UCCD2063 ARTIFICIAL INTELLIGENCE TECHNIQUES

Classification of Red Wine Quality using NeuralNetwork

Group ID: 36

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Data Exploration

In [1]:

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns

wine = pd.read_csv("./redwinequality.csv")
```

In [2]:

```
wine.head()
```

Out[2]:

	WineID	FixedAcidity	VolatileAcidity	CitricAcid	ResidualSugar	Chlorides	FreeSulfurDioxi
0	1	7.4	0.70	0.00	1.9	0.076	11
1	2	7.8	0.88	0.00	2.6	0.098	25
2	3	7.8	0.76	0.04	2.3	0.092	15
3	4	11.2	0.28	0.56	1.9	0.075	17
4	5	7.4	0.70	0.00	1.9	0.076	11

As per observed from above, 'WineID' is not part of the features and must not included in the model. There are total of 11 features and 'Quality' is the output values.

The features for input matrix have different scales. Standardization on the features is needed to get standard deviation of 1.

In [3]:

```
wine.drop("WineID", axis =1 , inplace = True)
```

In [4]:

```
wine.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1599 entries, 0 to 1598
Data columns (total 12 columns):
FixedAcidity          1599 non-null float64
VolatileAcidity       1599 non-null float64
CitricAcid            1599 non-null float64
ResidualSugar         1599 non-null float64
Chlorides             1599 non-null float64
FreeSulfurDioxide     1599 non-null float64
TotalSulfurDioxide    1599 non-null float64
Density               1599 non-null float64
PH                    1599 non-null float64
Sulphates             1599 non-null float64
Alcohol               1599 non-null float64
Quality               1599 non-null int64
dtypes: float64(11), int64(1)
memory usage: 149.9 KB
```

No empty or null values found in this dataset

In [5]:

