HW2_MLforBio_Ensemble Methods

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ML for Bioinformatics Computer Engineering Department Homework 2: Practical - Random Forest and XGboost Bahar Oveisgharan (bahar.oveis.2000@gmail.com) Ghazal Farahani (farahaniqazal@gmail.com)

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0.0.3 Breast Cancer

Most of us know someone who struggled with breast cancer, or at least heard about the struggles facing patients who are fighting against breast cancer.The most important part of a process of clinical decision-making in patients with cancers, in general, is the accurate estimation of prognosis and survival duration. Breast cancer patients with the same stage of the disease and the same clinical characteristics can have different treatment responses and overall survival. In this practical assignment, you are going to train a Random Forest and XGBoost model on breast_cancer.csv dataset.

Import all the libraries you may need here

[ ]:
```
import sklearn
import pandas as pd
import xgboost as xgb
```

Loading the Data

[ ]:
```
from sklearn import set_config

set_config(transform_output="pandas")
pd.set_option("display.max_columns", None)
pd.set_option("display.expand_frame_repr", False)
pd.set_option("max_colwidth", None)

# Load the dataset into a pandas dataframe
df = pd.read_csv("breast_cancer.csv")
```

0.0.4 Data Exploration

Let's start off by exploring the files we just imported. it's not necessary to do any visualization just a statistical summary of the data would be enough. split your data to train and test.

[ ]:
```python
from sklearn.model_selection import train_test_split


X = df.drop("overall_survival", axis=1)
y = df["overall_survival"]
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.2, random_state=92847
)

# Display a statistical summary of the data
print("Training set summary:")
print(X_train.describe())
print("*" * 20)
print("Test set summary:")
print(X_test.describe())
```

```
Training set summary:
       Unnamed: 0  age_at_diagnosis  chemotherapy       cohort
neoplasm_histologic_grade  hormone_therapy  lymph_nodes_examined_positive
mutation_count  nottingham_prognostic_index  radio_therapy   tumor_size
tumor_stage
count  1523.00000       1523.000000   1523.000000  1523.000000
1523.000000      1523.000000                    1523.000000     1523.000000
1523.000000     1523.000000  1523.000000  1523.000000
mean    959.58306         61.128431      0.210112     2.655942
2.415709         0.621799                       2.017728        5.782804
4.034162         0.598162     26.255389     1.752605
std     552.72670         12.956723      0.407521     1.222789
0.635067         0.485097                       4.109420        4.160442
1.132175         0.490431     15.103027     0.546869
min       1.00000         21.930000      0.000000     1.000000
1.000000         0.000000                       0.000000        1.000000
1.000000         0.000000      1.000000     0.000000
25%     486.50000         51.620000      0.000000     2.000000
2.000000         0.000000                       0.000000        3.000000
3.050000         0.000000     17.950000     1.000000
50%     960.00000         61.890000      0.000000     3.000000
2.415939         1.000000                       0.000000        5.000000
4.042000         1.000000     23.000000     1.750535
75%    1441.50000         70.520000      0.000000     3.000000
3.000000         1.000000                       2.000000        7.000000
5.040000         1.000000     30.000000     2.000000
max    1903.00000         96.290000      1.000000     5.000000
```

```
3.000000         1.000000                     45.000000       80.000000
6.360000       1.000000   182.000000     4.000000
********************
Test set summary:
        Unnamed: 0  age_at_diagnosis  chemotherapy      cohort
neoplasm_histologic_grade  hormone_therapy  lymph_nodes_examined_positive
mutation_count  nottingham_prognostic_index  radio_therapy  tumor_size
tumor_stage
count   381.000000        381.000000    381.000000  381.000000
381.000000       381.000000                    381.000000      381.000000
381.000000     381.000000  381.000000   381.000000
mean    919.188976         60.921654      0.199475    2.595801
2.416859         0.595801                      1.939633        5.357444
4.028447       0.593176   26.172119     1.742256
std     537.347659         13.082049      0.400131    1.252107
0.651345         0.491382                      3.964849        3.327810
1.193983       0.491887   15.012701     0.511646
min       0.000000         26.720000      0.000000    1.000000
1.000000         0.000000                      0.000000        1.000000
1.020000       0.000000    1.000000     0.000000
25%     451.000000         50.750000      0.000000    1.000000
2.000000         0.000000                      0.000000        3.000000
3.040000       0.000000   17.000000     1.750535
50%     915.000000         60.960000      0.000000    3.000000
2.415939         1.000000                      0.000000        5.000000
4.046000       1.000000   24.000000     2.000000
75%    1372.000000         71.110000      0.000000    3.000000
3.000000         1.000000                      2.000000        7.000000
5.050000       1.000000   30.000000     2.000000
max    1896.000000         92.140000      1.000000    5.000000
3.000000         1.000000                     41.000000       23.000000
6.300000       1.000000  150.000000     3.000000
```

0.0.5 Data Preparation

Creating two custom transformers to put on our pipeline:

- To split the data into categorical and numerical features and
- To preprocess the categorical features.
- Create the X feature matrix and the y target vector.
- split the data.

[ ]:
```
import pandas as pd
from sklearn.base import BaseEstimator, TransformerMixin
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler, OneHotEncoder, Normalizer
from sklearn.compose import ColumnTransformer, make_column_selector
from sklearn.model_selection import train_test_split
```

```python
# Load the dataset into a pandas dataframe
df = pd.read_csv("breast_cancer.csv").dropna()


# Define custom transformers
class CategoricalFeatureSelector(BaseEstimator, TransformerMixin):
    def __init__(self):
        pass

    def fit(self, X, y=None):
        return self

    def transform(self, X):
        return X.select_dtypes(include=["object"])


class CategoricalPreprocessor(BaseEstimator, TransformerMixin):
    def __init__(self):
        pass

    def fit(self, X, y=None):
        return self

    def transform(self, X):
        ohe = OneHotEncoder(
            handle_unknown="ignore", sparse_output=False, drop="if_binary"
        )
        return ohe.fit_transform(X)


# Create X feature matrix and y target vector
X = df.drop("overall_survival", axis=1)
y = df["overall_survival"]


# Split the data into training and testing sets
X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.2, random_state=92847
)

# Define the preprocessing pipeline
categorical_pipeline = Pipeline(
    [
        ("cat_selector", CategoricalFeatureSelector()),
        ("cat_preprocessor", CategoricalPreprocessor()),
        ("normalizer", Normalizer()),
```

```python
    ]
)

numerical_pipeline = Pipeline(
    [
        ("scaler", StandardScaler()),
    ]
)

preprocessor = ColumnTransformer(
    transformers=[
        ("cat", categorical_pipeline, X.columns),
        ("num", numerical_pipeline,␣
 ↪make_column_selector(dtype_exclude="object")),
    ],
    verbose_feature_names_out=False,
)


X_preprocessed = preprocessor.fit_transform(X, y)
y_preprocessed = y

(
    X_train_preprocessed,
    X_test_preprocessed,
    y_train_preprocessed,
    y_test_preprocessed,
) = train_test_split(X_preprocessed, y_preprocessed, test_size=0.2,␣
 ↪random_state=92847)

X_preprocessed.head()
```

