# Wang\_Miaohan\_HW2

#### February 2, 2020

```
[1]: import random
  import numpy as np
  import matplotlib.pyplot as plt
  import pandas as pd
  from sklearn.model_selection import train_test_split
  from sklearn.discriminant_analysis import LinearDiscriminantAnalysis
  from sklearn.discriminant_analysis import QuadraticDiscriminantAnalysis
  from sklearn.linear_model import LogisticRegression
  from sklearn.neighbors import KNeighborsClassifier
  from sklearn.naive_bayes import GaussianNB
  import sklearn.metrics as metrics
[2]: # auxiliary function for Q2, Q3, Q4
  def simulation(size, rep, model, linearity, random_state=1020):
      random.seed(random_state)
```

```
[2]: # auxiliary function for Q2, Q3, Q4
         train_err = np.array([])
         test_err = np.array([])
         assert(model in ['lda', 'qda']), print("Please only put 'lda' or 'qda' in⊔
      \hookrightarrowthe 'model' parameter.")
         for i in range(rep):
             X_1 = np.random.uniform(-1, 1, size)
             X_2 = np.random.uniform(-1, 1, size)
             X_data = np.stack((X_1, X_2), axis=-1)
             temp = X_1 + X_2 + np.random.normal(0, 1, size)
             if not linearity:
                 temp += X_1**2 + X_2**2
             y_data = np.array(temp > 0)
             X_train, X_test, y_train, y_test = train_test_split(X_data, y_data,_
      →test_size=0.3, random_state=random_state)
             mod = None
             if model == 'lda':
                 mod = LinearDiscriminantAnalysis()
             elif model == 'qda':
```

```
mod = QuadraticDiscriminantAnalysis()
        mod.fit(X_train, y_train)
        train_err = np.append(train_err, 1-mod.score(X_train, y_train))
        test_err = np.append(test_err, 1-mod.score(X_test, y_test))
    return train_err.mean(), test_err.mean()
# auxiliary function for Q5
def fit_model(split_dataset, model, k=0, random_state=1020):
    assert(model in ['log', 'lda', 'qda', 'nb', 'knn'])
    X_train, X_test, y_train, y_test = split_dataset
    title = 'ROC with '
    mod = None
    if model == 'log':
        mod = LogisticRegression(random_state=random_state)
        title += 'Logistic Regression'
    elif model == 'lda':
        mod = LinearDiscriminantAnalysis()
        title += 'LDA'
    elif model == 'qda':
        mod = QuadraticDiscriminantAnalysis()
        title += 'QDA'
    elif model == 'knn':
        mod = KNeighborsClassifier(n_neighbors = k)
        title += str(k) + ' Nearest Neighbor(s)'
    elif model == 'nb':
        mod = GaussianNB()
        title += 'Naive Bayes'
    mod.fit(X_train, y_train)
    fpr, tpr, threshold = metrics.roc_curve(y_test, mod.predict(X_test))
    roc_auc = metrics.auc(fpr, tpr)
    plt.plot(fpr, tpr, 'b', label = 'AUC = %0.2f' % roc_auc)
    plt.title(title, fontsize=15)
    plt.legend(loc = 'lower right')
    plt.plot([0, 1], [0, 1], 'r--')
    plt.xlim([0, 1])
    plt.ylim([0, 1])
    plt.ylabel('Sensitivity')
    plt.xlabel('1 - Specificity')
```

```
plt.show()
return 1-mod.score(X_train, y_train), 1-mod.score(X_test, y_test), roc_auc
```

