```
from google.colab import drive
drive.mount('/content/drive')
```

```
Drive already mounted at /content/drive; to attempt to forcibly remount, call drive.mount("/content/drive", force_remou
```

```
# libraries required
import pandas as pd
import numpy as np
# Matplotlib visualization
import matplotlib.pyplot as plt
# Seaborn for visualization
import seaborn as sns
import statsmodels.api as sm
from numpy.core.numeric import NaN
import warnings
warnings.simplefilter('ignore')
```

```
/usr/local/lib/python3.7/dist-packages/statsmodels/tools/_testing.py:19: FutureWarning: pandas.util.testing is deprecat
  import pandas.util.testing as tm
```

```
# Read in data into a dataframe
dfeature= pd.read_csv('/content/drive/My Drive/tox21_global_cdf_rdkit.csv')
df = pd.read_csv('/content/drive/My Drive/tox21.csv')
```

```
#show all of rows and columns
pd.set_option('display.max_columns', None)
pd.set_option('display.max_rows', None)
```

```
# shape of dataset
print(dfeature.shape)
print(df.shape)
```

```
(7831, 201)
(7831, 13)
```

```
df= df.drop('smiles', axis= 1)
df.head()
```

	NR-AR	NR-AR-LBD	NR-AhR	NR-Aromatase	NR-ER	NR-ER-LBD	NR-PPAR-gamma	SR-ARE	SR-ATAD5	SR-HSE	SR-MMP	SR-p53
0	0.0	0.0	1.0	NaN	NaN	0.0	0.0	1.0	0.0	0.0	0.0	0.0
1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	NaN	0.0	NaN	0.0	0.0
2	NaN	NaN	NaN	NaN	NaN	NaN	NaN	0.0	NaN	0.0	NaN	NaN

```
# Function to calculate missing values by column
def values_table(df):
        # Total missing values
        mis_val = df.isnull().sum()
        ones=df.sum()
        zeros=7832-(mis_val+ones)
        # Percentage of missing values
        mis_val_percent = 100 * df.isnull().sum() / len(df)

        # Make a table with the results
        mis_val_table = pd.concat([ones,zeros,mis_val, mis_val_percent], axis=1)

        # Rename the columns
        mis_val_table_ren_columns = mis_val_table.rename(
        columns = {2 : 'Missing Values', 3 : '% of Total Missing Values',0:'One labeled data',1:'Zero labeled data'})

        # Sort the table by percentage of missing descending
        mis_val_table_ren_columns = mis_val_table_ren_columns[
            mis_val_table_ren_columns.iloc[:,1] != 0].sort_values(
        'One labeled data', ascending=False).round(1)

        # Print some summary information
        print ("Your selected dataframe has " + str(df.shape[1]) + " columns.\n"
            "There are " + str(mis_val_table_ren_columns.shape[0]) +
              " columns that have missing values.")

        # Return the dataframe with missing information
        return mis_val_table_ren_columns
```

```
values_table(df)
```

```
Your selected dataframe has 12 columns.
There are 12 columns that have missing values.
