In []: !pip install ISLP
!pip install catboost

```
Collecting ISLP
 Downloading ISLP-0.4.0-py3-none-any.whl.metadata (7.0 kB)
Requirement already satisfied: numpy>=1.7.1 in /usr/local/lib/python3.10/dist-packages (from ISLP) (1.26.4)
Requirement already satisfied: scipy>=0.9 in /usr/local/lib/python3.10/dist-packages (from ISLP) (1.13.1)
Requirement already satisfied: pandas>=0.20 in /usr/local/lib/python3.10/dist-packages (from ISLP) (2.2.2)
Requirement already satisfied: lxml in /usr/local/lib/python3.10/dist-packages (from ISLP) (5.3.0)
Requirement already satisfied: scikit-learn>=1.2 in /usr/local/lib/python3.10/dist-packages (from ISLP) (1.5.2)
Requirement already satisfied: joblib in /usr/local/lib/python3.10/dist-packages (from ISLP) (1.4.2)
Requirement already satisfied: statsmodels>=0.13 in /usr/local/lib/python3.10/dist-packages (from ISLP) (0.14.4)
Collecting lifelines (from ISLP)
 Downloading lifelines-0.30.0-py3-none-any.whl.metadata (3.2 kB)
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Collecting torchmetrics (from ISLP)
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Requirement already satisfied: threadpoolctl>=3.1.0 in /usr/local/lib/python3.10/dist-packages (from scikit-learn>=1.2->ISLP)
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Requirement already satisfied: autograd>=1.5 in /usr/local/lib/python3.10/dist-packages (from lifelines->ISLP) (1.7.0)
Collecting autograd-gamma>=0.3 (from lifelines->ISLP)
 Downloading autograd-gamma-0.5.0.tar.gz (4.0 kB)
  Preparing metadata (setup.py) ... done
Collecting formulaic>=0.2.2 (from lifelines->ISLP)
  Downloading formulaic-1.0.2-py3-none-any.whl.metadata (6.8 kB)
Requirement already satisfied: progressbar2<5.0.0,>=4.2.0 in /usr/local/lib/python3.10/dist-packages (from pygam->ISLP) (4.5.0)
Collecting scipy>=0.9 (from ISLP)
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P) (4.12.2)
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 Downloading lightning_utilities-0.11.9-py3-none-any.whl.metadata (5.2 kB)
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Collecting interface-meta>=1.2.0 (from formulaic>=0.2.2->lifelines->ISLP)
 Downloading interface_meta-1.3.0-py3-none-any.whl.metadata (6.7 kB)
Requirement already satisfied: wrapt>=1.0 in /usr/local/lib/python3.10/dist-packages (from formulaic>=0.2.2->lifelines->ISLP)
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Requirement already satisfied: aiohttp!=4.0.0a0,!=4.0.0a1 in /usr/local/lib/python3.10/dist-packages (from fsspec[http]>=2022.
5.0->pytorch-lightning->ISLP) (3.11.9)
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-lightning->ISLP) (75.1.0)
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Requirement already satisfied: async-timeout<6.0,>=4.0 in /usr/local/lib/python3.10/dist-packages (from aiohttp!=4.0.0a0,!=4.0.
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Requirement already satisfied: multidict<7.0,>=4.5 in /usr/local/lib/python3.10/dist-packages (from aiohttp!=4.0.0a0,!=4.0.0a1-
```

```
>fsspec[http]>=2022.5.0->pytorch-lightning->ISLP) (6.1.0)
       Requirement already satisfied: propcache>=0.2.0 in /usr/local/lib/python3.10/dist-packages (from aiohttp!=4.0.0a0,!=4.0.0a1->fs
       spec[http]>=2022.5.0->pytorch-lightning->ISLP) (0.2.1)
       Requirement already satisfied: yarl<2.0,>=1.17.0 in /usr/local/lib/python3.10/dist-packages (from aiohttp!=4.0.0a0,!=4.0.0a1->f
       sspec[http]>=2022.5.0->pytorch-lightning->ISLP) (1.18.3)
       Requirement already satisfied: idna>=2.0 in /usr/local/lib/python3.10/dist-packages (from yarl<2.0,>=1.17.0->aiohttp!=4.0.0a0,!
       =4.0.0a1->fsspec[http]>=2022.5.0->pytorch-lightning->ISLP) (3.10)
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       Downloading lifelines-0.30.0-py3-none-any.whl (349 kB)
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       Downloading pygam-0.9.1-py3-none-any.whl (522 kB)
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       Downloading torchmetrics-1.6.0-py3-none-any.whl (926 kB)
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       Downloading lightning_utilities-0.11.9-py3-none-any.whl (28 kB)
       Downloading interface_meta-1.3.0-py3-none-any.whl (14 kB)
       Building wheels for collected packages: autograd-gamma
         Building wheel for autograd-gamma (setup.py) ... done
         Created wheel for autograd-gamma: filename=autograd_gamma-0.5.0-py3-none-any.whl size=4031 sha256=4f9e7490640d47feffb5257bb51
       58ba92c129d664024a22c9b3f84708c5784dc
         Stored in directory: /root/.cache/pip/wheels/25/cc/e0/ef2969164144c899fedb22b338f6703e2b9cf46eeebf254991
       Successfully built autograd-gamma
       Installing collected packages: scipy, lightning-utilities, interface-meta, autograd-gamma, torchmetrics, pygam, formulaic, life
       lines, pytorch-lightning, ISLP
         Attempting uninstall: scipy
           Found existing installation: scipy 1.13.1
           Uninstalling scipy-1.13.1:
             Successfully uninstalled scipy-1.13.1
       Successfully installed ISLP-0.4.0 autograd-gamma-0.5.0 formulaic-1.0.2 interface-meta-1.3.0 lifelines-0.30.0 lightning-utilitie
       s-0.11.9 pygam-0.9.1 pytorch-lightning-2.4.0 scipy-1.11.4 torchmetrics-1.6.0
       Collecting catboost
         Downloading catboost-1.2.7-cp310-cp310-manylinux2014_x86_64.whl.metadata (1.2 kB)
       Requirement already satisfied: graphviz in /usr/local/lib/python3.10/dist-packages (from catboost) (0.20.3)
       Requirement already satisfied: matplotlib in /usr/local/lib/python3.10/dist-packages (from catboost) (3.8.0)
       Requirement already satisfied: numpy<2.0,>=1.16.0 in /usr/local/lib/python3.10/dist-packages (from catboost) (1.26.4)
       Requirement already satisfied: pandas>=0.24 in /usr/local/lib/python3.10/dist-packages (from catboost) (2.2.2)
       Requirement already satisfied: scipy in /usr/local/lib/python3.10/dist-packages (from catboost) (1.11.4)
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       Requirement already satisfied: pillow>=6.2.0 in /usr/local/lib/python3.10/dist-packages (from matplotlib->catboost) (11.0.0)
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       Requirement already satisfied: tenacity>=6.2.0 in /usr/local/lib/python3.10/dist-packages (from plotly->catboost) (9.0.0)
       Downloading catboost-1.2.7-cp310-cp310-manylinux2014 x86_64.whl (98.7 MB)
                                                 - 98.7/98.7 MB 7.7 MB/s eta 0:00:00
       Installing collected packages: catboost
       Successfully installed catboost-1.2.7
In [ ]: import numpy as np
        import pandas as pd
        import matplotlib.pyplot as plt
        from matplotlib.pyplot import subplots
        import statsmodels.api as sm
        from ISLP import load_data
        from ISLP.models import (ModelSpec as MS,
        summarize)
        from ISLP import confusion_table
        from ISLP.models import contrast
        from sklearn.discriminant_analysis import \
        (LinearDiscriminantAnalysis as LDA,
        QuadraticDiscriminantAnalysis as QDA)
        from sklearn.naive bayes import GaussianNB
        from sklearn.neighbors import KNeighborsClassifier
        from sklearn.preprocessing import StandardScaler
        from sklearn.model_selection import train_test_split
        from sklearn.linear model import LogisticRegression
        from itertools import combinations
        import seaborn as sns
        from sklearn.tree import DecisionTreeClassifier
```

from sklearn.metrics import accuracy_score, f1_score, recall_score, balanced_accuracy_score,classification_report, confusion_m

