Project_final

April 3, 2021

1 Machine Learning Assignment

[30]:
```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
import warnings
warnings.simplefilter('ignore')
from matplotlib import colors
from sklearn.preprocessing import MinMaxScaler
from sklearn.model_selection import train_test_split, StratifiedKFold,␣
↪cross_val_score, validation_curve, GridSearchCV
from sklearn.neighbors import KNeighborsClassifier as kNN
from sklearn.linear_model import LogisticRegression as LogReg
from sklearn.discriminant_analysis import LinearDiscriminantAnalysis as LDA
from sklearn.discriminant_analysis import QuadraticDiscriminantAnalysis as QDA
from sklearn.tree import DecisionTreeClassifier as DTreeClass
from sklearn.metrics import accuracy_score, zero_one_loss, roc_auc_score,␣
↪roc_curve, classification_report, f1_score
from scipy import stats
import jupyterthemes
!jt -t grade3 -tfs 7 -nfs 7 -ofs 7 -fs 7
```

[31]:
```
names = ['Sequence␣
↪name','mcg','gvh','alm','mit','erl','pox','vac','nuc','class'];

data_yeast = pd.read_csv('yeast.data', header = None, sep = '\s+', names =␣
↪names);

data_pima = pd.read_csv('diabetes.csv');
```

1.1 Question 1

[32]:
```
cols = data_pima.columns[:8]
fig, ax = plt.subplots(2,4, sharex=False, sharey=False, figsize=(20, 8))
```

```
txt="Figure 1. Box plots for the values of the variables according to target class."
plt.figtext(0.5, 0.01, txt, wrap=True, horizontalalignment='center', fontsize=14)
for i in range(len(cols)):
    sns.boxplot(ax=ax[i//4, i%4], y=cols[i], x='Outcome', data=data_pima)
    ax[i//4, i%4].set(xlabel=cols[i])
plt.show();
```

