Classification Methods

January 27, 2019

```
In [1]: # import the packages
        import numpy as np
        import pandas as pd
        import matplotlib.pyplot as plt
        import statsmodels.api as sm

        from sklearn.discriminant_analysis import LinearDiscriminantAnalysis
        from sklearn.discriminant_analysis import QuadraticDiscriminantAnalysis
        from sklearn.linear_model import LogisticRegression
        from sklearn.naive_bayes import GaussianNB
        from sklearn.neighbors import KNeighborsClassifier
        from sklearn.metrics import roc_curve, auc
```

1 Conceptual exercises

1.1 Differences between LDA and QDA

1.1.1 If the Bayes decision boundary is linear, do we expect LDA or QDA to perform better on the training set? On the test set?

I would expect the QDA to perform better on the training sets, while LDA will perform better on the testing sets if the Bayes decision boundary is linear.

Repeat the following process 1000 times.

- (1) Simulate a dataset of 1000 observations with X_1, $X_2 \sim Uniform(1, +1)$. Y is a binary response variable defined by a Bayes decision boundary of $f(X) = X_1 + X_2$, where values 0 or greater are coded TRUE and values less than 0 or coded FALSE. Whereas your simulated Y is a function of $X_1 + X_2 + \epsilon$, where $\epsilon \sim N(0, 1)$. That is, your simulated Y is a function of the Bayes decision boundary plus some irreducible error.
- (2) Randomly split your dataset into 70/30% training/test sets.
- (3) Use the training dataset to estimate LDA and QDA models.
- (4) Calculate each model's training and test error rate.

```
In [2]: class DA_simulate:
    def __init__(self, seed = 1, data = None):
        self.data = data
        self.seed = seed

    def generate_data(self):
        np.random.seed(self.seed)
        X = np.random.uniform(-1,1,(2,1000))
        Y = ((X[0,:] + X[1,:] + np.random.normal(size = 1000))>=0)*1
        data = np.vstack((X, Y))
        self.data = data

    def split_data(self):
        seq = np.arange(1000)
        np.random.seed(self.seed)
        np.random.shuffle(seq)
        train_idx = seq[:700]; test_idx = seq[700:]
        return self.data[:,train_idx], self.data[:,test_idx]

    def LD(self, data, model):
        X_var = data[:2,:].T; y = data[2,:].T
        if model=='LDA':
            lda = LinearDiscriminantAnalysis(solver="svd", store_covariance=True)
            res = lda.fit(X_var, y)
        elif model=='QDA':
            qda = QuadraticDiscriminantAnalysis(store_covariance=True)
            res = qda.fit(X_var, y)
        else:
            raise ValueError('model must be either LDA or QDA')
        return res

    def error_rate(self):
        train, test = self.split_data()
        lda = self.LD(train,model='LDA'); qda = self.LD(train,model = 'QDA')
        lda_train = (lda.predict(train[:2,:].T)!=train[2,:]).sum()/train.shape[1]
        lda_test = (lda.predict(test[:2,:].T)!=test[2,:]).sum()/test.shape[1]
        qda_train = (qda.predict(train[:2,:].T)!=train[2,:]).sum()/train.shape[1]
        qda_test = (qda.predict(test[:2,:].T)!=test[2,:]).sum()/test.shape[1]
        return lda_train, lda_test, qda_train, qda_test
```

```
In [3]: # Try the simulation
        sim = DA_simulate(1)
        sim.generate_data()
        error_rate = np.array([sim.error_rate()])

In [4]: error_rate

Out[4]: array([[0.27285714, 0.26333333, 0.26142857, 0.27333333]])

In [5]: # Proceed with additional 999 trials
        for seed in range(2, 1001):
```

```
        sim = DA_simulate(seed)
        sim.generate_data()
        error_rate = np.vstack((error_rate, np.array([sim.error_rate()])))
```

```
In [6]: error_rate
```

```
Out[6]: array([[0.27285714, 0.26333333, 0.26142857, 0.27333333],
               [0.26714286, 0.30666667, 0.26      , 0.30666667],
               [0.28857143, 0.27      , 0.28571429, 0.27      ],
               ...,
               [0.26142857, 0.27333333, 0.26428571, 0.27      ],
               [0.27142857, 0.25333333, 0.27428571, 0.25      ],
               [0.30142857, 0.23333333, 0.30142857, 0.23666667]])
```

