# Project\_final

### April 3, 2021

```
[45]: import pandas as pd
      import matplotlib.pyplot as plt
      import numpy as np
      import seaborn as sns
      # ^^^ pyforest auto-imports - don't write above this line
      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, u
      →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, u
      →roc_curve, classification_report, f1_score
      from scipy import stats
```

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

## 0.1 Question 1

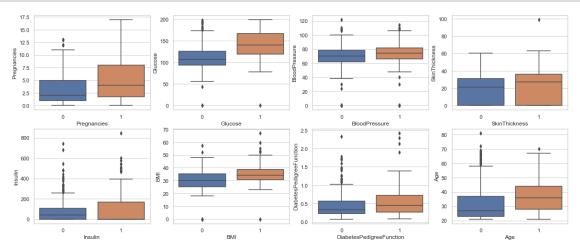
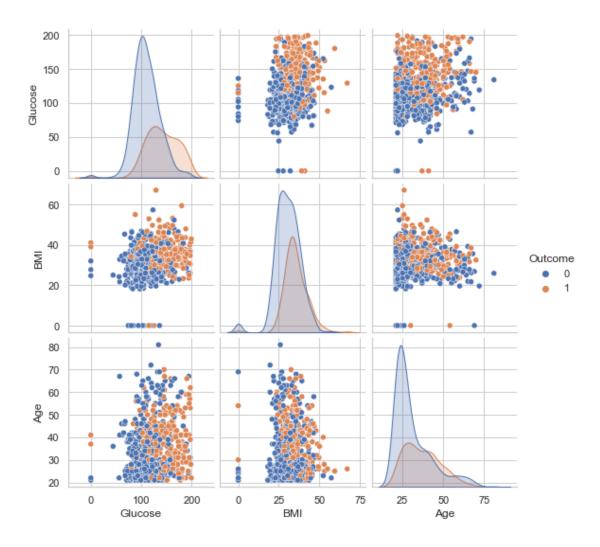


Figure 1. Box plots for the values of the variables according to target class.

```
[48]: data_pima_sel = data_pima.drop(columns = ['BloodPressure', 'SkinThickness', \_ \to '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.

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

```
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, u)

random_state=123, stratify= y)
```

## 0.2.1 Logistic Regression

```
F1 score on training set: 0.5943
F1 score on test set: 0.5455
F1 score on 5-fold test data: 0.5262 +/- 0.1354
```

#### 0.2.2 Quadratic Discriminant Analysis

```
[53]: modelQDA = QDA()
modelQDA.fit(x_train, y_train)
y_pred_trainQDA = modelQDA.predict(x_train)
y_pred_testQDA = modelQDA.predict(x_test)
print('F1 score on training set: ',round(f1_score(y_train, y_pred_trainQDA),4),
→'\nF1 score on test set: ',round(f1_score(y_test, y_pred_testQDA), 4))

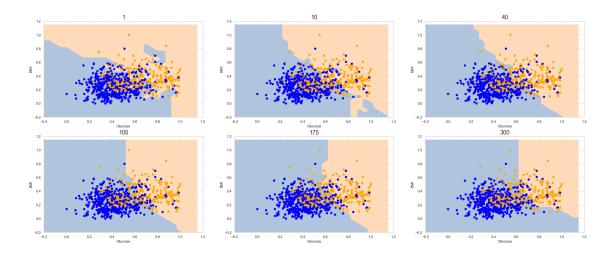
SKF = StratifiedKFold(n_splits=5, shuffle=True, random_state=1)
score_QDA = []
for train_index, test_index in SKF.split(x_test, y_test):
    x_test1 = x_train[test_index]
    y_test1 = y_train[test_index]
    score_QDA.append(f1_score(y_test1, modelQDA.predict(x_test1)))
print('F1 score on 5-fold test data: ',round(np.mean(score_QDA),4),'+/-',
→round(np.std(score_QDA),4))
```

```
F1 score on training set: 0.6129
F1 score on test set: 0.5495
F1 score on 5-fold test data: 0.4902 +/- 0.1367
```

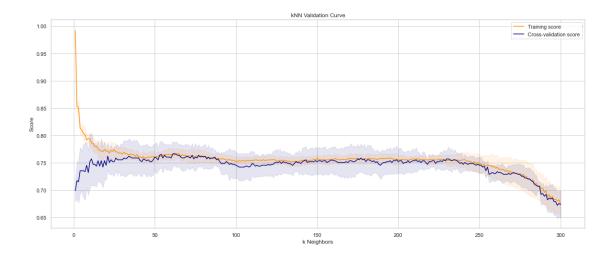
#### 0.2.3 kNN

