# Project_final

April 3, 2021

## 1 Machine Learning Assignment

[1]:
```
import pyforest
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 -tfs 7 -ofs 7 -fs 7
```

[2]:
```
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');
```

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```

### 1.1 Question 1

[3]:
```
cols = data_pima.columns[:8]
fig, ax = plt.subplots(2,4, sharex=False, sharey=False, figsize=(20, 8))
```

```python
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();
```

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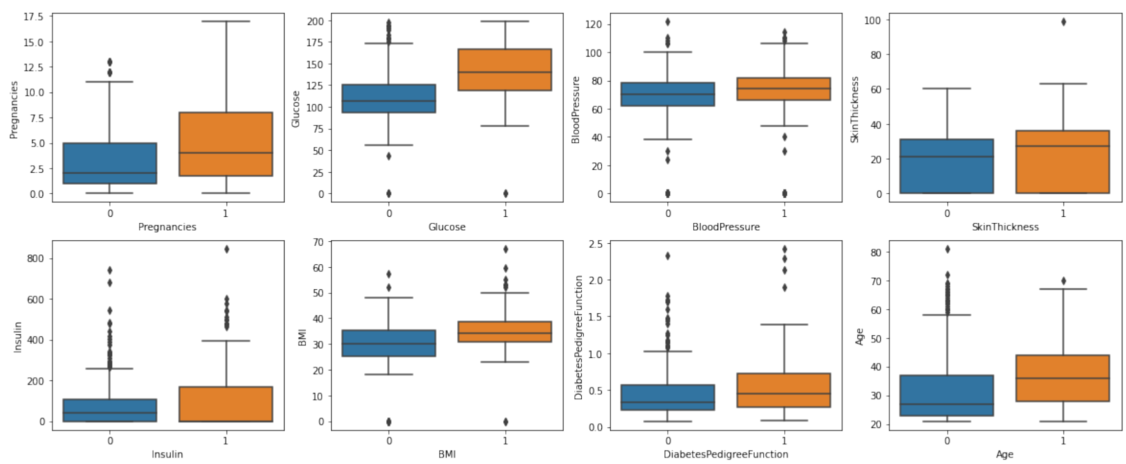


Figure 1. Box plots for the values of the variables according to target class.