## 1 Question 1

```
[3]: # setting random seed
random.seed(1020)

# simulate dataset
X1 = np.random.uniform(-1, 1, 200)
X2 = np.random.uniform(-1, 1, 200)

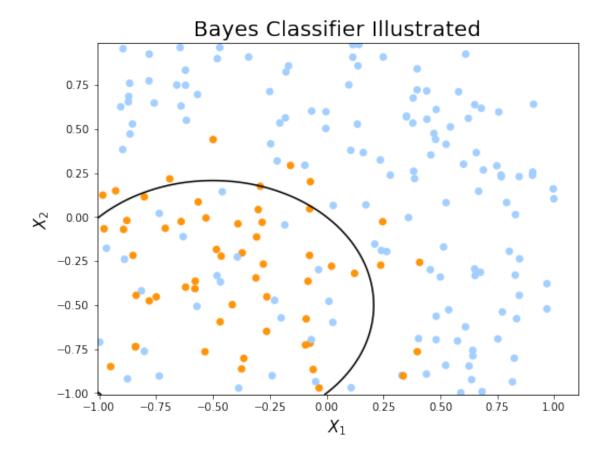
# calculating Y and probabilty derived from Y
Y = X1 + X1**2 + X2 + X2**2 + np.random.normal(0, 0.5, 200)
prob = np.exp(Y) / (1 + np.exp(Y))
[4]: plt.figure(figsize=(8,6))

# scatter plot of X1 against X2
categories = np.array([1 if p > 0.5 else 0 for p in prob])
plt.scatter(X1, X2, c=np.where(prob > 0.5, '#a2cffe', '#ff9408'))
```

```
[4]: plt.figure(figsize=(8,6))

# scatter plot of X1 against X2
categories = np.array([1 if p > 0.5 else 0 for p in prob])
plt.scatter(X1, X2, c=np.where(prob > 0.5, '#a2cffe', '#ff9408'))
plt.xlabel('$X_1$', fontsize=15)
plt.ylabel('$X_2$', fontsize=15)
plt.title('Bayes Classifier Illustrated', fontsize=20)

# drawing bayesian decision boundary
a = np.arange(-1.01, 1, 0.01)
b = np.arange(-1.01, 1, 0.01)
A, B = np.meshgrid(a, b)
C = A + A**2 + B + B**2
prob_C = np.exp(C) / (1 + np.exp(C))
plt.contour(A, B, prob_C, levels=[0.5], colors='black');
```



# 2 Question 2

We expect the LDA to work better than QDA in both test error since the data we generated is strictly linear, but the train error of QDA might be better than LDA since it might take noises as quadratic relationships, resulting in overfitting the data. First we simulate 1000 times the LDA and QDA models of  $f(X) = X_1 + X_2 + \epsilon$ , we obtain the average train and test error rates in the following table:

[5]: LDA QDA Train Error 0.274826 0.272263

```
Test Error 0.276997 0.276873
```

We observe that with  $f(X) = X_1 + X_2 + \epsilon$ , train error rate of LDA is higher than that of QDA and test error rate of LDA is slightly lower than that of QDA. This conforms with our expectation. Since the data given by f(X) here is linear, which fulfills assumptions of LDA that all classes shares the same covariance matrix. LDA would perform better than QDA when the relationshop in the data is indeed linear.

#### 3 Question 3

We would expect QDA to perform better than LDA in both train and test error rates given the relationship in the data is quadratic. Here, we simulate 1000 times the LDA and QDA models of  $f(X) = X_1 + X_1^2 + X_2 + X_2^2 + \epsilon$ , we obtain the average train and test error rates in the following table:

```
[6]: LDA QDA
Train Error 0.273210 0.258609
Test Error 0.274353 0.261380
```

When we switch to  $f(X) = X_1 + X_1^2 + X_2 + X_2^2 + \epsilon$ , the performances of QDA is better than that of LDA, same as what we expected. QDA has both a lower train error rate and a lower test error rate. This is because the data here has a quadratic relationship, so that QDA captures the perculiarities of the data much better than LDA. Hence QDA performs better in both training and test scenarios. The LDA model suffers from unequal variance across f(X), yielding a less satisfactory performance than in the linear case.