```
[54]: fig = plt.figure(figsize=(30,12))
k = [1,10,40,100,175,300]

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');
```



```
[55]: #Determination of k
     modelkNN = kNN()
     param_range = [*range(1,301)]
     rg = np.array([*range(1,301)])
     train_scores, test_scores = validation_curve(modelkNN, x_train, y_train, __
      →param_name="n_neighbors", param_range=param_range, scoring="accuracy",
      \rightarrown_jobs=6)
     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", u
      ⇔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", __
      plt.fill_between(param_range, test_scores_mean - test_scores_std,_u
      →test_scores_mean + test_scores_std, alpha=0.1, color="navy")
     plt.legend(loc="best")
     plt.show();
     print("Best K is %d" %rg[np.where(test_scores_mean ==__
       →max(test_scores_mean))][0])
```

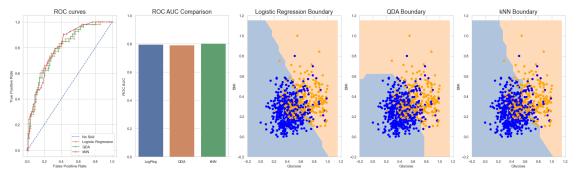


#### Best K is 62

```
[56]: modelkNN = kNN(n_neighbors=40)
      modelkNN.fit(x_train, y_train)
      y_pred_train_kNN = modelkNN.predict(x_train)
      y_pred_test_kNN = modelkNN.predict(x_test)
      print('F1 score on training set: ',round(f1_score(y_train,__
      →y_pred_train_kNN),4), '\nF1 score on test set: ',round(f1_score(y_test,_
      →y_pred_test_kNN), 4))
      SKF = StratifiedKFold(n_splits=5, shuffle=True, random_state=1)
      score_kNN = []
      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_kNN.append(f1_score(y_test1, modelkNN.predict(x_test1)))
      print('F1 score on 5-fold test data: ',round(np.mean(score_kNN),4),'+/-',__
       →round(np.std(score_kNN),4))
     F1 score on training set: 0.6006
     F1 score on test set: 0.5435
     F1 score on 5-fold test data: 0.5324 +/- 0.1118
[57]: #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)
```

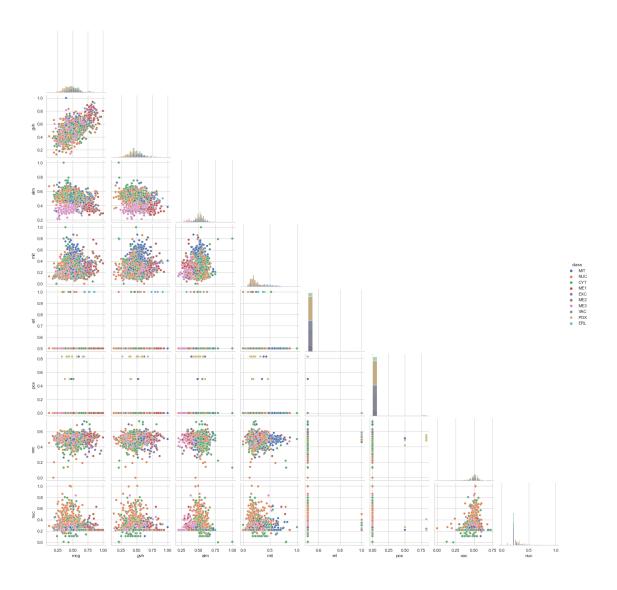
```
LogReg_auc = roc_auc_score(y_test, LogReg_probs)
      QDA_auc = roc_auc_score(y_test, QDA_probs)
      kNN_auc = roc_auc_score(y_test, kNN_probs)
      # summarize scores
      #print('No Skill: ROC AUC=%.3f' % (ns_auc))
      print('LR ROC AUC=%.3f' % (LogReg_auc))
      print('QDA ROC AUC=%.3f' % (QDA_auc))
      print('kNN ROC AUC=%.3f' % (kNN_auc))
     LR ROC AUC=0.797
     QDA ROC AUC=0.792
     kNN ROC AUC=0.804
[58]: #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');
      #plot LogReg decision boundary
      axs = figs.add_subplot(1, 5, 3)
      plot_classifier_boundary(modelLogReg,X)
      axs.scatter(X[:,0],X[:,1],color=cmap(y))
      axs.set xlabel('Glucose')
      axs.set_ylabel('BMI');
      axs.set title('Logistic Regression Boundary', fontsize = 18)
      #plot QDA decision boundary
      axs = figs.add_subplot(1, 5, 4)
      plot classifier boundary(modelQDA,X)
```

