12/28/22, 4:24 PM

```
In [ ]: import numpy as np
        from matplotlib import pyplot as plt
        import pandas as pd
        import random
        from sklearn.neighbors import KNeighborsClassifier
        from sklearn.tree import DecisionTreeClassifier
        from sklearn.ensemble import AdaBoostClassifier
        from sklearn.svm import SVC
        from sklearn.ensemble import RandomForestClassifier
        from sklearn.metrics import accuracy score
        from sklearn.metrics import f1 score
        from sklearn.metrics import roc auc score
        from sklearn.metrics import precision_score
        from sklearn.metrics import recall score
        from sklearn.model selection import cross validate
        from sklearn.model selection import RepeatedKFold
        from sklearn.model selection import GridSearchCV
        from sklearn.model_selection import RandomizedSearchCV
        # randomizedSearchCV
```

Importing training and testing data sets, eploratory analysis of features

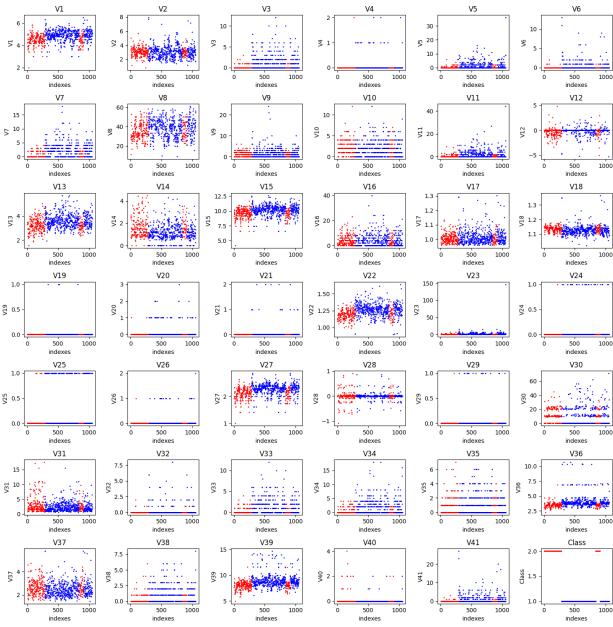
```
In [ ]: train = pd.read_csv('train.csv')
         test = pd.read csv('test.csv')
         train.head() # display a few samples
Out[]:
                       V3 V4 V5 V6 V7
                                             V8 V9 V10 ... V33 V34 V35
                                                                             V36
                                                                                   V37 V38
                                                                                              V39
         3 3.932 3.2512
                          0.0
                                 0
                                     0
                                         0
                                            26.7
                                                  2
                                                                0
                                                                     0
                                                                            3.076 2.417
                                                                                           0 7.601
         5 4.236 3.3944
                          0.0
                                 0
                                     0
                                         0 29.4
                                                  2
                                                                0
                                                                          0 3.351 2.405
                                                                                           0 8.003
         6 4.236 3.4286
                          0.0
                                 0
                                     0
                                         0 28.6
                                                  2
                                                       4 ...
                                                                0
                                                                     0
                                                                          0 3.351 2.556
                                                                                           0 7.904
         7 5.000 5.0476
                          1 0.0
                                 0
                                     0
                                         0 11.1
                                                                          1 4.712 4.583
                                                                                           0 9.303
         8 4.525 3.8301
                         0.0
                                 0
                                     0
                                         0 31.6
                                                  3
                                                       2 ...
                                                                0
                                                                     0
                                                                          0 3.379 2.143
                                                                                           0 7.950
        5 rows × 42 columns
```

```
In [ ]: f = plt.figure(figsize=(15, 15))

for i, col in enumerate(train.columns):
    print(col, len(train[col].unique()), end="; ")
    f.add_subplot(7, 6, i+1)
    plt.title(col)
    plt.ylabel(col)
    plt.xlabel("indexes")
```

```
plt.tight_layout()
plt.plot(train[col][train['Class'] == 1], "bo", markersize="1")
plt.plot(train[col][train['Class'] == 2], "ro", markersize="1")
```