[4]:
```python
data_pima_sel = data_pima.drop(columns = ['BloodPressure', 'SkinThickness',␣
↪'Pregnancies', 'DiabetesPedigreeFunction', 'Insulin'])
sns.pairplot(data_pima_sel, hue = 'Outcome');
```

```
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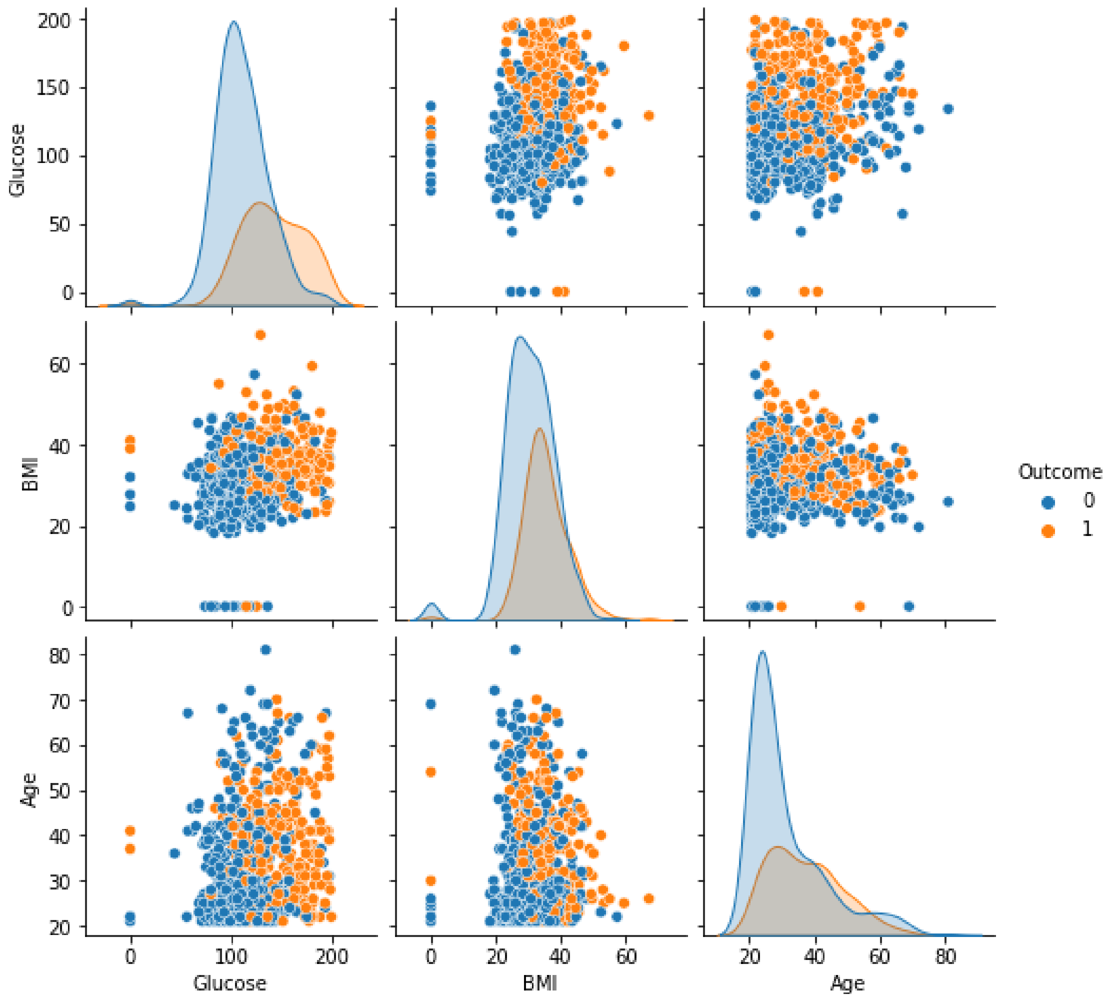


Após análise aos gráficos apresentados, podemos observar rapidamente que as variáveis que melhor "separam" a variável alvo são a Glucose, BMI e Age. Contudo, as duas escolhidas (como requisitado pelo exercicio) foram a Glucose e BMI. A variável Age foi descartada pois tinha mais outliars.

### 1.2 Methods comparison (kNN, Logistic Regression, QDA)

[5]:
```
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)
```

[6]:
```
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)
```

[7]:
```
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'])
```

[8]:
```
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

[9]:
```
modelLogReg = LogReg()
modelLogReg.fit(x_train, y_train)
StratKF(modelLogReg,5, x_train, y_train, x_test, y_test)
```

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```
F1 score on 5-fold test data:  0.5417 +/- 0.0708
F1 score on training set:  0.5886
F1 score on test set:  0.5682
```

### 1.2.2 Quadratic Discriminant Analysis

[10]:
```python
modelQDA = QDA()
modelQDA.fit(x_train, y_train)
StratKF(modelQDA,5, x_train, y_train, x_test, y_test)
```

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```
F1 score on 5-fold test data:  0.5688 +/- 0.0568
F1 score on training set:  0.6192
F1 score on test set:  0.5682
```