```
wine.describe()
```

Out[5]:

	FixedAcidity	VolatileAcidity	CitricAcid	ResidualSugar	Chlorides	FreeSulfurDioxi
count	1599.000000	1599.000000	1599.000000	1599.000000	1599.000000	1599.0000
mean	8.319637	0.527821	0.270976	2.538806	0.087467	15.8749
std	1.741096	0.179060	0.194801	1.409928	0.047065	10.4601
min	4.600000	0.120000	0.000000	0.900000	0.012000	1.0000
25%	7.100000	0.390000	0.090000	1.900000	0.070000	7.0000
50%	7.900000	0.520000	0.260000	2.200000	0.079000	14.0000
75%	9.200000	0.640000	0.420000	2.600000	0.090000	21.0000
max	15.900000	1.580000	1.000000	15.500000	0.611000	72.0000

In [6]:

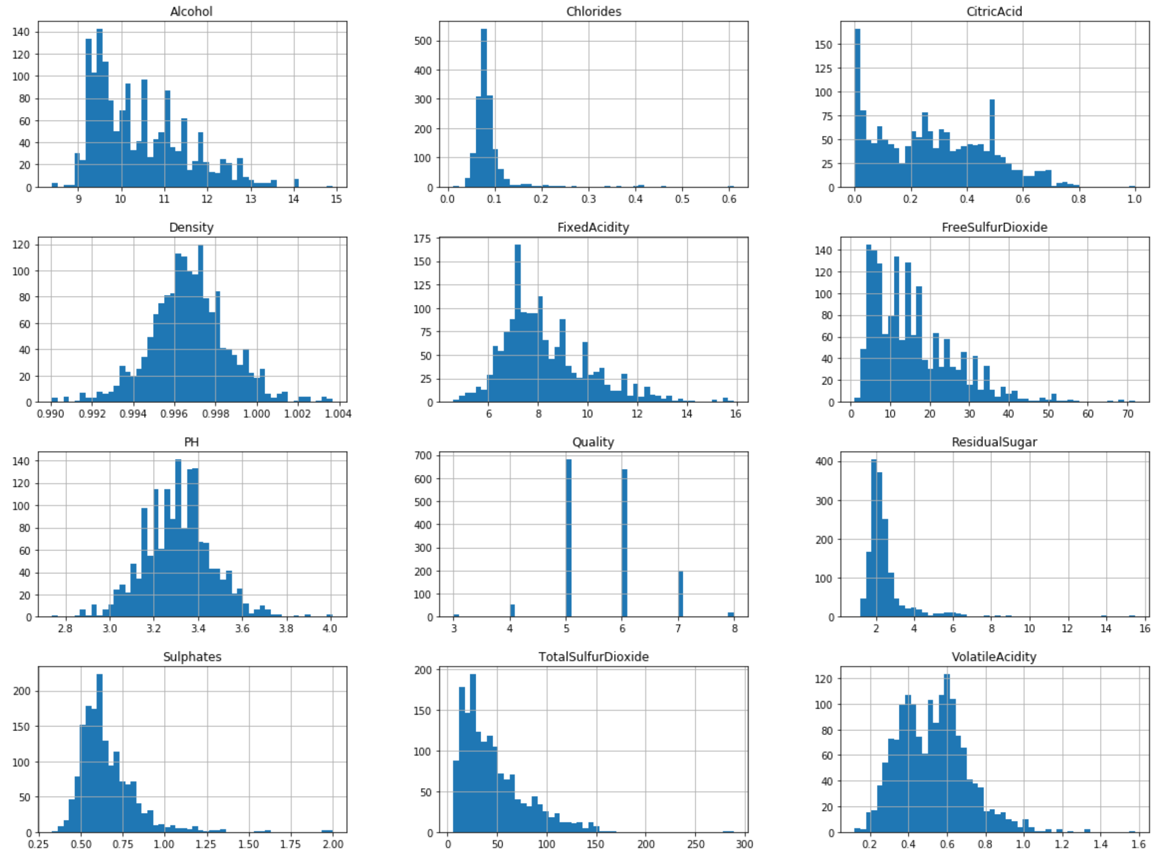
```
wine.corr()
```

Out[6]:

	FixedAcidity	VolatileAcidity	CitricAcid	ResidualSugar	Chlorides	FreeSul
FixedAcidity	1.000000	-0.256131	0.671703	0.114777	0.093705	
VolatileAcidity	-0.256131	1.000000	-0.552496	0.001918	0.061298	
CitricAcid	0.671703	-0.552496	1.000000	0.143577	0.203823	
ResidualSugar	0.114777	0.001918	0.143577	1.000000	0.055610	
Chlorides	0.093705	0.061298	0.203823	0.055610	1.000000	
FreeSulfurDioxide	-0.153794	-0.010504	-0.060978	0.187049	0.005562	
TotalSulfurDioxide	-0.113181	0.076470	0.035533	0.203028	0.047400	
Density	0.668047	0.022026	0.364947	0.355283	0.200632	
PH	-0.682978	0.234937	-0.541904	-0.085652	-0.265026	
Sulphates	0.183006	-0.260987	0.312770	0.005527	0.371260	
Alcohol	-0.061668	-0.202288	0.109903	0.042075	-0.221141	
Quality	0.124052	-0.390558	0.226373	0.013732	-0.128907	

In [7]:

```
wine.hist(bins=50,figsize=(20,15))
plt.show()
```



In [8]:

```
wine.isnull().sum()
```

Out[8]:

```
FixedAcidity          0
VolatileAcidity       0
CitricAcid            0
ResidualSugar         0
Chlorides             0
FreeSulfurDioxide     0
TotalSulfurDioxide    0
Density               0
PH                    0
Sulphates             0
Alcohol               0
Quality               0
dtype: int64
```

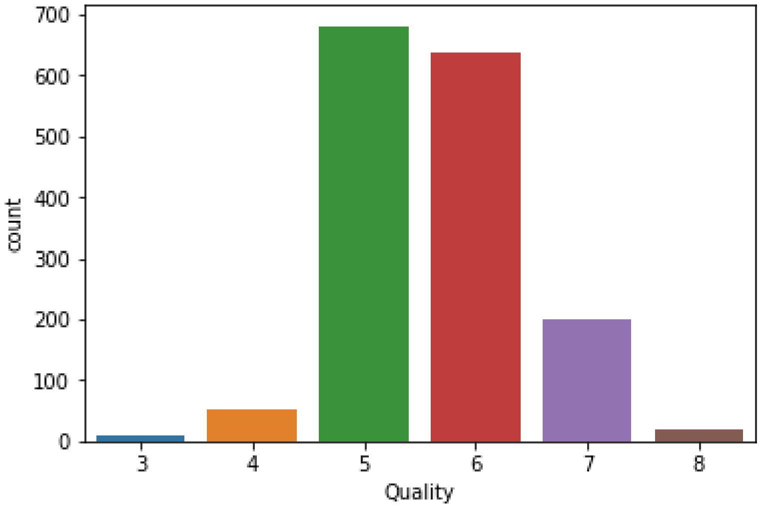
In [9]:

```
print(wine.Quality.value_counts())
```

```
5    681
6    638
7    199
4     53
8     18
3     10
Name: Quality, dtype: int64
```

In [10]:

```
sns.countplot(x="Quality", data=wine)
plt.show()
```



The output values is skewed(right).

Preprocessing

To obtained a more accurate data, the output value is divided into 2 categories which 3-5 are categorized as 0(Low Quality), and 1(High Quality)

In [11]:

```
wine['Quality'] = pd.cut(wine['Quality'], bins=2, labels=False)
```

In [12]:

```
X = wine.drop('Quality', axis = 1)
y = wine["Quality"]
```

In [13]:

```
y.value_counts()
```

Out[13]:

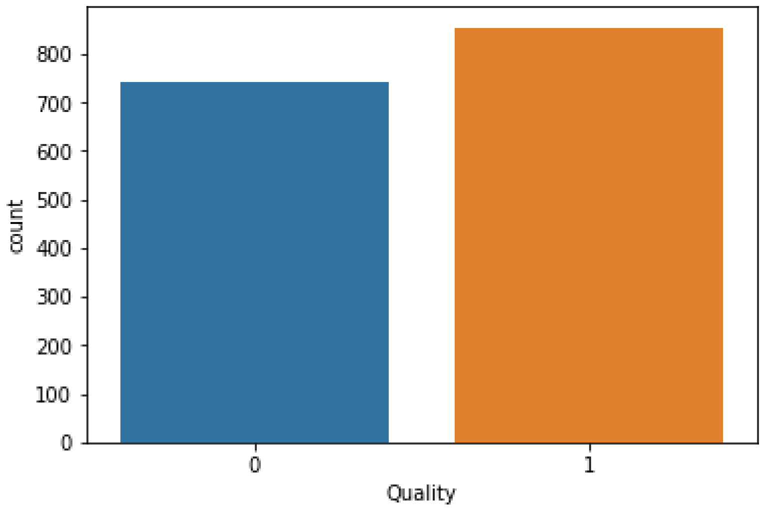
```
1    855
0    744
Name: Quality, dtype: int64
```

In [14]:

```
sns.countplot(y)
```

Out[14]:

```
<matplotlib.axes._subplots.AxesSubplot at 0xbc90a30>
```



The output values are more balance after converted to 0 and 1

In [15]:

```
print ('X: shape=', X.shape)
print ('y: shape=', y.shape)
```

```
X: shape= (1599, 11)
y: shape= (1599,)
```

The datasets are splited into 80% training set and 20% test set.

In [16]:

```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=4
2)
print ('train shape=', X_train.shape)
print ('test shape=', X_test.shape)
```

```
train shape= (1279, 11)
test shape= (320, 11)
```

Standardization on the features needed to be performed as the features have different scales.

In [17]:

```
from sklearn.preprocessing import StandardScaler

scaler = StandardScaler(copy = False)
scaler.fit(X_train)
X_train_tr = scaler.transform(X_train)
y_train = y_train.values
```

Training

Neural Network

Create the model using MLPClassifier in Neural Network.

In [18]:

```
from sklearn.neural_network import MLPClassifier

mlp = MLPClassifier(random_state=42)
mlp.fit(X_train_tr, y_train)
y_pred = mlp.predict(X_train_tr)
```

```
C:\ProgramData\Anaconda3\lib\site-packages\sklearn\neural_network\multilay
er_perceptron.py:562: ConvergenceWarning: Stochastic Optimizer: Maximum it
erations (200) reached and the optimization hasn't converged yet.
  % self.max_iter, ConvergenceWarning)
```

In [19]:

```
def peek_results(actual, predicted, num = 20):
    print('Actual | Predicted')
    print('------------------')
    for i in range(num):
        sel = np.random.randint(0, len(y_train))
        print(actual[sel], '     |    ', predicted[sel])

peek_results(y_train, y_pred)
```

```
Actual | Predicted
------------------
0      |     0
1      |     1
0      |     0
1      |     1
1      |     1
0      |     0
1      |     0
0      |     1
1      |     1
1      |     1
1      |     1
1      |     1
0      |     0
1      |     1
0      |     0
1      |     1
0      |     0
0      |     0
1      |     1
1      |     1
```

Validation

Import all the libraries that required later.

In [20]:

```
from sklearn.metrics import accuracy_score
from sklearn.metrics import classification_report
from sklearn.model_selection import cross_validate
from sklearn.model_selection import cross_val_predict
from sklearn.metrics import confusion_matrix
from sklearn.metrics import precision_score, recall_score, f1_score
from sklearn.metrics import precision_recall_curve
from sklearn.metrics import roc_curve
from sklearn.metrics import roc_auc_score
```

PCA

Principal Component Analysis (PCA) is used to reduce the number of features of the data. Some output of the dataset is affected by only few main features, thus PCA is applied in this datasets to test whether reducing number of fetures will increase the accuracy of data.

In [21]:

```
from sklearn.decomposition import PCA

pca = PCA(n_components=3)
pca.fit(X_train_tr, y_train)
X_train_tr_pca = pca.transform(X_train_tr)

mlp.fit(X_train_tr_pca, y_train)
pca_pred = mlp.predict(X_train_tr_pca)
print('Training Accuracy with PCA = ', accuracy_score(y_train, pca_pred))
```

```
Training Accuracy with PCA =  0.7498045347928068

C:\ProgramData\Anaconda3\lib\site-packages\sklearn\neural_network\multilay
er_perceptron.py:562: ConvergenceWarning: Stochastic Optimizer: Maximum it
erations (200) reached and the optimization hasn't converged yet.
  % self.max_iter, ConvergenceWarning)
```

The training accuracy is around 75% after reducing to 3 features for the data.

Accuracy

In [22]:

```
train_acc = accuracy_score(y_train, y_pred)

print("Training accuracy without PCA: {:.4f}".format(train_acc))
```

```
Training accuracy without PCA: 0.8139
```

The training accuracy without applying PCA is around 81%. Thus all features in this datasets are important and contribute much to the output values.

The model is fitted again with the original dataset.

In [23]:

```
mlp.fit(X_train_tr, y_train)
```

```
C:\ProgramData\Anaconda3\lib\site-packages\sklearn\neural_network\multilay
er_perceptron.py:562: ConvergenceWarning: Stochastic Optimizer: Maximum it
erations (200) reached and the optimization hasn't converged yet.
  % self.max_iter, ConvergenceWarning)
```

Out[23]:

```
MLPClassifier(activation='relu', alpha=0.0001, batch_size='auto', beta_1=
0.9,
       beta_2=0.999, early_stopping=False, epsilon=1e-08,
       hidden_layer_sizes=(100,), learning_rate='constant',
       learning_rate_init=0.001, max_iter=200, momentum=0.9,
       n_iter_no_change=10, nesterovs_momentum=True, power_t=0.5,
       random_state=42, shuffle=True, solver='adam', tol=0.0001,
       validation_fraction=0.1, verbose=False, warm_start=False)
```

Cross Validation

The training accuracy is measured with cross-validation to evaluate the model. 4-folds is set for this model.

In [24]:

```
kfold_result = cross_validate (mlp, X_train_tr, y_train, cv=4, scoring='accuracy', retu
rn_train_score=True)

print('Average training accuracy = {:.4f}'.format(kfold_result['train_score'].mean()))
print('Average validation accuracy = {:.4f}'.format(kfold_result['test_score'].mean()))
```

```
C:\ProgramData\Anaconda3\lib\site-packages\sklearn\neural_network\multilay
er_perceptron.py:562: ConvergenceWarning: Stochastic Optimizer: Maximum it
erations (200) reached and the optimization hasn't converged yet.
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C:\ProgramData\Anaconda3\lib\site-packages\sklearn\neural_network\multilay
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C:\ProgramData\Anaconda3\lib\site-packages\sklearn\neural_network\multilay
er_perceptron.py:562: ConvergenceWarning: Stochastic Optimizer: Maximum it
erations (200) reached and the optimization hasn't converged yet.
  % self.max_iter, ConvergenceWarning)

Average training accuracy = 0.8108
Average validation accuracy = 0.7577

C:\ProgramData\Anaconda3\lib\site-packages\sklearn\neural_network\multilay
er_perceptron.py:562: ConvergenceWarning: Stochastic Optimizer: Maximum it
erations (200) reached and the optimization hasn't converged yet.
  % self.max_iter, ConvergenceWarning)
```

Confusion Matrix

In [25]:

```
y_pred_cv = cross_val_predict (mlp, X_train_tr, y_train, cv=4)

from sklearn.metrics import confusion_matrix
cm = confusion_matrix (y_train, y_pred_cv)
print(cm)
```

```
C:\ProgramData\Anaconda3\lib\site-packages\sklearn\neural_network\multilay
er_perceptron.py:562: ConvergenceWarning: Stochastic Optimizer: Maximum it
erations (200) reached and the optimization hasn't converged yet.
  % self.max_iter, ConvergenceWarning)
C:\ProgramData\Anaconda3\lib\site-packages\sklearn\neural_network\multilay
er_perceptron.py:562: ConvergenceWarning: Stochastic Optimizer: Maximum it
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  % self.max_iter, ConvergenceWarning)
C:\ProgramData\Anaconda3\lib\site-packages\sklearn\neural_network\multilay
er_perceptron.py:562: ConvergenceWarning: Stochastic Optimizer: Maximum it
erations (200) reached and the optimization hasn't converged yet.
  % self.max_iter, ConvergenceWarning)

[[456 147]
 [163 513]]

C:\ProgramData\Anaconda3\lib\site-packages\sklearn\neural_network\multilay
er_perceptron.py:562: ConvergenceWarning: Stochastic Optimizer: Maximum it
erations (200) reached and the optimization hasn't converged yet.
  % self.max_iter, ConvergenceWarning)
```

Precision, Recall, F1 Score

In [26]:

```
print(classification_report(y_train, y_pred_cv))
```

```
              precision    recall  f1-score   support

           0       0.74      0.76      0.75       603
           1       0.78      0.76      0.77       676

   micro avg       0.76      0.76      0.76      1279
   macro avg       0.76      0.76      0.76      1279
weighted avg       0.76      0.76      0.76      1279
```

In [27]:

```
print('Precision = {:.4f}'.format(precision_score(y_train, y_pred_cv)))
print('Recall = {:.4f}'.format(recall_score (y_train, y_pred_cv)))
print('F1 Score = {:.4f}'.format(f1_score(y_train, y_pred_cv)))
```

```
Precision = 0.7773
Recall = 0.7589
F1 Score = 0.7680
```

In [28]:

```
kfold_scores = cross_validate (mlp, X_train_tr, y_train, cv=4, scoring = ['precision',
'recall', 'f1'], return_train_score=False)

print('Average cross-validation recall = {:.4f}'.format(kfold_scores['test_recall'].mea
n()))
print('Average cross-validation precision = {:.4f}'.format(kfold_scores['test_precisio
n'].mean()))
print('Average cross-validation f1 = {:.4f}'.format(kfold_scores['test_f1'].mean()))
```

```
C:\ProgramData\Anaconda3\lib\site-packages\sklearn\neural_network\multilay
er_perceptron.py:562: ConvergenceWarning: Stochastic Optimizer: Maximum it
erations (200) reached and the optimization hasn't converged yet.
  % self.max_iter, ConvergenceWarning)
C:\ProgramData\Anaconda3\lib\site-packages\sklearn\neural_network\multilay
er_perceptron.py:562: ConvergenceWarning: Stochastic Optimizer: Maximum it
erations (200) reached and the optimization hasn't converged yet.
  % self.max_iter, ConvergenceWarning)
C:\ProgramData\Anaconda3\lib\site-packages\sklearn\neural_network\multilay
er_perceptron.py:562: ConvergenceWarning: Stochastic Optimizer: Maximum it
erations (200) reached and the optimization hasn't converged yet.
  % self.max_iter, ConvergenceWarning)

Average cross-validation recall = 0.7589
Average cross-validation precision = 0.7775
Average cross-validation f1 = 0.7679

