Welcome to the module 6b coding part: Grading Boosted Tree!

This notebook was created at San Francisco State University (SFSU) for the Promoting INclusivity and Computing (PINC) and gSTAR programs by Dr. Pleuni Pennings (SFSU biology professor), Lucy Moctezuma Tan (California State University, East Bay CSUEB master student) and Lorena Benitez-Rivera (SFSU master students). All members of the COde to understand Drug resistance Evolution (CODE) lab in 2023.

OBJECTIVE OF THIS NOTEBOOK:

In this notebook we will learn how to create a **Gradient Boosted Tree** model using different functions that will allow us to get predicted labels for each type of drug instead of doing it one drug at a time.

The objective of this notebook is to learn how to apply what we have been learning in a more complex project, so you can think of different ways in which machine learning could be used. In this case we will try to recreate specifically some of the results from the **Gradient Boosted Tree** model that was used in Moragadivand's 2018 paper.

In this notebook you will learn:

- How to create different functions that will let us run our **Gradient Boosted Tree** model per drug and per feature combinations.
- How to link all functions together to create a cohesive workflow and get our results.

Step 1) Importing packages needed

Just like before we will be loading up the previous packages and functions we have seen so far.

```
# Data manipulation imports for ML
import pandas as pd
import numpy as np
from sklearn.model_selection import train_test_split

# Import packages for Gradient Boosted Tree model
from xgboost import XGBClassifier
from sklearn import preprocessing

# Imports for model evaluation
from sklearn import metrics
from sklearn.metrics import classification_report, confusion_matrix, ConfusionMatrixDisplay

# Imports for data visualization
```

```
import matplotlib.pyplot as plt

# Imports for file management
import os
from google.colab import drive
drive.mount('/content/drive')
```

```
Mounted at /content/drive
```

Step 2) Loading CSV file and creating dataframes for each antibiotic

a) Loading CSV created from previous notebook (6a)

Let's first load our merged dataframe, created by notebook 6a, containing each feature and labels for all our drugs. The datataframe contains:

1. **Year features as a matrix**
2. **Population structure features**
3. **Presence and absence of specific genes**

We will learn in the following steps how to select different combinations of these 3 features.

```
# Loads csv file as a dataframe
filepath= '/content/drive/MyDrive/EColi_ML_CSV_files/'
# reads csv file as a dataframe
All_Drugs_df = pd.read_csv(filepath+"EColi_Merged_dfs.csv", na_values="NaN")
All_Drugs_df.head()
```

```
<ipython-input-2-36e031182889>:4: DtypeWarning: Columns (4,5,6) have mixed types. Spe
  All_Drugs_df = pd.read_csv(filepath+"EColi_Merged_dfs.csv", na_values="NaN")
```

	Isolate	CTZ	CTX	AMP	AMX	AMC	TZP	CXM	CET	GEN	...	cutoff_25459	cutoff_
0	11657_5#10	S	S	S	NaN	S	S	S	S	S	...	0	
1	11657_5#11	S	S	R	NaN	R	S	S	S	S	...	0	
2	11657_5#12	S	S	S	NaN	S	S	S	S	S	...	0	
3	11657_5#13	S	S	R	NaN	R	S	S	S	S	...	0	
4	11657_5#14	S	S	R	NaN	S	S	S	S	S	...	0	

5 rows × 18304 columns

b) Creating dataframes for each drug

Below we will be creating the function **makeDF**, this will allow us to create one dataframe for each antibiotic drug, by joining the labels of one group and the features corresponding to it.

```
# creating a list of antibiotic names
drug_list = All_Drugs_df.iloc[:,1:13].columns
drug_list
```

```
Index(['CTZ', 'CTX', 'AMP', 'AMX', 'AMC', 'TZP', 'CXM', 'CET', 'GEN', 'TBM',
       'TMP', 'CIP'],
      dtype='object')
```

```
# creating a function that makes dataframes for each antibiotic and dropping NaN valu
def makeDF(drug):
    df_list = [All_Drugs_df[["Isolate",drug]],All_Drugs_df.iloc[:,13:]]
    Drug_df = pd.concat(df_list, axis=1)
    Drug_df = Drug_df.dropna()
    return Drug_df
```