### 1.2.3 kNN

[11]:
```python
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');
```

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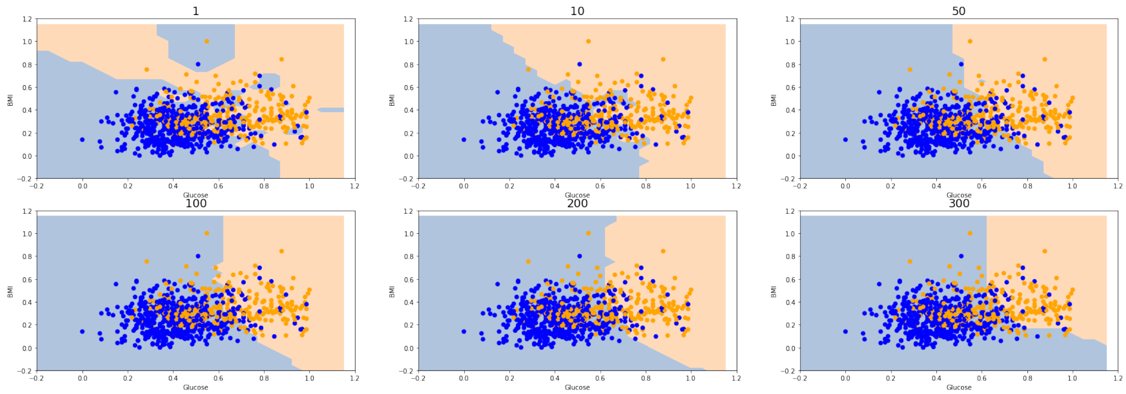


[12]:
```python
def valid_curve(model, x_train, y_train, n_jobs, scoring, param_range = np.array([*range(1,301)]), param_name="n_neighbors"):
    np.random.seed(1)
    train_scores, test_scores = validation_curve(model, x_train, y_train, param_name=param_name, param_range=param_range, scoring=scoring, 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]
```

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[13]:
```python
#Determination of k
modelkNN = kNN()
k_best = valid_curve(modelkNN, x_train, y_train, 6, 'accuracy')
```

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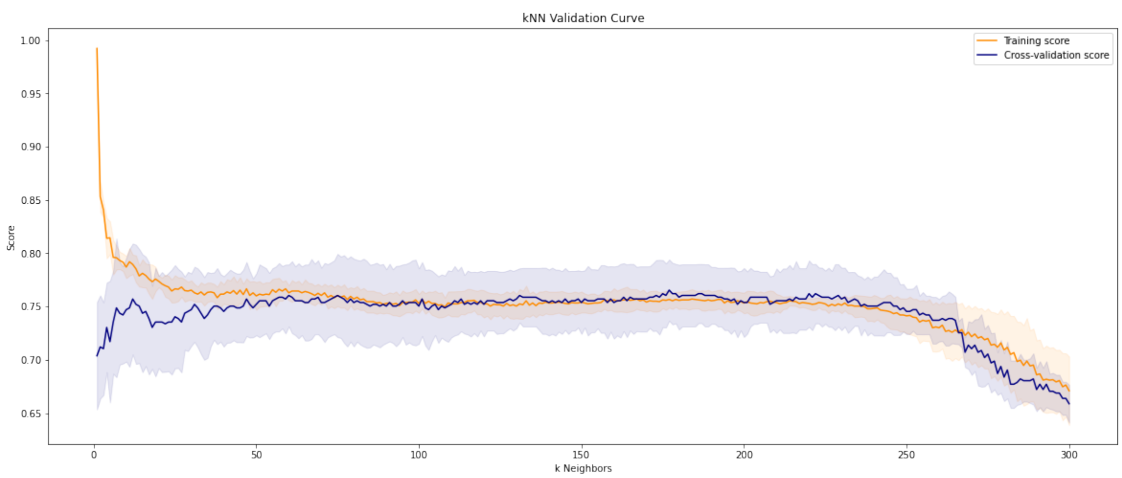


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Best K is 177

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[14]:
```
modelkNN = kNN(n_neighbors=k_best)
modelkNN.fit(x_train, y_train)
StratKF(modelkNN,5, x_train, y_train, x_test, y_test)
```

```
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F1 score on 5-fold test data:  0.4868 +/- 0.113
F1 score on training set:  0.5698
F1 score on test set:  0.5185
```

[15]:
```
#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=0.821
QDA ROC AUC=0.808
kNN ROC AUC=0.827
```

[16]:
```
#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')
```

```python
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();
```

