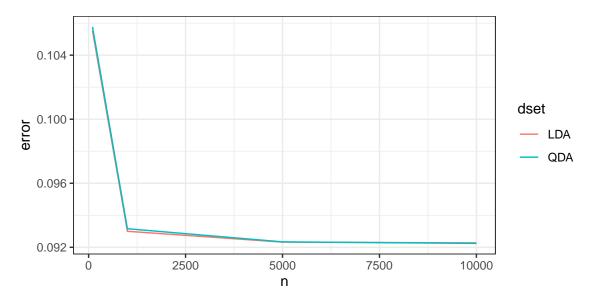
## QDA Test Data Error Rate



#### 4. Increasing the sample size

```
train_lda4_mean = c()
test_lda4_mean = c()
train_qda4_mean = c()
test_qda4_mean = c()
for (n in c(100, 1000, 5000, 10000)) {
  train 1da4 = c()
  test_1da4 = c()
  train_qda4 = c()
  test_qda4 = c()
  for (i in 1:1000) {
    # i data generation
    x_1 = runif(n, -1, 1)
    x_2 = runif(n, -1, 1)
    ep = rnorm(n, 0, 0.25)
    y = case\_when(x_1 + x_2 + ep >= 0 \sim TRUE,
                   x_1 + x_2 + ep < 0 \sim FALSE
    df \leftarrow data.frame(x_1, x_2, y)
    # ii split
    split <- initial_split(df, prop = .7)</pre>
    train <- training(split)</pre>
    test <- testing(split)</pre>
    # iii training
    1da4 \leftarrow MASS::1da(y \sim x_1 + x_2, data = train)
    qda4 \leftarrow MASS::qda(y \sim x_1 + x_2, data = train)
    # iv error
    train_lda4 = c(train_lda4, sum(predict(lda4, train)$class != train$y)
                    /(0.7*n)
    test_lda4 = c(test_lda4, sum(predict(lda4, test)$class != test$y)
                   /(0.3*n)
```

### b. Summarize the results



### Modeling voter turnout

### 5. Building classifiers

### a. Split data

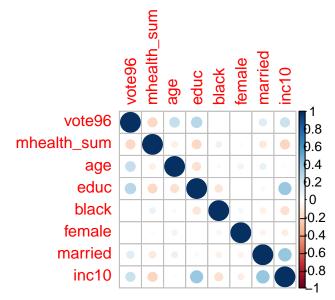
Since there are NAs in the data, I first omit those observations that contains NAs, then split them into training set and test set.

```
df5 <- read.csv('mental_health.csv')
# Drop NAs
df5 <- df5 %>%
    drop_na()
split <- initial_split(df5, prop = .7)</pre>
```

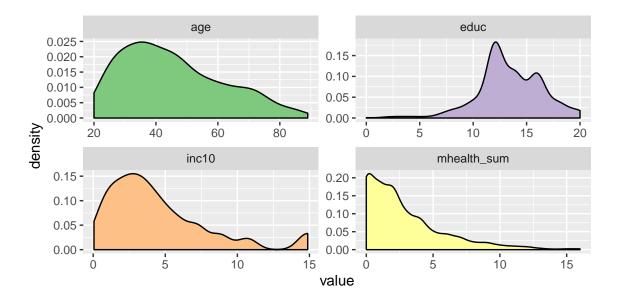
```
train <- training(split)
test <- testing(split)</pre>
```

From the Lab notebook, below is some simple EDA.

```
# checking correlation across several features
train %>%
   select_if(is.numeric) %>%
   cor() %>%
   corrplot::corrplot()
```



```
# checking normality assumption for continuous features
train %>%
  dplyr::select(age, educ, inc10, mhealth_sum) %>%
  gather(metric, value) %>%
  ggplot(aes(value, fill = metric)) +
  geom_density(show.legend = FALSE) +
  scale_fill_brewer(type = "qual") +
  facet_wrap(~ metric, scales = "free")
```



#### b. Estimation

For the following training and predicting, I use caret package.