 $\textbf{from} \ \, \textbf{sklearn.model_selection} \ \, \textbf{import} \ \, \textbf{GridSearchCV}$

from imblearn.over_sampling import SMOTE
from sklearn.ensemble import RandomForestClassifier

import xgboost as xgb
from sklearn.linear_model import LogisticRegression

In []: df = pd.read_csv("train.csv")

df.head(5)

Out[]:		PatientID	Age	Gender	Ethnicity	EducationLevel	ВМІ	Smoking	AlcoholConsumption	PhysicalActivity	DietQuality	•••	Memor
,	0	1	67	0	3	0	37.205177	0	12.215677	7.780544	6.433890		
	1	2	65	1	0	0	35.141843	1	17.111404	6.645284	1.112379		
	2	3	62	0	1	1	17.875103	0	13.525546	9.585769	4.266008		
	3	4	67	0	0	1	37.503437	1	19.952014	1.953946	6.797333		
	4	5	65	1	0	2	29.187863	1	0.533209	8.759570	6.364302		

5 rows × 35 columns

Exploratory Data Analysis (EDA)

In []: #Checking for NULL values
df.isna().sum()

```
Out[]:
                                 0
                       PatientID 0
                            Age 0
                         Gender 0
                        Ethnicity 0
                  EducationLevel 0
                            BMI 0
                        Smoking 0
             AlcoholConsumption 0
                  PhysicalActivity 0
                     DietQuality 0
                    SleepQuality 0
          FamilyHistoryAlzheimers 0
            Cardiovascular Disease 0
                        Diabetes 0
                      Depression 0
                      HeadInjury 0
                    Hypertension 0
                      SystolicBP 0
                      DiastolicBP 0
                 CholesterolTotal 0
                  CholesterolLDL 0
                  CholesterolHDL 0
          CholesterolTriglycerides 0
                          MMSE 0
            FunctionalAssessment 0
              MemoryComplaints 0
              BehavioralProblems 0
                            ADL 0
                      Confusion 0
                   Disorientation 0
              PersonalityChanges 0
        DifficultyCompletingTasks 0
                    Forgetfulness 0
                       Diagnosis 0
                  DoctorInCharge 0
        dtype: int64
```

```
duplicates = df[df[list(df.columns)].duplicated()].index
duplicates

Out[]: Index([], dtype='int64')

The dataset got no duplicates and no null values

In []: def reset_df():
    # 0.8-0.2 Train-val split
    df_train, df_val = train_test_split(df, test_size=0.2, random_state=5, stratify=df['Diagnosis'])

    train_diagnosis = df_train['Diagnosis'].reset_index(drop = True)
    val_diagnosis = df_val['Diagnosis'].reset_index(drop = True)

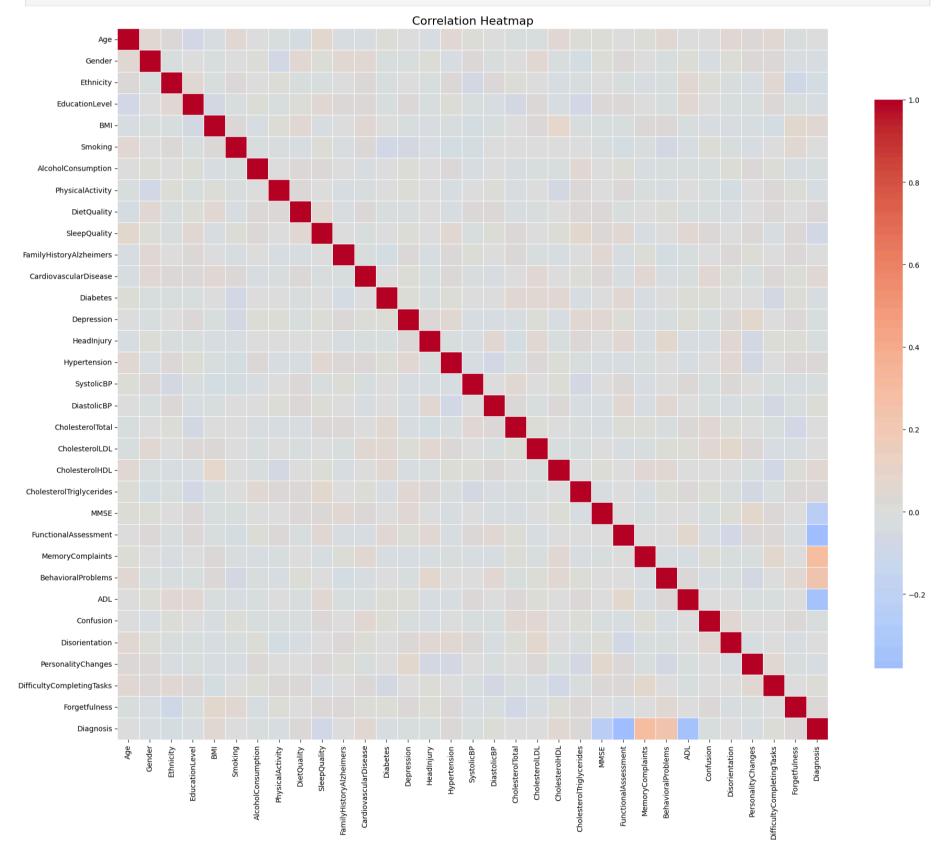
#Dropping Irrelevant columns
    df_train = df_train.drop(['PatientID', 'DoctorInCharge', 'Diagnosis'], axis=1)
    df_val = df_val.drop(['PatientID', 'DoctorInCharge', 'Diagnosis'], axis=1)
```

In []: #Checking for duplicates

```
#Standardizing every column except diagnosis
scaler = StandardScaler()

df_train = pd.DataFrame(scaler.fit_transform(df_train), columns=df_train.columns)
df_val = pd.DataFrame(scaler.transform(df_val), columns = df_val.columns)

#Adding diagnosis column which is not standardized
df_train['Diagnosis'] = train_diagnosis
df_val['Diagnosis'] = val_diagnosis
return df_train, df_val, scaler
df_train, df_val, scaler = reset_df()
```



```
In []: def top_correlated_features(data, target_feature, top_n=10):
    # Identifies the top correlated features to a given target feature.

# Calculate the correlation matrix
    correlation_matrix = data.corr()

# Extract correlation values for the target feature
    target_correlation = correlation_matrix[target_feature].drop(labels=[target_feature])

# Get the top N correlated features (absolute value to account for both positive and negative correlations)
    top_correlations = target_correlation.abs().sort_values(ascending=False).head(top_n)

# Return the correlation values with original signs
    return target_correlation[top_correlations.index]
    top_correlated_features(df_train, "BehavioralProblems")
```