V1 379; V2 823; V3 11; V4 4; V5 16; V6 10; V7 14; V8 172; V9 15; V10 11; V11 21; V12 307; V13 638; V14 321; V15 436; V16 24; V17 158; V18 115; V19 2; V20 4; V21 3; V22 32 2; V23 13; V24 2; V25 2; V26 3; V27 291; V28 174; V29 3; V30 372; V31 468; V32 8; V33 11; V34 16; V35 8; V36 603; V37 536; V38 8; V39 711; V40 5; V41 16; Class 2;

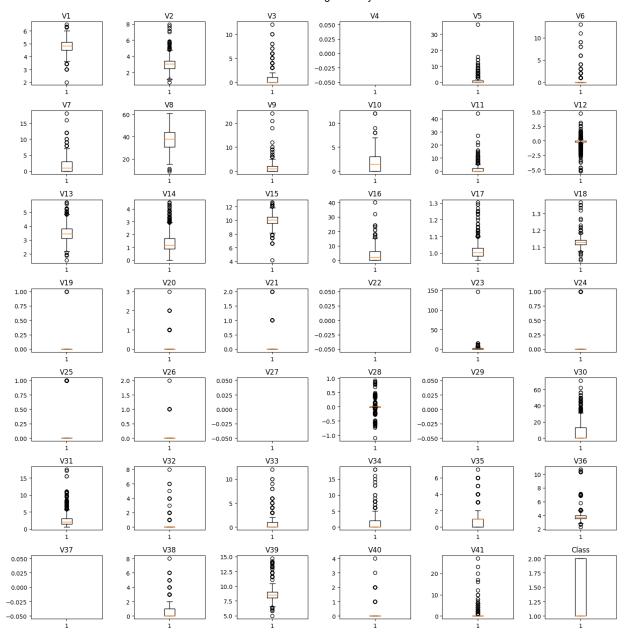


```
In []: f = plt.figure(figsize=(10, 8))

b = [26, 35, 38, 0]
a = train.columns[b]

counter = 1
    for i, col in enumerate(a):
        for j, col2 in enumerate(a[i+1:]):
            f.add_subplot(2, 3, counter)
            plt.title(col + " " + col2)
            plt.ylabel(col2)
            plt.xlabel(col)
```

```
plt.tight_layout()
                  plt.plot(train[col][train['Class'] == 1], train[col2][train['Class'] == 1],
                  plt.plot(train[col][train['Class'] == 2], train[col2][train['Class'] == 2], "r
                  counter += 1
         plt.show()
                                                         V27 V39
                                                                                          V27 V1
                        V27 V36
                                             14
           10
                                            12
            8
         V36
                                          ရ<del>ွ</del> 10
                                                                            7
            6
                                             8
                                                                              2
              1.0
                     1.5
                                 2.5
                                               1.0
                                                      1.5
                                                            2.0
                                                                   2.5
                                                                                 1.0
                                                                                       1.5
                                                                                             2.0
                                                                                                    2.5
                                                           V27
                                                                                            V27
                        V36 V39
                                                         V36 V1
                                                                                           V39 V1
           14
           12
         £ 10
                                           7
                                                                            7
                                                                              3
            6
                                     10
                                                                      10
                                                                                        8
                                                                                                  12
                                                                                                       14
                          6
                                                           6
                                                                                             10
                          V36
                                                           V36
                                                                                            V39
In [ ]: f = plt.figure(figsize=(15, 15))
         for i, col in enumerate(train.columns):
              f.add_subplot(7, 6, i+1)
              plt.title(col)
              plt.tight_layout()
              plt.boxplot(train[col])
```



2.1 Exploration

Inspect the dataset. How balanced is the target variable? Are there any missing values present? If there are, choose a strategy that takes this into account. Most of your data is of the numeric type. Can you identify, by adopting exploratory analysis, whether some features are directly related to the target? What about feature pairs? Produce at least three types of visualizations of the feature space and be prepared to argue why these visualizations were useful for your subsequent analysis.

Target variable distributions in test and training sets are close to [2/3 1/3].

Yes, there are some missing values. One possible strategy is to drop those that don't have all values. Some classifiers however don't really need all information, so you can just ignore missing rows for that specific attributes.

The visualizations are above. I haven't found anything very concrete some of the features are more and some less releted to target.