The arguments of the function can be found in https://topepo.github.io/caret/available-models.html

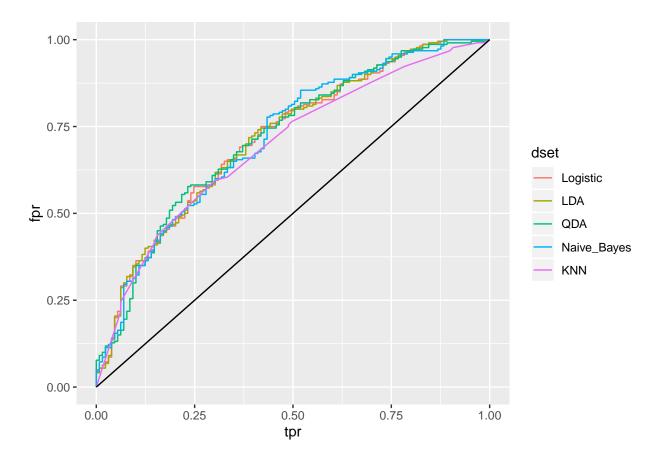
#### c. Performance metrics

```
dset = 'Logistic')
colnames(roc.lr) <- c('tpr', 'fpr', 'dset')</pre>
lr.perf <- data.frame(Logistic = c(</pre>
  confusionMatrix(pred.c, as.factor(test$vote96))[3]$overall['Accuracy'],
  confusionMatrix(pred.c, as.factor(test$vote96))[4]$byClass,
  AUC = as.numeric(auc.tmp@y.values)))
# LDA
pred.c <- predict(m5.lda, newdata = test)</pre>
pred.p <- predict(m5.lda, newdata = test, type = 'prob')</pre>
pred.roc <- prediction(pred.p['1'], as.factor(test$vote96))</pre>
auc.tmp <- performance(pred.roc, 'auc')</pre>
perf <- performance(pred.roc, 'tpr', 'fpr')</pre>
roc.lda <- data.frame(x = slot(perf, 'x.values'),</pre>
                       y = slot(perf, 'y.values'),
                       dset = 'LDA')
colnames(roc.lda) <- c('tpr', 'fpr', 'dset')</pre>
lda.perf <- data.frame(LDA = c(</pre>
  confusionMatrix(pred.c, as.factor(test$vote96))[3]$overall['Accuracy'],
  confusionMatrix(pred.c, as.factor(test$vote96))[4]$byClass,
  AUC = as.numeric(auc.tmp@y.values)))
# QDA
pred.c <- predict(m5.qda, newdata = test)</pre>
pred.p <- predict(m5.qda, newdata = test, type = 'prob')</pre>
pred.roc <- prediction(pred.p['1'], as.factor(test$vote96))</pre>
auc.tmp <- performance(pred.roc, 'auc')</pre>
perf <- performance(pred.roc, 'tpr', 'fpr')</pre>
roc.qda <- data.frame(x = slot(perf, 'x.values'),</pre>
                        y = slot(perf, 'y.values'),
                        dset = 'QDA')
colnames(roc.qda) <- c('tpr', 'fpr', 'dset')</pre>
qda.perf <- data.frame(QDA = c(</pre>
  confusionMatrix(pred.c, as.factor(test$vote96))[3]$overall['Accuracy'],
  confusionMatrix(pred.c, as.factor(test$vote96))[4]$byClass,
  AUC = as.numeric(auc.tmp@y.values)))
# Naive Bayes
pred.c <- predict(m5.nb, newdata = test)</pre>
pred.p <- predict(m5.nb, newdata = test, type = 'prob')</pre>
pred.roc <- prediction(pred.p['1'], as.factor(test$vote96))</pre>
auc.tmp <- performance(pred.roc, 'auc')</pre>
perf <- performance(pred.roc, 'tpr', 'fpr')</pre>
roc.nb <- data.frame(x = slot(perf, 'x.values'),</pre>
                       y = slot(perf, 'y.values'),
                       dset = 'Naive_Bayes')
colnames(roc.nb) <- c('tpr', 'fpr', 'dset')</pre>
nb.perf <- data.frame(Naive_Bayes = c(</pre>
  confusionMatrix(pred.c, as.factor(test$vote96))[3]$overall['Accuracy'],
```

```
confusionMatrix(pred.c, as.factor(test$vote96))[4]$byClass,
  AUC = as.numeric(auc.tmp@y.values)))
# K-NN with Euclidean distance metrics
pred.c <- predict(m5.knn, newdata = test)</pre>
pred.p <- predict(m5.knn, newdata = test, type = 'prob')</pre>
pred.roc <- prediction(pred.p['1'], as.factor(test$vote96))</pre>
auc.tmp <- performance(pred.roc, 'auc')</pre>
perf <- performance(pred.roc, 'tpr', 'fpr')</pre>
roc.knn <- data.frame(x = slot(perf, 'x.values'),</pre>
                       y = slot(perf, 'y.values'),
                       dset = 'KNN')
colnames(roc.knn) <- c('tpr', 'fpr', 'dset')</pre>
knn.perf <- data.frame(KNN = c(</pre>
  confusionMatrix(pred.c, as.factor(test$vote96))[3]$overall['Accuracy'],
  confusionMatrix(pred.c, as.factor(test$vote96))[4]$byClass,
  AUC = as.numeric(auc.tmp@y.values)))
d \leftarrow data.frame(x=c(0, 1), y=c(0, 1))
cbind(lr.perf, lda.perf, qda.perf, nb.perf, knn.perf)
```