Out[]: **BehavioralProblems** Diagnosis 0.239710 HeadInjury 0.064203 **PersonalityChanges** -0.060831 **Forgetfulness** 0.060083 **Smoking** -0.058980 0.054790 Age **FamilyHistoryAlzheimers** -0.050267 **CholesterolHDL** 0.047882 CardiovascularDisease -0.044209 **DiastolicBP** 0.041060

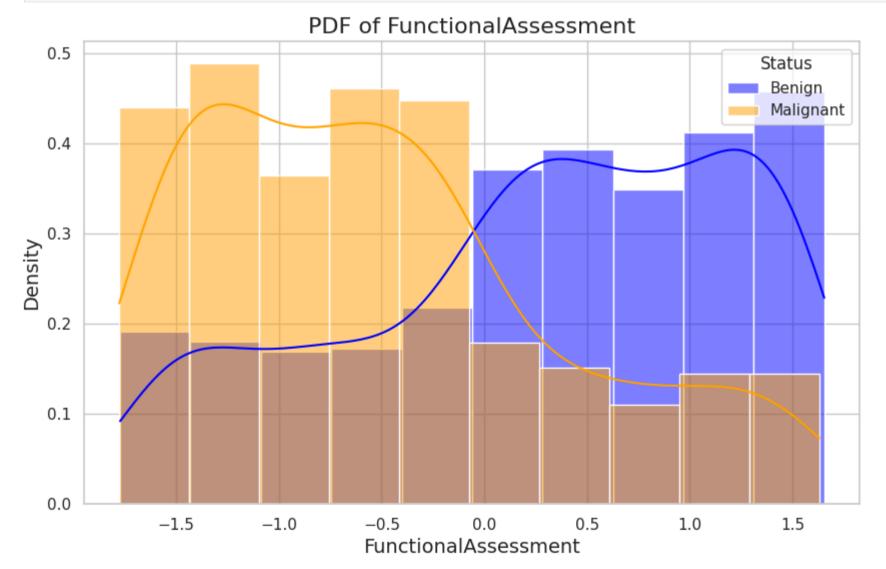
dtype: float64

```
In []:
    def plot_pdf(df, col):
        #PLot two pdf: pdf of specific column given diagnosis = 0, pdf of specific column given diagnosis = 1
        sns.set(style="whitegrid")

# Plot the PDF using Seaborn's kdeplot
    plt.figure(figsize=(10, 6))
    sns.histplot(df[df['Diagnosis'] == 0][col], kde=True, color='blue', label='Benign', stat="density", bins=10, alpha=0.5)
    sns.histplot(df[df['Diagnosis'] == 1][col], kde=True, color='orange', label='Malignant', stat="density", bins=10, alpha=0.

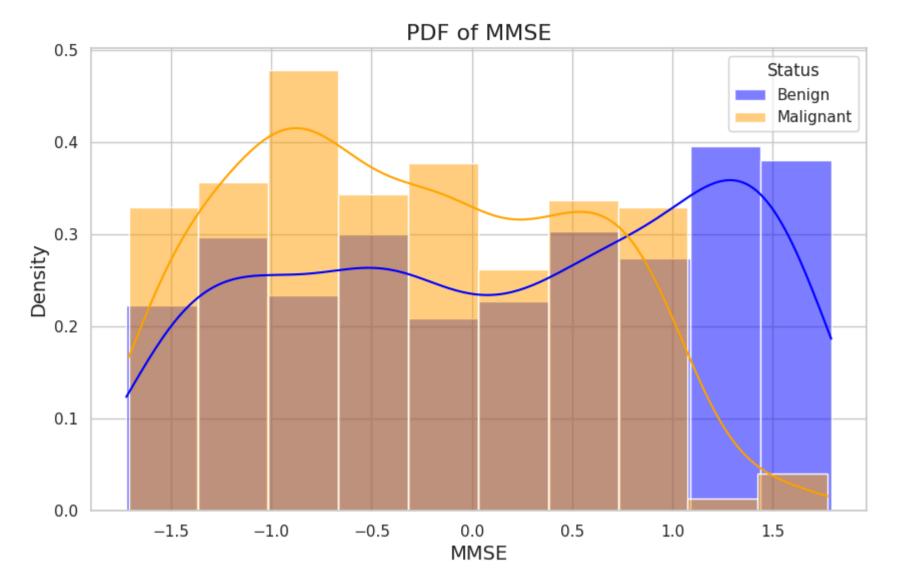
    plt.title(f"PDF of {col}", fontsize=16)
    plt.xlabel(f"{col}", fontsize=14)
    plt.ylabel("Density", fontsize=14)
    plt.legend(title="Status")
    plt.grid(True)

    plt.show()
    plot_pdf(df_train, "FunctionalAssessment")
```



- 1. FunctionalAssessment > 0, tend to be Benign FunctionalAssessment < 0, tend to be Malignant
- 2. Graph overlaps, so additional features are needed to classify Benign/Malignant

```
In [ ]: plot_pdf(df_train,'MMSE')
```



```
In []: def plot_box(df,col):
    #PLotting box plot of specific column for diagnosis = 0, diagnosis = 1

plt.figure(figsize=(10, 6))
    sns.boxplot(data=df, x='Diagnosis', y=col, palette={'0': 'blue', '1': 'orange'})

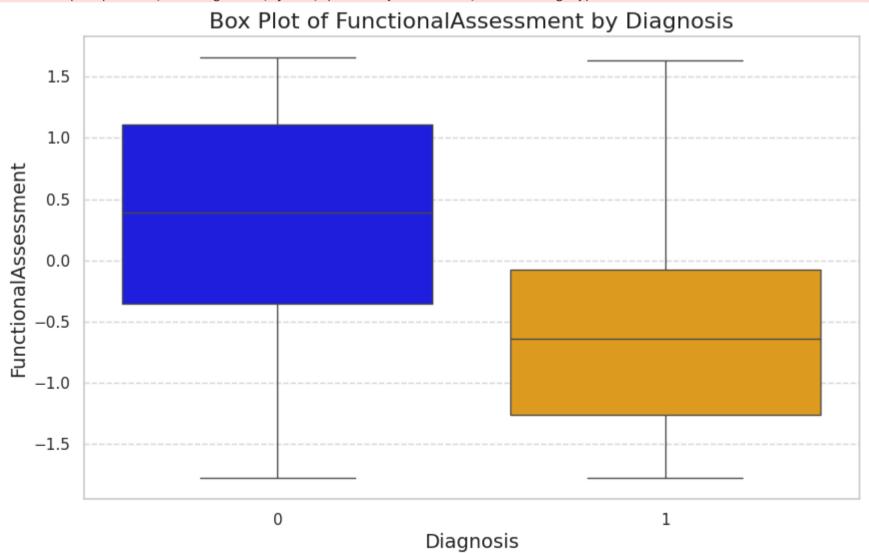
plt.title(f'Box Plot of {col} by Diagnosis', fontsize=16)
    plt.xlabel('Diagnosis', fontsize=14)
    plt.ylabel(col, fontsize=14)

plt.grid(axis='y', linestyle='--', alpha=0.7)
    plt.show()
    plot_box(df_train, "FunctionalAssessment")
```