[ ]:

```
   type_of_breast_surgery_MASTECTOMY  cancer_type_detailed_Breast
cancer_type_detailed_Breast Invasive Ductal Carcinoma
cancer_type_detailed_Breast Invasive Lobular Carcinoma
cancer_type_detailed_Breast Invasive Mixed Mucinous Carcinoma
cancer_type_detailed_Breast Mixed Ductal and Lobular Carcinoma  cellularity_High
cellularity_Low  cellularity_Moderate  pam50_+_claudin-low_subtype_Basal
pam50_+_claudin-low_subtype_Her2  pam50_+_claudin-low_subtype_LumA
pam50_+_claudin-low_subtype_LumB  pam50_+_claudin-low_subtype_NC
pam50_+_claudin-low_subtype_Normal  pam50_+_claudin-low_subtype_claudin-low
er_status_measured_by_ihc_Positve  er_status_Positive
her2_status_measured_by_snp6_GAIN  her2_status_measured_by_snp6_LOSS
her2_status_measured_by_snp6_NEUTRAL  her2_status_measured_by_snp6_UNDEF
her2_status_Positive  tumor_other_histologic_subtype_Ductal/NST
tumor_other_histologic_subtype_Lobular  tumor_other_histologic_subtype_Medullary
tumor_other_histologic_subtype_Mixed  tumor_other_histologic_subtype_Mucinous
```

```
tumor_other_histologic_subtype_Other  tumor_other_histologic_subtype_Tubular/
cribriform  inferred_menopausal_state_Pre  integrative_cluster_1
integrative_cluster_10  integrative_cluster_2  integrative_cluster_3
integrative_cluster_4ER+  integrative_cluster_4ER-  integrative_cluster_5
integrative_cluster_6  integrative_cluster_7  integrative_cluster_8
integrative_cluster_9  primary_tumor_laterality_Right  oncotree_code_BREAST
oncotree_code_IDC  oncotree_code_ILC  oncotree_code_IMMC  oncotree_code_MDLC
pr_status_Positive  3-gene_classifier_subtype_ER+/HER2- High Prolif
3-gene_classifier_subtype_ER+/HER2- Low Prolif
3-gene_classifier_subtype_ER-/HER2-  3-gene_classifier_subtype_HER2+  Unnamed: 0
age_at_diagnosis  chemotherapy   cohort  neoplasm_histologic_grade
hormone_therapy  lymph_nodes_examined_positive  mutation_count
nottingham_prognostic_index  radio_therapy  tumor_size  tumor_stage
1                           0.000000                          0.0
0.277350                                              0.000000
0.0                                                       0.00000
0.277350              0.0               0.000000
0.0                          0.000000                            0.27735
0.000000                            0.0                                   0.0
0.0                           0.277350            0.277350
0.000000                          0.000000
0.277350                                0.0                   0.0
0.277350                               0.000000
0.0                              0.00000
0.0                                  0.0
0.0                        0.27735                    0.0
0.0                   0.0               0.000000                    0.27735
0.0                   0.0                    0.0               0.000000
0.0              0.000000                       0.277350                   0.0
0.277350          0.000000                0.0             0.00000
0.277350                                       0.277350
0.0                                 0.0                                0.0
-1.787999        -1.382285     -0.505135 -1.327344                   0.918582
0.787699                     -0.502713       -0.903557
-0.011661       0.825479   -1.068241    -1.367789
4                           0.277350                          0.0
0.000000                                              0.000000
0.0                                                       0.27735
0.277350              0.0               0.000000
0.0                          0.000000                            0.00000
0.277350                            0.0                                   0.0
0.0                           0.277350            0.277350
0.000000                          0.000000
0.277350                                0.0                   0.0
0.000000                               0.000000
0.0                              0.27735
0.0                                  0.0
```

```
0.0          0.00000          0.0
0.0          0.0          0.000000          0.00000
0.0          0.0          0.0          0.000000
0.0          0.277350          0.277350          0.0
0.000000          0.000000          0.0          0.27735
0.277350          0.277350
0.0          0.0          0.0
-1.782329          1.210528          1.979670 -1.327344          0.918582
0.787699          1.564581          -0.903557
1.802388          0.825479          0.891764          0.449647
5          0.288675          0.0
0.288675          0.000000
0.0          0.00000
0.000000          0.0          0.288675
0.0          0.000000          0.00000
0.288675          0.0          0.0
0.0          0.288675          0.288675
0.000000          0.000000
0.288675          0.0          0.0
0.288675          0.000000
0.0          0.00000
0.0          0.0
0.0          0.00000          0.0
0.0          0.0          0.000000          0.00000
0.0          0.0          0.0          0.288675
0.0          0.000000          0.000000          0.0
0.288675          0.000000          0.0          0.00000
0.288675          0.288675
0.0          0.0          0.0
-1.780440          1.348689          -0.505135 -1.327344          0.918582
0.787699          -0.502713          -0.419821
0.025324          0.825479          0.303762          4.084519
8          0.000000          0.0
0.301511          0.000000
0.0          0.00000
0.000000          0.0          0.301511
0.0          0.000000          0.00000
0.301511          0.0          0.0
0.0          0.301511          0.301511
0.301511          0.000000
0.000000          0.0          0.0
0.301511          0.000000
0.0          0.00000
0.0          0.0
0.0          0.00000          0.0
0.0          0.0          0.000000          0.00000
0.0          0.0          0.0          0.000000
```

```
0.0                 0.301511                                0.301511                          0.0
0.301511             0.000000                         0.0              0.00000
0.000000                                                  0.301511
0.0                                    0.0                                       0.0
-1.774770            1.935104      -0.505135 -1.327344                           0.918582
0.787699                          -0.244301        -0.419821
0.879512        0.825479    -0.676240      0.449647
9                           0.316228                           0.0
0.000000                                                         0.316228
0.0                                                                  0.00000
0.316228              0.0                0.000000
0.0                          0.316228                                0.00000
0.000000                               0.0                                  0.0
0.0                               0.000000             0.316228
0.000000                               0.316228
0.000000                                     0.0                     0.0
0.000000                                       0.316228
0.0                                   0.00000
0.0                                       0.0
0.0                         0.00000                         0.0
0.0                     0.0                  0.316228                    0.00000
0.0                     0.0                       0.0                0.000000
0.0                 0.000000                                0.000000                          0.0
0.000000             0.316228                         0.0              0.00000
0.000000                                                  0.316228
0.0                                    0.0                                       0.0
-1.772880            1.767008      -0.505135 -1.327344                          -0.654582
-1.269521                          -0.502713        -0.177952
-0.860566       -1.211418     0.107762      0.449647
```