```

	One labeled data	Zero labeled data	Missing Values	% of Total Missing Values
SR-ARE	942.0	4891.0	1999	25.5
SR-MMP	918.0	4893.0	2021	25.8
NR-ER	793.0	5401.0	1638	20.9
NR-AhR	768.0	5782.0	1282	16.4
SR-p53	423.0	6352.0	1057	13.5
SR-HSE	372.0	6096.0	1364	17.4
NR-ER-LBD	350.0	6606.0	876	11.2
NR-AR	309.0	6957.0	566	7.2
NR-Aromatase	300.0	5523.0	2010	25.7

```
dlabel= pd.read_csv('/content/drive/My Drive/tox21label.csv') #this file contains smiles and 'SR-ARE' label

data0=pd.concat([dfeature,dlabel],axis=1)
data1 = data0.iloc[:,1:]
dataf= data1.dropna(how='any')#data was cleaned


xdata = dataf.iloc[:,:-2] #features
ydata = dataf.iloc[:,-2:] # smile & target label
ydata=pd.DataFrame(ydata)
xdata
```

```
from sklearn.model_selection import train_test_split

X_trainingdata, X_test, y_trainingdata, y_test =train_test_split(xdata,ydata, stratify=ydata['SR-ARE'],test_size=0.10)
```

```
X_trainingdata.describe()
```

	('BalabanJ', <class	('BertzCT', <class	('Chi0', <class 'numpy.float64'>)	('Chi0n', <class 'numpy.float64'>)

```
X_test.describe()
```

	('BalabanJ', <class 'numpy.float64'>)	('BertzCT', <class 'numpy.float64'>)	('Chi0', <class 'numpy.float64'>)	('Chi0n', <class 'numpy.float64'>)
count	577.000000	577.000000	5.770000e+02	5.770000e+02
mean	0.825332	0.132312	1.624583e-01	1.653808e-01
std	0.253309	0.205895	2.452118e-01	2.427365e-01
min	0.000020	0.000577	3.875255e-15	2.722966e-11
25%	0.814424	0.006040	5.815540e-03	5.572814e-03
50%	0.942433	0.032431	3.005244e-02	3.721124e-02
75%	0.976435	0.160505	2.184949e-01	2.541685e-01
max	0.997048	1.000000	9.990553e-01	9.971261e-01

```
# Function to calculate 0 and 1 labels in test and train
def labels_counter(df1):
        # count of 1 & 0 labels
        ones1=df1.sum()
        zeros1=df1.shape[0]-ones1
             # Make a table with the results
        label_val_table1 = pd.concat([ones1,zeros1], axis=1)
           # Rename the columns
        label_val_table_ren_columns1= label_val_table1.rename(
        columns = {0:'Label:1',1:'Label:0'} )
              # Return the dataframe with missing information
        return label_val_table_ren_columns1
```

```
label_train=labels_counter(pd.DataFrame(y_trainingdata['SR-ARE']))
label_test=labels_counter(pd.DataFrame(y_test['SR-ARE']))
print('trainingset labels:\n \n ',label_train,'\n \n \n testset labels : \n  \n' ,label_test)
```

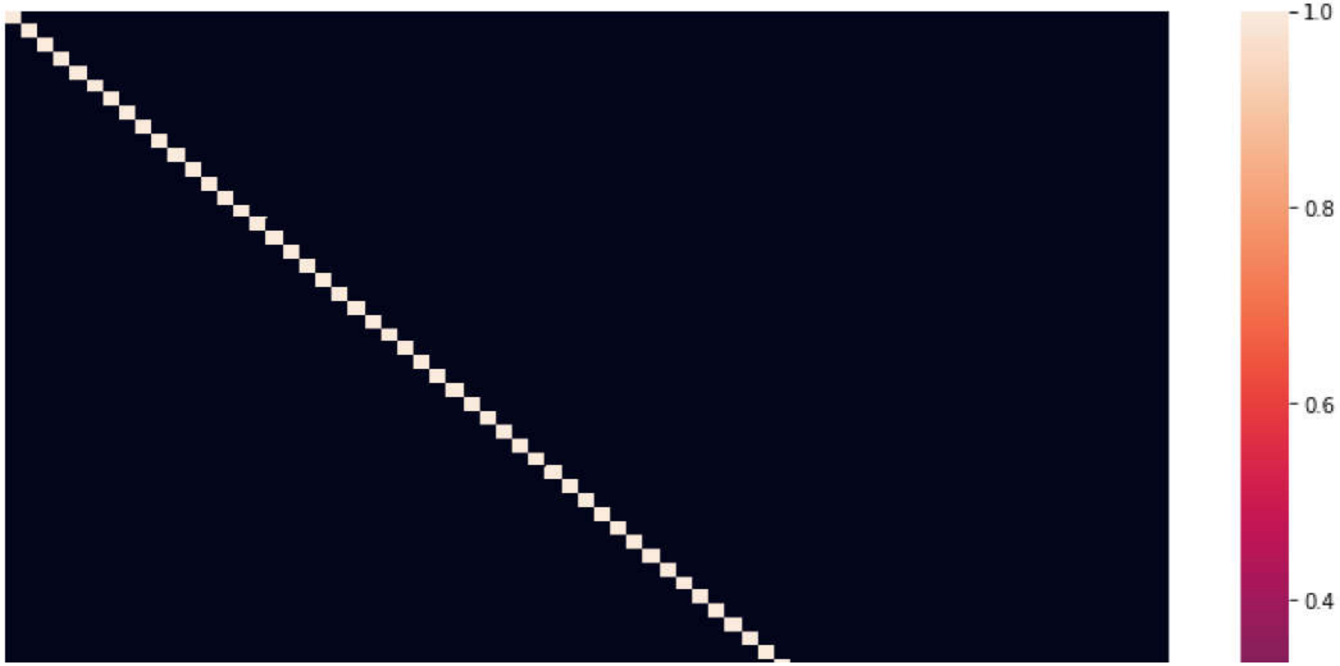
```
trainingset labels:

          Label:1  Label:0