# 4 Question 4

```
qda_errors = simulation(size=int(size), rep=1000, model='qda',⊔

→linearity=False)

qda_results[str(size)] = qda_errors[1]
```

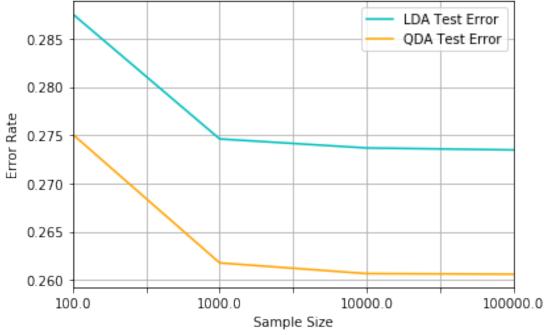
```
[8]: # creating table for visualization
df_lda = pd.DataFrame(lda_results, index=['LDA Test Error']).T
df_qda = pd.DataFrame(qda_results, index=['QDA Test Error']).T
df_Q4 = df_lda.merge(df_qda, left_index=True, right_index=True)

# Error Comparison of LDA and QDA with Increasing Sample Sizes (Non-linear Case)
df_Q4
```

```
[8]: LDA Test Error QDA Test Error 100.0 0.287533 0.275067 1000.0 0.274597 0.261757 10000.0 0.273664 0.260651 100000.0 0.273460 0.260584
```

```
[9]: # in graphical form
    df_Q4.plot(color=['c','orange'], grid=True)
    plt.title('LDA & QDA Error Rates with Increasing Sample Size', fontsize=15)
    plt.xlabel('Sample Size')
    plt.ylabel('Error Rate');
```

# LDA & QDA Error Rates with Increasing Sample Size



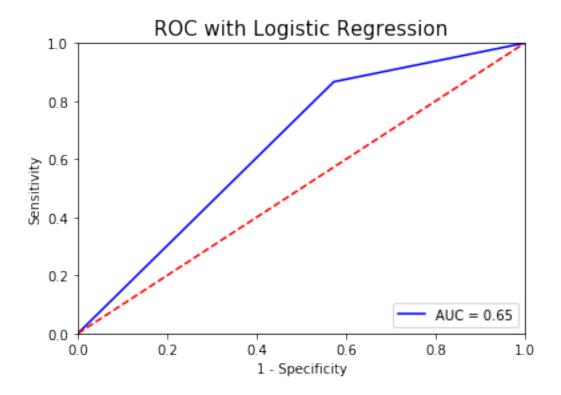
Both LDA and QDA have their test error decreasing when sample size increases, but LDA did not necessarily get better than QDA. The distance in test error between LDA and QDA remains unchanged. This confirms that the larger the sample size, the more generalizable the model to new data (less overfitting) which leads to a lower test error. The test error rate plateaus after n = 10000, where the sample size is large enough that the size does not affect model fitting anymore. However, the QDA model, no matter how large the sample size is, always performs better than LDA model with a lower test error rate. Given we retrieved our data from a quadratic random variable, QDA in theory would have greater predictive power than LDA. Our result confirmed this. LDA does not work well under non-linearity, when covariance matrix is not universal across all classes.