Majority classifier

```
majority = train['Class'].value counts()
majorityArr = np.array(majority)
print("Class distribution (train)")
print(majority)
print("Percentage:")
print(np.array(majorityArr[0] / np.sum(majorityArr)))
majorityTest = test['Class'].value counts()
majorityTestArr = np.array(majorityTest)
print("Class distribution (test)")
print(majorityTest)
print("Percentage:")
print(np.array(majorityTestArr[0] / np.sum(majorityTestArr)))
Class distribution (train)
1
    564
2
    282
Name: Class, dtype: int64
Percentage:
Class distribution (test)
1
    135
     74
Name: Class, dtype: int64
Percentage:
0.645933014354067
```

Random classifier

There are two classes if we choose between them randomly accuracy is 1/2

Preprocessing

```
In []: # removing NA values from train dataframe
    train = train.dropna()
    # Separate input features (X) and target variable (y)
    y = train.Class
    X = train.drop('Class', axis=1)

    testY = test.Class
    testX = test.drop('Class', axis=1)

# le = LabelEncoder()
# y = le.fit_transform(y)
# testY = le.fit_transform(testY)
```

Decision tree

12/28/22, 4:24 PM biodegradability

```
In []: clf_decitionTree = DecisionTreeClassifier(random_state=0)
    clf_decitionTree.fit(X, y)

pred_y_decitionTree = clf_decitionTree.predict(testX)
    print(accuracy_score(testY, pred_y_decitionTree))
    prob_y_decisionTree = clf_decitionTree.predict_proba(testX)
    prob_y_decisionTree = [p[1] for p in prob_y_decisionTree]
    print(roc_auc_score(testY, prob_y_decisionTree))
    print(f1_score(testY, pred_y_decitionTree))
    print(precision_score(testY, pred_y_decitionTree))
    print(recall_score(testY, pred_y_decitionTree))

0.8181818181818182
    0.8043043043043043
    0.8582089552238805
    0.8646616541353384
    0.8518518518518519
```

KNN

```
In []: clf_knn = KNeighborsClassifier(n_neighbors=9)
    clf_knn.fit(X, y)

    pred_y_knn = clf_knn.predict(testX)
    print(accuracy_score(testY, pred_y_knn))
    prob_y_knn = clf_knn.predict_proba(testX)
    prob_y_knn = [p[1] for p in prob_y_knn]
    print(roc_auc_score(testY, prob_y_knn))
    print(fl_score(testY, pred_y_knn))
    print(precision_score(testY, pred_y_knn))
    print(recall_score(testY, pred_y_knn))

0.7894736842105263
    0.8444944944944945
    0.8307692307692307
    0.864
    0.8
```

SVC / SVM

```
In [ ]: clf_svc = SVC(kernel='linear', class_weight='balanced', probability=True)
    clf_svc.fit(X, y)

    pred_y_svc = clf_svc.predict(testX)
    print(accuracy_score(testY, pred_y_svc))
    prob_y_svc = clf_svc.predict_proba(testX)
    prob_y_svc = [p[1] for p in prob_y_svc]
    print(roc_auc_score(testY, prob_y_svc))
    print(fl_score(testY, pred_y_svc))
    print(precision_score(testY, pred_y_svc))
    print(recall_score(testY, pred_y_svc))
```

```
0.8564593301435407
0.917917917917918
0.8846153846153846
0.92
0.8518518518518519
```

Random forest

```
In [ ]: clf_randomForest = RandomForestClassifier(random_state=1234)
    clf_randomForest.fit(X, y)
    pred_y_randomForest = clf_randomForest.predict(testX)
    print(accuracy_score(testY, pred_y_randomForest))
    prob_y_randomForest = clf_randomForest.predict_proba(testX)
    prob_y_randomForest = [p[1] for p in prob_y_randomForest]
    print(roc_auc_score(testY, prob_y_randomForest))
    print(f1_score(testY, pred_y_randomForest))
    print(precision_score(testY, pred_y_randomForest))
    print(recall_score(testY, pred_y_randomForest))

0.8373205741626795
    0.925025025025025
    0.8740740740740742
    0.87407407407474741
    0.8740740740740741
```