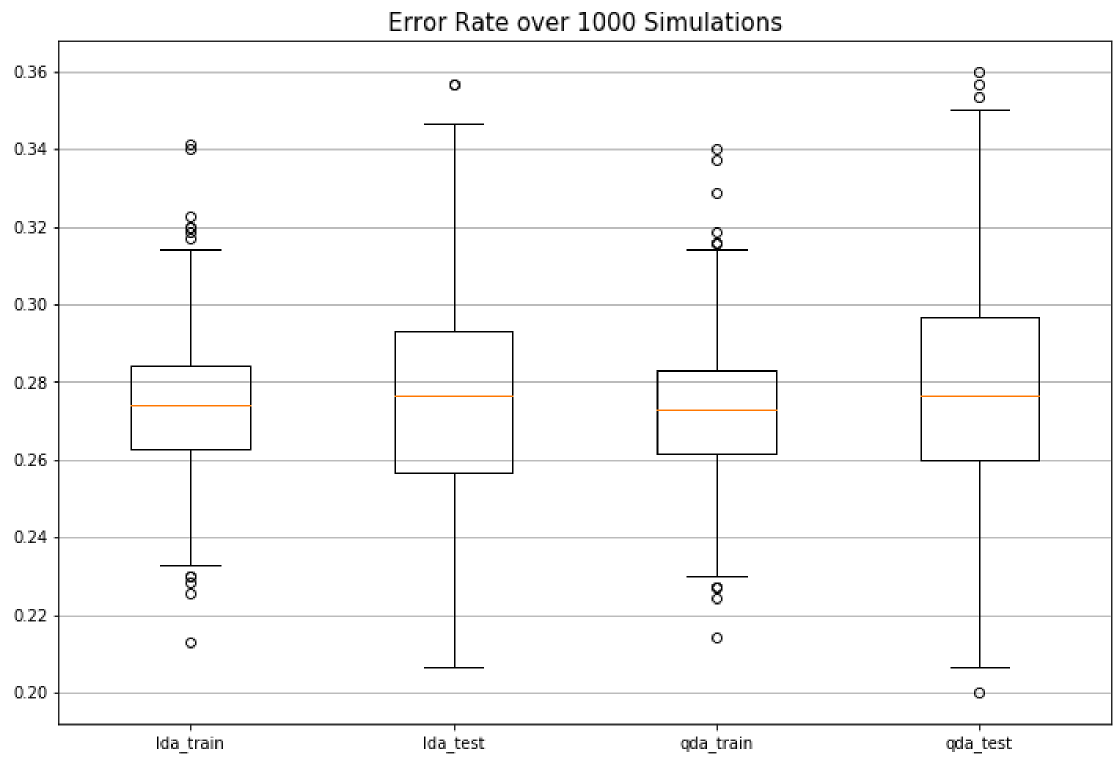
Summarize all the simulations' error rates and report the results in tabular and graphical form. Use this evidence to support your answer.

```
In [7]: error_rate.mean(axis = 0)
```

```
Out[7]: array([0.27369857, 0.27612333, 0.27261286, 0.27694667])
```

Group	Error Rate
LDA_train	27.36%
LDA_test	27.61%
QDA_train	27.26%
QDA_test	27.69%

```
In [8]: # Draw the boxplot
        fig, ax = plt.subplots()
        fig.set_size_inches(12, 8)
        ax.boxplot((error_rate.T[0], error_rate.T[1], error_rate.T[2], error_rate.T[3]), vert=
        ax.set_xticklabels(["lda_train", "lda_test", "qda_train", "qda_test"])
        ax.yaxis.grid(True)
        plt.title("Error Rate over 1000 Simulations", size = 15)
        plt.show()
```



As calculated, the average error rate of **Linear Discrimination** is **27.37%** for the training sets, **27.61%** for the testing sets; the the average error rate of **Quadratic Discrimination** is **27.26%** for the training sets, **27.69%** for the testing sets. Plus what we see from the boxplots, we now have solid evidence that **LDA can predict better on the testing set**, while **QDA can fit the training sets better**(better on the training set).

1.1.2 If the Bayes decision boundary is non-linear, do we expect LDA or QDA to perform better on the training set? On the test set?

I would expect the QDA to perform better on both the training sets and the testing sets.

Repeat the following process 1000 times.