Below we will demonstrate how **makeDF** works by creating a single dataframe using the the drug AMP that contains the labels for AMP and all the features we are interested in.

```
# implementing function using as example the drug AMP
AMP_df = makeDF("AMP")

# looking at the shape of AMP dataframe
print("AMP dataframe shape: ", AMP_df.shape)

# looking at the first 5 rows of this dataframe
AMP_df.head()
```

```
AMP dataframe shape:  (841, 18293)
```

	Isolate	AMP	Year_1970.0	Year_1977.0	Year_1994.0	Year_1997.0	Year_1998.0
0	11657_5#10	S	False	False	False	False	False
1	11657_5#11	R	False	False	False	False	False
2	11657_5#12	S	False	False	False	False	False
3	11657_5#13	R	False	False	False	False	False
4	11657_5#14	R	False	False	False	False	False

5 rows × 18293 columns

Step 3) Separating each drug dataframe into sections

The dataframe will be separated into 4 sections:

1. **Training features**

2. **Training labels**
3. **Testing features**
4. **Testing labels**

a) Creating testing and training datasets for each antibiotic drug

Below we will be creating the function **Split_train_test**, which will allow us to split the dataset of each of the dataframes created by our previous function, and store these splits into a single python dictionary. Then we will test this function by splitting only the dataframe we created before using the drug AMP.

```
# Separating each dataframe into Labels and Features
def Split_train_test(Drug_df,drug):
    Train_test_dic = {}
    labels = Drug_df[drug]
    features = Drug_df.drop(columns=[drug])
    features_train, features_test, labels_train, labels_test = train_test_split(features, la

    Train_test_dic['labels_train'] = labels_train
    Train_test_dic['features_train'] = features_train
    Train_test_dic['labels_test'] = labels_test
    Train_test_dic['features_test'] = features_test

    return Train_test_dic
```

Task 1:

Below we implement the function we just created and accessed specifically the training features of the AMP dataset. Try accessing the other three key-value pairs of this dictionary, such as the features of the testing dataset. What do you think are some of the benefits of using a dictionary to store the different parts of the dataset?

Answer to Task 1: I think that using a dictionary allows you to keep different parts of the dataset organized in a single structure, making it easier to pass around and access.And it can avoid managing separate variables for each dataset.

```
# Implementing the function Split_train_test() for AMP example
AMP_Train_test_dic = Split_train_test(AMP_df,"AMP")
AMP_Train_test_dic["features_train"]
```

	Isolate	Year_1970.0	Year_1977.0	Year_1994.0	Year_1997.0	Year_1998.0	Y
755	11658_8#26	False	False	False	False	False	
1837	24742_1#282	False	False	False	False	False	
1678	18090_8#7	False	False	False	False	False	
1520	18090_6#44	False	False	False	False	False	
1684	24742_1#103	False	False	False	False	False	
...	...	...	...	...	...	...	
266	11657_7#7	False	False	False	False	False	
392	11658_4#24	False	False	False	False	False	
761	11658_8#32	False	False	False	False	False	
1530	18090_6#54	False	False	False	False	False	
388	11658_4#20	False	False	False	False	False	

563 rows × 18292 columns

```
# Access the features testing of the dictionary
AMP_Test_features = AMP_Train_test_dic['features_test']
AMP_Test_features.head()
```

	Isolate	Year_1970.0	Year_1977.0	Year_1994.0	Year_1997.0	Year_1998.0	Y
1580	18090_7#32	False	False	False	False	False	
1912	24742_1#381	False	False	False	False	False	
100	11657_6#15	False	False	False	False	False	
1646	18090_7#94	False	False	False	False	False	
382	11658_4#15	False	False	False	False	False	

5 rows × 18292 columns

Below you can also access all the Python dictionary elements we have created for this specific AMP dataset. Below I decided to print the shape for each of the data chunks we have split.

```
# checking the shape of each dataframe or series stored in the dictionary created fo
print("AMP")
for k, df in AMP_Train_test_dic.items():
    print(k, df.shape)
```

```
AMP
labels_train (563,)
```

```
features_train (563, 18292)
labels_test (278,)
features_test (278, 18292)
```