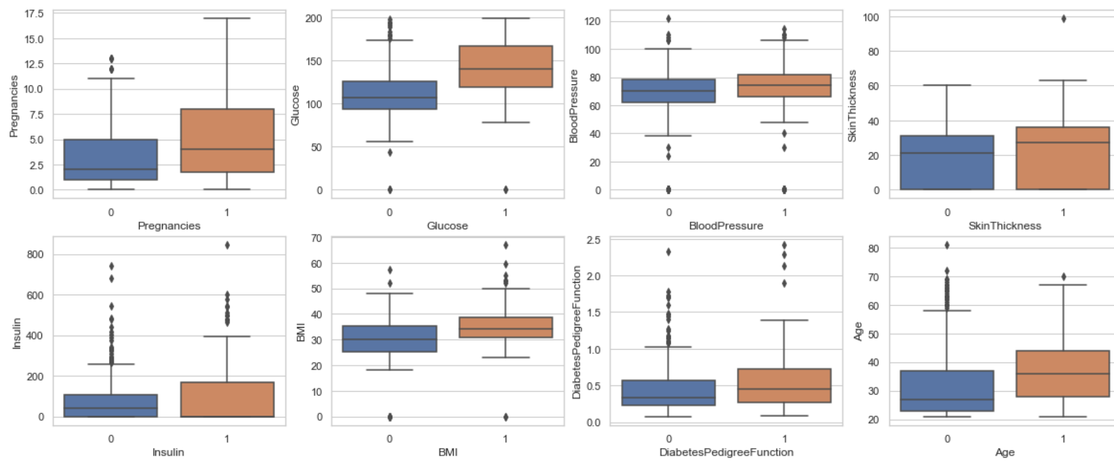
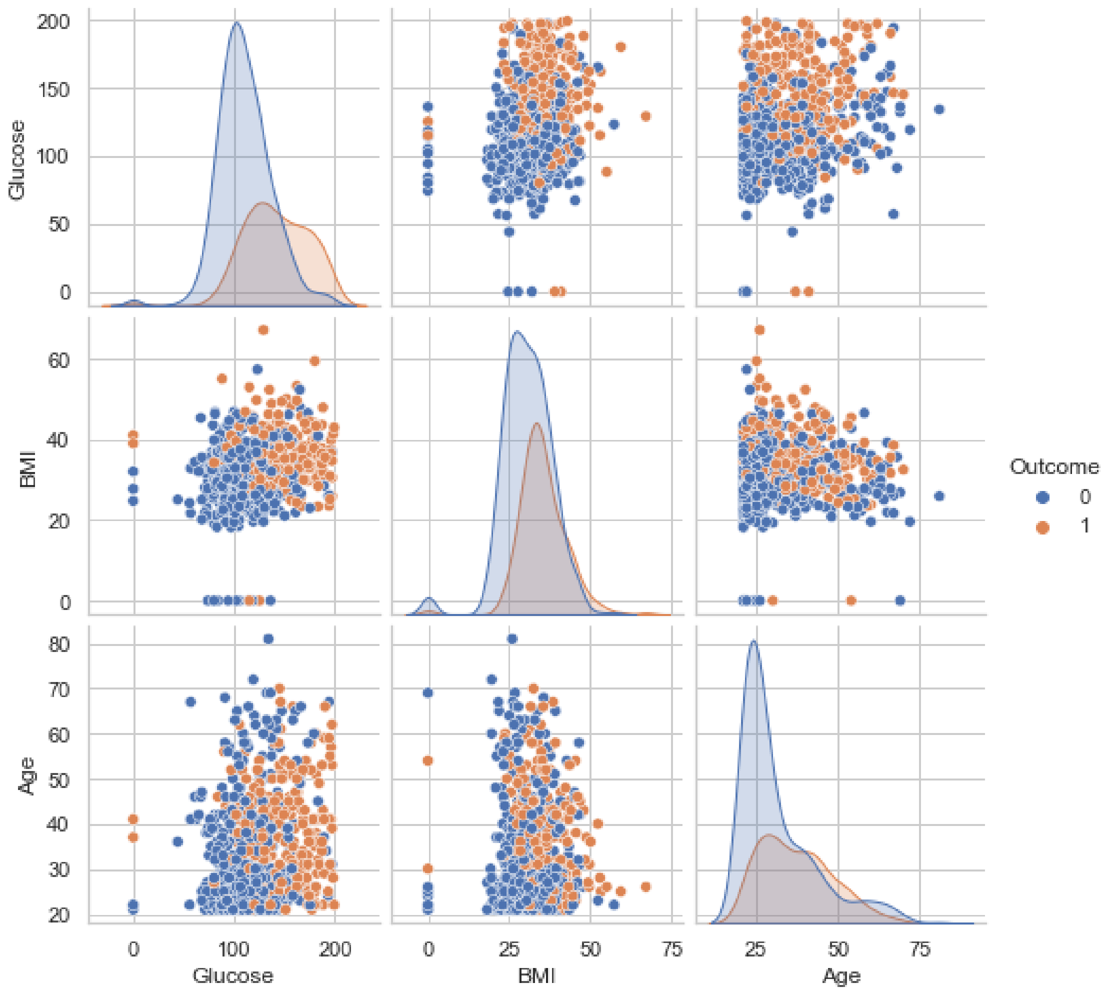


Figure 1. Box plots for the values of the variables according to target class.

[33]:
```
data_pima_sel = data_pima.drop(columns = ['BloodPressure', 'SkinThickness', 'Pregnancies', 'DiabetesPedigreeFunction', 'Insulin'])
sns.pairplot(data_pima_sel, hue = 'Outcome');
```



Após análise aos gráficos apresentados, podemos observar rapidamente que as variáveis que melhor "separam" a variável alvo são a Glucose, BMI e Age. Contudo, as duas escolhidas (como requisitado pelo exercicio) foram a Glucose e BMI. A variável Age foi descartada pois tinha mais outliars.