### 5 Question 5

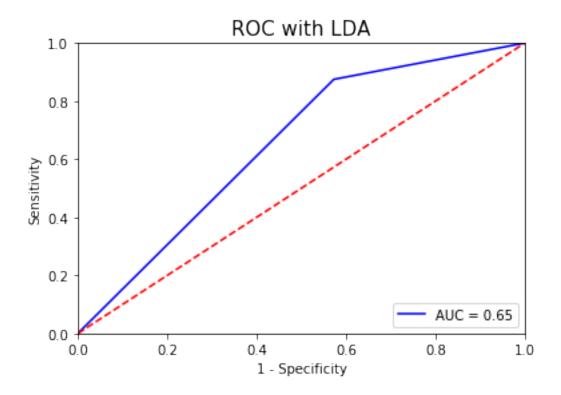
After preparing the data, we fit different models including Logistic Regression, LDA, QDA, Naives Bayes (Gaussian) and K1~10 Nearest Neighbors:

```
[11]: # collecting error rates and AUC scores
mod_errors = {}

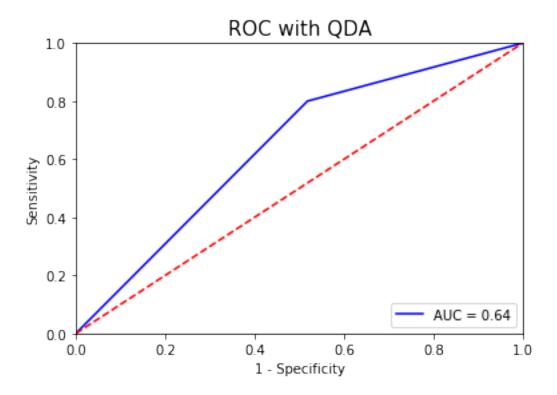
# Logistic Regression
log_err = fit_model(split_dataset=split_dataset, model='log')
mod_errors['Logistic Regression'] = log_err
```



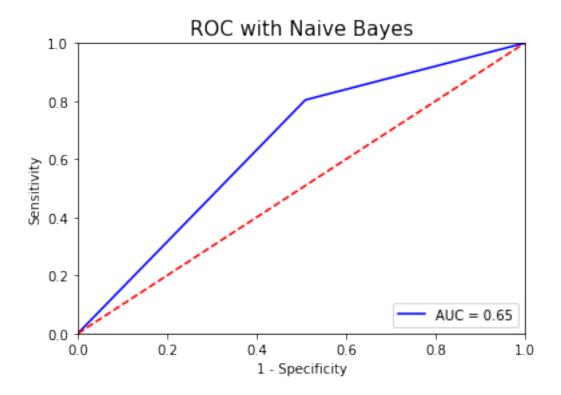
```
[12]: # Linear Discriminant Analysis
lda_err = fit_model(split_dataset=split_dataset, model='lda')
mod_errors['LDA'] = lda_err
```



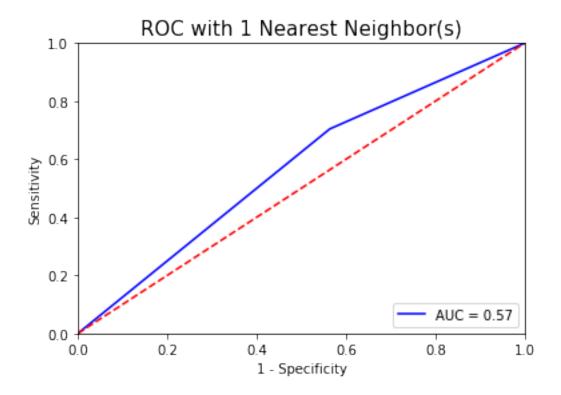
```
[13]: # Quadratic Discriminant Analysis
qda_err = fit_model(split_dataset=split_dataset, model='qda')
mod_errors['QDA'] = qda_err
```



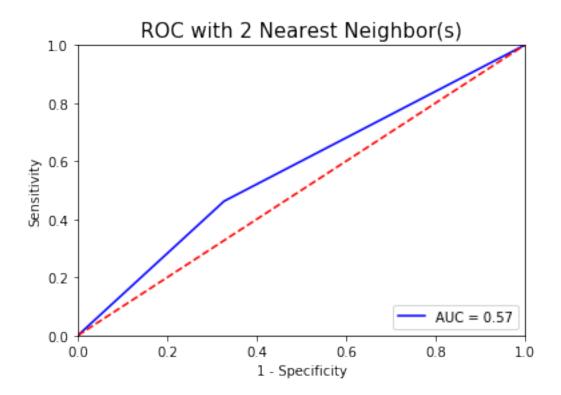
```
[14]: # Naive Bayes
nb_err = fit_model(split_dataset=split_dataset, model='nb')
mod_errors['Naive Bayes'] = nb_err
```