- (1) Simulate a dataset of 1000 observations with X_1, $X_2 \sim Uniform(1, +1)$. Y is a binary response variable defined by a Bayes decision boundary of $f(X) = X_1 + X_1^2 + X_2 + X_2^2$, where values 0 or greater are coded TRUE and values less than 0 or coded FALSE. Whereas your simulated Y is a function of $X_1 + X_1^2 + X_2 + X_2^2 + \epsilon$, where $\epsilon \sim N(0, 1)$. That is, your simulated Y is a function of the Bayes decision boundary plus some irreducible error.
- (2) Randomly split your dataset into 70/30% training/test sets.
- (3) Use the training dataset to estimate LDA and QDA models.
- (4) Calculate each model's training and test error rate.

```
In [9]: class DA_simulate_nonlinear:

            def __init__(self, seed = 1, data = None):
                self.data = data
                self.seed = seed

            def generate_data(self):
                np.random.seed(self.seed)
                X = np.random.uniform(-1,1,(2,1000))
                Y = ((X[0,:] + X[0,:]**2 + X[1,:] + X[1,:]**2 + np.random.normal(size = 1000))
                data = np.vstack((X, Y))
                self.data = data

            def split_data(self):
                seq = np.arange(1000)
                np.random.seed(self.seed)
                np.random.shuffle(seq)
                train_idx = seq[:700]; test_idx = seq[700:]
                return self.data[:,train_idx], self.data[:,test_idx]

            def LD(self, data, model):
                X_var = data[:2,:].T; y = data[2,:].T
                if model=='LDA':
                    lda = LinearDiscriminantAnalysis(solver="svd", store_covariance=True)
                    res = lda.fit(X_var, y)
                elif model=='QDA':
                    qda = QuadraticDiscriminantAnalysis(store_covariance=True)
                    res = qda.fit(X_var, y)
                else:
                    raise ValueError('model must be either LDA or QDA')
                return res

            def error_rate(self):
                train, test = self.split_data()
                lda = self.LD(train,model='LDA'); qda = self.LD(train,model = 'QDA')
                lda_train = (lda.predict(train[:2,:].T)!=train[2,:]).sum()/train.shape[1]
                lda_test = (lda.predict(test[:2,:].T)!=test[2,:]).sum()/test.shape[1]
                qda_train = (qda.predict(train[:2,:].T)!=train[2,:]).sum()/train.shape[1]
                qda_test = (qda.predict(test[:2,:].T)!=test[2,:]).sum()/test.shape[1]
                return lda_train, lda_test, qda_train, qda_test

In [10]: # Try the simulation
         sim = DA_simulate_nonlinear(1)
         sim.generate_data()
         error_rate = np.array([sim.error_rate()])

In [11]: error_rate

Out[11]: array([[0.25857143, 0.26      , 0.26142857, 0.23666667]])
```

```
In [12]: # Proceed with additional 999 trials
         for seed in range(2, 1001):
             sim = DA_simulate_nonlinear(seed)
             sim.generate_data()
             error_rate = np.vstack((error_rate, np.array([sim.error_rate()])))
```

```
In [13]: error_rate
```

```
Out[13]: array([[0.25857143, 0.26      , 0.26142857, 0.23666667],
                [0.25571429, 0.27      , 0.24      , 0.27666667],
                [0.29714286, 0.23      , 0.27285714, 0.23333333],
                ...,
                [0.29571429, 0.26      , 0.27285714, 0.27333333],
                [0.27      , 0.27666667, 0.27142857, 0.27      ],
                [0.28285714, 0.3       , 0.26571429, 0.29      ]])
```

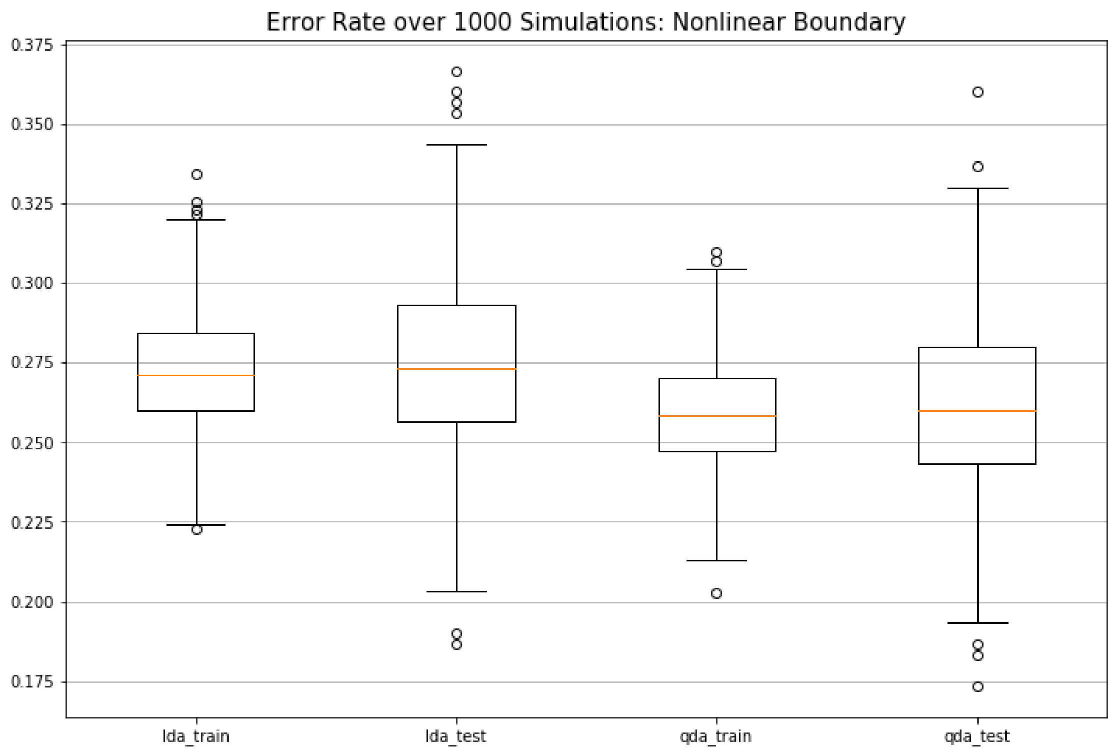
Summarize all the simulations' error rates and report the results in tabular and graphical form. Use this evidence to support your answer.

```
In [14]: error_rate.mean(axis = 0)
```

```
Out[14]: array([0.27218286, 0.27514667, 0.25898714, 0.26201   ])
```