SR-ARE    821.0   4367.0


 testset labels :

         Label:1  Label:0
SR-ARE     91.0    486.0
```

```
from sklearn.decomposition import PCA
pca = PCA(n_components=71)
principalComponents = pca.fit_transform(X_trainingdata)
X_trainingdata_PCA = pd.DataFrame(data = principalComponents)
X_trainingdata_PCA
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
%matplotlib inline
plt.figure(figsize=(13,9))
a=sns.heatmap(X_trainingdata_PCA.corr(),xticklabels=False, yticklabels=False)
```



```
print(np.sum(pca.explained_variance_ratio_))

     0.9520798546956848
```

```
y_trainingdata_PCA=pd.DataFrame(data =y_trainingdata.to_numpy()[:,1],columns=['SR-ARE'])
y_trainingdata_PCA
```

```
from sklearn.ensemble import AdaBoostClassifier
clf=AdaBoostClassifier()
clf.fit(X_trainingdata,y_trainingdata['SR-ARE'])
cptrain=clf.score(X_trainingdata,y_trainingdata['SR-ARE'])
print('training score adaboost= ',cptrain)
cptest=clf.score(X_test,y_test['SR-ARE'])
print('test score = ',cptest)

     training score adaboost=  0.8583269082498073
     test score =  0.8509532062391681
```

```
from sklearn.metrics import accuracy_score

for clf in (log_clf, rnd_clf):
    clf.fit(X_trainingdata, y_trainingdata['SR-ARE'])
    y_pred = clf.predict(X_test)
    print(clf.__class__.__name__, accuracy_score(y_test['SR-ARE'], y_pred))
```

```
LogisticRegression 0.854419410745234
RandomForestClassifier 0.8648180242634316
```

```
# ...bagging dessicion
bag_clf = BaggingClassifier(
    DecisionTreeClassifier(splitter="random", max_leaf_nodes=16, random_state=42),
    n_estimators=500, max_samples=1.0, bootstrap=True, n_jobs=-1, random_state=42)
bag_clf.fit(X_trainingdata, y_trainingdata['SR-ARE'])
y_pred = bag_clf.predict(X_test)
print(accuracy_score(y_test['SR-ARE'], y_pred))
```

```
0.8440207972270364
```

```
# ...PCA of bagging dessicion
from sklearn.ensemble import BaggingClassifier
from sklearn.tree import DecisionTreeClassifier
from sklearn.metrics import accuracy_score
bag_clf = BaggingClassifier(
    DecisionTreeClassifier(splitter="random", max_leaf_nodes=16, random_state=42),
    n_estimators=500, max_samples=1.0, bootstrap=True, n_jobs=-1, random_state=42)
bag_clf.fit(X_trainingdata_PCA.to_numpy().astype('float'),np.transpose(y_trainingdata_PCA.to_numpy().astype('int'))[0])
#need xtest PCA
principalComponents = pca.fit_transform(X_test)
X_test_PCA = pd.DataFrame(data = principalComponents)
y_pred = bag_clf.predict(X_test_PCA)