Step 4) Creating different combination of features before training

Below we will be creating the function **combo_feat**, which will allow us to choose what are the specific combinations we want to use to train our model. As you can see we have decided to test all the ones present in the **combo_list** list.

```
# making a list of combinations of data sources we would like to test in oul
combo_list = ['G','S', 'GS', 'GYS']

# making a function that creates different feature combinations of the predictoı
def combo_feat(features_df, drug, combo):

    # creating Year column filters for features_df
    year_filter = [col for col in features_df if col.startswith("Year")]
    year_feat = features_df[year_filter]

    # creating Population structure column filters for features_df
    pop_str_filter = [col for col in features_df if col.startswith("cutoff")]
    pop_struc_feat = features_df[pop_str_filter]

    # creating Gene precence column filters for features_df
    gene_presc_filter = [col for col in features_df.columns if col not in pop_st
    gene_presc_feat = features_df[gene_presc_filter]

    if combo == 'G':
        df_list = [features_df['Isolate'], gene_presc_feat]
        G_feat_df = pd.concat(df_list, axis=1)
        G_feat_df = G_feat_df.drop(columns=['Isolate'])
        return G_feat_df

    if combo == 'S':
        df_list = [features_df['Isolate'], pop_struc_feat]
        S_feat_df = pd.concat(df_list, axis=1)
        S_feat_df = S_feat_df.drop(columns=['Isolate'])
        return S_feat_df

    if combo == 'GY':
        df_list = [features_df['Isolate'], gene_presc_feat, year_feat]
        GY_feat_df = pd.concat(df_list, axis=1)
        GY_feat_df = GY_feat_df.drop(columns=['Isolate'])
        return GY_feat_df

    if combo== "GS":
        df_list = [features_df['Isolate'], gene_presc_feat, pop_struc_feat]
        GS_feat_df = pd.concat(df_list, axis=1)
        GS_feat_df = GS_feat_df.drop(columns=['Isolate'])
        return GS_feat_df

    if combo == 'SY':
        df_list = [features_df['Isolate'], pop_struc_feat, year_feat]
        SY_feat_df = pd.concat(df_list, axis=1)
        SY_feat_df = SY_feat_df.drop(columns=['Isolate'])
        return SY_feat_df

    if combo == 'GYS':
        df_list = [features_df['Isolate'], gene_presc_feat, pop_struc_feat, year_feat
        GYS_feat_df = pd.concat(df_list, axis=1)
        GYS_feat_df = GYS_feat_df.drop(columns=['Isolate'])
        return GYS_feat_df
```

Following the example of working with a single drug AMP, we can see below that we can actually test and access a specific part of the dictionary we created in the previous step and also choose specifically what feature combination we are interested in training. In this case is **GS (Gene Presence and Absence and Population Structure)**

```
# Implementing combo_feat() function created for training data
AMP_GS_train_df = combo_feat(AMP_Train_test_dic['features_train'],"AMP","GS")

# looking only at the feature column names for the combination for "GS" for drug "
AMP_GS_train_df.columns
```

```
Index(['yeiU', 'yhhS', 'ybaE', 'eutR', 'ibrB', 'ytfP', 'aslB', 'narQ', 'tolR',
       'galM',
       ...
       'cutoff_25459', 'cutoff_25654', 'cutoff_25772', 'cutoff_25979',
       'cutoff_26792', 'cutoff_27119', 'cutoff_27236', 'cutoff_27248',
       'cutoff_27690', 'cutoff_45092'],
      dtype='object', length=18269)
```

Step 5) Creating Gradient Boosted Trees model and training it per feature combination

Below we will create another function called **run_GB** that will let us create and train our Gradient Boosted Tree, by assigning a training data (features, labels and what feature combination) we would like to train.

```
# creating Gradient Boosted Trees model function
def run_GB(feat_train_df, lab_train, drug, combo):
    labels = lab_train
    le = preprocessing.LabelEncoder()
    le.fit(labels)
    labels_t = le.transform(labels)
    print(drug +" Training combo: "+ combo)
    GB = XGBClassifier(random_state = 42)
    GB = GB.fit(feat_train_df, labels_t)
    return GB
```

Below we will test our function by:

- Using the **training features** we specified in the previously **(step 4)**.
- Getting our **training labels** from the python dictionary we created before **(step 3)**
- Specifying the feature combination we want, in this example, **GS**.

```
# implementing run_GB() for specific drug feature combination dataframe
GB_AMP_GS_model = run_GB(AMP_GS_train_df, AMP_Train_test_dic['labels_train'],"AMP","GS")
GB_AMP_GS_model
```

```
AMP Training combo: GS
```

```
XGBClassifier

XGBClassifier(base_score=None, booster=None, callbacks=None,
              colsample_bylevel=None, colsample_bynode=None,
              colsample_bytree=None, device=None, early_stopping_rounds=None,
              enable_categorical=False, eval_metric=None, feature_types=None,
              gamma=None, grow_policy=None, importance_type=None,
              interaction_constraints=None, learning_rate=None, max_bin=None,
              max_cat_threshold=None, max_cat_to_onehot=None,
              max_delta_step=None, max_depth=None, max_leaves=None,
              min_child_weight=None, missing=nan, monotone_constraints=None,
              multi_strategy=None, n_estimators=None, n_jobs=None,
              num_parallel_tree=None, random_state=42, ...)
```

Step 6) Making predictions from Gradient Boosted Trees model

We will create here another function called **predict** to make our predictions using:

- The model we trained on **(step 5)**
- Choosing the test features chunks we made from **(step 3)**

```
# creating a function using the model created and trained and the feature combinatior
def predict(GB_combo_Model, features_test):
    labels_pred = GB_combo_Model.predict(features_test)
    return labels_pred
```

Below we will be resusing our function **combo_feat** to specify that we want to use only specific features from out test dataset, because it has to be based on what our model was trained with. In this case we only want **GS combination**.

```
# Implementing combo_feat() function created for testing data
AMP_GS_test_df = combo_feat(AMP_Train_test_dic['features_test'],"AMP","GS")
```

```
# looking only at the feature column names for the combination for "GS" for drug "A
AMP_GS_test_df.columns
```

```
Index(['yeiU', 'yhhS', 'ybaE', 'eutR', 'ibrB', 'ytfP', 'aslB', 'narQ', 'tolR',
       'galM',
       ...
       'cutoff_25459', 'cutoff_25654', 'cutoff_25772', 'cutoff_25979',
       'cutoff_26792', 'cutoff_27119', 'cutoff_27236', 'cutoff_27248',
       'cutoff_27690', 'cutoff_45092'],
      dtype='object', length=18269)
```

Finally we will use our function with the correct model and correct testing dataset, where the only combination we want to make predictions with is GS. We will also print out how many did our model predict Resistance(R) and how many were predicted as Susceptible(S). In this case we got 210 Resistant E.Coli Predicted and 68 E.Coli Susceptible Predicted to the AMP drug, using only the feature combination GS.

```
# Implementation of the predict() function using the feature combination "GS"
AMP_GS_labels_pred = predict(GB_AMP_GS_model,AMP_GS_test_df)

# transforming back our labels for interpretation in the next output
labels_pred = np.where(AMP_GS_labels_pred<1,"R","S")

# observe how many predictions were made for each category "R" and "S"
print("Labels predicted: ", np.unique(labels_pred, return_counts=True))
```

```
Labels predicted:  (array(['R', 'S'], dtype='<U1'), array([210,  68]))
```