Ada boost

```
In [ ]: clf adaboost = AdaBoostClassifier(n estimators = 50, learning rate = 0.2)
        clf adaboost.fit(X, y)
        pred y adaboost = clf adaboost.predict(testX)
        print(accuracy_score(testY, pred_y_adaboost))
        prob_y_adaboost = clf_adaboost.predict_proba(testX)
        prob y adaboost = [p[1] for p in prob y adaboost]
        print(roc auc score(testY, prob y adaboost))
        print(f1_score(testY, pred_y_adaboost))
        print(precision score(testY, pred y adaboost))
        print(recall_score(testY, pred_y_adaboost))
        0.8516746411483254
        0.8983483483483484
        0.8888888888888888
        0.8611111111111112
        0.9185185185185
In [ ]: def printScores(scores):
            avgAccuracy = np.mean(scores['test accuracy'])
            stdAccuracy = np.std(scores['test_accuracy'])
            avgF1 = np.mean(scores['test f1 macro'])
            stdF1 = np.std(scores['test_f1_macro'])
            avgRecall = np.mean(scores['test_recall_macro'])
            stdRecall = np.std(scores['test recall macro'])
            avgAUC = np.mean(scores['test roc auc'])
            stdAUC = np.std(scores['test roc auc'])
            print(f"Precision average {avgAccuracy} with standard deviation {stdAccuracy}")
            print(f"F1 average {avgF1} with standard deviation {stdF1}")
```

```
print(f"Recall average {avgRecall} with standard deviation {stdRecall}")
print(f"AUC average {avgAUC} with standard deviation {stdAUC}")
return avgAccuracy, avgF1, avgRecall, avgAUC
```

```
In [ ]: scoring = ['accuracy', 'f1_macro', 'recall_macro', 'roc_auc']
        rkf = RepeatedKFold(n_splits=5, n_repeats=10, random_state=1234)
        print("DecisionTree:")
        scores = cross_validate(clf_decitionTree, X, y, cv=rkf.split(X), scoring=scoring)
        accDT, f1DT, recallDT, aucDT = printScores(scores)
        print("KNN:")
        scores = cross_validate(clf_knn, X, y, cv=rkf.split(X), scoring=scoring)
        accKNN, f1KNN, recallKNN, aucKNN = printScores(scores)
        print("SVC:")
        scores = cross_validate(clf_svc, X, y, cv=rkf.split(X), scoring=scoring)
        accSVC, f1SVC, recallSVC, aucSVC = printScores(scores)
        print("Random forest:")
        scores = cross validate(clf randomForest, X, y, cv=rkf.split(X), scoring=scoring)
        accRF, f1RF, recallRF, aucRF = printScores(scores)
        print("Ada boost:")
        scores = cross validate(clf adaboost, X, y, cv=rkf.split(X), scoring=scoring)
        accAB, f1AB, recallAB, aucAB = printScores(scores)
        accArr = np.array([accDT, accKNN, accSVC, accRF, accAB])
        f1Arr = np.array([f1DT, f1KNN, f1SVC, f1RF, f1AB])
        recallArr = np.array([recallDT, recallKNN, recallSVC, recallRF, recallAB])
        aucArr = np.array([aucDT, aucKNN, aucSVC, aucRF, aucAB])
```

DecisionTree:

Precision average 0.812156862745098 with standard deviation 0.02854376403060423 F1 average 0.784408516342152 with standard deviation 0.03202103986272087 Recall average 0.7846760605124242 with standard deviation 0.032710517604903296 AUC average 0.7846760605124244 with standard deviation 0.0327105176049033 KNN:

Precision average 0.8037908496732026 with standard deviation 0.03176470588235294 F1 average 0.7830756361992742 with standard deviation 0.03501761634187004 Recall average 0.7948762190469268 with standard deviation 0.03443701598610628 AUC average 0.8695242325608025 with standard deviation 0.029821877354123717 SVC:

Precision average 0.8483660130718953 with standard deviation 0.02449018822901332 F1 average 0.8334307934166105 with standard deviation 0.025822140023746137 Recall average 0.8494180778534464 with standard deviation 0.02297552655916109 AUC average 0.9172983682699644 with standard deviation 0.021409121779670134 Random forest:

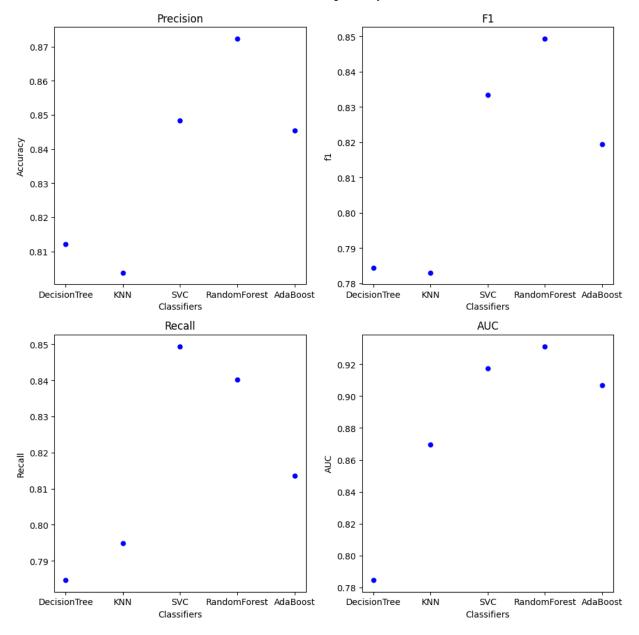
Precision average 0.8722875816993464 with standard deviation 0.026507599397837152 F1 average 0.8493273984299182 with standard deviation 0.030395319693460075 Recall average 0.8401993072677727 with standard deviation 0.03133459395358015 AUC average 0.931217265590636 with standard deviation 0.022160026982249132

Precision average 0.8454901960784312 with standard deviation 0.02781458537908356 F1 average 0.8194661758682241 with standard deviation 0.03067931648303135 Recall average 0.8135451479407578 with standard deviation 0.030293738100877578 AUC average 0.9067507600767993 with standard deviation 0.02745133093093605

```
In [ ]: xAxis = ['DecisionTree', 'KNN', 'SVC', 'RandomForest', 'AdaBoost']
f = plt.figure(figsize=(10, 10))
f.add_subplot(2, 2, 1)
```

```
plt.title("Precision")
plt.ylabel("Accuracy")
plt.xlabel("Classifiers")
plt.tight layout()
plt.plot(xAxis, accArr, "bo", markersize="5")
f.add_subplot(2, 2, 2)
plt.title("F1")
plt.ylabel("f1")
plt.xlabel("Classifiers")
plt.tight layout()
plt.plot(xAxis, f1Arr, "bo", markersize="5")
f.add_subplot(2, 2, 3)
plt.title("Recall")
plt.ylabel("Recall")
plt.xlabel("Classifiers")
plt.tight_layout()
plt.plot(xAxis, recallArr, "bo", markersize="5")
f.add_subplot(2, 2, 4)
plt.title("AUC")
plt.ylabel("AUC")
plt.xlabel("Classifiers")
plt.tight_layout()
plt.plot(xAxis, aucArr, "bo", markersize="5")
```

Out[]: [<matplotlib.lines.Line2D at 0x19fd5c46470>]



Comment on the performance of algorithms and visualize their final scores. How do they perform against the random baseline? What about the constant one? How do different learning scenarios impact the final score? Are the differences between the models statistically significant?

Random forest performed the best then SVC and AdaBoost. DecisionTree and KNN performed significantly worse than others. They all perform better than random and constant baseline (50%/66% accuracy). Different parameters will change final scores and also different preprocessing of data might improve the final score (less noise/outliers, more accurate data,...). Differences of the RandomForest, SVC, AdaBoost are not very big, but depending on the needs of the classification different classification model might be more desirable.