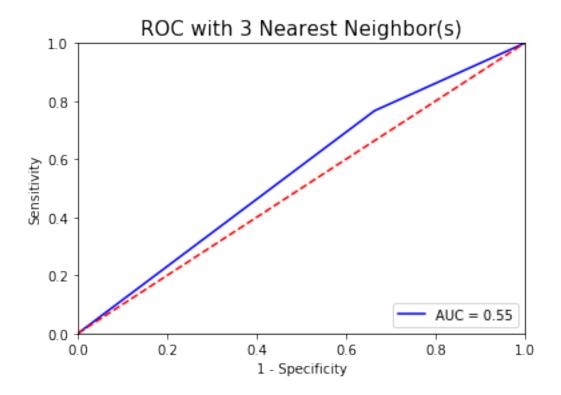
```
[15]: # 1 Nearest Neighbor
k1_err = fit_model(split_dataset=split_dataset, model='knn', k=1)
mod_errors['1 Nearest Neighbor'] = k1_err
```



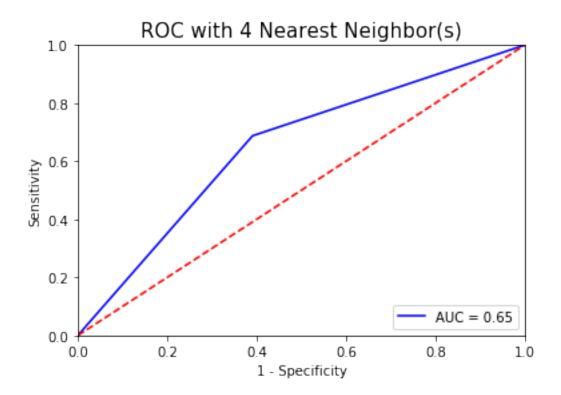
```
[16]: # 2 Nearest Neighbors
k2_err = fit_model(split_dataset=split_dataset, model='knn', k=2)
mod_errors['2 Nearest Neighbors'] = k2_err
```



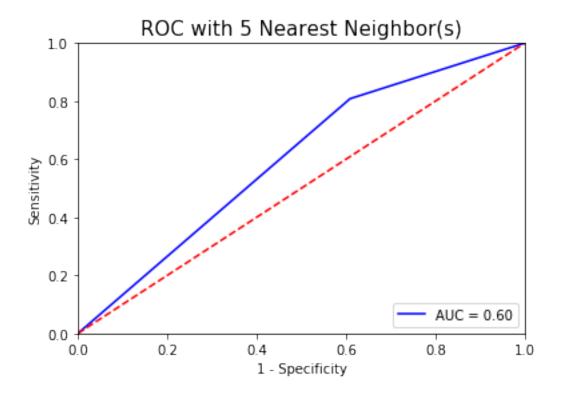
```
[17]: # 3 Nearest Neighbors
k3_err = fit_model(split_dataset=split_dataset, model='knn', k=3)
mod_errors['3 Nearest Neighbors'] = k1_err
```



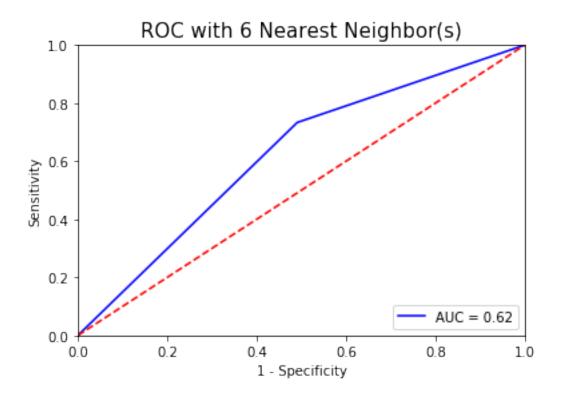
```
[18]: # 4 Nearest Neighbors
k4_err = fit_model(split_dataset=split_dataset, model='knn', k=4)
mod_errors['4 Nearest Neighbors'] = k4_err
```