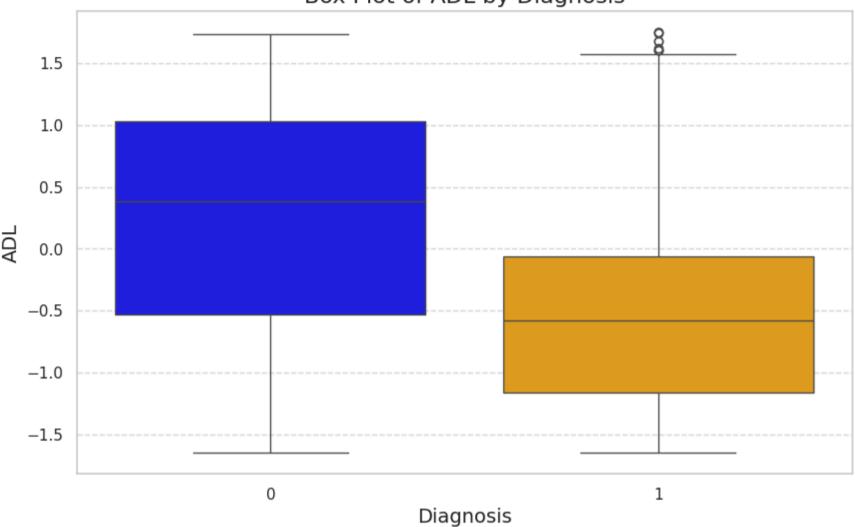
<ipython-input-11-4e68a1b26e33>:5: FutureWarning:

Passing `palette` without assigning `hue` is deprecated and will be removed in v0.14.0. Assign the `x` variable to `hue` and se t `legend=False` for the same effect.

sns.boxplot(data=df, x='Diagnosis', y=col, palette={'0': 'blue', '1': 'orange'})



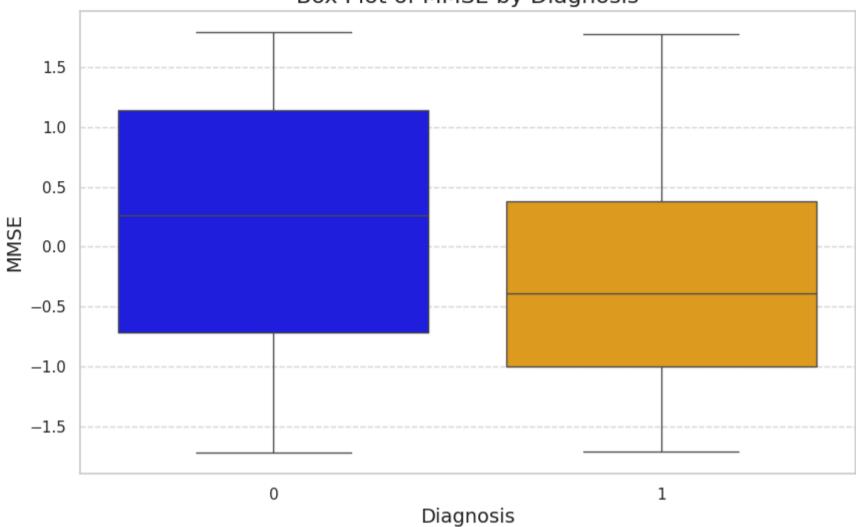
Box Plot of ADL by Diagnosis

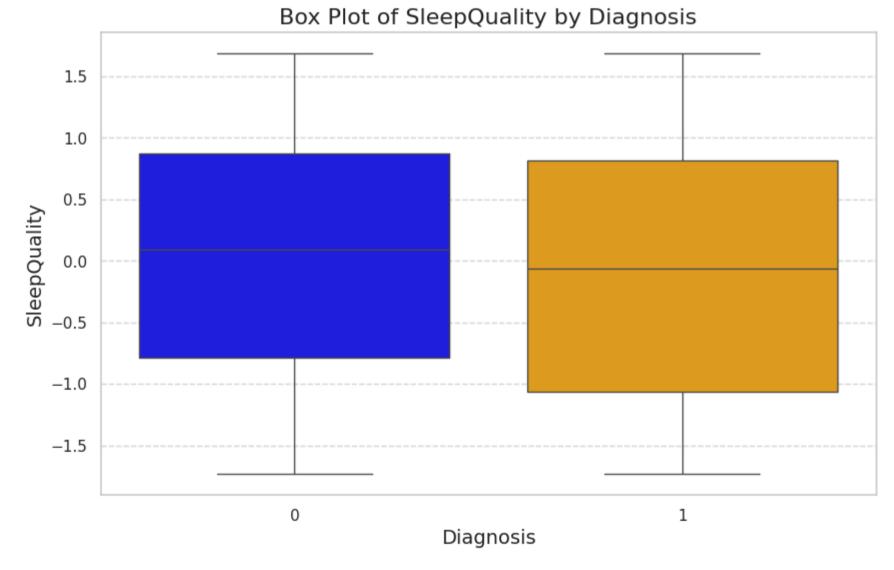


```
In [ ]: #Finding upper bound for group 1
        grouped = df_train.groupby('Diagnosis')['ADL']
        # For Diagnosis = 1 (orange box)
        Q1 = grouped.quantile(0.25).loc[1]
        Q3 = grouped.quantile(0.75).loc[1]
        IQR = Q3 - Q1
        upper_bound = Q3 + 1.5 * IQR
        # Print results for Diagnosis = 1
        print("For Diagnosis = 1:")
        print("Q1:", Q1)
        print("Q3:", Q3)
        print("IQR:", IQR)
        print("Upper Bound:", upper_bound)
       For Diagnosis = 1:
       Q1: -1.1616764567839484
       Q3: -0.059578148261666145
       IQR: 1.1020983085222822
       Upper Bound: 1.593569314521757
In [ ]: len(df_train[(df_train['ADL'] > upper_bound) & (df_train['Diagnosis'] == 1)])
Out[]: 9
In [ ]: plot_box(df_train,"MMSE")
       <ipython-input-11-4e68a1b26e33>:5: FutureWarning:
       Passing `palette` without assigning `hue` is deprecated and will be removed in v0.14.0. Assign the `x` variable to `hue` and se
       t `legend=False` for the same effect.
```

sns.boxplot(data=df, x='Diagnosis', y=col, palette={'0': 'blue', '1': 'orange'})

Box Plot of MMSE by Diagnosis





```
In []: class_counts = df_train['Diagnosis'].value_counts()

# Print the distribution
print("Class Distribution:")
print(class_counts)

# Plot the distribution
plt.figure(figsize=(8, 6))
class_counts.plot(kind='bar', color=['skyblue', 'salmon'])
plt.title('Class Distribution in Diagnosis Column')
plt.xlabel('Class (0: Benign, 1: Malignant)')
```

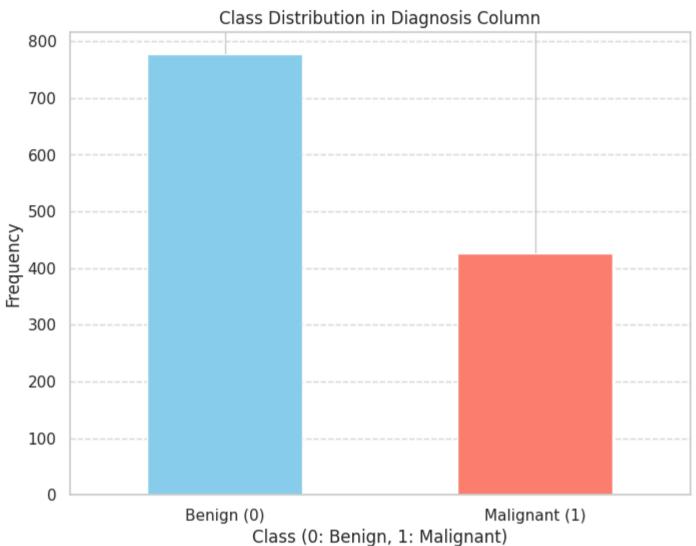
```
plt.ylabel('Frequency')
 plt.xticks([0, 1], ['Benign (0)', 'Malignant (1)'], rotation=0)
 plt.grid(axis='y', linestyle='--', alpha=0.7)
 plt.show()
Class Distribution:
```