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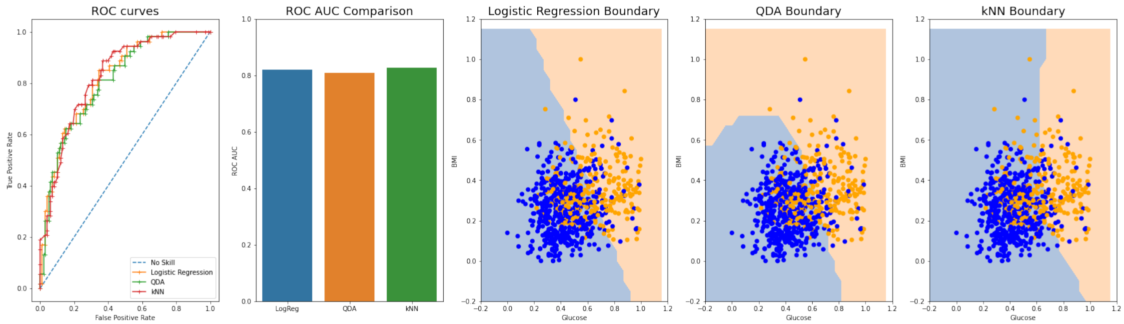


## 1.3 Question 2

### 1.3.1 normalization

[17]:
```
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

[18]:
```
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)
```

[19]:
```
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

[20]:
```
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

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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

[21]:
```
k_best = valid_curve(modelkNN, X_train, Y_train, 6, 'accuracy')
```

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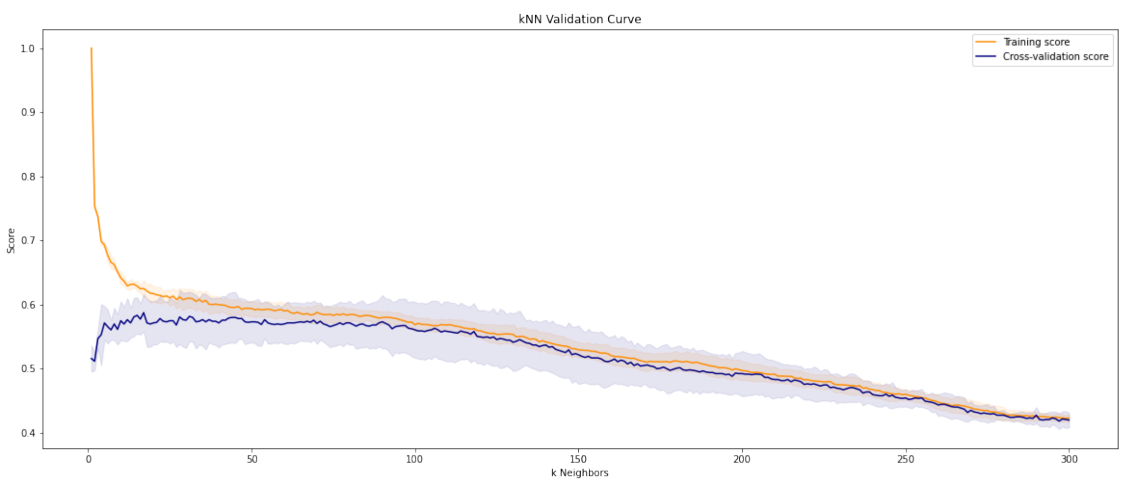

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Best K is 17

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```

[22]:

```
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

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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

[23]:

```
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
```

```
<IPython.core.display.Javascript object>
```

```
<IPython.core.display.Javascript object>
```

```
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
```

[24]:
```
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_
```

[25]:
```
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}
```

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[26]:
```
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)
  Best score: 0.5662322898481822
 Best Params: {'ccp_alpha': 0.01, 'criterion': 'entropy', 'max_depth': 5,
'min_samples_leaf': 4, 'min_samples_split': 2, 'splitter': 'best'}
```

[27]:
```
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
```

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```
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

[28]:
```
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)
```

[29]:
```
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]);
```

```
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<IPython.core.display.Javascript object>

<IPython.core.display.Javascript object>

<IPython.core.display.Javascript object>
```