Step 7) Evaluating our model using a confusion matrix and metrics

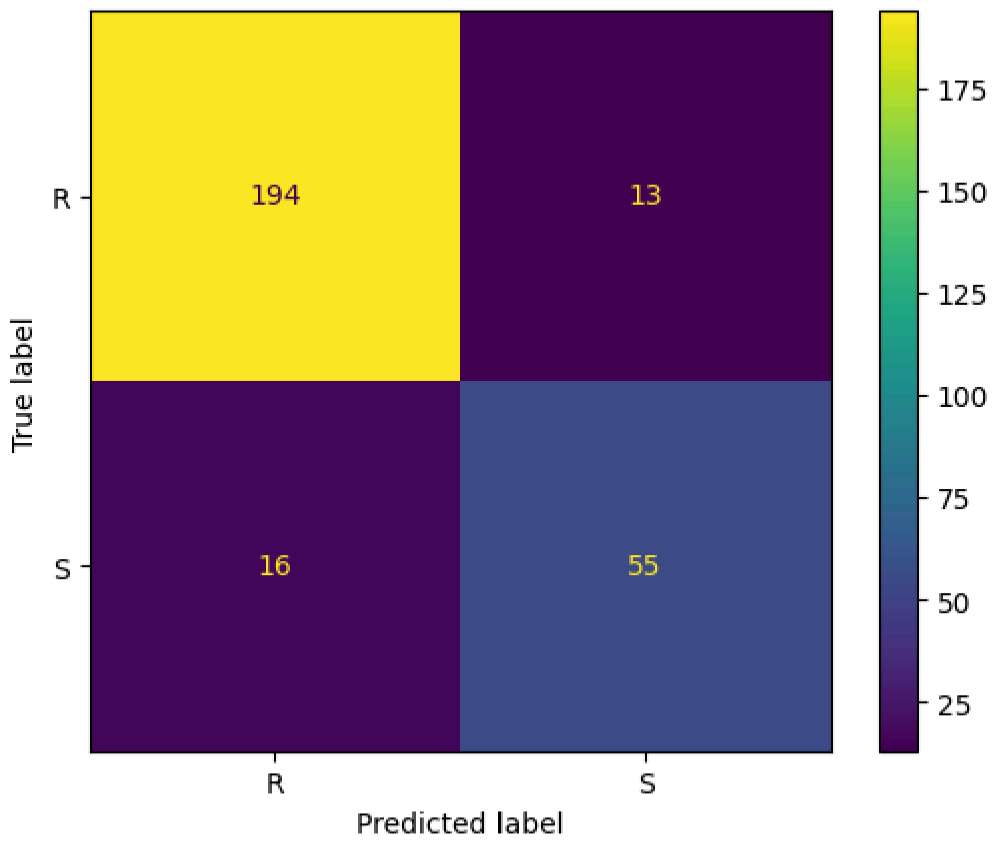
Below we create our last function **evaluate**, where we are able to extract our accuracy, f-scores for Resistant and Susceptible E.Coli, plus a Confusion Matrix. Notice that within the function, we had to convert the labels test into numbers as well in order to be able to be compared with our predicted labels.

```
# Creating a function that evaluates our model using our actual and predicted data
def evaluate(GB_combo_model, labels_test, labels_pred, cf= True):
    labels = labels_test
    le = preprocessing.LabelEncoder()
    le.fit(labels)
    labels_t = le.transform(labels)
    report = classification_report(labels_t, labels_pred, output_dict = True)
    accuracy = report['accuracy']
    R_recall = report["0"]['recall']# Resistant
    S_recall = report["1"]['recall']# Susceptible
    if cf == True:
        labels_pred = np.where(labels_pred<1,"R","S")
        cm = confusion_matrix(labels_test, labels_pred, labels=np.where(GB_combo_model.classes
        disp = ConfusionMatrixDisplay(confusion_matrix=cm, display_labels=np.where(GB_combo_moc
        disp.plot()
        plt.show()
    return [accuracy,R_recall,S_recall]
```

Below we will be testing our function using:

- The model we trained in **(step 5)**
- The test labels we separated and put into a data dictionary in **(Step 3)**
- The predicted labels that we got from **(Step 6)**

```
# implementing the evaluate() function
Model_Report = evaluate(GB_AMP_GS_model, AMP_Train_test_dic['labels_test'],AMP_GS_labels_pred)
print("Results from Model for drug: AMP")
print("Using feature combination: GS")
print("Accuracy: ", Model_Report[0])
print("R_recall: ", Model_Report[1])
print("S_recall: ", Model_Report[2])
```



```
Results from Model for drug: AMP
Using feature combination: GS
Accuracy:  0.89568345323741
R_recall:  0.9371980676328503
S_recall:  0.7746478873239436
```

Task 2:

As a review, list all the functions we have created so far in this notebook. Write a one-sentence description in your own words for each of the functions. We will use those functions in step 8.

Step 8) Use all functions and evaluate every drug in every feature combination!

Alright this is the part where we put all our created functions into use by creating a for loop, that chains each of the steps we have done so far.