Group	Error Rate
LDA_train	27.37%
LDA_test	27.51%
QDA_train	25.90%
QDA_train	26.20%

```
In [15]: # Draw the boxplot
         fig, ax = plt.subplots()
         fig.set_size_inches(12, 8)
         ax.boxplot((error_rate.T[0], error_rate.T[1], error_rate.T[2], error_rate.T[3]), vert=
         ax.set_xticklabels(["lda_train", "lda_test", "qda_train", "qda_test"])
         ax.yaxis.grid(True)
         plt.title("Error Rate over 1000 Simulations: Nonlinear Boundary", size = 15)
         plt.show()
```



As calculated, the average error rate of **Linear Discrimination** is **27.22%** for the training sets, **27.51%** for the testing sets; the the average error rate of **Quadratic Discrimination** is **25.90%** for the training sets, **26.20%** for the testing sets. Plus what we see from the boxplots, we now have solid evidence that **QDA both fit the training data better and predict the testing sets better**, when the Bayes boundary is not linear.

1.1.3 In general, as sample size n increases, do we expect the test error rate of QDA relative to LDA to improve, decline, or be unchanged? Why?

Whtn the sample size increases, I would expect the both QDA and LDA to frow their prediction capabilities, and QDA may have a greater improvement.

```
In [16]: class DA_simulate_nonlinear_vobs:

             def __init__(self, seed = 1, nobs = 1000, data = None):
                 self.data = data
                 self.seed = seed
                 self.nobs = nobs

             def generate_data(self):
                 np.random.seed(self.seed)
                 X = np.random.uniform(-1,1,(2, self.nobs))
                 Y = ((X[0,:] + X[0,:]**2 + X[1,:] + X[1,:]**2 + np.random.normal(size = self.r
                 data = np.vstack((X, Y))
```

```
            self.data = data

        def split_data(self):
            seq = np.arange(self.nobs)
            np.random.seed(self.seed)
            np.random.shuffle(seq)
            train_idx = seq[:int(0.7*self.nobs)]; test_idx = seq[int(0.7*self.nobs):]
            return self.data[:,train_idx], self.data[:,test_idx]

        def LD(self, data, model):
            X_var = data[:2,:].T; y = data[2,:].T
            if model=='LDA':
                lda = LinearDiscriminantAnalysis(solver="svd", store_covariance=True)
                res = lda.fit(X_var, y)
            elif model=='QDA':
                qda = QuadraticDiscriminantAnalysis(store_covariance=True)
                res = qda.fit(X_var, y)
            else:
                raise ValueError('model must be either LDA or QDA')
            return res

        def error_rate(self):
            train, test = self.split_data()
            lda = self.LD(train,model='LDA'); qda = self.LD(train,model = 'QDA')
            lda_train = (lda.predict(train[:2,:].T)!=train[2,:]).sum()/train.shape[1]
            lda_test = (lda.predict(test[:2,:].T)!=test[2,:]).sum()/test.shape[1]
            qda_train = (qda.predict(train[:2,:].T)!=train[2,:]).sum()/train.shape[1]
            qda_test = (qda.predict(test[:2,:].T)!=test[2,:]).sum()/test.shape[1]
            return lda_train, lda_test, qda_train, qda_test
```

Use the non-linear Bayes decision boundary approach from part (2) and vary n across your simulations.

```
In [17]: errors = []

         for n in [10**2, 10**3, 10**4, 10**5]:
             sim = DA_simulate_nonlinear_vobs(1, n)
             sim.generate_data()
             error_rate = np.array([sim.error_rate()])
             for seed in range(2, 1001):
                 sim = DA_simulate_nonlinear_vobs(seed, n)
                 sim.generate_data()
                 error_rate = np.vstack((error_rate, np.array([sim.error_rate()])))
             errors.append(error_rate.mean(axis = 0))
```

```
In [18]: errors = np.array(errors)
```

```
In [19]: errors
```

```
Out[19]: array([[0.26155714, 0.291     , 0.23847143, 0.2754    ],
                [0.27218286, 0.27514667, 0.25898714, 0.26201   ],
                [0.27351743, 0.273386  , 0.260696  , 0.26059433],
                [0.27346231, 0.27342533, 0.26062903, 0.26057177]])
```