Diagnosis 0 777

426

1

Name: count, dtype: int64



Model

```
In [ ]: def evaluate(model, X, y, class_report = True):
            y_pred = model.predict(X)
            accuracy = accuracy_score(y,y_pred)
            f1 = f1_score(y,y_pred, average='weighted')
            sensitivity = recall_score(y,y_pred,average='weighted')
            balanced_accuracy = balanced_accuracy_score(y,y_pred)
            if class_report:
                print(classification_report(y, y_pred, target_names=["Benign","Malignant"]))
            return accuracy, f1, sensitivity, balanced_accuracy
In [ ]: def evaluate_model(model, X_train, y_train, X_val, y_val, class_report = True):
            train_accuracy, train_f1, train_sensitivity, train_balanced_accuracy = evaluate(model, X_train, y_train, class_report)
            validation_accuracy, validation_f1, validation_sensitivity, validation_balanced_accuracy = evaluate(model, X_val, y_val, c
            print(f"Training Metrics: Accuracy = {train_accuracy}, F1 score = {train_f1}, Sensitivity = {train_sensitivity}")
            print(f"Validation Metrics: Accuracy = {validation_accuracy}, F1 score = {validation_f1}, Sensitivity = {validation_sensit
In [ ]: def prepare_X_y(X_col, resample = True):
            #prepare X, y given arbitrary training features with SMOTE resampling
            X_train = df_train[X_col]
            y_train = df_train['Diagnosis']
            X_{val} = df_{val}[X_{col}]
            y_val = df_val['Diagnosis']
            #Apply SMOTE resampling
            if resample == True:
                smote = SMOTE(random_state=0)
                X_train, y_train = smote.fit_resample(X_train, y_train)
            return X_train, y_train, X_val, y_val
```

Logistic Regression

```
In [ ]: #Try using MMSE, FunctionalAssessment, MemoryComplaints, BehavioralProblems, ADL for fitting (5 most important features)
        X_train, y_train, X_val, y_val = prepare_X_y(['MMSE', 'FunctionalAssessment', 'MemoryComplaints', 'BehavioralProblems', 'ADL',
        lr_model = LogisticRegression(
            penalty='12', # L2 regularization (ridge)
            C=1.0,
            solver='liblinear', # Good for small datasets
            random_state=42,
            max_iter=1000,
```

```
# Fit the model
 lr_model.fit(X_train, y_train)
 evaluate_model(lr_model, X_train, y_train, X_val, y_val)
             precision
                           recall f1-score support
     Benign
                   0.84
                             0.82
                                       0.83
                                                  777
  Malignant
                   0.82
                             0.84
                                       0.83
                                                  777
                                       0.83
                                                 1554
   accuracy
   macro avg
                   0.83
                             0.83
                                       0.83
                                                 1554
weighted avg
                   0.83
                             0.83
                                       0.83
                                                 1554
                           recall f1-score
             precision
                                              support
      Benign
                   0.88
                             0.80
                                       0.84
                                                  195
                                                  106
  Malignant
                   0.69
                             0.80
                                       0.74
   accuracy
                                       0.80
                                                  301
  macro avg
                   0.78
                             0.80
                                       0.79
                                                  301
weighted avg
                   0.81
                             0.80
                                       0.80
                                                  301
Training Metrics: Accuracy = 0.832046332046332, F1 score = 0.8320262301382366, Sensitivity = 0.832046332046332
Validation Metrics: Accuracy = 0.8006644518272426, F1 score = 0.803641904264886, Sensitivity = 0.8006644518272426
```

Decision Tree

```
In [ ]: #Decision Tree
    clf = DecisionTreeClassifier(random_state=0, max_depth = 5, min_samples_split = 2)
    clf.fit(X_train, y_train)
    evaluate_model(clf, X_train, y_train, X_val, y_val)
```

	precision	recall	f1-score	support
Benign	0.95	0.98	0.97	777
Malignant	0.98	0.95	0.96	777
accuracy			0.96	1554
macro avg	0.96	0.96	0.96	1554
weighted avg	0.96	0.96	0.96	1554
	precision	recall	f1-score	support
Benign	precision 0.96	recall 0.92	f1-score 0.94	support 195
Benign Malignant				• •
•	0.96	0.92	0.94	195
Malignant	0.96	0.92	0.94 0.90	195 106

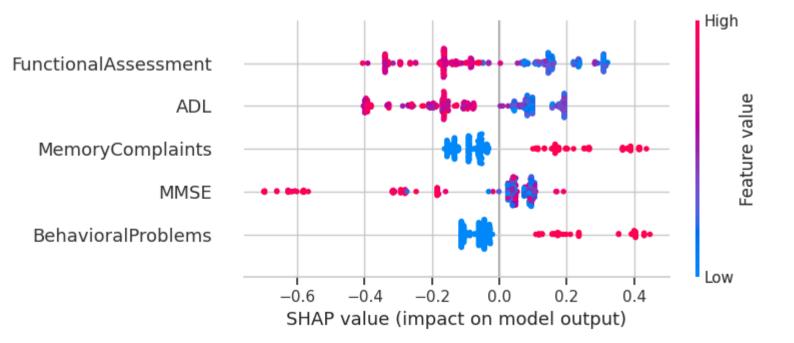
Training Metrics: Accuracy = 0.9646074646074646, F1 score = 0.9646010002174386, Sensitivity = 0.9646074646074646 Validation Metrics: Accuracy = 0.9269102990033222, F1 score = 0.927473865474596, Sensitivity = 0.9269102990033222

```
In []: import shap

# Initialize SHAP explainer
explainer = shap.TreeExplainer(clf)

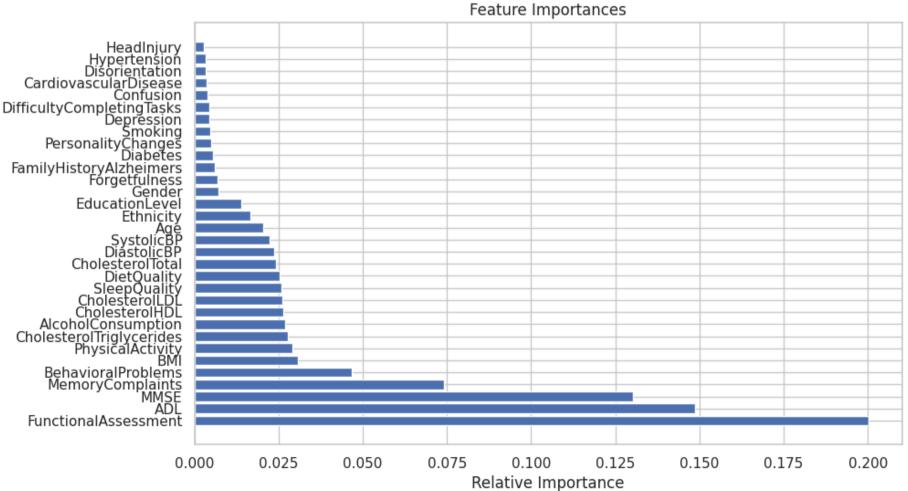
# Get SHAP values for the entire dataset
shap_values = explainer.shap_values(X_val)

# Visualize SHAP values
shap.summary_plot(shap_values[:,:,1], X_val) # For binary classification (class 1)
```