print(accuracy_score(y_test['SR-ARE'], y_pred))
```

```
0.8422876949740035
```

```
from sklearn.ensemble import RandomForestClassifier

rnd_clf = RandomForestClassifier(n_estimators=500, max_leaf_nodes=16, n_jobs=-1, random_state=42)
rnd_clf.fit(X_trainingdata, y_trainingdata['SR-ARE'])

y_pred_rf = rnd_clf.predict(X_test)
np.sum(y_pred == y_pred_rf) / len(y_pred)  # almost identical predictions
```

```
     0.9982668977469671
```

```
from sklearn.ensemble import BaggingClassifier
from sklearn.tree import DecisionTreeClassifier

bag_clf = BaggingClassifier(
    DecisionTreeClassifier(random_state=42), n_estimators=500,
    max_samples=100, bootstrap=True, n_jobs=-1, random_state=42)
bag_clf.fit(X_trainingdata, y_trainingdata['SR-ARE'])
y_pred = bag_clf.predict(X_test)

from sklearn.metrics import accuracy_score
print(accuracy_score(y_test['SR-ARE'], y_pred))
```

```
     0.8440207972270364
```

```
bag_clf2 = BaggingClassifier(
    DecisionTreeClassifier(random_state=42), n_estimators=500,
    max_samples=1, bootstrap=True, n_jobs=-1, random_state=42)
bag_clf2.fit(X_trainingdata, y_trainingdata['SR-ARE'])
y_pred2 = (bag_clf2).predict(X_test)
print(accuracy_score(y_test['SR-ARE'], y_pred2))
```

```
     0.8422876949740035
```

```
from sklearn.ensemble import RandomForestClassifier
from sklearn.ensemble import VotingClassifier
from sklearn.linear_model import LogisticRegression
from sklearn.svm import SVC
```

```
log_clf = LogisticRegression(solver="liblinear", random_state=42) # See the following link for a very good review on the dif
# and see this https://scikit-learn.org/stable/modules/linear_model.html#logistic-regression
rnd_clf = RandomForestClassifier(n_estimators=20, random_state=42)
svm_clf = SVC(gamma="auto", random_state=42)

voting_clf = VotingClassifier(
    estimators=[('lr', log_clf), ('rf', rnd_clf), ('svc', svm_clf)],
    voting='hard')

from sklearn.metrics import accuracy_score

for clf in (log_clf, rnd_clf, svm_clf, voting_clf):
    clf.fit(X_trainingdata, y_trainingdata['SR-ARE'])
    y_pred = clf.predict(X_test)
    print(clf.__class__.__name__, accuracy_score(y_test['SR-ARE'], y_pred))
```

```
LogisticRegression 0.854419410745234
RandomForestClassifier 0.8648180242634316
SVC 0.8422876949740035
VotingClassifier 0.8526863084922011
```

```
log_clf = LogisticRegression(solver="liblinear", random_state=42)
rnd_clf = RandomForestClassifier(n_estimators=20, random_state=42)