Here we tabulate the error rates' changes over numbers of simulations:

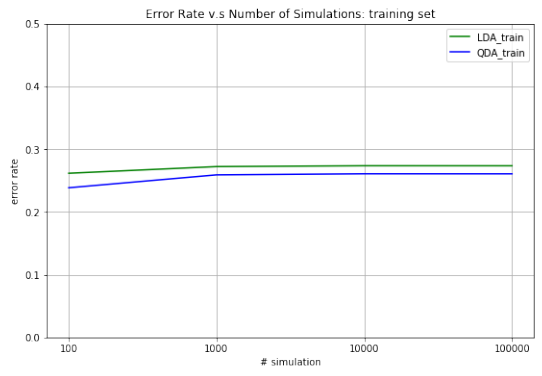
Error Rate
Simulations
100
1000
10000
100000

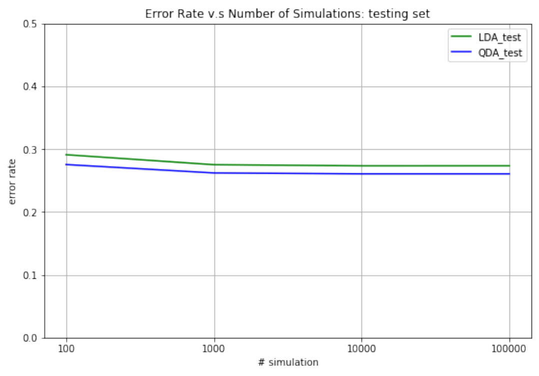
```
In [20]: # Graphical Interpretation

         fig, axes = plt.subplots(1,2)
         x = np.log10([100, 1000, 10000, 100000])
         fig.set_size_inches(20,6)
         ax = axes[0]
         ax.plot(x, errors[:,0], color = 'g', label = 'LDA_train')
         ax.plot(x, errors[:,2], color = 'b', label = 'QDA_train')
         ax.set_xticks([2, 3, 4, 5]); ax.set_xticklabels([100, 1000, 10000, 100000])
         ax.set_title("Error Rate v.s Number of Simulations: training set")
         ax.set_xlabel("# simulation"); ax.set_ylabel("error rate")
         ax.set_ylim(0, 0.5)
         ax.legend(); ax.grid()

         ax = axes[1]
         ax.plot(x, errors[:,1], color = 'g', label = 'LDA_test')
         ax.plot(x, errors[:,3], color = 'b', label = 'QDA_test')
         ax.set_xticks([2, 3, 4, 5]); ax.set_xticklabels([100, 1000, 10000, 100000])
         ax.set_title("Error Rate v.s Number of Simulations: testing set")
         ax.set_xlabel("# simulation"); ax.set_ylabel("error rate")
         ax.set_ylim(0, 0.5)
         ax.legend(); ax.grid()

         plt.show()
```





As the table and the graphs indicate, for the training sets, both LDA and QDA tend to have bigger error rates as N increases. This is because larger samples are harder to fit with relatively inflexible models. While both models predict better on the testing sets, as the models we estimate now are closer to the true model, with more observations. And QDA seems to increase faster in terms of predicting accuracy, and the relative error rate to LDA declines.

1.1.4 True or False: Even if the Bayes decision boundary for a given problem is linear, we will probably achieve a superior test error rate using QDA rather than LDA because QDA is flexible enough to model a linear decision boundary. Justify your answer.

I think the statement is false. The QDA might be able to fit the training set better, as it is more flexible. But it might in the meantime overfit the training data and perform worse in doing out of sample prediction, especially when the true Bayes decision boundary is linear.

2 Modeling voter turnout

```
In [21]: # import the data
         mh = pd.read_csv("data/mental_health.csv")
```

```
In [22]: # remove the NANs
         mh = mh.dropna(axis = 0, how='any')
```

```
In [23]: mh.head()
```

```
Out[23]:     vote96  mhealth_sum   age  educ  black  female  married    inc10
         0      1.0          0.0  60.0  12.0      0       0      0.0   4.8149
         2      1.0          1.0  36.0  12.0      0       0      1.0   8.8273
         3      0.0          7.0  21.0  13.0      0       0      0.0   1.7387
         7      0.0          6.0  29.0  13.0      0       0      0.0  10.6998
         11     1.0          1.0  41.0  15.0      1       1      1.0   8.8273
```

2.1 Split the data into a training and test set (70/30).

```
In [24]: np.random.seed(30100)
         idx = np.arange(mh.shape[0])
```

```
        np.random.shuffle(idx)
        idx_train = idx[:int(mh.shape[0]*0.7)]; idx_test = idx[int(mh.shape[0]*0.7):]
        train = mh.iloc[idx_train,:]; test = mh.iloc[idx_test,:]
```

2.2 Using the training set and all available predictors, estimate the following models with vote96 as the response variable:

2.2.1 Logistic regression model

```
In [25]: x_train = train.iloc[:,1:]; y_train = train['vote96']

         m_logit = LogisticRegression()
         res_logit = m_logit.fit(sm.add_constant(x_train), y_train)
```

2.2.2 Linear discriminant model

```
In [26]: m_lda = LinearDiscriminantAnalysis(solver="svd", store_covariance=True)
         res_lda = m_lda.fit(x_train, y_train)
```

2.2.3 Quadratic discriminant model

```
In [27]: m_qda = QuadraticDiscriminantAnalysis(store_covariance=True)
         res_qda = m_qda.fit(x_train, y_train)
```

2.2.4 Naive Bayes - you can use the default hyperparameter settings

```
In [28]: m_nb = GaussianNB()
         res_nb = m_nb.fit(x_train, y_train)
```

2.2.5 K-nearest neighbors with $K = 1, 2, ..., 10$ (that is, 10 separate models varying K) and Euclidean distance metrics

```
In [29]: m_knn = []; res_knn = []
         for k in range(1,11):
             m = KNeighborsClassifier(n_neighbors=k)
             res = m.fit(x_train, y_train)
             m_knn.append(m); res_knn.append(res)
```

2.3 Using the test set, calculate the following model performance metrics:

```
In [30]: x_test = test.iloc[:,1:]; y_test = test['vote96']

In [31]: # Compute the error rates of all the previous models, using the testing dataset
         pred_logit = res_logit.predict(sm.add_constant(x_test))
         pred_lda = res_lda.predict(x_test)
         pred_qda = res_qda.predict(x_test)
         pred_nb = res_nb.predict(x_test)
         pred_knn = []
         for i in range(10):
             pred_knn.append(res_knn[i].predict(x_test))
```

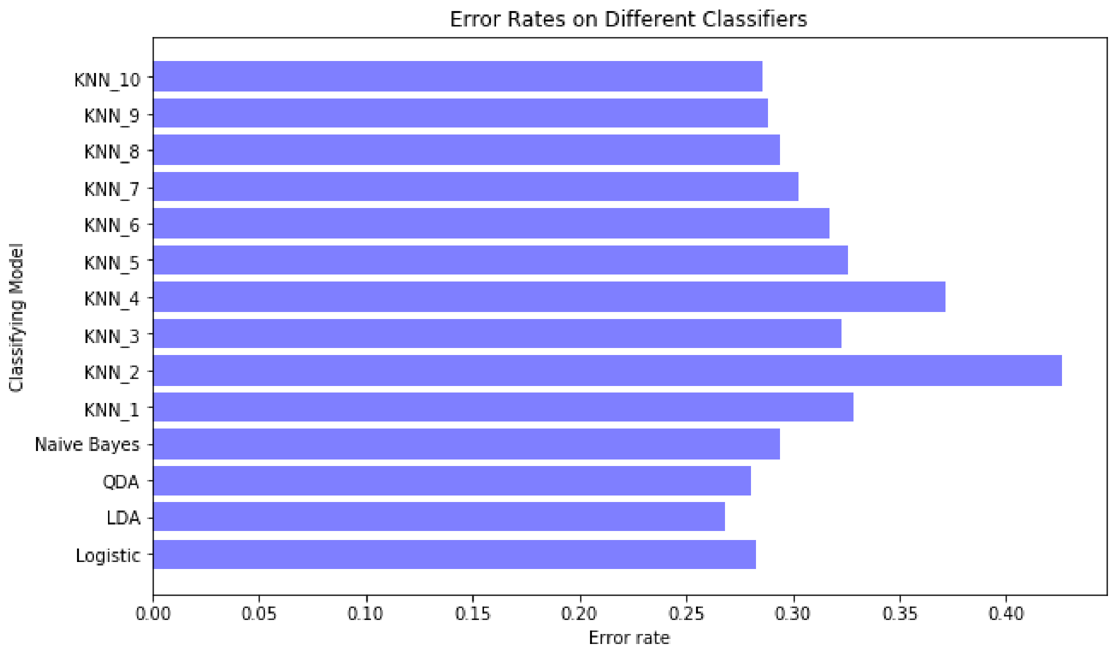
2.3.1 Error rate

```
In [32]: l = y_test.shape[0]
         error_logit = (np.array(pred_logit) != y_test).sum()/l
         error_lda = (np.array(pred_lda) != y_test).sum()/l
         error_qda = (np.array(pred_qda) != y_test).sum()/l
         error_nb = (np.array(pred_nb) != y_test).sum()/l
         error_knn = []
         for i in range(10):
             error_knn.append((np.array(pred_knn[i]) != y_test).sum()/l)

         error_rates = [error_logit, error_lda, error_qda, error_nb] + error_knn
```

```
In [33]: model = ['Logistic', 'LDA', 'QDA', 'Naive Bayes'] + ['KNN_'+str(i) for i in range(1,1

         fig, ax = plt.subplots()
         fig.set_size_inches(10, 6)
         ax.barh(range(len(model)), error_rates, color = 'b', alpha = 0.5)
         ax.set_yticks(range(len(model)))
         ax.set_yticklabels(model)
         ax.set_xlabel('Error rate'); ax.set_ylabel('Classifying Model')
         ax.set_title('Error Rates on Different Classifiers')
         plt.show()
```