1.2 Methods comparison (kNN, Logistic Regression, QDA)

[34]:
```
data_pima_clean = data_pima_sel[(data_pima['Glucose'] != 0) & (data_pima['BMI']␣
↪!= 0)]

data_pima_clean = data_pima_clean.sample(frac=1).reset_index(drop=True)
```

[35]:
```
data_pima_sel_final = data_pima_clean.drop(columns = 'Age')

column_names = ['Glucose', 'BMI']
temp = data_pima_sel_final[column_names].values
temp_scaled = MinMaxScaler().fit_transform(temp)
```

```
data_pima_sel_final[column_names] = temp_scaled

X = data_pima_sel_final.drop(columns = 'Outcome').values

y = data_pima_sel_final.loc[:,'Outcome'].values
x_train, x_test, y_train, y_test = train_test_split(X, y, test_size=0.20,␣
↪random_state=123, stratify= y)
```

[36]:
```
def plot_classifier_boundary(model,x,h = .05): #kindly provided in class
    cmap_light = colors.ListedColormap(['lightsteelblue', 'peachpuff'])
    x_min, x_max = x[:, 0].min()-.2, x[:, 0].max()+.2
    y_min, y_max = x[:, 1].min()-.2, x[:, 1].max()+.2
    xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                         np.arange(y_min, y_max, h))
    Z = model.predict(np.c_[xx.ravel(), yy.ravel()])
    Z = Z.reshape(xx.shape)
    plt.contourf(xx, yy, Z, cmap=cmap_light)
    plt.xlim((x_min,x_max))
    plt.ylim((y_min,y_max))
cmap = colors.ListedColormap(['blue','orange'])
```

[37]:
```
def StratKF(model, splits,x_train, y_train, x_test, y_test):         #fitted␣
↪model necessary
    SKF = StratifiedKFold(n_splits=splits, shuffle=True, random_state=1)
    score = []
    y_pred_train = model.predict(x_train)
    y_pred_test = model.predict(x_test)
    for train_index, test_index in SKF.split(x_test, y_test):
        x_test1 = x_train[test_index]
        y_test1 = y_train[test_index]
        score.append(f1_score(y_test1, model.predict(x_test1)))
    print(f'F1 score on {splits}-fold test data: ',round(np.mean(score),4),'+/
↪-', round(np.std(score),4))
    print('F1 score on training set: ',round(f1_score(y_train,␣
↪y_pred_train),4), '\nF1 score on test set: ',round(f1_score(y_test,␣
↪y_pred_test), 4))
```

1.2.1 Logistic Regression

[38]:
```
modelLogReg = LogReg()
modelLogReg.fit(x_train, y_train)
StratKF(modelLogReg,5, x_train, y_train, x_test, y_test)
```

```
F1 score on 5-fold test data:  0.524 +/- 0.1142
F1 score on training set:  0.6067
F1 score on test set:  0.5116
```

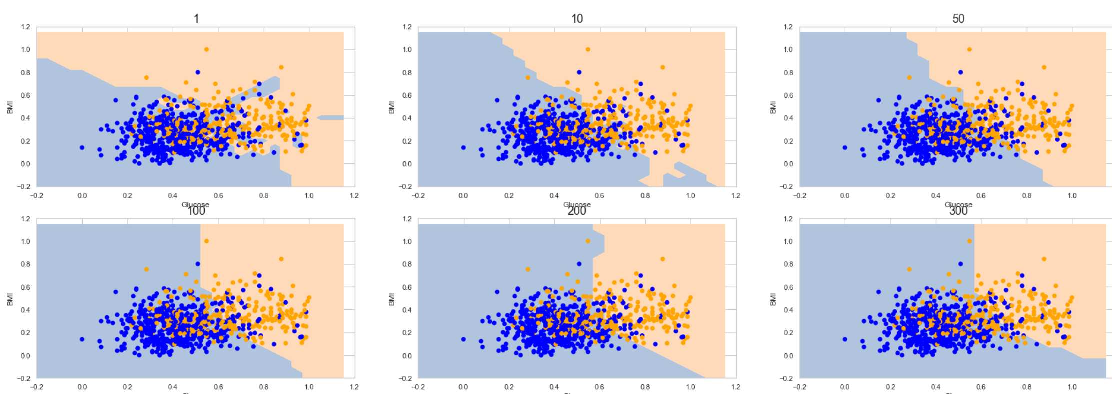
1.2.2 Quadratic Discriminant Analysis

[39]:
```
modelQDA = QDA()
modelQDA.fit(x_train, y_train)
StratKF(modelQDA,5, x_train, y_train, x_test, y_test)
```

```
F1 score on 5-fold test data:  0.5145 +/- 0.0953
F1 score on training set:  0.6458
F1 score on test set:  0.5169
```