Complete Task 2 here

- makeDF(drug)
- Split_train_test(Drug_df, drug)
- combo_feat(features_df, drug, combo)
- run_GB(feat_train_df, lab_train, drug, combo)
- predict(GB_combo_Model, features_test)
- evaluate(GB_combo_model, labels_test, labels_pred, cf=True)

a) Lets recall the list of drugs we have available and the combination of features we are interested in

```
# let's check all drugs
drug_list
```

```
Index(['CTZ', 'CTX', 'AMP', 'AMX', 'AMC', 'TZP', 'CXM', 'CET', 'GEN', 'TBM',
       'TMP', 'CIP'],
      dtype='object')
```

```
# let's see all combinations we are interested in
combo_list
```

```
['G', 'S', 'GS', 'GYS']
```

b) Create a loop that will go through all our functions using the lists above

Below is how we chose to chain these functions in order to get all our results and store them in a dictionary called **GB_model_metrics**. Note that this will take a long time as it is training for each drug every combination of features we have specified, so just sit back and grab something to drink as the computer does it's job. You can check the print out to see what model it's currently training.

Note: This loop will take some time to run. Lucy Moctezuma who wrote the code says it took 42 minutes when she last did it. If that is too long for you, feel free to focus on fewer of the drugs and fewer of the combintions. For example, you could loop over part of the drug_list (for drug in drug_list[:3]

```
# Lets use all our functions this time and save our report into a single data stru
GB_model_metrics = {}

for drug in drug_list:
    print(drug)
    Drug_df = makeDF(drug) # creates one df per drug
    Test_Train_dic = Split_train_test(Drug_df, drug) # splits each drug df into a dicti
    for combo in combo_list:
        # Training each drug_combo features
        labels_train = Test_Train_dic["labels_train"]
        features_train = combo_feat(Test_Train_dic["features_train"], drug, combo) # create
        GB_combo_model = run_GB(features_train, labels_train, drug, combo) # runs gradient

        # Predicting each drug_combo features
        features_test = combo_feat(Test_Train_dic["features_test"], drug, combo) # create c
        labels_pred = predict(GB_combo_model, features_test) # generate predictions based

        # Evaluating our models
        labels_test = Test_Train_dic["labels_test"]
        report = evaluate(GB_combo_model, labels_test, labels_pred, cf=False) #extracting t
        GB_model_metrics[drug+"_"+combo] = report #saving these metrics into dictionary

        print(report)
```

```
[0.9655712050078247, 0.8080808080808081, 0.9944444444444445]
GEN Training combo: S
[0.8982785602503912, 0.494949494949495, 0.9722222222222222]
GEN Training combo: GS
[0.9655712050078247, 0.797979797979798, 0.9962962962962963]
GEN Training combo: GYS
[0.9655712050078247, 0.797979797979798, 0.9962962962962963]
TBM
TBM Training combo: G
[0.9136690647482014, 0.8202247191011236, 0.9576719576719577]
TBM Training combo: S
[0.7877697841726619, 0.6067415730337079, 0.873015873015873]
TBM Training combo: GS
[0.9280575539568345, 0.8314606741573034, 0.9735449735449735]
TBM Training combo: GYS
[0.9280575539568345, 0.8314606741573034, 0.9735449735449735]
TMP
TMP Training combo: G
[0.9244604316546763, 0.9243697478991597, 0.9245283018867925]
TMP Training combo: S
[0.7194244604316546, 0.6302521008403361, 0.7861635220125787]
TMP Training combo: GS
[0.9280575539568345, 0.9243697478991597, 0.9308176100628931]
TMP Training combo: GYS
[0.935251798561151, 0.9411764705882353, 0.9308176100628931]
CIP
CIP Training combo: G
[0.9530516431924883, 0.8493150684931506, 0.9837728194726166]
CIP Training combo: S
```

c) Store the metrics report for all drugs and features combinations as a csv file

After running our code is only necessary for us to save it as a csv file, that way we can access it later on!

```
# convert dictionary into a dataframe
GB_metrics = pd.DataFrame.from_dict(GB_model_metrics, orient='index',columns=["Accuracy'
GB_metrics = GB_metrics.rename(columns = {'index':'Drug_combo'})

# saving our metric results into a CSV file
GB_metrics.to_csv(filepath+"GB_metrics_df.csv", index= False)
GB_metrics
```