Random Forest

```
In [ ]: #Random Forest using all features & Grid search
        features = [col for col in df_train.columns if col != 'Diagnosis']
        X_train, y_train, X_val, y_val = prepare_X_y(features)
In [ ]: param_grid = {
            'n_estimators': [100, 200],
            'max_depth': [None, 10],
            'min_samples_split': [2, 5],
            'min_samples_leaf': [1, 2, 3],
            'max_features': ['log2','sqrt'],
            'bootstrap': [True]
In [ ]: | rf = RandomForestClassifier(random_state=42)
        grid_search = GridSearchCV(estimator=rf, param_grid=param_grid, cv=5, scoring='precision', verbose=1) #Accuracy
        grid_search.fit(X_train, y_train)
       Fitting 5 folds for each of 48 candidates, totalling 240 fits
       /usr/local/lib/python3.10/dist-packages/numpy/ma/core.py:2820: RuntimeWarning: invalid value encountered in cast
         _data = np.array(data, dtype=dtype, copy=copy,
Out[]: | >
                        GridSearchCV
          ▶ best_estimator_: RandomForestClassifier
                   RandomForestClassifier
In [ ]: print("Best Parameters:", grid_search.best_params_)
        print("Best Accuracy:", grid_search.best_score_)
        best_rf = grid_search.best_estimator_
       Best Parameters: {'bootstrap': True, 'max_depth': None, 'max_features': 'log2', 'min_samples_leaf': 1, 'min_samples_split': 2,
       'n_estimators': 100}
       Best Accuracy: 0.9760440649975571
In [ ]: #Feature importances from our Random Forest
        importances = best_rf.feature_importances_
        feature_names = X_train.columns
        indices = np.argsort(importances)[::-1]
        # Plot the feature importances
        plt.figure(figsize=(10, 6))
        plt.title("Feature Importances")
        plt.barh(range(len(importances)), importances[indices], align="center")
        plt.yticks(range(len(importances)), np.array(feature_names)[indices])
        plt.xlabel("Relative Importance")
        plt.show()
```



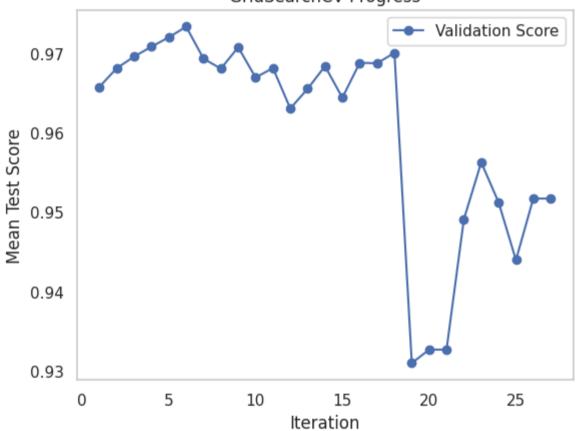
In []: validation_accuracy, validation_f1, validation_sensitivity, validation_balanced_accuracy = evaluate(best_rf, X_val, y_val)
print(f"Validation Metrics: Accuracy = {validation_accuracy}, F1 score = {validation_f1}, Sensitivity = {validation_sensitivity}

```
precision
                                  recall f1-score
                                                    support
                          0.93
             Benign
                                    0.95
                                              0.94
                                                         195
          Malignant
                          0.90
                                    0.87
                                              0.88
                                                         106
                                              0.92
                                                         301
           accuracy
          macro avg
                          0.92
                                    0.91
                                              0.91
                                                         301
       weighted avg
                          0.92
                                    0.92
                                              0.92
                                                         301
       Validation Metrics: Accuracy = 0.920265780730897, F1 score = 0.9199038477754095, Sensitivity = 0.920265780730897
        XGBoost
In [ ]: #Fitting XGBoost on 30 most important features
        X_train, y_train, X_val, y_val = prepare_X_y(np.array(feature_names)[indices][:30])
        xgb_clf = xgb.XGBClassifier(
            objective='binary:logistic',
            random_state=42,
            n_jobs=-1, # Use all available cores
        xgb_clf.fit(X_train,y_train)
        evaluate_model(xgb_clf,X_train, y_train, X_val, y_val)
                                  recall f1-score
                     precision
                                                     support
                          1.00
                                   1.00
                                              1.00
                                                         777
             Benign
          Malignant
                          1.00
                                    1.00
                                              1.00
                                                         777
                                              1.00
                                                        1554
           accuracy
                                    1.00
                                                        1554
          macro avg
                          1.00
                                              1.00
       weighted avg
                          1.00
                                    1.00
                                              1.00
                                                        1554
                                  recall f1-score
                     precision
                                                     support
             Benign
                          0.97
                                    0.93
                                              0.95
                                                         195
          Malignant
                          0.88
                                    0.94
                                              0.91
                                                         106
           accuracy
                                              0.93
                                                         301
          macro avg
                          0.92
                                    0.94
                                              0.93
                                                         301
                          0.94
                                    0.93
                                              0.93
       weighted avg
       Training Metrics: Accuracy = 1.0, F1 score = 1.0, Sensitivity = 1.0
       Validation Metrics: Accuracy = 0.9335548172757475, F1 score = 0.9340671504314509, Sensitivity = 0.9335548172757475
In [ ]: #XGBoost with grid search
        param_grid = {
                       'n_estimators': [50, 100, 200],
                       'learning_rate': [0.01, 0.1, 1],
                       'max_depth': [3, 5, 7],
        # Create the XGBoost classifier
        xgb_clf = xgb.XGBClassifier(
            objective='binary:logistic',
            random_state=42,
            n_jobs=-1 # Use all available cores
        grid_search = GridSearchCV(estimator=xgb_clf, param_grid=param_grid, cv=5, scoring='precision', verbose=1)
        grid_search.fit(X_train, y_train)
       Fitting 5 folds for each of 27 candidates, totalling 135 fits
GridSearchCV
          ▶ best_estimator_: XGBClassifier
                   ▶ XGBClassifier
In [ ]: print("Best Parameters:", grid_search.best_params_)
        print("Best Accuracy:", grid_search.best_score_)
        best_xgb = grid_search.best_estimator_
       Best Parameters: {'learning_rate': 0.01, 'max_depth': 5, 'n_estimators': 100}
       Best Accuracy: 0.9735702856249894
In [ ]: validation_accuracy, validation_f1, validation_sensitivity, validation_balanced_accuracy = evaluate(best_xgb, X_val, y_val)
        print(f"Validation Metrics: Accuracy = {validation accuracy}, F1 score = {validation f1}, Sensitivity = {validation sensitivit
```

```
precision
                                  recall f1-score support
             Benign
                          0.96
                                    0.95
                                              0.95
                                                         195
          Malignant
                          0.91
                                    0.92
                                              0.92
                                                         106
                                              0.94
                                                         301
           accuracy
          macro avg
                          0.93
                                    0.94
                                              0.93
                                                         301
       weighted avg
                          0.94
                                    0.94
                                              0.94
                                                         301
       Validation Metrics: Accuracy = 0.9401993355481728, F1 score = 0.9403246524815795, Sensitivity = 0.9401993355481728
In [ ]: #SKLearn gradient boosting + Grid search
        from sklearn.ensemble import GradientBoostingClassifier
        model = GradientBoostingClassifier(random_state = 0)
        grid_search = GridSearchCV(model, param_grid, cv = 5, scoring = 'precision')
        grid_search.fit(X_train,y_train)
        best_gb = grid_search.best_estimator_
In [ ]: | print("Best Parameters:", grid_search.best_params_)
        print("Best Accuracy:", grid_search.best_score_)
       Best Parameters: {'learning_rate': 0.01, 'max_depth': 5, 'n_estimators': 50}
       Best Accuracy: 0.9643439784819096
In [ ]: validation_accuracy, validation_f1, validation_sensitivity, validation_balanced_accuracy = evaluate(best_gb, X_val, y_val)
        print(f"Validation Metrics: Accuracy = {validation_accuracy}, F1 score = {validation_f1}, Sensitivity = {validation_sensitivit
                     precision
                                  recall f1-score
                                                     support
                                              0.94
                          0.96
                                    0.93
             Benign
                                                         195
          Malignant
                          0.88
                                    0.92
                                              0.90
                                                         106
           accuracy
                                              0.93
                                                         301
                          0.92
                                    0.93
                                                         301
                                              0.92
          macro avg
       weighted avg
                          0.93
                                    0.93
                                              0.93
                                                         301
       Validation Metrics: Accuracy = 0.9269102990033222, F1 score = 0.9273451072876345, Sensitivity = 0.9269102990033222
In [ ]: #CatBoost + Gridsearch
        from catboost import CatBoostClassifier
        cbc = CatBoostClassifier(verbose=0)
        grid_search = GridSearchCV(estimator=cbc, param_grid=param_grid, cv=5, scoring='precision', verbose=1)
        grid_search.fit(X_train,y_train)
        best_cbc = grid_search.best_estimator_
       Fitting 5 folds for each of 27 candidates, totalling 135 fits
        Gridsearch Visualization (Edited)
In [ ]: # taking results
        results = grid_search.cv_results_
        # checking result tables
        results_df = pd.DataFrame(results)
        print(results_df[['param_learning_rate', 'param_max_depth', 'param_n_estimators', 'mean_test_score']])
        # compute score
        scores = results['mean_test_score']
        iterations = range(1, len(scores) + 1)
        # line graph
        plt.plot(iterations, scores, marker='o', label='Validation Score')
        plt.xlabel('Iteration')
        plt.ylabel('Mean Test Score')
        plt.title('GridSearchCV Progress')
        plt.grid()
        plt.legend()
        plt.show()
```