1.2.3 kNN

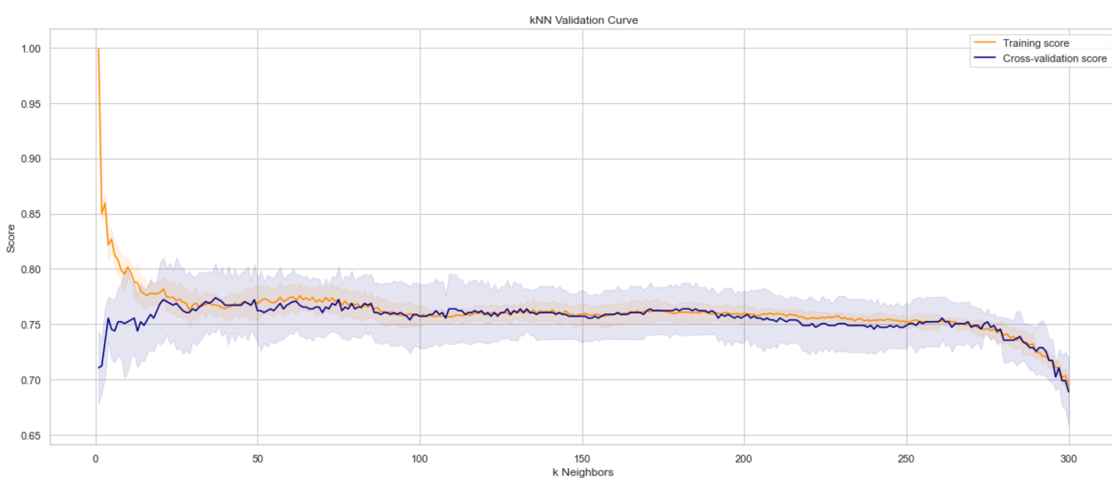
[40]:
```
fig = plt.figure(figsize=(30,10))
k = [1,10,50,100,200,300]

for i in range(len(k)):
    modelkNN = kNN(n_neighbors=k[i])
    modelkNN.fit(x_train, y_train)
    ax = fig.add_subplot(2, 3, i+1)
    plot_classifier_boundary(modelkNN, X)
    ax.scatter(X[:,0],X[:,1],color=cmap(y))
    ax.set_title(k[i], fontsize = 18)
    ax.set_xlabel('Glucose')
    ax.set_ylabel('BMI');
```



[41]:
```
def valid_curve(model, x_train, y_train, n_jobs, scoring, param_range = np.
↪array([*range(1,301)]), param_name="n_neighbors"):
    np.random.seed(1)
    train_scores, test_scores = validation_curve(model, x_train, y_train,␣
↪param_name=param_name, param_range=param_range, scoring=scoring,␣
↪n_jobs=n_jobs)
    train_scores_mean = np.mean(train_scores, axis=1)
    train_scores_std = np.std(train_scores, axis=1)
```

```
    test_scores_mean = np.mean(test_scores, axis=1)
    test_scores_std = np.std(test_scores, axis=1)

    plt.figure(figsize=(20, 8))
    plt.title("kNN Validation Curve")
    plt.xlabel("k Neighbors")
    plt.ylabel("Score")
    plt.plot(param_range, train_scores_mean, label="Training score",␣
↪color="darkorange")
    plt.fill_between(param_range, train_scores_mean - train_scores_std,␣
↪train_scores_mean + train_scores_std, alpha=0.1, color="darkorange")
    plt.plot(param_range, test_scores_mean, label="Cross-validation score",␣
↪color="navy")
    plt.fill_between(param_range, test_scores_mean - test_scores_std,␣
↪test_scores_mean + test_scores_std, alpha=0.1, color="navy")
    plt.legend(loc="best")
    plt.show();

    print("Best K is %d" %param_range[np.where(test_scores_mean ==␣
↪max(test_scores_mean))][0])
    return param_range[np.where(test_scores_mean == max(test_scores_mean))][0]
```