1 Implementing two different models

1.1 Random Forest

1.1.1 train the model

[ ]:
```python
# Train a Random Forest model on the preprocessed data
from sklearn.ensemble import RandomForestClassifier

# We will store the accurary report of different models in this dictionary
model_comparison_dict = {}

rf_model = RandomForestClassifier(n_estimators=100, random_state=92847)
rf_model.fit(X_train_preprocessed, y_train_preprocessed)
```

[ ]:
```
RandomForestClassifier(random_state=92847)
```

1.1.2 Model assessment

Print Train Accuracy, Test Accuracy and classification Report.

[ ]:
```
from sklearn.metrics import classification_report

# For train set
y_train_pred = rf_model.predict(X_train_preprocessed)

train_clf_report = classification_report(
    y_train_preprocessed, y_train_pred, output_dict=True
)
pd.DataFrame(train_clf_report)
```

[ ]:

	0	1	accuracy	macro avg	weighted avg
precision	1.0	1.0	1.0	1.0	1.0
recall	1.0	1.0	1.0	1.0	1.0
f1-score	1.0	1.0	1.0	1.0	1.0
support	674.0	542.0	1.0	1216.0	1216.0

[ ]:
```
# For test set
from sklearn.metrics import accuracy_score


y_test_pred = rf_model.predict(X_test_preprocessed)

vanilla_rf_score = accuracy_score(y_test_preprocessed, y_test_pred)
model_comparison_dict['DefaultRandomForest'] = vanilla_rf_score

test_clf_report = classification_report(
    y_test_preprocessed, y_test_pred, output_dict=True
)
pd.DataFrame(test_clf_report)
```

[ ]:

	0	1	accuracy	macro avg	weighted avg
precision	0.756757	0.596639	0.694079	0.676698	0.695659
recall	0.744681	0.612069	0.694079	0.678375	0.694079
f1-score	0.750670	0.604255	0.694079	0.677463	0.694801
support	188.000000	116.000000	0.694079	304.000000	304.000000

1.1.3 Hyperparameter tuning :

Randomized Search Cross Validation and Grid Search Cross Validation report best hyperparameters in each part.

[ ]:
```
# Define the parameter grid for Randomized Search Cross Validation
from sklearn.metrics import classification_report, accuracy_score
from sklearn.model_selection import GridSearchCV, RandomizedSearchCV
```

```python
param_distributions = {
    "n_estimators": [50, 200, 500],
    "max_depth": [None, 3, 5, 10, 15],
    "min_samples_split": [2, 5, 10],
    "min_samples_leaf": [1, 2, 4, 8],
    "max_features": ["sqrt", "log2", None],
    "bootstrap": [True, False],
}

# Perform Randomized Search Cross Validation to find the best hyperparameters
rf_random = RandomizedSearchCV(
    estimator=RandomForestClassifier(random_state=92847),
    param_distributions=param_distributions,
    n_iter=100,
    cv=5,
    random_state=92847,
    n_jobs=-1,
    verbose=1,
    refit=True,
)
rf_random.fit(X_train_preprocessed, y_train_preprocessed)
print("Randomized Search CV best parameters:", rf_random.best_params_)
print("Randomized Search CV best score:", rf_random.best_score_)
```

```
Fitting 5 folds for each of 100 candidates, totalling 500 fits
Randomized Search CV best parameters: {'n_estimators': 200, 'min_samples_split':
2, 'min_samples_leaf': 8, 'max_features': None, 'max_depth': 5, 'bootstrap':
True}
Randomized Search CV best score: 0.709748364028874
```

[ ]:
```python
# Define the parameter grid for Grid Search Cross Validation
param_grid = {
    "n_estimators": [100, 150, 200],
    "max_depth": [None, 10, 15],
    "min_samples_split": [2, 5],
    "min_samples_leaf": [1, 2],
    "max_features": ["sqrt", "log2"],
}

# Perform Grid Search Cross Validation to find the best hyperparameters
rf_grid = GridSearchCV(
    estimator=RandomForestClassifier(random_state=38294),
    param_grid=param_grid,
    cv=5,
    n_jobs=-1,
    verbose=1,
```

```
    refit=True,
)
rf_grid.fit(X_train_preprocessed, y_train_preprocessed)
print("Grid Search CV best parameters:", rf_grid.best_params_)
print("Grid Search CV best score:", rf_grid.best_score_)
```

```
Fitting 5 folds for each of 72 candidates, totalling 360 fits
Grid Search CV best parameters: {'max_depth': 10, 'max_features': 'log2',
'min_samples_leaf': 1, 'min_samples_split': 2, 'n_estimators': 100}
Grid Search CV best score: 0.7064966605950213
```

[ ]:
```
# Make predictions on the test data using the trained model with best␣
↪hyperparameters
rf_best_cv = rf_grid if rf_grid.best_score_ > rf_random.best_score_ else␣
↪rf_random

rf_best_model = RandomForestClassifier(**rf_best_cv.best_params_,␣
↪random_state=92847)
rf_best_model.fit(X_train_preprocessed, y_train_preprocessed)
y_test_pred = rf_best_model.predict(X_test_preprocessed)

gs_rf_score = accuracy_score(y_test_preprocessed, y_test_pred)
model_comparison_dict['GridSearchRandomForest'] = gs_rf_score

pd.DataFrame(classification_report(y_test_preprocessed, y_test_pred,␣
↪output_dict=True))
```

[ ]:

	0	1	accuracy	macro avg	weighted avg
precision	0.752747	0.581967	0.684211	0.667357	0.687581
recall	0.728723	0.612069	0.684211	0.670396	0.684211
f1-score	0.740541	0.596639	0.684211	0.668590	0.685631
support	188.000000	116.000000	0.684211	304.000000	304.000000

[ ]:
```
# Comparison between RF model with default parameters, and RF model obtained
# using the best of grid search and randomized grid search
pd.DataFrame(model_comparison_dict, index=['Accuracy'])
```

[ ]:

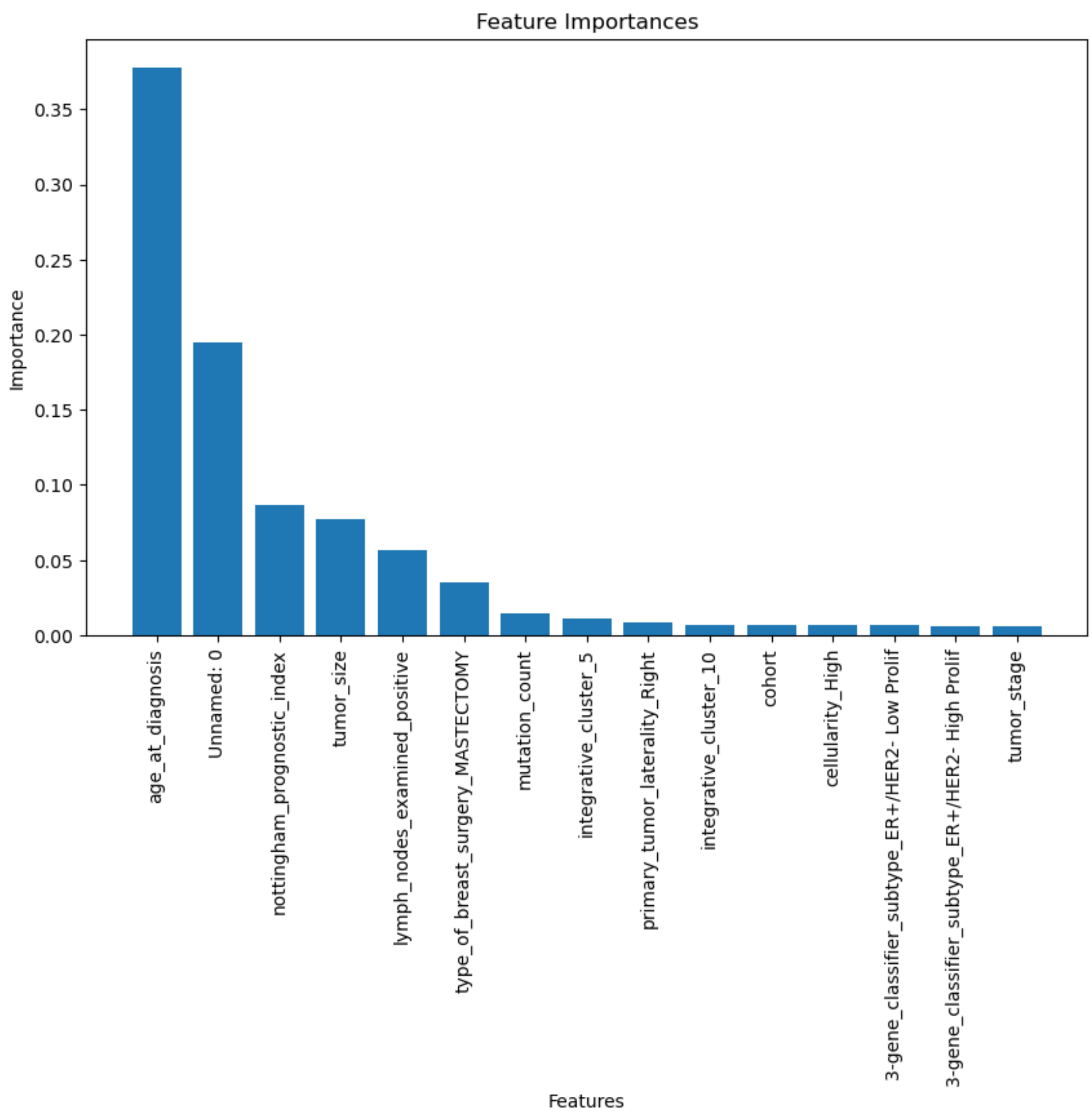
	DefaultRandomForest	GridSearchRandomForest
Accuracy	0.694079	0.684211

1.1.4 Find important features with Random Forest model

Visualize feature scores of the features

[ ]:
```
from matplotlib import pyplot as plt



# Get the feature importances and sort them in descending order
feature_importances = pd.DataFrame(
```

```
    rf_best_model.feature_importances_,
    index=X_preprocessed.columns,
    columns=["importance"],
).sort_values("importance", ascending=False)
feature_importances = feature_importances.iloc[:15,]

# Visualize the feature importances as a bar plot
plt.figure(figsize=(10, 6))
plt.bar(feature_importances.index, feature_importances["importance"])
plt.xticks(rotation=90)
plt.xlabel("Features")
plt.ylabel("Importance")
plt.title("Feature Importances")
plt.show()
```



1.1.5 * Improve Model (Bonus)

In this bonus part, you can add your ideas for improving your model's performance. implement it and compare the results.

We use bagging ensemble method. Bagging can reduce the variance of the model by training multiple instances of the same model on different subsets of the data and aggregating their predictions.

As you can see in the classification report, the model marginally outperforms the previous best one that was obtained using grid search.