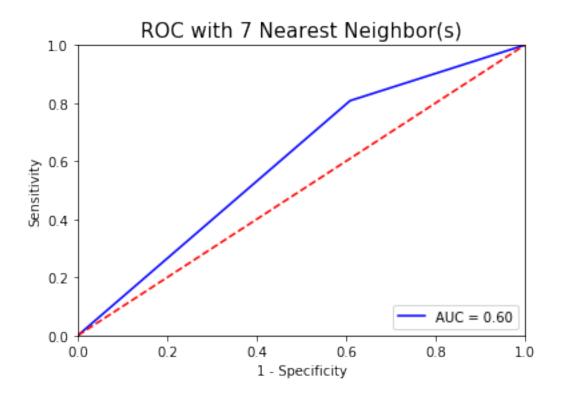
```
[19]: # 5 Nearest Neighbors
k5_err = fit_model(split_dataset=split_dataset, model='knn', k=5)
mod_errors['5 Nearest Neighbors'] = k5_err
```



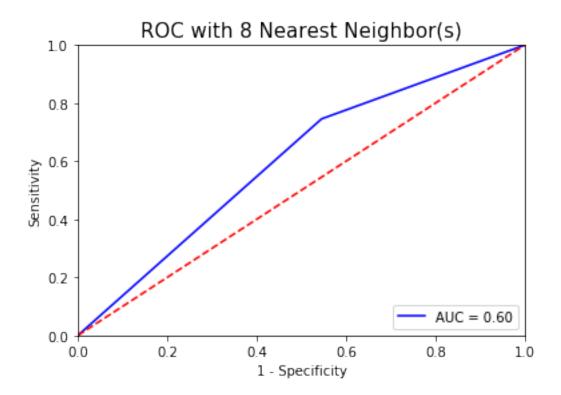
```
[20]: # 6 Nearest Neighbors
k6_err = fit_model(split_dataset=split_dataset, model='knn', k=6)
mod_errors['6 Nearest Neighbors'] = k6_err
```



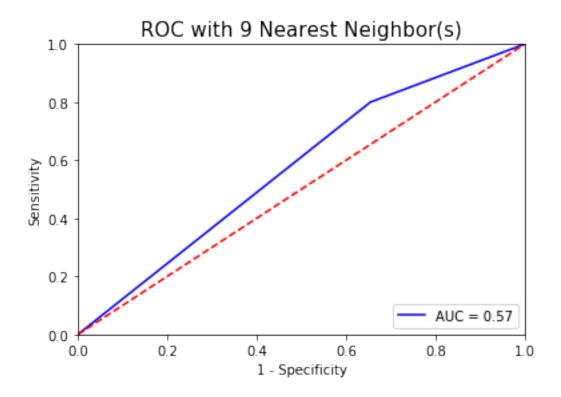
```
[21]: # 7 Nearest Neighbors
k7_err = fit_model(split_dataset=split_dataset, model='knn', k=7)
mod_errors['7 Nearest Neighbors'] = k7_err
```