[42]:
```
#Determination of k
modelkNN = kNN()
k_best = valid_curve(modelkNN, x_train, y_train, 6, 'accuracy')
```




```
Best K is 37
```

[43]:
```
modelkNN = kNN(n_neighbors=k_best)
modelkNN.fit(x_train, y_train)
StratKF(modelkNN,5, x_train, y_train, x_test, y_test)
```

```
F1 score on 5-fold test data:  0.5293 +/- 0.1105
F1 score on training set:  0.6273
F1 score on test set:  0.5227
```

[44]:

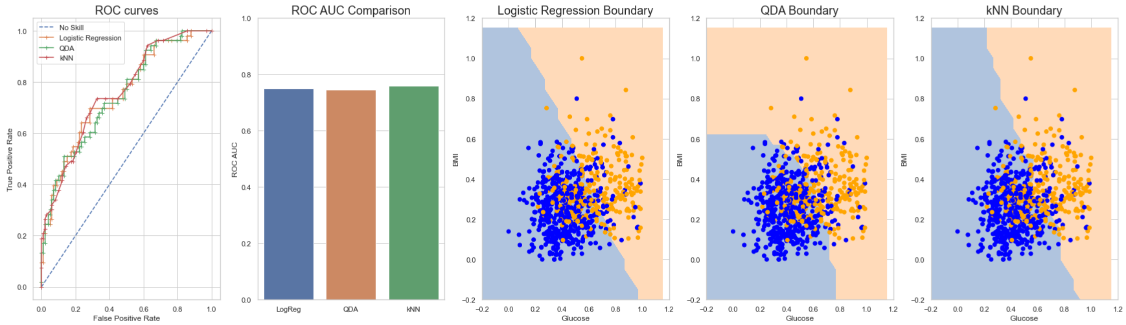
```
#ROC AUC
ns_probs = [0 for _ in range(len(y_test))]
# probabilities for the positive outcome
LogReg_probs = modelLogReg.predict_proba(x_test)[:, 1]
QDA_probs = modelQDA.predict_proba(x_test)[:, 1]
kNN_probs = modelkNN.predict_proba(x_test)[:, 1]
# calculate scores
ns_auc = roc_auc_score(y_test, ns_probs)
LogReg_auc = roc_auc_score(y_test, LogReg_probs)
QDA_auc = roc_auc_score(y_test, QDA_probs)
kNN_auc = roc_auc_score(y_test, kNN_probs)
# summarize scores
#print('No Skill: ROC AUC=%.3f' % (ns_auc))
print('LR ROC AUC=%.3f' % (LogReg_auc))
print('QDA ROC AUC=%.3f' % (QDA_auc))
print('kNN ROC AUC=%.3f' % (kNN_auc))
```

```
LR ROC AUC=0.751
QDA ROC AUC=0.746
kNN ROC AUC=0.759
```

[45]:

```
#ROC curves
# calculate roc curves
ns_fpr, ns_tpr, _ = roc_curve(y_test, ns_probs, pos_label=None)
LogReg_fpr, LogReg_tpr, _ = roc_curve(y_test, LogReg_probs)
QDA_fpr, QDA_tpr, _ = roc_curve(y_test, QDA_probs)
kNN_fpr, kNN_tpr, _ = roc_curve(y_test, kNN_probs)

figs = plt.figure(figsize=(30,8))
# plot the roc curves
axs = figs.add_subplot(1, 5, 1)
axs.plot(ns_fpr, ns_tpr, linestyle='--', label='No Skill')
axs.plot(LogReg_fpr,LogReg_tpr, marker='+', label='Logistic Regression')
axs.plot(QDA_fpr,QDA_tpr, marker='+', label='QDA')
axs.plot(kNN_fpr,kNN_tpr, marker='+', label='kNN')
axs.set_xlabel('False Positive Rate')
axs.set_ylabel('True Positive Rate')
axs.set_title('ROC curves', fontsize = 18)
axs.legend();
##Barplot of AUCs
axs = figs.add_subplot(1, 5, 2)
sns.barplot(y=[LogReg_auc,QDA_auc,kNN_auc], x=['LogReg', 'QDA', 'kNN'], ax=axs)
axs.set_ylim(0,1)
```

```
axs.set_title('ROC AUC Comparison', fontsize = 18)
axs.set_ylabel('ROC AUC');

model_list = [(modelLogReg,'Logistic Regression Boundary') , (modelQDA, 'QDA␣
↪Boundary'), (modelkNN, 'kNN Boundary')]

for i in range(3,6,1):
    axs = figs.add_subplot(1, 5, i)
    plot_classifier_boundary(model_list[i-3][0],X)
    axs.scatter(X[:,0],X[:,1],color=cmap(y))
    axs.set_xlabel('Glucose')
    axs.set_ylabel('BMI');
    axs.set_title(model_list[i-3][1], fontsize = 18)

plt.show();
```