[ ]:
```
from sklearn.decomposition import PCA
from sklearn.ensemble import BaggingClassifier
from sklearn.metrics import accuracy_score

bagging_model = BaggingClassifier(
    estimator=rf_best_model, n_estimators=100, n_jobs=-1, verbose=1,␣
 ↪random_state=92847
)
bagging_model.fit(X_train_preprocessed, y_train_preprocessed)

# Get the accuracy of the model on the test data
y_pred = bagging_model.predict(X_test_preprocessed)
improvevd_rf_accuracy = accuracy_score(y_test_preprocessed, y_pred)
model_comparison_dict['ImprovedRandomForest'] = improvevd_rf_accuracy

improved_rf_clf_report = classification_report(y_test_preprocessed, y_pred,␣
 ↪output_dict=True)
pd.DataFrame(improved_rf_clf_report)
```

```
[Parallel(n_jobs=8)]: Using backend LokyBackend with 8 concurrent workers.
[Parallel(n_jobs=8)]: Done   2 out of   8 | elapsed:   39.8s remaining:  2.0min
[Parallel(n_jobs=8)]: Done   8 out of   8 | elapsed:   45.7s finished
[Parallel(n_jobs=8)]: Using backend LokyBackend with 8 concurrent workers.
[Parallel(n_jobs=8)]: Done   2 out of   8 | elapsed:    1.8s remaining:    5.7s
[Parallel(n_jobs=8)]: Done   8 out of   8 | elapsed:    5.7s finished
```

[ ]:

	0	1	accuracy	macro avg	weighted avg
precision	0.769231	0.606557	0.703947	0.687894	0.707158
recall	0.744681	0.637931	0.703947	0.691306	0.703947
f1-score	0.756757	0.621849	0.703947	0.689303	0.705279
support	188.000000	116.000000	0.703947	304.000000	304.000000

[ ]:
```
# Compare the performance of the models trained so far
pd.DataFrame(model_comparison_dict, index=['Accuracy'])
```

[ ]:

	DefaultRandomForest	GridSearchRandomForest	ImprovedRandomForest
Accuracy	0.694079	0.684211	0.703947

1.2 XGBoost

1.2.1 Train the model

[ ]:
```
import pandas as pd
import xgboost as xgb
from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score

# Convert the data to an XGBoost DMatrix
dtrain = xgb.DMatrix(X_train_preprocessed, label=y_train_preprocessed)
dtest = xgb.DMatrix(X_test_preprocessed, label=y_test_preprocessed)

# Set the XGBoost parameters
params = {
    "max_depth": 3,
    "eta": 0.1,
    "objective": "binary:logistic",
    "eval_metric": "error",
}

# Train the XGBoost model
num_rounds = 100
xgb_model = xgb.train(params, dtrain, num_rounds)

# Make predictions on the test data
y_pred = xgb_model.predict(dtest)
y_pred_binary = [round(pred) for pred in y_pred]

# Evaluate the accuracy of the model on the test data
vanilla_xgb_accuracy = accuracy_score(y_test_preprocessed, y_pred_binary)

print(f"Accuracy of XGBoost Model: {vanilla_xgb_accuracy}")
```

```
Accuracy of XGBoost Model: 0.6842105263157895
```

1.2.2 Model assessment

Print Train Accuracy, Test Accuracy and classification Report.

[ ]:
```
# Accuracy and Classification Report for Train Data
import pandas as pd
import xgboost as xgb
from sklearn.model_selection import train_test_split
from sklearn.metrics import accuracy_score, classification_report
```

```
y_train_pred = xgb_model.predict(dtrain)
y_train_pred_binary = [round(pred) for pred in y_train_pred]

# Evaluate the accuracy of the model on the train data
train_accuracy = accuracy_score(y_train_preprocessed, y_train_pred_binary)

print("Train Accuracy:", train_accuracy)

# Print the classification report
clf_report_train = classification_report(
    y_train_preprocessed, y_train_pred_binary, output_dict=True
)
pd.DataFrame(clf_report_train)
```

```
Train Accuracy: 0.8297697368421053
```

[ ]:

	0	1	accuracy	macro avg	weighted avg
precision	0.832148	0.826511	0.82977	0.829329	0.829635
recall	0.867953	0.782288	0.82977	0.825120	0.829770
f1-score	0.849673	0.803791	0.82977	0.826732	0.829223
support	674.000000	542.000000	0.82977	1216.000000	1216.000000

[ ]:

```
# Evaluate the accuracy of the model on the test data
test_accuracy = accuracy_score(y_test_preprocessed, y_pred_binary)

print("Test Accuracy:", test_accuracy)

# Print the classification report
clf_report_test = classification_report(
    y_test_preprocessed, y_pred_binary, output_dict=True
)
pd.DataFrame(clf_report_test)
```

```
Test Accuracy: 0.6842105263157895
```

[ ]:

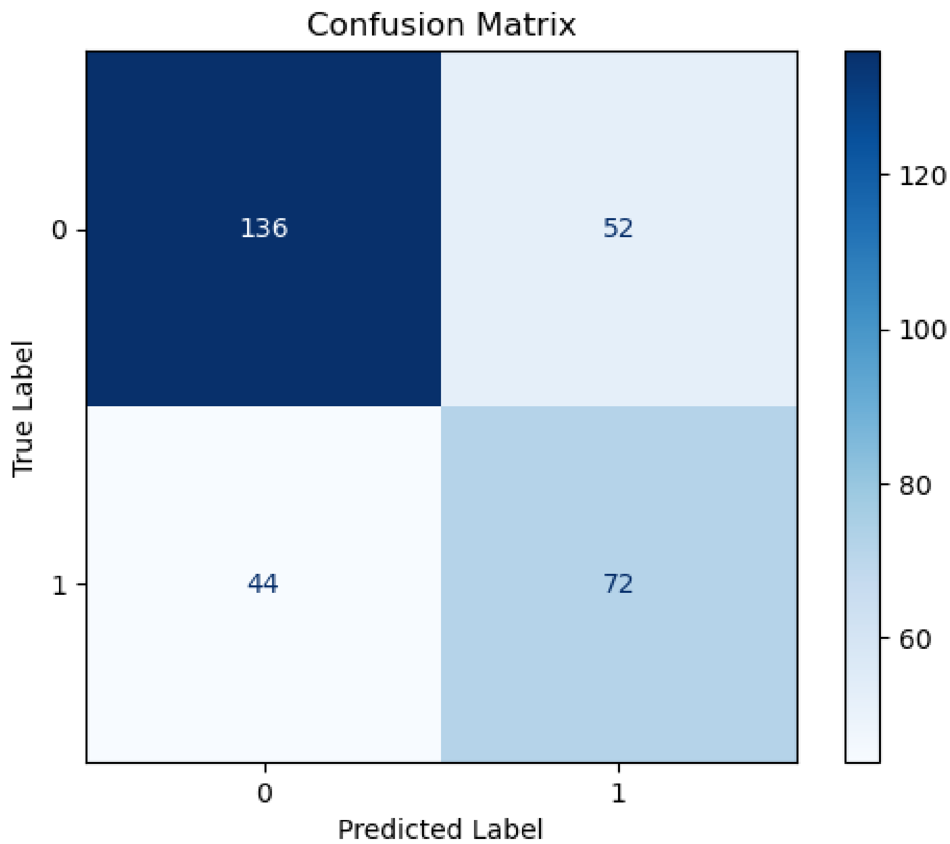
	0	1	accuracy	macro avg	weighted avg
precision	0.755556	0.580645	0.684211	0.668100	0.688813
recall	0.723404	0.620690	0.684211	0.672047	0.684211
f1-score	0.739130	0.600000	0.684211	0.669565	0.686041
support	188.000000	116.000000	0.684211	304.000000	304.000000