svm_clf = SVC(gamma="auto", probability=True, random_state=42)

voting_clf = VotingClassifier(
    estimators=[('lr', log_clf), ('rf', rnd_clf), ('svc', svm_clf)],
    voting='soft')
voting_clf.fit(X_trainingdata, y_trainingdata['SR-ARE'])
```

```
VotingClassifier(estimators=[('lr',
                              LogisticRegression(random_state=42,
                                                 solver='liblinear')),
                             ('rf',
                              RandomForestClassifier(n_estimators=20,
                                                     random_state=42)),
                             ('svc',
                              SVC(gamma='auto', probability=True,
                                 random_state=42))],
                         voting='soft')
```

```
###### ..     GRID SEARCH CV   .. #####
```

```
from sklearn.neighbors import KNeighborsClassifier
from sklearn.model_selection import GridSearchCV
from sklearn.metrics import confusion_matrix,plot_confusion_matrix
knn = KNeighborsClassifier()
param_grid={'n_neighbors':np.arange(1,100,2),'metric':['euclidean','cosine','manhattan']}
grid=GridSearchCV(knn,param_grid=param_grid,cv=10,scoring='balanced_accuracy',return_train_score=False)
grid.fit(X_trainingdata_PCA.to_numpy().astype('float'),np.transpose(y_trainingdata_PCA.to_numpy().astype('int'))[0])
print("best mean cv score= ",grid.best_score_)
print("best parameters= ",grid.best_params_)
```

```
best mean cv score=  0.6640470378287008
best parameters=  {'metric': 'cosine', 'n_neighbors': 1}
```

```
X_test_pca=pd.DataFrame(data=pca.transform(X_test))
grid.score(X_test_pca,y_test['SR-ARE'])
```

```
0.5543571654682766
```

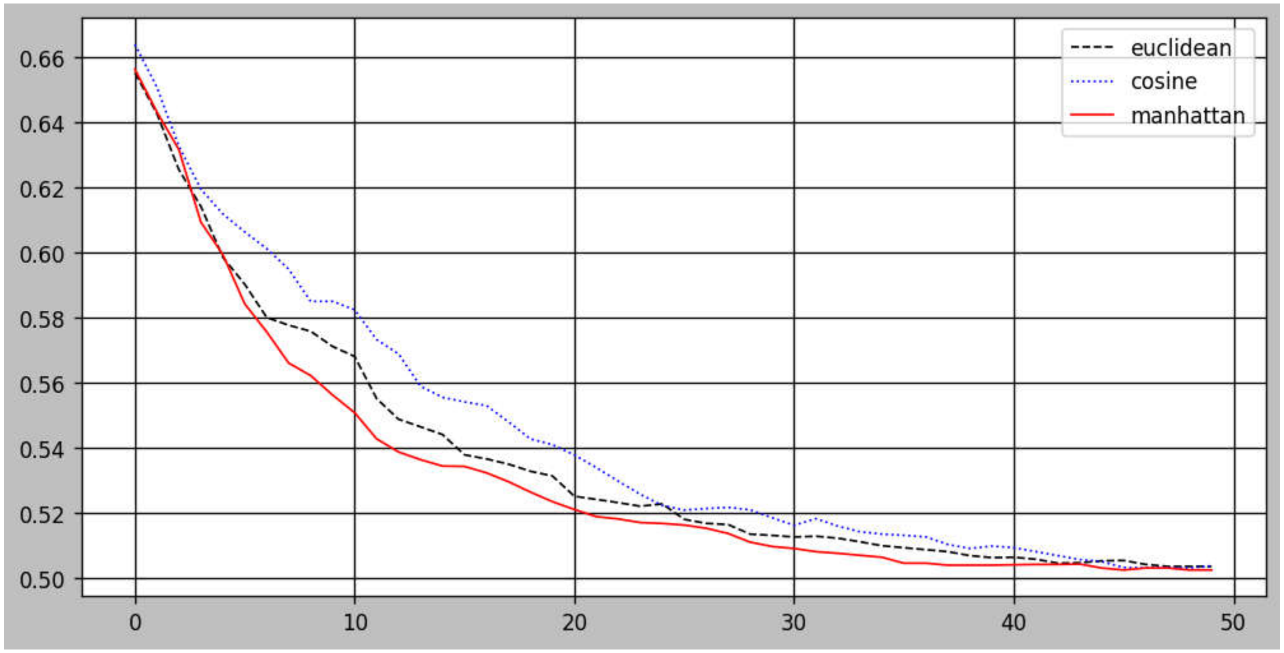
```
y_pred_knn=grid.best_estimator_.predict(X_test_pca)
print(confusion_matrix(y_test['SR-ARE'],np.transpose(np.matrix(y_pred_knn))))
```

```
[[416  70]
 [ 68  23]]
```

```
knn_cv_results=grid.cv_results_
```

```
plt.style.use('grayscale')
plt.figure(figsize=(10,5),dpi=120)
plt.plot(np.arange(0,50,1),knn_cv_results['mean_test_score'][0:50],lw=1,label='euclidean',ls='--')
plt.plot(np.arange(0,50,1),knn_cv_results['mean_test_score'][50:100],lw=1,label='cosine',ls=":",c='blue')
plt.plot(np.arange(0,50,1),knn_cv_results['mean_test_score'][100:150],lw=1,label='manhattan',ls='-',c='red')
plt.legend()
plt.grid()
plt.show()
import matplotlib.pyplot as plt

fig = plt.figure()
fig.canvas.manager.full_screen_toggle() # toggle fullscreen mode