	Drug_combo	Accuracy	R_recall	S_recall
0	CTZ_G	0.956182	0.764045	0.987273
1	CTZ_S	0.893584	0.449438	0.965455
2	CTZ_GS	0.951487	0.741573	0.985455
3	CTZ_GYS	0.949922	0.741573	0.983636
4	CTX_G	0.982085	0.926230	0.995935
5	CTX_S	0.928339	0.811475	0.957317
6	CTX_GS	0.977199	0.918033	0.991870
7	CTX_GYS	0.972313	0.918033	0.985772
8	AMP_G	0.895683	0.951691	0.732394
9	AMP_S	0.762590	0.888889	0.394366
10	AMP_GS	0.895683	0.937198	0.774648
11	AMP_GYS	0.913669	0.956522	0.788732
12	AMX_G	0.886740	0.892857	0.876812
13	AMX_S	0.651934	0.700893	0.572464
14	AMX_GS	0.886740	0.910714	0.847826
15	AMX_GYS	0.881215	0.906250	0.840580
16	AMC_G	0.792793	0.600000	0.877922
17	AMC_S	0.711712	0.441176	0.831169
18	AMC_GS	0.800000	0.570588	0.901299
19	AMC_GYS	0.805405	0.576471	0.906494
20	TZP_G	0.933213	0.060606	0.988484
21	TZP_S	0.918773	0.090909	0.971209
22	TZP_GS	0.929603	0.060606	0.984645
23	TZP_GYS	0.936823	0.060606	0.992322
24	CXM_G	0.881064	0.648045	0.971739
25	CXM_S	0.841941	0.625698	0.926087
26	CXM_GS	0.887324	0.659218	0.976087
27	CXM_GYS	0.885759	0.648045	0.978261
28	CET_G	0.917266	0.886957	0.938650
29	CET_S	0.848921	0.756522	0.914110
30	CET_GS	0.913669	0.869565	0.944785
31	CET_GYS	0.920863	0.869565	0.957055

32	GEN_G	0.965571	0.808081	0.994444
33	GEN_S	0.898279	0.494949	0.972222
34	GEN_GS	0.965571	0.797980	0.996296
35	GEN_GYS	0.965571	0.797980	0.996296
36	TBM_G	0.913669	0.820225	0.957672
37	TBM_S	0.787770	0.606742	0.873016
38	TBM_GS	0.928058	0.831461	0.973545
39	TBM_GYS	0.928058	0.831461	0.973545
40	TMP_G	0.924460	0.924370	0.924528
41	TMP_S	0.719424	0.630252	0.786164
42	TMP_GS	0.928058	0.924370	0.930818
43	TMP_GYS	0.935252	0.941176	0.930818
44	CIP_G	0.953052	0.849315	0.983773
45	CIP_S	0.915493	0.787671	0.953347
46	CIP_GS	0.949922	0.828767	0.985801
47	CIP_GYS	0.951487	0.842466	0.983773

後續步驟: 使用 GB_metrics生成程式碼 查看建議的圖表 New interactive sheet

d) Create a bar graph showing accuracies of all drugs when using all features (GS)

Below we will create a quick bar graph checking at how each of the drugs performed using the specific combination of GS. (Gene Absence and Presence + Population Structure)

```
# filtering for all the rows that contain GS combination only
GS_filter = [drug_combo for drug_combo in GB_metrics['Drug_combo'] if drug_combo.endswith(
GS_df = GB_metrics.loc[GB_metrics["Drug_combo"].isin(GS_filter)]



# plotting bar graph of only

# Figure Size
fig = plt.figure(figsize =(20, 8))

# Adding title
plt.title('Accuracy, R_recall and S_recall', fontsize = 12)

# Variables to be plotted
x = np.arange(len(GS_df["Drug_combo"]))
acc = list(GS_df["Accuracy"])
```