```
axs.scatter(X[:,0],X[:,1],color=cmap(y))
axs.set_xlabel('Glucose')
axs.set_ylabel('BMI');
axs.set_title('QDA Boundary', fontsize = 18)
#plot kNN decision boundary
axs = figs.add_subplot(1, 5, 5)
plot_classifier_boundary(modelkNN,X)
axs.scatter(X[:,0],X[:,1],color=cmap(y))
axs.set_xlabel('Glucose')
axs.set_ylabel('BMI');
axs.set_title('kNN Boundary', fontsize = 18)
plt.show();
```



## 0.3 Question 2

```
[59]: sns.pairplot(data_yeast, hue='class', diag_kind="hist", corner=True);
```



#### 0.3.1 normalization

```
[60]: 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']])
```

## 0.3.2 Separation in train data and test data

```
[61]: X = data_yeast.loc[:, ['mcg', 'gvh', 'alm', 'mit', 'erl', 'pox', 'vac', 'nuc']].

⇒values
Y = data_yeast.loc[:,'class'].values
```

## 0.3.3 Logistic regression

```
[62]: modelLR = LogReg()
      modelLR.fit(X_train, Y_train)
      Y_pred_trainLogReg = modelLR.predict(X_train)
      Y_pred_testLogReg = modelLR.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 LogReg = []
      accscore_LogReg = []
      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_LogReg.append(f1_score(Y_test1, modelLR.predict(X_test1),__
       →average='weighted'))
          accscore_LogReg.append(accuracy_score(Y_test1, modelLR.predict(X_test1)))
      print('Weighted F1 score on 5-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))
```

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

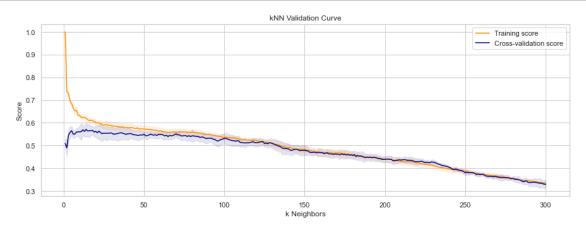
## Classification report:

	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
```

#### 0.3.4 kNN

```
[63]: modelknn = kNN()
     param range = [*range(1,301)]
     rg = np.array([*range(1,301)])
     train scores, test scores = validation curve(modelknn, X train, Y train, ...
      →param_name="n_neighbors", param_range=param_range, cv = 4,
      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=(15, 5))
     plt.title("kNN Validation Curve")
     plt.xlabel("k Neighbors")
     plt.ylabel("Score")
     plt.plot(param_range, train_scores_mean, label="Training score", __
      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", |
      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" %rg[np.where(test_scores_mean ==_
      →max(test scores mean))][0])
```



#### Best K is 14

```
[64]: modelknn = kNN(n_neighbors=14)
      modelknn.fit(X train, Y train)
      Y_pred_trainknn = modelknn.predict(X_train)
      Y_pred_testknn = modelknn.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 knn = []
      accscore_knn = []
      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_knn.append(f1_score(Y_test1, modelknn.predict(X_test1),_
      →average='weighted'))
          accscore_knn.append(accuracy_score(Y_test1, modelknn.predict(X_test1)))
      print('Weighted F1 score on 5-fold test data: ',round(np.
      →mean(f1score_knn),4),'+/-', round(np.std(f1score_knn),4))
      print('\nClassification report:\n',classification_report(Y_test,__
       →Y_pred_testknn, digits=3))
     Weighted F1 score on training set: 0.5564
     Weighted F1 score on test set: 0.5406
     Weighted F1 score on 5-fold test data: 0.5592 +/- 0.0471
```

#### Classification report:

	precision	recall	f1-score	support
CYT	0.522	0.634	0.573	93
ERL	1.000	1.000	1.000	1
EXC	0.667	0.571	0.615	7
ME1	0.429	0.667	0.522	9
ME2	0.500	0.200	0.286	10
ME3	0.710	0.688	0.698	32
MIT	0.652	0.612	0.632	49
NUC	0.557	0.512	0.533	86
POX	0.667	0.500	0.571	4
VAC	0.000	0.000	0.000	6
accuracy			0.572	297
macro avg	0.570	0.538	0.543	297
weighted avg	0.567	0.572	0.564	297