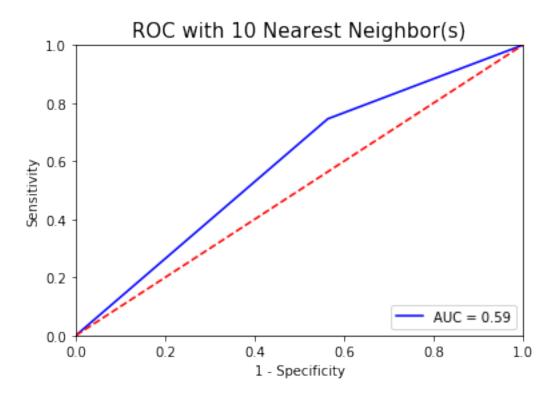
```
[22]: # 8 Nearest Neighbors
k8_err = fit_model(split_dataset=split_dataset, model='knn', k=8)
mod_errors['8 Nearest Neighbors'] = k8_err
```



```
[23]: # 9 Nearest Neighbors
k9_err = fit_model(split_dataset=split_dataset, model='knn', k=9)
mod_errors['9 Nearest Neighbors'] = k9_err
```



```
[24]: # 10 Nearest Neighbors
k10_err = fit_model(split_dataset=split_dataset, model='knn', k=10)
mod_errors['10 Nearest Neighbors'] = k10_err
```



Then we compare the models by their error rates and AUC:

```
[25]: errors_df = pd.DataFrame(mod_errors, index=['Train Err', 'Test Err', __ 

→'AUC-ROC']).T
errors_df.sort_values(by='Test Err', axis=0) # sorted by test error rate
```

```
[25]:
                            Train Err
                                       Test Err
                                                  AUC-ROC
     LDA
                             0.278528
                                       0.265714
                                                 0.651136
     Logistic Regression
                                       0.271429
                             0.268712
                                                 0.646970
     Naive Bayes
                             0.300613
                                       0.294286
                                                 0.647538
     QDA
                             0.269939
                                       0.300000
                                                 0.640909
      5 Nearest Neighbors
                             0.218405 0.322857
                                                 0.599621
      7 Nearest Neighbors
                             0.239264
                                       0.322857
                                                 0.599621
      4 Nearest Neighbors
                             0.235583 0.337143
                                                 0.648295
      6 Nearest Neighbors
                             0.241718
                                       0.337143
                                                 0.621212
      9 Nearest Neighbors
                             0.250307
                                       0.342857
                                                 0.572727
      8 Nearest Neighbors
                             0.235583
                                       0.345714
                                                 0.600189
      10 Nearest Neighbors
                             0.256442
                                       0.351429
                                                 0.591098
      1 Nearest Neighbor
                             0.001227
                                       0.380000
                                                 0.570265
      3 Nearest Neighbors
                             0.001227
                                       0.380000
                                                 0.570265
      2 Nearest Neighbors
                             0.168098 0.471429
                                                 0.567614
```

[26]: errors\_df.sort\_values(by='AUC-ROC', axis=0, ascending=False) # sorted by AUC-ROC

#### [26]: Train Err Test Err AUC-ROC LDA 0.278528 0.265714 0.651136 4 Nearest Neighbors 0.235583 0.337143 0.648295 Naive Bayes 0.294286 0.647538 0.300613 Logistic Regression 0.268712 0.271429 0.646970 QDA 0.300000 0.640909 0.269939 6 Nearest Neighbors 0.241718 0.337143 0.621212 8 Nearest Neighbors 0.235583 0.345714 0.600189 5 Nearest Neighbors 0.322857 0.218405 0.599621 7 Nearest Neighbors 0.239264 0.322857 0.599621 10 Nearest Neighbors 0.256442 0.351429 0.591098 9 Nearest Neighbors 0.342857 0.250307 0.572727 1 Nearest Neighbor 0.001227 0.380000 0.570265 3 Nearest Neighbors 0.380000 0.001227 0.570265 2 Nearest Neighbors 0.168098 0.471429 0.567614

When choosing a classifier model, we first want it to have low test error rate, so that it has good generalizability whenever it meets new data. Second, we want the classifier to predict actual 0's as 0 and actual 1's as 1, in another word, to produce as little false positives as possible. Hence, we are looking for the model with the lowest test error rate possible and largest AUC score possible. In our case, LDA possesses both the lowest test error rate and the highest AUC score. Therefore, in my opinion, LDA is the best-performing model in this scenario.