1.2.3 Plot the results

[ ]:

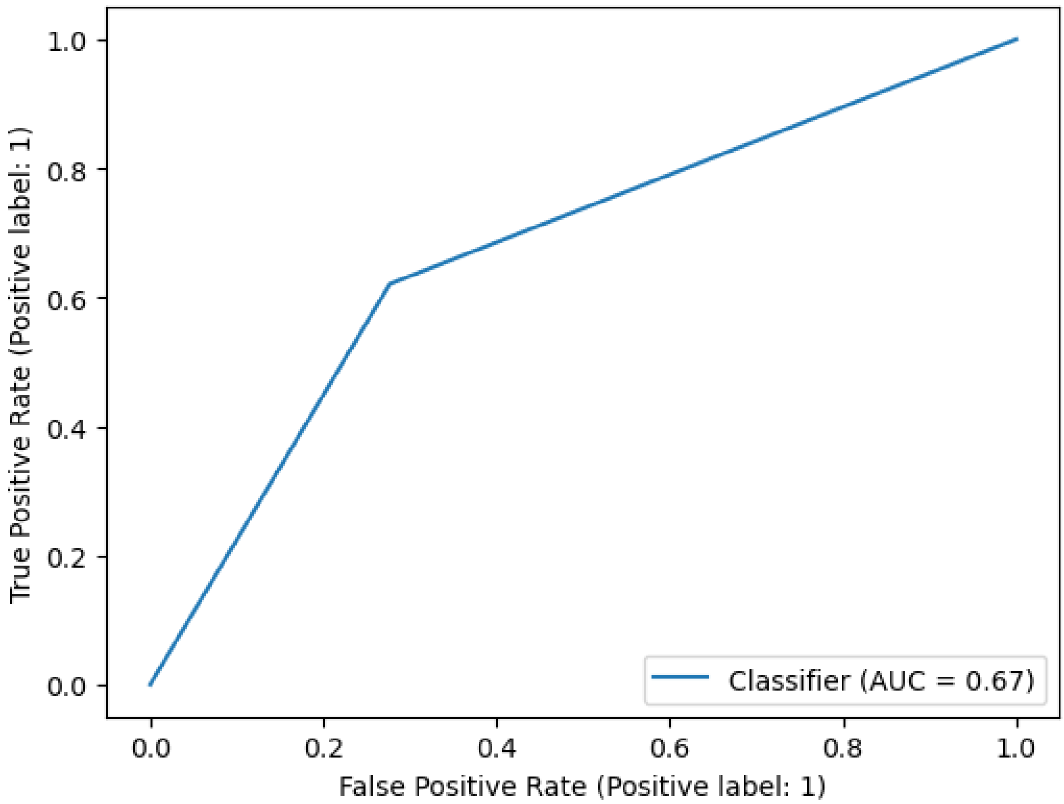
```
import pandas as pd
import xgboost as xgb
from sklearn.model_selection import train_test_split
from sklearn.metrics import ConfusionMatrixDisplay, RocCurveDisplay,␣
 ↪confusion_matrix
```

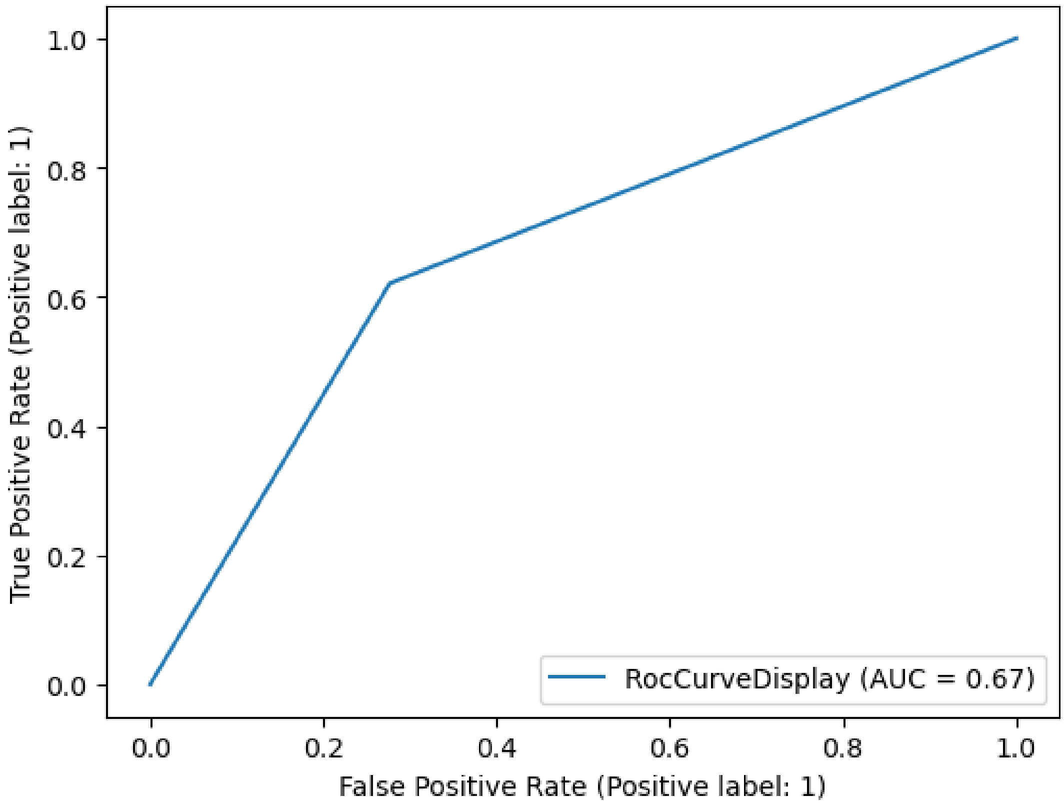
```python
cm = confusion_matrix(y_test_preprocessed, y_pred_binary)
disp = ConfusionMatrixDisplay(confusion_matrix=cm)

# plot confusion matrix
disp.plot(cmap="Blues")

# add title and axis labels
plt.title("Confusion Matrix")
plt.xlabel("Predicted Label")
plt.ylabel("True Label")
plt.show()
```



[ ]:
```python
from sklearn.metrics import RocCurveDisplay

disp_roc_curve = RocCurveDisplay.from_predictions(
    y_true=y_test_preprocessed, y_pred=y_pred_binary
)

# plot roc curve
```

```
disp_roc_curve.plot(name="RocCurveDisplay")

plt.show()
```





1.2.4 Hyperparameter tuning: Grid Search and Cross validation

- create a default XGBoost classifier.
- create the Kfold object. You can use tratifiedKFold from sklearn.model_selection.
- create the grid search object. You can use RandomizedSearchCV from sklearn.model_selection.
- fit grid search.