1.3 Question 2

1.3.1 normalization

[46]:
```
MinMaxSca = MinMaxScaler()
data_yeast[['mcg', 'gvh', 'alm', 'mit', 'erl', 'pox', 'vac', 'nuc']] =␣
↪MinMaxSca.fit_transform(data_yeast.loc[:,['mcg', 'gvh', 'alm', 'mit', 'erl',␣
↪'pox', 'vac', 'nuc']])
```

1.3.2 Separation in train data and test data

```
[47]: X = data_yeast.loc[:, ['mcg', 'gvh', 'alm', 'mit', 'erl', 'pox', 'vac', 'nuc']].
      ↪values
      Y = data_yeast.loc[:,'class'].values

      X_train, X_test, Y_train, Y_test = train_test_split(X, Y, test_size = 0.2,␣
      ↪random_state = 1, stratify = Y, shuffle=True)

      SKF = StratifiedKFold(n_splits=5, shuffle=True, random_state=1)
```

```
[48]: def StratKFW(model, splits, X_train, Y_train, X_test, Y_test):
          Y_pred_trainLogReg = model.predict(X_train)
          Y_pred_testLogReg = model.predict(X_test)
          print('Weighted F1 score on training set: ',round(f1_score(Y_train,␣
      ↪Y_pred_trainLogReg, average='weighted'),4),
              '\nWeighted F1 score on test set: ',round(f1_score(Y_test,␣
      ↪Y_pred_testLogReg, average='weighted'), 4))
          f1score = []
          accscore = []
          for train_index, test_index in SKF.split (X_test, Y_test):
              X_test1 = X_test[test_index]
              Y_test1 = Y_test[test_index]
              f1score.append(f1_score(Y_test1, model.predict(X_test1),␣
      ↪average='weighted'))
              accscore.append(accuracy_score(Y_test1, model.predict(X_test1)))
          print(f'Weighted F1 score on {splits}-fold test data: ',round(np.
      ↪mean(f1score_LogReg),4),'+/-', round(np.std(f1score_LogReg),4))
          print('\nClassification report:\n',classification_report(Y_test,␣
      ↪Y_pred_testLogReg, digits=3))
          return f1score, accscore
```