#### 0.3.5 Decision tree

```
[65]: modeltree = DTreeClass()
      modeltree.fit(X_train, Y_train)
      Y_pred_traintree = modeltree.predict(X_train)
      Y_pred_testtree = modeltree.predict(X_test)
      print('Weighted F1 score on training set: ',round(f1_score(Y_train,_
       →Y_pred_traintree, average='weighted'),4),
            '\nWeighted F1 score on test set: ',round(f1_score(Y_test,_
      →Y_pred_testtree, average='weighted'), 4))
      f1score_tree = []
      accscore_tree = []
      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_tree.append(f1_score(Y_test1, modeltree.predict(X_test1),__
       →average='weighted'))
          accscore_tree.append(accuracy_score(Y_test1, modeltree.predict(X_test1)))
      print('Weighted F1 score on 5-fold test data: ',round(np.
       →mean(f1score_tree),4),'+/-', round(np.std(f1score_tree),4))
      print('\nClassification report:\n',classification_report(Y_test,__
       →Y_pred_testtree, digits=3))
```

Weighted F1 score on training set: 1.0
Weighted F1 score on test set: 0.4806
Weighted F1 score on 5-fold test data: 0.4739 +/- 0.0456

#### Classification report:

precision	recall	f1-score	support
0.526	0.538	0.532	93
0.000	0.000	0.000	1
0.300	0.429	0.353	7
0.556	0.556	0.556	9
0.222	0.200	0.211	10
0.667	0.625	0.645	32
0.488	0.408	0.444	49
0.472	0.488	0.480	86
0.000	0.000	0.000	4
0.000	0.000	0.000	6
		0.478	297
0.323	0.324	0.322	297
0.485	0.478	0.481	297
	0.526 0.000 0.300 0.556 0.222 0.667 0.488 0.472 0.000 0.000	0.526	0.526

```
[66]: 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_
[67]: \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}
[68]: 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: 0.5669393207369835
      Best Params: {'ccp_alpha': 0.01, 'criterion': 'entropy', 'max_depth': 5,
     'min_samples_leaf': 4, 'min_samples_split': 2, 'splitter': 'best'}
[69]: modeltree = tree grid
      Y pred traintree = modeltree.predict(X train)
      Y_pred_testtree = modeltree.predict(X_test)
      print('Weighted F1 score on training set: ',round(f1_score(Y_train,_
       →Y_pred_traintree, average='weighted'),4),
            '\nWeighted F1 score on test set: ',round(f1_score(Y_test,_
       →Y_pred_testtree, average='weighted'), 4))
      f1score_tree = []
      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_tree append(f1_score(Y_test1, modeltree predict(X_test1),_
       →average='weighted'))
      print('Weighted F1 score on 5-fold test data: ',round(np.
       \rightarrowmean(f1score tree),4),'+/-', round(np.std(f1score tree),4))
```

```
Weighted F1 score on training set: 0.5986
Weighted F1 score on test set: 0.5512
Weighted F1 score on 5-fold test data: 0.5519 +/- 0.0611
```

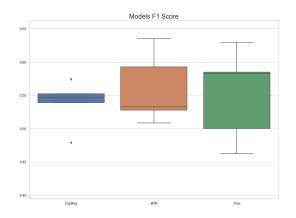
#### Classification report:

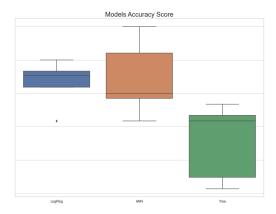
	precision	recall	f1-score	support
CY	T 0.526	0.538	0.532	93
ER	L 0.000	0.000	0.000	1
EX	C 0.571	0.571	0.571	7
ME	1 0.571	0.889	0.696	9
ME	2 0.500	0.300	0.375	10
ME	3 0.711	0.844	0.771	32
MI	T 0.617	0.592	0.604	49
NU	C 0.522	0.547	0.534	86
PO	X 0.000	0.000	0.000	4
VA	C 0.000	0.000	0.000	6
accurac	у		0.566	297
macro av	g 0.402	0.428	0.408	297
weighted av	g 0.542	0.566	0.551	297

#### 0.3.6 Achieved results comparison

```
[70]: stats_f1,pvalue_f1 = stats.f_oneway(f1score_LogReg, f1score_knn, f1score_tree) stats_acc, pvalue_acc = stats.f_oneway(accscore_LogReg, accscore_knn, u 

accscore_tree)
```





[]:	
[]:	