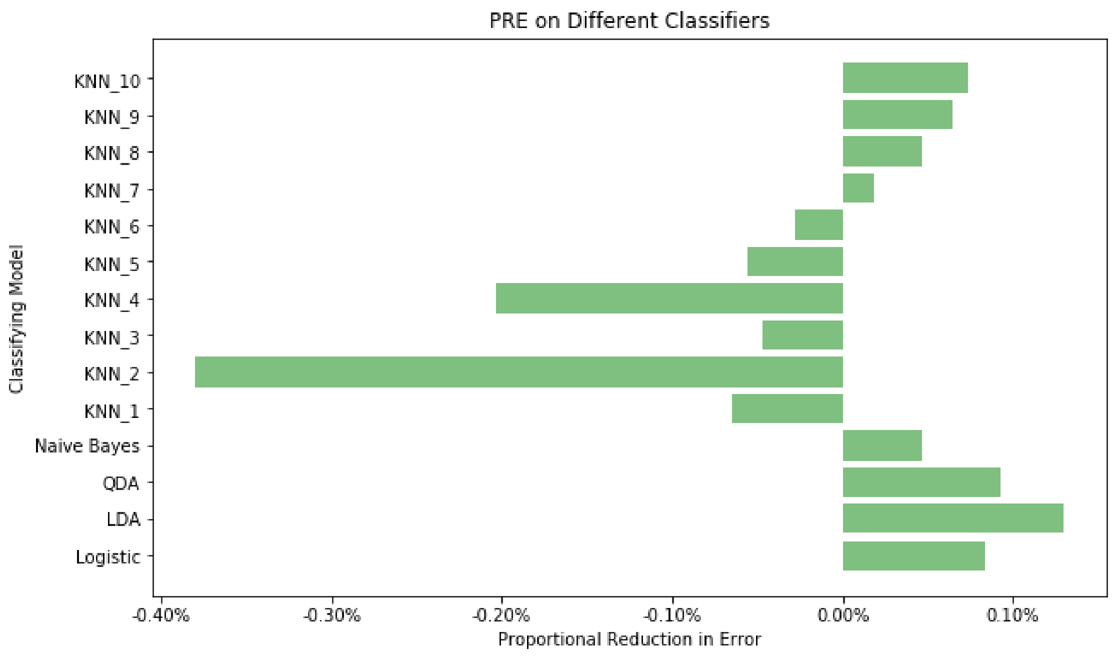


2.3.2 Proporitional Reduction in Error

```
In [34]: error_null = 1 - y_test.sum()/y_test.shape[0]
         PRE = [(error_null - i)/error_null for i in error_rates]
```

```
In [35]: import matplotlib.ticker as ticker

         fig, ax = plt.subplots()
         fig.set_size_inches(10, 6)
         ax.barh(range(len(model)), PRE, color = 'g', alpha = 0.5)
         ax.set_yticks(range(len(model)))
         ax.set_yticklabels(model)
         ax.xaxis.set_major_formatter(ticker.PercentFormatter())
         ax.set_xlabel('Proportional Reduction in Error'); ax.set_ylabel('Classifying Model')
         ax.set_title('PRE on Different Classifiers')
         plt.show()
```