1.3.3 Logistic regression

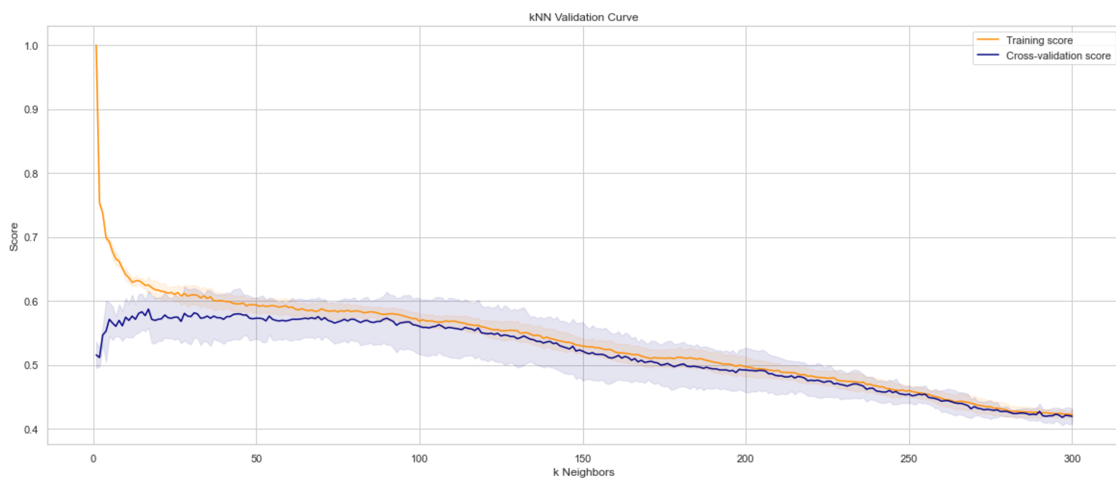
```
[49]: modelLR = LogReg()
      modelLR.fit(X_train, Y_train)
      f1score_LogReg, accscore_LogReg = [], []
      f1score_LogReg, accscore_LogReg = StratKFW(modelLR, 5, X_train, Y_train,␣
      ↪X_test, Y_test)
```

```
Weighted F1 score on training set:  0.5564
Weighted F1 score on test set:  0.5406
Weighted F1 score on 5-fold test data:  nan +/- nan

Classification report:
               precision    recall  f1-score   support

         CYT      0.504     0.742     0.600        93
         ERL      0.000     0.000     0.000         1
```

```
         EXC      0.000     0.000     0.000         7
         ME1      0.455     0.556     0.500         9
         ME2      0.000     0.000     0.000        10
         ME3      0.667     0.688     0.677        32
         MIT      0.617     0.592     0.604        49
         NUC      0.631     0.477     0.543        86
         POX      0.667     0.500     0.571         4
         VAC      0.000     0.000     0.000         6

    accuracy                          0.566       297
   macro avg      0.354     0.355     0.350       297
weighted avg      0.537     0.566     0.541       297
```

1.3.4 kNN

[50]:
```python
k_best = valid_curve(modelkNN, X_train, Y_train, 6, 'accuracy')
```




```
Best K is 17
```

[51]:
```python
modelknn = kNN(n_neighbors=k_best)
modelknn.fit(X_train, Y_train)
f1score_knn, accscore_knn = [], []
f1score_knn, accscore_knn = StratKFW(modelknn, 5, X_train, Y_train, X_test,␣
 ↪Y_test)
```

```
Weighted F1 score on training set:  0.6207
Weighted F1 score on test set:  0.5658
Weighted F1 score on 5-fold test data:  0.5383 +/- 0.0319

Classification report:
               precision    recall  f1-score   support
```

```
         CYT      0.526     0.656     0.584        93
         ERL      0.000     0.000     0.000         1
         EXC      0.667     0.571     0.615         7
         ME1      0.462     0.667     0.545         9
         ME2      0.333     0.200     0.250        10
         ME3      0.719     0.719     0.719        32
         MIT      0.681     0.653     0.667        49
         NUC      0.554     0.477     0.513        86
         POX      0.667     0.500     0.571         4
         VAC      0.000     0.000     0.000         6

    accuracy                          0.576       297
   macro avg      0.461     0.444     0.446       297
weighted avg      0.565     0.576     0.566       297
```

1.3.5 Decision tree

[52]:
```
modeltree = DTreeClass()
modeltree.fit(X_train, Y_train)
f1score_tree, accscore_tree = [], []
f1score_tree, accscore_tree = StratKFW(modeltree, 5, X_train, Y_train, X_test,␣
 ↪Y_test)
```

```
Weighted F1 score on training set:  1.0
Weighted F1 score on test set:  0.4973
Weighted F1 score on 5-fold test data:  0.5383 +/- 0.0319

Classification report:
               precision    recall  f1-score   support

         CYT      0.515     0.548     0.531        93
         ERL      0.000     0.000     0.000         1
         EXC      0.300     0.429     0.353         7
         ME1      0.727     0.889     0.800         9
         ME2      0.111     0.100     0.105        10
         ME3      0.688     0.688     0.688        32
         MIT      0.556     0.408     0.471        49
         NUC      0.489     0.500     0.494        86
         POX      0.000     0.000     0.000         4
         VAC      0.000     0.000     0.000         6

    accuracy                          0.498       297
   macro avg      0.339     0.356     0.344       297
weighted avg      0.501     0.498     0.497       297
```