C:\ProgramData\Anaconda3\lib\site-packages\sklearn\neural_network\multilay
er_perceptron.py:562: ConvergenceWarning: Stochastic Optimizer: Maximum it
erations (200) reached and the optimization hasn't converged yet.
  % self.max_iter, ConvergenceWarning)
```

Precision-Recal Graph

In [29]:

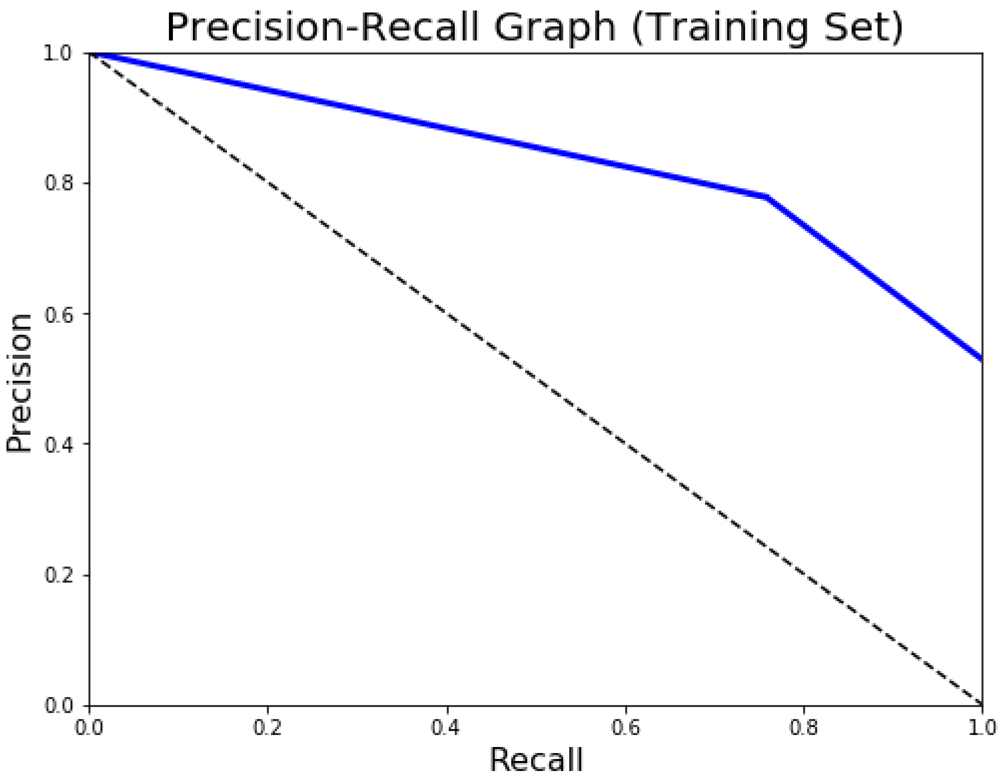
```
y_scores_cv = cross_val_predict (mlp, X_train_tr, y_train, cv=4)
precisions, recalls, thresholds = precision_recall_curve (y_train, y_scores_cv)
```

```
C:\ProgramData\Anaconda3\lib\site-packages\sklearn\neural_network\multilay
er_perceptron.py:562: ConvergenceWarning: Stochastic Optimizer: Maximum it
erations (200) reached and the optimization hasn't converged yet.
  % self.max_iter, ConvergenceWarning)
C:\ProgramData\Anaconda3\lib\site-packages\sklearn\neural_network\multilay
er_perceptron.py:562: ConvergenceWarning: Stochastic Optimizer: Maximum it
erations (200) reached and the optimization hasn't converged yet.
  % self.max_iter, ConvergenceWarning)
C:\ProgramData\Anaconda3\lib\site-packages\sklearn\neural_network\multilay
er_perceptron.py:562: ConvergenceWarning: Stochastic Optimizer: Maximum it
erations (200) reached and the optimization hasn't converged yet.
  % self.max_iter, ConvergenceWarning)
C:\ProgramData\Anaconda3\lib\site-packages\sklearn\neural_network\multilay
er_perceptron.py:562: ConvergenceWarning: Stochastic Optimizer: Maximum it
erations (200) reached and the optimization hasn't converged yet.
  % self.max_iter, ConvergenceWarning)
```

In [30]:

```
def plot_precision_vs_recall(precisions, recalls):
    plt.plot(recalls, precisions, "b-", linewidth=3)
    plt.plot(np.linspace(0, 1, 20), np.linspace(1, 0, 20), 'k--')
    plt.xlabel("Recall", fontsize=16)
    plt.ylabel("Precision", fontsize=16)
    plt.axis([0, 1, 0, 1])

plt.figure(figsize=(8, 6))
plot_precision_vs_recall(precisions, recalls)
plt.title ('Precision-Recall Graph (Training Set)', fontsize = 20)
plt.show()
```

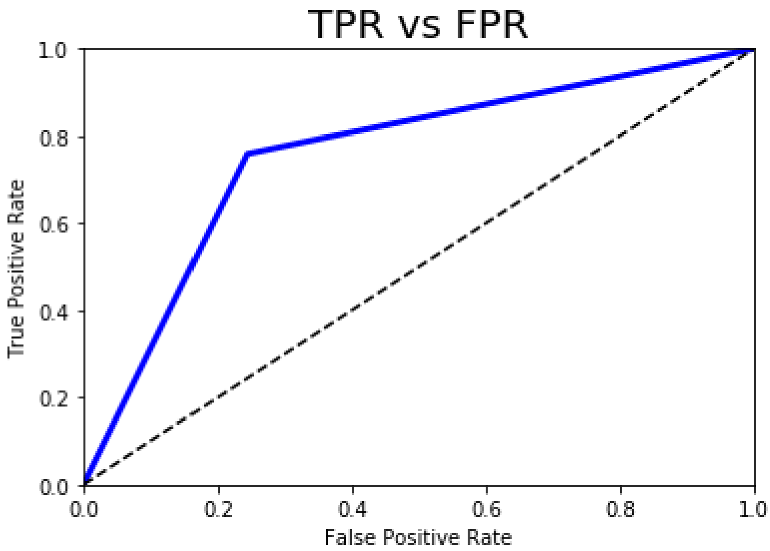


In [31]:

```
fpr, tpr, thresholds = roc_curve(y_train, y_scores_cv)

def plot_roc_curve (fpr, tpr, style = 'b-', label = None):
    plt.plot(fpr, tpr, style, linewidth = 3, label = label)
    plt.plot([0,1], [0, 1], 'k--')
    plt.axis([0, 1, 0, 1])
    plt.xlabel ('False Positive Rate')
    plt.ylabel ('True Positive Rate')
    plt.title('TPR vs FPR', fontsize=20)

plot_roc_curve(fpr, tpr)
```



In [32]:

```
auc = roc_auc_score(y_train, y_scores_cv)
print('AUC = {:.4f}'.format(auc))
```

```
AUC = 0.7575
```

Fine Tune

GridSearchCV

To get the best hyperparameters, GridSearchCV is used.

In [33]:

```
import time
from sklearn.model_selection import GridSearchCV

start_time = time.time()
param = {'solver':['lbfgs'], 'max_iter':[500,1000,1500], 'alpha':10.0**-np.arange(1,10
), 'hidden_layer_sizes':np.arange(10,15)}
grid_search = GridSearchCV(mlp, param, cv=4, scoring='accuracy')
print ('Performing grid search...', end = '')
grid_search.fit(X_train_tr, y_train)
print('Completed', end = '  ')
print('{:.2f}s'.format(time.time()-start_time))
```

```
Performing grid search...Completed  444.38s
```

In [34]:

```
best_model = grid_search.best_estimator_
best_model
```

Out[34]:

```
MLPClassifier(activation='relu', alpha=0.1, batch_size='auto', beta_1=0.9,
       beta_2=0.999, early_stopping=False, epsilon=1e-08,
       hidden_layer_sizes=12, learning_rate='constant',
       learning_rate_init=0.001, max_iter=1000, momentum=0.9,
       n_iter_no_change=10, nesterovs_momentum=True, power_t=0.5,
       random_state=42, shuffle=True, solver='lbfgs', tol=0.0001,
       validation_fraction=0.1, verbose=False, warm_start=False)
```

In [35]:

```
print('Accuracy of the best model =', grid_search.best_score_)
```

```
Accuracy of the best model = 0.7505863956215794
```

Testing

In [36]:

```
X_test_tr = scaler.transform(X_test)
y_test = y_test.values
```

Use the best model to predict test data.

In [37]:

```
y_pred_test = best_model.predict(X_test_tr)

print('Test data Accuracy= ', accuracy_score(y_test, y_pred_test))
```

```
Test data Accuracy=  0.778125
```

In [38]:

```
print('Test precision = {:.4f}'.format(precision_score(y_test, y_pred_test)))
print('Test recall = {:.4f}'.format(recall_score (y_test, y_pred_test)))
print('Test f1 score = {:.4f}'.format(f1_score(y_test, y_pred_test)))
```