fig.show()
```



```
<Figure size 432x288 with 0 Axes>
```

```
from sklearn.tree import DecisionTreeClassifier, export_graphviz
DecisionTree = DecisionTreeClassifier()
param_grid={'criterion':['gini','entropy'],'max_depth':[5,10,15,20,25,30]}
grid=GridSearchCV(DecisionTree,param_grid=param_grid,cv=8,scoring='balanced_accuracy',return_train_score=False)
grid.fit(X_trainingdata_PCA.to_numpy().astype('float'),np.transpose(y_trainingdata_PCA.to_numpy().astype('int'))[0])
print('DecisionTree')
print("best mean cv score= ",grid.best_score_)
print("best parameters= ",grid.best_params_)
y_pred_dt=grid.best_estimator_.predict(X_test_pca)
print(confusion_matrix(y_test['SR-ARE'],np.transpose(np.matrix(y_pred_dt))))
print('test score',grid.score(X_test_pca,y_test['SR-ARE']))
```

```
DecisionTree
best mean cv score=  0.6185195808733015
best parameters=  {'criterion': 'gini', 'max_depth': 30}
[[417  69]
 [ 65  26]]
test score 0.5718694885361553
```

```
tree_clf = DecisionTreeClassifier(random_state=42)
tree_clf.fit(X_trainingdata, y_trainingdata['SR-ARE'])
y_pred_tree = tree_clf.predict(X_test)
print('DecisionTree',accuracy_score(y_test['SR-ARE'], y_pred_tree))
```

```
DecisionTree 0.7989601386481803
```

```
from sklearn.ensemble import RandomForestClassifier
from sklearn.datasets import make_classification
RFC = RandomForestClassifier()
param_grid={'n_estimators':[300],'criterion':['gini','entropy'],'max_depth':[3,4,5,6], 'max_features':['auto','sqrt','log2']
grid=GridSearchCV(RFC,param_grid=param_grid,cv=5,scoring='balanced_accuracy',return_train_score=False)
grid.fit(X_trainingdata.to_numpy().astype('float'),y_trainingdata['SR-ARE'])
print("best mean cv score= ",grid.best_score_)
print("best parameters= ",grid.best_params_)
```

```
from sklearn.ensemble import AdaBoostClassifier
from sklearn.model_selection import GridSearchCV
from sklearn.metrics import confusion_matrix,plot_confusion_matrix
Adabost = AdaBoostClassifier()
param_grid={'n_estimators':np.arange(1,100,5)}
grid=GridSearchCV(Adabost,param_grid=param_grid,cv=10,scoring='balanced_accuracy',return_train_score=False)
grid.fit(X_trainingdata_PCA.to_numpy().astype('float'),(np.transpose(y_trainingdata_PCA.to_numpy().astype('int')))[0])
print("best mean cv score= ",grid.best_score_)
print("best parameters= ",grid.best_params_)
```

```
best mean cv score=  0.5937254770114919
best parameters=  {'n_estimators': 91}
```

✓ 1s completed at 12:59 AM