[ ]:
```
import pandas as pd
import xgboost as xgb
from sklearn.model_selection import StratifiedKFold, RandomizedSearchCV

# Create DMatrix
x_DMatrix = xgb.DMatrix(X_preprocessed, label=y_preprocessed)

# Define the hyperparameter grid for RandomizedSearchCV
param_grid = {
    "max_depth": [3, 5, 7, 9],
    "learning_rate": [0.01, 0.1, 0.5, 1],
    "n_estimators": [50, 100, 200, 500],
    "gamma": [0, 0.1, 0.5, 1],
```

```
    "subsample": [0.5, 0.7, 1],
    "colsample_bytree": [0.5, 0.7, 1],
    "reg_alpha": [0, 0.1, 0.5, 1],
    "reg_lambda": [0, 0.1, 0.5, 1],
}

# Create the grid search object
grid_search = RandomizedSearchCV(
    estimator=xgb.XGBClassifier(),
    param_distributions=param_grid,
    n_iter=100,
    cv=5,
    n_jobs=-1,
    random_state=92847,
    refit=True,
    verbose=1,
)

# Fit the grid search object
grid_search.fit(X_train_preprocessed, y_train_preprocessed)

# Print the best hyperparameters and accuracy score
print("Best Hyperparameters:", grid_search.best_params_)
print("Best Score:", grid_search.best_score_)
```

```
Fitting 5 folds for each of 100 candidates, totalling 500 fits
Best Hyperparameters: {'subsample': 0.5, 'reg_lambda': 0.1, 'reg_alpha': 1,
'n_estimators': 50, 'max_depth': 9, 'learning_rate': 0.01, 'gamma': 0.5,
'colsample_bytree': 0.7}
Best Score: 0.7081157660392633
```

1.2.5 Assessing model performance using the best model from grid search

Print Train Accuracy, Test Accuracy and Classification Report.

[ ]:
```
import pandas as pd
import xgboost as xgb
from sklearn.metrics import accuracy_score, classification_report

# Get the best model from grid search
xgb_best_model = xgb.XGBClassifier(**grid_search.best_params_)
xgb_best_model.fit(X_train_preprocessed, y_train_preprocessed)

# Make predictions on the train and test data using the best model
y_train_pred = xgb_best_model.predict(X_train_preprocessed)
y_test_pred = xgb_best_model.predict(X_test_preprocessed)

# Evaluate the accuracy of the model on the train and test data
train_accuracy = accuracy_score(y_train_preprocessed, y_train_pred)
```

```python
test_accuracy = accuracy_score(y_test_preprocessed, y_test_pred)

print("Train Accuracy:", train_accuracy)
print("Test Accuracy:", test_accuracy)

model_comparison_dict['GridSearchXGB'] = test_accuracy

# Print the classification report
xgb_clf_report = classification_report(
    y_test_preprocessed, y_test_pred, output_dict=True
)
pd.DataFrame(xgb_clf_report)
```

```
Train Accuracy: 0.8445723684210527
Test Accuracy: 0.6973684210526315
```

[ ]:

	0	1	accuracy	macro avg	weighted avg
precision	0.742424	0.613208	0.697368	0.677816	0.693118
recall	0.781915	0.560345	0.697368	0.671130	0.697368
f1-score	0.761658	0.585586	0.697368	0.673622	0.694472
support	188.000000	116.000000	0.697368	304.000000	304.000000

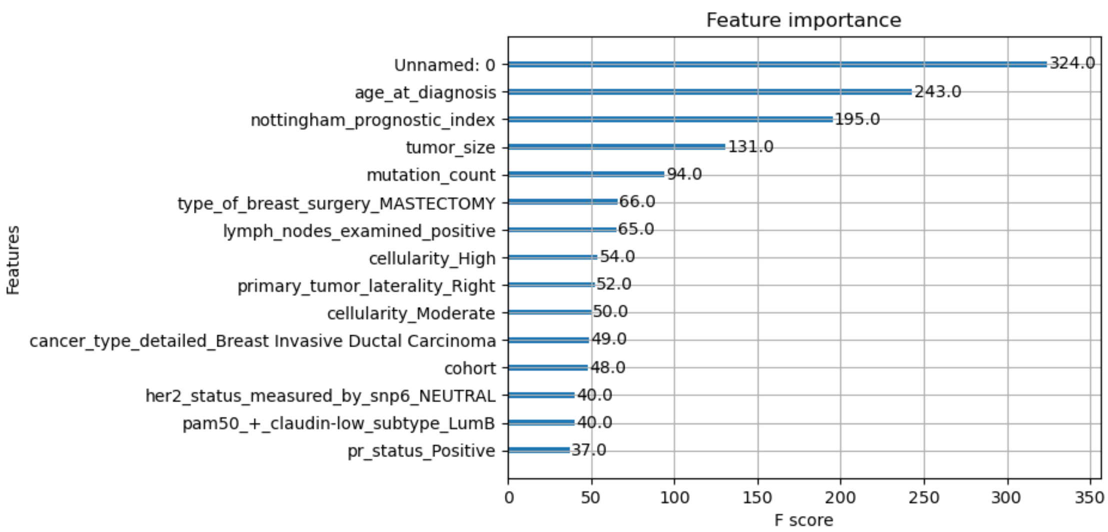
[ ]:
```python
# Comparison Between Models Trained So Far
pd.DataFrame(model_comparison_dict, index=['Accuracy'])
```

[ ]:

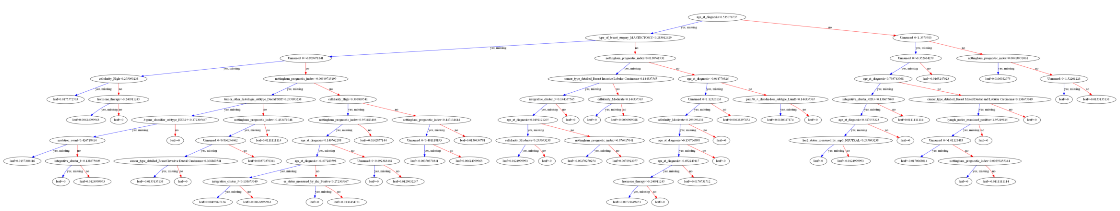
	DefaultRandomForest	GridSearchRandomForest	ImprovedRandomForest	GridSearchXGB
Accuracy	0.694079	0.684211	0.703947	0.697368

1.2.6 Create the feature importances plot, plot a decision tree from the booster.

[ ]:
```python
import matplotlib.pyplot as plt
from xgboost import plot_importance

# Plot the feature importances
plot_importance(xgb_best_model, max_num_features=15)
plt.show()
```



[ ]:
```python
from xgboost import plot_tree
import matplotlib.pyplot as plt

fig, ax = plt.subplots(figsize=(30, 30))
plot_tree(xgb_best_model, ax=ax)
plt.savefig("./decision_tree.png", dpi=600)
plt.show()
```



1.2.7 * Improve Model (Bonus)

In this bonus part, you can add your ideas for improving your model's performance. You can implement your model and compare the results.

We try to improve the model using parameter regularization. We adjust the regularization parameters of the XGBoost model to reduce overfitting and improve generalization performance. For example, we could increase the values of the reg_alpha and reg_lambda hyperparameters.

[ ]:
```python
import pandas as pd
import xgboost as xgb
from sklearn.model_selection import (
    RandomizedSearchCV,
```

```
)
from sklearn.metrics import accuracy_score, classification_report

param_grid = {
    "max_depth": [3, 5, 7, 9],
    "learning_rate": [0.01, 0.1, 0.5, 1],
    "n_estimators": [50, 100, 200, 500],
    "gamma": [0, 0.1, 0.5, 1],
    "subsample": [0.5, 0.7, 1],
    "colsample_bytree": [0.5, 0.7, 1],
    "reg_alpha": [0, 0.1, 0.5, 1],
    "reg_lambda": [0, 0.1, 0.5, 1],
}

# Create the grid search object
grid_search_impr = RandomizedSearchCV(
    estimator=xgb.XGBClassifier(),
    param_distributions=param_grid,
    n_iter=100,
    cv=5,
    n_jobs=-1,
    random_state=83728,
    verbose=1,
    refit=True,
)

# Fit the grid search object
grid_search_impr.fit(X_train_preprocessed, y_train_preprocessed)

# Get the best model from grid search
best_model_impr = xgb.XGBClassifier(**grid_search_impr.best_params_)
best_model_impr.fit(X_train_preprocessed, y_train_preprocessed)

# Make predictions on the train and test data using the best model
y_train_pred = best_model_impr.predict(X_train_preprocessed)
y_test_pred = best_model_impr.predict(X_test_preprocessed)

# Evaluate the accuracy of the model on the train and test data
train_accuracy = accuracy_score(y_train_preprocessed, y_train_pred)
test_accuracy = accuracy_score(y_test_preprocessed, y_test_pred)

model_comparison_dict['ImprovedXGB'] = test_accuracy

print("Train Accuracy:", train_accuracy)
print("Test Accuracy:", test_accuracy)

xgb_improved_clf_report = classification_report(
```

```
    y_test_preprocessed, y_test_pred, output_dict=True
)
pd.DataFrame(xgb_improved_clf_report)
```

```
Fitting 5 folds for each of 100 candidates, totalling 500 fits
Train Accuracy: 0.796875
Test Accuracy: 0.6907894736842105
```

[ ]:

	0	1	accuracy	macro avg	weighted avg
precision	0.747368	0.596491	0.690789	0.671930	0.689797
recall	0.755319	0.586207	0.690789	0.670763	0.690789
f1-score	0.751323	0.591304	0.690789	0.671314	0.690263
support	188.000000	116.000000	0.690789	304.000000	304.000000

1.3 Comparison between XGBoost and Random Forest Classifier

Compare the results from these two models. How Would you rate each method in terms of its performance? What's the difference between these models? explain.

Performance: Here is an overall comparison on the performance of models we trained in this homework:

[ ]:

```
# Comparison Between Models Trained So Far
pd.DataFrame(model_comparison_dict, index=['Accuracy'])
```

[ ]:

```
          DefaultRandomForest  GridSearchRandomForest  ImprovedRandomForest
GridSearchXGB  ImprovedXGB
Accuracy             0.694079                0.684211              0.703947
0.697368     0.690789
```

It seems that both XGBoost and Random Forest had moderate performance on this dataset. From the accuracy report, none of the models outperformed the other. Also, it appears that both random forest and XGBoost performed as-well as the best model obtained using grid-search and other techniques like bagging.

In general, XGBoost tends to perform slightly better than Random Forest Classifier on many datasets, especially when the dataset is large and complex. XGBoost is known for its ability to handle high-dimensional data and learn complex interactions between features.

However, Random Forest Classifier can sometimes perform better than XGBoost on smaller datasets or datasets with simpler relationships between features. Random Forest Classifier is also known for its ability to handle noisy data and outliers.

Difference between models: The main difference between XGBoost and Random Forest Classifier is in how they build their decision trees.

Random Forest Classifier builds decision trees independently of each other, using a random subset of the features at each split. This helps to reduce overfitting and increase the diversity of the trees in the ensemble.

XGBoost builds decision trees sequentially, using the residuals of the previous trees to guide the construction of the next tree. This allows XGBoost to focus on the samples that are most difficult to classify and can lead to better performance.

XGBoost also includes additional regularization parameters, such as L1 and L2 regularization, that can help to further reduce overfitting and improve generalization performance.

Another difference is that XGBoost uses a gradient boosting approach, while Random Forest Classifier uses a bagging approach. This means that XGBoost tries to minimize the errors of the previous trees, while Random Forest Classifier tries to reduce the variance of the ensemble by averaging the predictions of the trees.

Conclusion Overall, both XGBoost and Random Forest Classifier are powerful methods that can be effective for classification tasks. On this specific dataset, both models had very similar performance.