	param_learning_rate	param_max_depth	param_n_estimators	mean_test_score
0	0.01	3	50	0.965752
1	0.01	3	100	0.968102
2	0.01	3	200	0.969561
3	0.01	5	50	0.970811
4	0.01	5	100	0.971982
5	0.01	5	200	0.973323
6	0.01	7	50	0.969303
7	0.01	7	100	0.968049
8	0.01	7	200	0.970737
9	0.10	3	50	0.966932
10	0.10	3	100	0.968125
11	0.10	3	200	0.963040
12	0.10	5	50	0.965520
13	0.10	5	100	0.968360
14	0.10	5	200	0.964393
15	0.10	7	50	0.968784
16	0.10	7	100	0.968724
17	0.10	7	200	0.970035
18	1.00	3	50	0.931027
19	1.00	3	100	0.932732
20	1.00	3	200	0.932717
21	1.00	5	50	0.949115
22	1.00	5	100	0.956269
23	1.00	5	200	0.951239
24	1.00	7	50	0.943992
25	1.00	7	100	0.951719
26	1.00	7	200	0.951717

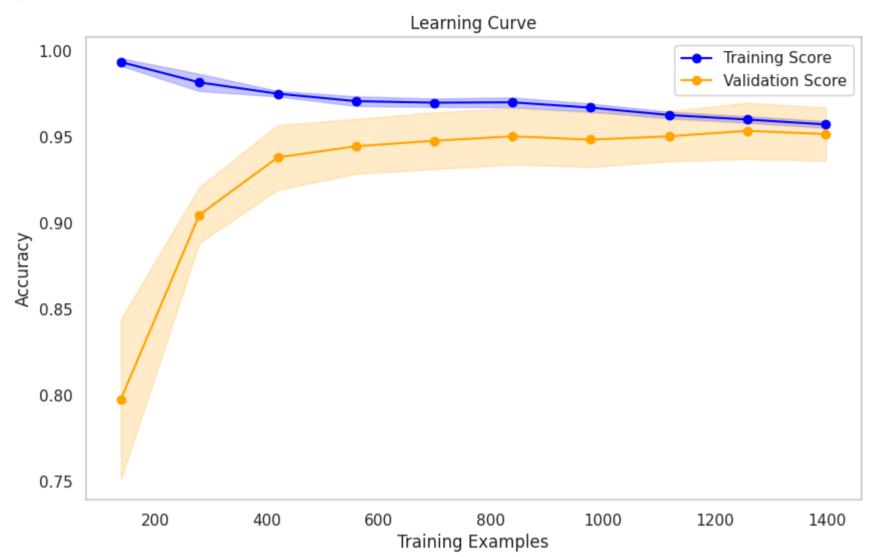
GridSearchCV Progress



Learning curve (Edited)

```
In [ ]: from sklearn.model_selection import learning_curve
        # define model
        model = CatBoostClassifier(**best_cbc.get_params())
        # calculating learning curve
        train_sizes, train_scores, test_scores = learning_curve(
            model, X_train, y_train, cv=10, scoring='accuracy', n_jobs=-1, train_sizes=np.linspace(0.1, 1.0, 10)
        train_mean = np.mean(train_scores, axis=1)
        train_std = np.std(train_scores, axis=1)
        test_mean = np.mean(test_scores, axis=1)
        test_std = np.std(test_scores, axis=1)
        # plot
        plt.figure(figsize=(10, 6))
        plt.plot(train_sizes, train_mean, 'o-', color='blue', label='Training Score')
        plt.plot(train_sizes, test_mean, 'o-', color='orange', label='Validation Score')
        # std area
        plt.fill_between(train_sizes, train_mean - train_std, train_mean + train_std, alpha=0.2, color='blue')
        plt.fill_between(train_sizes, test_mean - test_std, test_mean + test_std, alpha=0.2, color='orange')
        plt.title('Learning Curve')
        plt.xlabel('Training Examples')
        plt.ylabel('Accuracy')
        plt.legend(loc='best')
```

plt.grid()
plt.show()