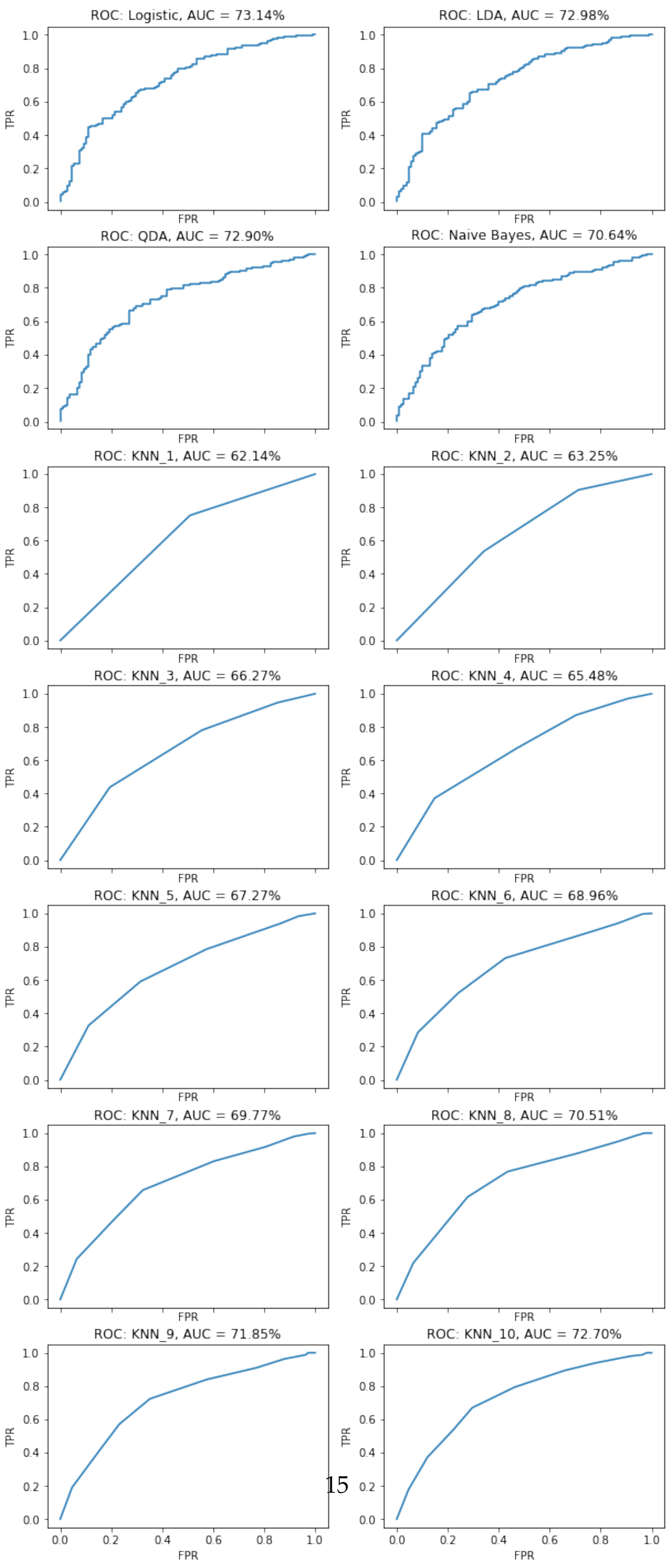


2.3.3 ROC curve & AUC

```
In [36]: res = [res_logit, res_lda, res_qda, res_nb] + res_knn

         fig, axes = plt.subplots(7, 2,sharex=True)
         fig.set_size_inches(10, 25)
         ax = axes[0][0]
         y_score = res_logit.decision_function(sm.add_constant(x_test))
         fpr, tpr, _ = roc_curve(y_test, y_score)
```

```python
ax.plot(fpr, tpr)
ax.set_xlabel('FPR'); ax.set_ylabel('TPR')
ax.set_title('ROC: Logistic, AUC = {:.2%}'.format(auc(fpr, tpr)))
ax = axes[0][1]
y_score = res_lda.decision_function(x_test)
fpr, tpr, _ = roc_curve(y_test, y_score)
ax.plot(fpr, tpr)
ax.set_xlabel('FPR'); ax.set_ylabel('TPR')
ax.set_title('ROC: LDA, AUC = {:.2%}'.format(auc(fpr, tpr)))
for i in range(1,7):
    for j in range(2):
        ax = axes[i][j]
        y_score = res[2*i+j].predict_proba(x_test)[:,1]
        fpr, tpr, _ = roc_curve(y_test, y_score)
        ax.plot(fpr, tpr)
        ax.set_xlabel('FPR'); ax.set_ylabel('TPR')
        ax.set_title('ROC: {}, AUC = {:.2%}'.format(model[2*i+j], auc(fpr, tpr)))
plt.show()
```


ROC: Logistic, AUC = 73.14%
ROC: LDA, AUC = 72.98%
ROC: QDA, AUC = 72.90%
ROC: Naive Bayes, AUC = 70.64%
ROC: KNN_1, AUC = 62.14%
ROC: KNN_2, AUC = 63.25%
ROC: KNN_3, AUC = 66.27%
ROC: KNN_4, AUC = 65.48%
ROC: KNN_5, AUC = 67.27%
ROC: KNN_6, AUC = 68.96%
ROC: KNN_7, AUC = 69.77%
ROC: KNN_8, AUC = 70.51%
ROC: KNN_9, AUC = 71.85%
ROC: KNN_10, AUC = 72.70%
TPR
FPR
0.0
0.2
0.4
0.6
0.8
1.0

2.4 Which model performs the best? Be sure to define what you mean by "best" and identify supporting evidence to support your conclusion(s).

Since our main goal here is to reach the best prediction, I would take these predicting diagnostics more seriously. Therefore, my best-performance model is the **LDA model**, which has the lowest error rate (26.86%), the most PRE (12.96%) and the second best AUC (72.98%). In addition, since it is a linear model and we have coefficient estimates, it is also quite interpretable in a way.