Paramaters tuning (Random forest)

```
'max depth': [2,4], # Maximum number of levels in tree
                        'min_samples_split': [2, 5], # Minimum number of samples required to s
                        'min_samples_leaf': [1, 2], # Minimum number of samples required at eac
                        'bootstrap': [True, False]} # Method of selecting samples for training
        rf Model = RandomForestClassifier()
        rf_Grid = GridSearchCV(estimator = rf_Model, param_grid = params, cv = 10, verbose=2,
        rf Grid.fit(X, y)
        rf_Grid.best_params_
        rf_Random = RandomizedSearchCV(estimator = rf_Model, param_distributions = params, cv
        rf Random.fit(X, y)
        rf Random.best params
        Fitting 10 folds for each of 160 candidates, totalling 1600 fits
        Fitting 10 folds for each of 10 candidates, totalling 100 fits
Out[]: {'n_estimators': 25,
         'min samples split': 5,
         'min samples leaf': 1,
         'max_features': 'sqrt',
         'max depth': 4,
         'bootstrap': False}
In [ ]: print (f'Train Accuracy - : {rf_Grid.score(X,y):.3f}')
        print (f'Test Accuracy - : {rf Grid.score(testX,testY):.3f}')
        print (f'Train Accuracy - : {rf_Random.score(X,y):.3f}')
        print (f'Test Accuracy - : {rf_Random.score(testX,testY):.3f}')
        Train Accuracy - : 0.914
        Test Accuracy - : 0.854
        Train Accuracy - : 0.926
        Test Accuracy - : 0.861
```

Parameter tuning (AdaBoost)

```
In [ ]: adaBoostModel = AdaBoostClassifier(base_estimator=DecisionTreeClassifier())
        params = {'base estimator max depth':[i for i in range(2,11,2)],
                       'base_estimator__min_samples_leaf':[5,10],
                       'n estimators':[10,50,250,1000],
                       'learning_rate':[0.01,0.1]}
        adaBoost Grid = GridSearchCV(adaBoostModel, params, verbose=3, scoring='f1', n jobs=-1
        adaBoost Grid.fit(X,y)
        adaBoost_Grid.best_params_
        adaBoost Random = RandomizedSearchCV(estimator = adaBoostModel, param distributions =
        adaBoost Random.fit(X, y)
        adaBoost_Random.best_params_
        Fitting 5 folds for each of 80 candidates, totalling 400 fits
        Fitting 5 folds for each of 10 candidates, totalling 50 fits
Out[]: {'n estimators': 250,
         'learning rate': 0.1,
         'base_estimator__min_samples_leaf': 5,
         'base_estimator__max_depth': 2}
In [ ]: | print (f'Train Accuracy - : {adaBoost_Grid.score(X,y):.3f}')
        print (f'Test Accuracy - : {adaBoost_Grid.score(testX,testY):.3f}')
```

```
print (f'Train Accuracy - : {adaBoost_Random.score(X,y):.3f}')
print (f'Test Accuracy - : {adaBoost_Random.score(testX,testY):.3f}')

Train Accuracy - : 0.998
Test Accuracy - : 0.887
Train Accuracy - : 0.997
Test Accuracy - : 0.871
```

Parameter tuning (SVC)

```
In [ ]: from scipy import stats
        svcModel = SVC(kernel='linear', class_weight='balanced', probability=True)
        params = {"C": np.arange(2, 10, 2),
                     "gamma": np.arange(0.1, 1, 0.2)}
        svc_Grid = GridSearchCV(svcModel, param_grid = params, n_jobs = 4, cv = 3, scoring='f1
        svc_Grid.fit(X, y)
        svc_Grid.best_params_
        params = {"C": stats.uniform(2, 10),
                    "gamma": stats.uniform(0.1, 1)}
        svc_Random = RandomizedSearchCV(svcModel, param_distributions = params, n_iter = 20, r
        svc Random.fit(X, y)
        svc_Random.best_params_
Out[]: {'C': 6.479197998006022, 'gamma': 0.22054161556730448}
In [ ]: print (f'Train Accuracy - : {svc_Grid.score(X,y):.3f}')
        print (f'Test Accuracy - : {svc_Grid.score(testX,testY):.3f}')
        print (f'Train Accuracy - : {svc Random.score(X,y):.3f}')
        print (f'Test Accuracy - : {svc_Random.score(testX,testY):.3f}')
        Train Accuracy - : 0.911
        Test Accuracy - : 0.869
        Train Accuracy - : 0.913
        Test Accuracy - : 0.893
```