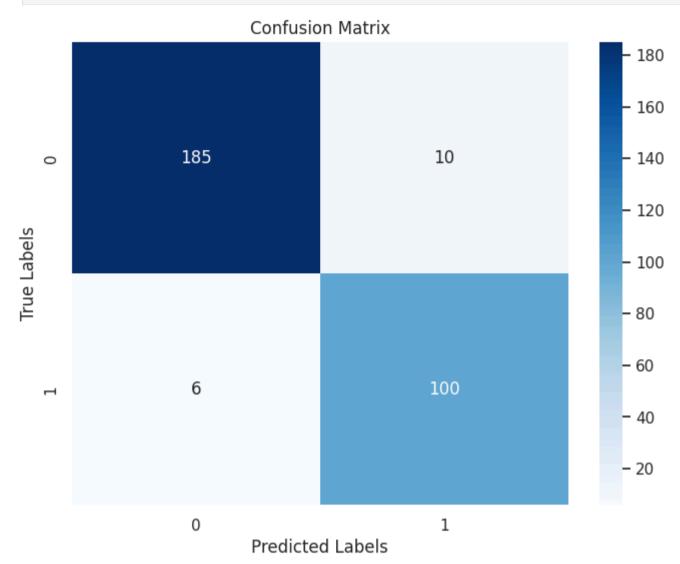
Malignant 0.91 0.94 0.93 106 accuracy 0.95 301 0.94 0.95 0.94 301 macro avg weighted avg 0.95 0.95 0.95 301

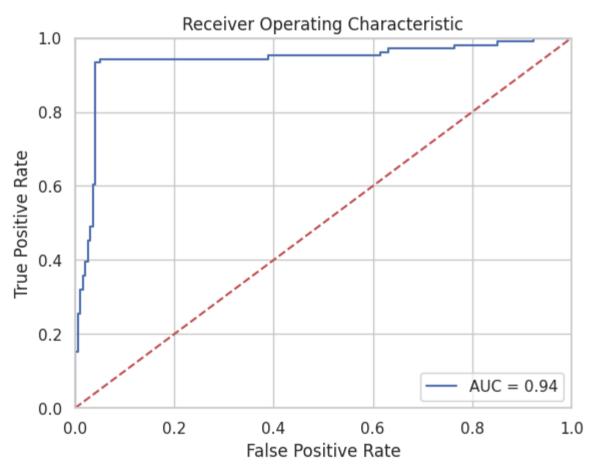
Validation Metrics: Accuracy = 0.946843853820598, F1 score = 0.9470606199127708, Sensitivity = 0.946843853820598

Confusion Matrix and AUC (Edited)

```
In [ ]: #addded for confusion matrix
        from sklearn.metrics import confusion_matrix, ConfusionMatrixDisplay
        import matplotlib.pyplot as plt
        y_true = y_val
        y_pred = best_cbc.predict(X_val)
        #compute
        cm = confusion_matrix(y_true, y_pred)
        #display
        plt.figure(figsize=(8, 6))
        sns.heatmap(cm, annot=True, fmt='d', cmap='Blues')
        plt.xlabel('Predicted Labels')
        plt.ylabel('True Labels')
        plt.title('Confusion Matrix')
        plt.show()
        #AUC
        import sklearn.metrics as metrics
        probs = best_cbc.predict_proba(X_val)
        preds = probs[:,1]
        fpr, tpr, threshold = metrics.roc_curve(y_true, preds)
        roc_auc = metrics.auc(fpr, tpr)
        #method: plt
        import matplotlib.pyplot as plt
        plt.title('Receiver Operating Characteristic')
        plt.plot(fpr, tpr, 'b', label = 'AUC = %0.2f' % roc_auc)
```

```
plt.legend(loc = 'lower right')
plt.plot([0, 1], [0, 1], 'r--')
plt.xlim([0, 1])
plt.ylim([0, 1])
plt.ylabel('True Positive Rate')
plt.xlabel('False Positive Rate')
plt.show()
```





```
In []: #Refitting the model on whole data

#Top 30 features
features = list(X_train.columns)

diag = df['Diagnosis'].reset_index(drop = True)

#Drop Irrelevant Columns

df_scaled = df.drop(['PatientID', 'DoctorInCharge','Diagnosis'], axis=1)

#Standardizing every column except diagnosis

df_scaled = pd.DataFrame(scaler.transform(df_scaled), columns=df_scaled.columns)

#Adding unscaled diagnosis column back

df_scaled['Diagnosis'] = diag

#Get X,y

X = df_scaled[features]
```

```
y = df_scaled['Diagnosis']
        smote = SMOTE(random_state=20)
        #Resample
        X, y = smote.fit_resample(X, y)
        #Refit the model on whole data
        best_model = CatBoostClassifier(**best_cbc.get_params())
        best_model.fit(X, y)
Out[ ]: <catboost.core.CatBoostClassifier at 0x7bedacefca30>
        Ensembling
In [ ]: X_train, y_train, X_val, y_val = prepare_X_y(['MMSE', 'FunctionalAssessment', 'MemoryComplaints', 'BehavioralProblems', 'ADL',
        #Logistic regression
        lr_pred = lr_model.predict_proba(X_val)
        #Decision Tree
        dt_pred = clf.predict_proba(X_val)
        #Random Forest
        features = [col for col in df_train.columns if col != 'Diagnosis']
        X_train, y_train, X_val, y_val = prepare_X_y(features)
        rf_pred = best_rf.predict_proba(X_val)
        #Tree Boosting
        X_train, y_train, X_val, y_val = prepare_X_y(np.array(feature_names)[indices][:30])
        xgb_pred = best_xgb.predict_proba(X_val)
        gb_pred = best_gb.predict_proba(X_val)
        cbc_pred = best_cbc.predict_proba(X_val)
In [ ]: |#Weighted Averaging
        y_pred_prob = (0.05*lr_pred + 0.05*dt_pred + 0.2*rf_pred + 0.2*xgb_pred + 0.2*xgb_pred + 0.2*xgb_pred + 0.3*cbc_pred)
        y_pred = np.argmax(y_pred_prob, axis=1)
        print(f"Accuracy: {accuracy_score(y_val,y_pred)}")
        print(f"Recall: {recall_score(y_val,y_pred, average='weighted')}")
       Accuracy: 0.9435215946843853
       Recall: 0.9435215946843853
        Model Submission
In [ ]: df_bf = pd.read_csv('best_submission.csv')
        df_test = pd.read_csv("test.csv")
In [ ]: def get_submission(model, features_used,scaler):
            df_test = pd.read_csv("test.csv")
            pat_ID = pd.DataFrame(df_test['PatientID'])
            df_test = df_test.drop(['PatientID', 'DoctorInCharge'], axis=1)
            df_test = pd.DataFrame(scaler.transform(df_test), columns=df_test.columns)
            X_t = df_test[features_used]
            y_test_pred = model.predict(X_t)
            pat_ID['Diagnosis'] = y_test_pred
            pat_ID.to_csv('submission.csv', index=False)
            accuracy, f1, sensitivity, _ = evaluate(model, X_t, df_bf['Diagnosis'])
            print(f"Comparing best result: Accuracy = {accuracy}, F1 score = {f1}, Sensitivity = {sensitivity}")
            print("Submission File Downloaded")
In [ ]: get_submission(best_model, list(X_train.columns), scaler)
                     precision recall f1-score
             Benign
                          1.00
                                    1.00
                                              1.00
                                                         426
          Malignant
                          1.00
                                    1.00
                                              1.00
                                                         219
           accuracy
                                              1.00
                                                         645
          macro avg
                          1.00
                                    1.00
                                              1.00
                                                         645
       weighted avg
                          1.00
                                    1.00
                                              1.00
                                                         645
       Comparing best result: Accuracy = 1.0, F1 score = 1.0, Sensitivity = 1.0
       Submission File Downloaded
In [ ]: %%shell
        jupyter nbconvert --to html /content/Colab_downladed_file_name.ipynb
```