[53]:
```
def model_grid_search(model, param_grid, cv, scoring, n_jobs): # "cv - integer,␣
↪to specify the number of folds in a `(Stratified) KFold`,"
    model_grid = GridSearchCV(estimator = model, param_grid = param_grid, cv =␣
↪cv, refit = True, scoring= scoring, n_jobs = n_jobs)
    model_grid.fit(X_train, Y_train)
    print(f"Best estimator: {model_grid.best_estimator_} \n  Best score:␣
↪{model_grid.best_score_} \n Best Params: {model_grid.best_params_}")
    return model_grid.best_estimator_
```

[54]:
```
max_depth = [None] + [x for x in np.arange(1,20,4)]
min_sample_split= np.arange(2, 10,2)
min_sample_leaf = np.arange(1,5)
ccp_alpha = np.arange(0.01,100, 10)

param_grid_tree = {"criterion": ['gini', "entropy"],\
              "splitter": ['best',"random"],\
              "max_depth": max_depth,\
              "min_samples_split": min_sample_split,\
              "min_samples_leaf": min_sample_leaf, \
              "ccp_alpha": ccp_alpha}
```

[55]:
```
tree_grid = model_grid_search(modeltree, param_grid_tree, 5, "f1_weighted", 2)
```

```
Best estimator: DecisionTreeClassifier(ccp_alpha=0.01, criterion='entropy',
max_depth=5,
                       min_samples_leaf=4, min_samples_split=4)
  Best score: 0.5669393207369835
 Best Params: {'ccp_alpha': 0.01, 'criterion': 'entropy', 'max_depth': 5,
'min_samples_leaf': 4, 'min_samples_split': 4, 'splitter': 'best'}
```

[56]:
```
modeltree = tree_grid
f1score_tree, accscore_tree = StratKFW(modelLR, 5, X_train, Y_train, X_test,␣
↪Y_test)
```

```
Weighted F1 score on training set:  0.5564
Weighted F1 score on test set:  0.5406
Weighted F1 score on 5-fold test data:  0.5383 +/- 0.0319

Classification report:
               precision    recall  f1-score   support

         CYT      0.504     0.742     0.600        93
         ERL      0.000     0.000     0.000         1
         EXC      0.000     0.000     0.000         7
         ME1      0.455     0.556     0.500         9
         ME2      0.000     0.000     0.000        10
         ME3      0.667     0.688     0.677        32
```

```
         MIT       0.617     0.592     0.604        49
         NUC       0.631     0.477     0.543        86
         POX       0.667     0.500     0.571         4
         VAC       0.000     0.000     0.000         6

    accuracy                           0.566       297
   macro avg       0.354     0.355     0.350       297
weighted avg       0.537     0.566     0.541       297
```

1.3.6 Achieved results comparison

[57]:
```python
stats_f1,pvalue_f1 = stats.f_oneway(f1score_LogReg, f1score_knn, f1score_tree)
stats_acc, pvalue_acc = stats.f_oneway(accscore_LogReg, accscore_knn,␣
↪accscore_tree)
```

[58]:
```python
fig, ax = plt.subplots(nrows=1, ncols=2, figsize=(15, 5), sharey=True)
sns.set_theme(style="whitegrid")
ax[0].set_title('Models F1 Score', fontsize = 20)
ax[1].set_title('Models Accuracy Score', fontsize = 20)
sns.boxplot(y=f1score_LogReg + f1score_knn + f1score_tree,␣
↪x=['LogReg']*5+['kNN']*5+['Tree']*5, ax=ax[0])
sns.boxplot(y=accscore_LogReg + accscore_knn + accscore_tree,␣
↪x=['LogReg']*5+['kNN']*5+['Tree']*5, ax=ax[1]);
```