```
Test precision = 0.8068
Test recall = 0.7933
Test f1 score = 0.8000
```

Compare with Other Classifiers

RandomForestClassifier

In [39]:

```
from sklearn.ensemble import RandomForestClassifier


forest = RandomForestClassifier(n_estimators=10, random_state=42)
forest.fit(X_train_tr, y_train)
y_pred_forest = forest.predict(X_train_tr)

print('Accuracy = ', accuracy_score(y_train, y_pred_forest))
```

```
Accuracy =  0.9929632525410477
```

The model fitted very well on the training set with accuracy 99%.

In [40]:

```
print(classification_report(y_train, y_pred_forest))
```

```
              precision    recall  f1-score   support

           0       0.99      1.00      0.99       603
           1       1.00      0.99      0.99       676

   micro avg       0.99      0.99      0.99      1279
   macro avg       0.99      0.99      0.99      1279
weighted avg       0.99      0.99      0.99      1279
```

In [41]:

```
y_pred_test_forest = forest.predict(X_test_tr)

print('Test data Accuracy= ', accuracy_score(y_test, y_pred_test_forest))
```

```
Test data Accuracy=  0.778125
```

However, the model doesn't fitted so well on the test set. This may caused by the model is slightly overfitting.

In [42]:

```
kfold_result = cross_validate (forest, X_train_tr, y_train, cv=5, scoring='accuracy', r
eturn_train_score=True)
print('Average training accuracy = {:.4f}'.format(kfold_result['train_score'].mean()))
print('Average validation accuracy = {:.4f}'.format(kfold_result['test_score'].mean()))
```

```
Average training accuracy = 0.9893
Average validation accuracy = 0.7764
```

RandomForestClassifier seem like perform better than MLPClassifier. However, the model is slightly overfitting the datasets.

SVClassifier

In [43]:

```
from sklearn.svm import SVC

svc = SVC()
svc.fit(X_train_tr, y_train)
y_pred_svc = svc.predict(X_train_tr)

print('Accuracy = ', accuracy_score(y_train, y_pred))
```

```
Accuracy =  0.8139171227521501
```

In [44]:

```
print(classification_report(y_train, y_pred_svc))
```

```
              precision    recall  f1-score   support

           0       0.78      0.81      0.79       603
           1       0.82      0.80      0.81       676

   micro avg       0.80      0.80      0.80      1279
   macro avg       0.80      0.80      0.80      1279
weighted avg       0.80      0.80      0.80      1279
```

In [45]:

```
y_pred_test_svc = svc.predict(X_test_tr)

print('Accuracy = ', accuracy_score(y_test, y_pred_test_svc))
```

```
Accuracy =  0.771875
```

In [46]:

```
kfold_result = cross_validate (svc, X_train_tr, y_train, cv=5, scoring='accuracy', retu
rn_train_score=True)
print('Average training accuracy = {:.4f}'.format(kfold_result['train_score'].mean()))
print('Average validation accuracy = {:.4f}'.format(kfold_result['test_score'].mean()))
```

```
C:\ProgramData\Anaconda3\lib\site-packages\sklearn\svm\base.py:196: Future
Warning: The default value of gamma will change from 'auto' to 'scale' in
version 0.22 to account better for unscaled features. Set gamma explicitly
to 'auto' or 'scale' to avoid this warning.
  "avoid this warning.", FutureWarning)
C:\ProgramData\Anaconda3\lib\site-packages\sklearn\svm\base.py:196: Future
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  "avoid this warning.", FutureWarning)
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version 0.22 to account better for unscaled features. Set gamma explicitly
to 'auto' or 'scale' to avoid this warning.
  "avoid this warning.", FutureWarning)


Average training accuracy = 0.8030
Average validation accuracy = 0.7546

C:\ProgramData\Anaconda3\lib\site-packages\sklearn\svm\base.py:196: Future
Warning: The default value of gamma will change from 'auto' to 'scale' in
version 0.22 to account better for unscaled features. Set gamma explicitly
to 'auto' or 'scale' to avoid this warning.
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to 'auto' or 'scale' to avoid this warning.
  "avoid this warning.", FutureWarning)
```

The training accuracy of SVClassifier is quite same as MLPClassifier. MLPClassifier have slightly better performace during prediction of test data.