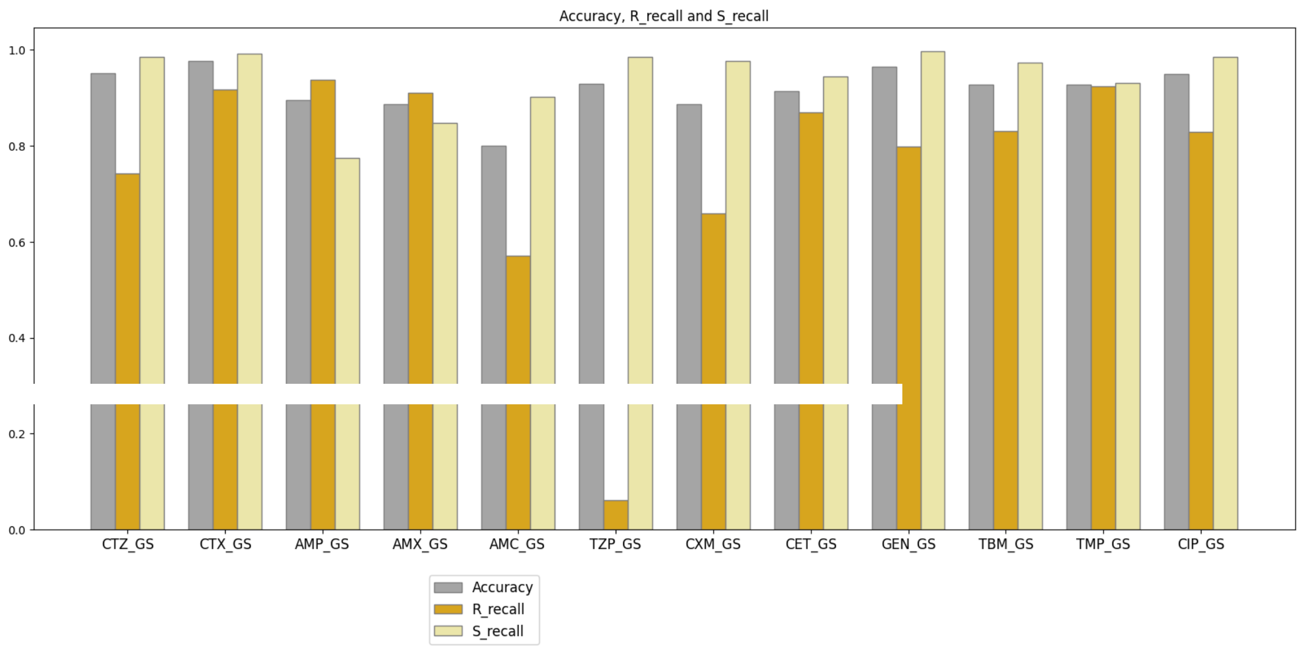
```
R_rec  =  list(GS_df["R_recall"])
S_rec  =  list(GS_df["S_recall"])

#  Plotting  barcharts
acc_bar=plt.bar(x-0.25,  height=  acc,  width=0.25,  color="darkgrey",  edgecolor="gray")
r_rec_bar=plt.bar(x,  height=  R_rec,  width=0.25,  color="goldenrod",  align="center",  edgecolor
s_rec_bar=plt.bar(x+0.25,  height=  S_rec,  width=0.25,  color="palegoldenrod",  edgecolor="gray")

plt.xticks([r  for  r  in  range(len(GS_df["Drug_combo"]))],
                GS_df["Drug_combo"],  fontsize  =  12)

#legend
fig.legend([acc_bar,r_rec_bar,s_rec_bar],["Accuracy",  "R_recall",  "S_recall"],  bbox_to_anchor=(

#  Show  Plot
plt.show()
```



Task 3:

Looking at the Graph above and the barplots for percentage resistance you made in 6A, why do you think TZP had such a high accuracy but such low Resistance Recall Score?

Answer your question here TZP's high accuracy but low Resistance Recall could be due to class imbalance in the dataset. If there are significantly more "Susceptible" (S) instances compared to "Resistant" (R) ones, the model may predict the majority class ("Susceptible") more often to optimize overall accuracy. This would result in a high accuracy score, as most predictions are correct due to the imbalance, but the recall for the minority class ("Resistant") will suffer since the model fails to correctly identify a significant number of "Resistant" cases.

Task 4:

Now that you have seen how creating different functions and stringing them together allows you to tackle a more complex project. Try to challenge yourself and do the same but using a Random Forest Model!

- Feel free to use this code as a general guide.
- Create your own functions and see if you can get as an end result to recreate the final dataframe and csv file with all the results stored.
- Remember there are many ways to tackle this problem.

```
from sklearn.ensemble import RandomForestClassifier

def run_RF(feat_train_df, lab_train, drug, combo):
        labels = lab_train
        le = preprocessing.LabelEncoder()
        le.fit(labels)
        labels_t = le.transform(labels)
        print(drug + " Training combo: " + combo)
        RF = RandomForestClassifier(random_state=42)
        RF = RF.fit(feat_train_df, labels_t)
```