|                      | Logistic  | LDA       | QDA       | Naive_Bayes | KNN       |
|----------------------|-----------|-----------|-----------|-------------|-----------|
| Accuracy             | 0.6762178 | 0.6790831 | 0.6848138 | 0.6905444   | 0.6676218 |
| Sensitivity          | 0.3178295 | 0.3255814 | 0.4418605 | 0.33333333  | 0.3255814 |
| Specificity          | 0.8863636 | 0.8863636 | 0.8272727 | 0.9000000   | 0.8681818 |
| Pos Pred Value       | 0.6212121 | 0.6268657 | 0.6000000 | 0.6615385   | 0.5915493 |
| Neg Pred Value       | 0.6890459 | 0.6914894 | 0.7165354 | 0.6971831   | 0.6870504 |
| Precision            | 0.6212121 | 0.6268657 | 0.6000000 | 0.6615385   | 0.5915493 |
| Recall               | 0.3178295 | 0.3255814 | 0.4418605 | 0.33333333  | 0.3255814 |
| F1                   | 0.4205128 | 0.4285714 | 0.5089286 | 0.4432990   | 0.4200000 |
| Prevalence           | 0.3696275 | 0.3696275 | 0.3696275 | 0.3696275   | 0.3696275 |
| Detection Rate       | 0.1174785 | 0.1203438 | 0.1633238 | 0.1232092   | 0.1203438 |
| Detection Prevalence | 0.1891117 | 0.1919771 | 0.2722063 | 0.1862464   | 0.2034384 |
| Balanced Accuracy    | 0.6020965 | 0.6059725 | 0.6345666 | 0.6166667   | 0.5968816 |
| AUC                  | 0.7171952 | 0.7181818 | 0.7186399 | 0.7171600   | 0.6949789 |

```
rbind(roc.lr, roc.lda, roc.qda, roc.nb, roc.knn) %>%
   ggplot(aes(x=tpr, y=fpr)) +
   geom_line(aes(color=dset)) +
   geom_line(data=d, aes(x=x, y=y))
```



### d. Results

The results above show that the best method is using QDA since its balanced accuracy is the highest (0.6346), and its AUC is the largest (0.7186). Each model has its strength and weakness