

```
!pip install \
    scikit-learn==1.2.2 \
    numpy==1.25.2 \
    pandas==2.0.3 \
    scipy==1.11.2 \
    joblib==1.2.0 \
    threadpoolctl==3.1.0 \
    cython==0.29.36 \
    imbalanced-learn==0.12.0
```

```
➞ Requirement already satisfied: scikit-learn==1.2.2 in /usr/local/lib/python
Requirement already satisfied: numpy==1.25.2 in /usr/local/lib/python3.11/d
Requirement already satisfied: pandas==2.0.3 in /usr/local/lib/python3.11/d
Requirement already satisfied: scipy==1.11.2 in /usr/local/lib/python3.11/d
Requirement already satisfied: joblib==1.2.0 in /usr/local/lib/python3.11/d
Requirement already satisfied: threadpoolctl==3.1.0 in /usr/local/lib/pytho
Requirement already satisfied: cython==0.29.36 in /usr/local/lib/python3.11
Requirement already satisfied: imbalanced-learn==0.12.0 in /usr/local/lib/p
Requirement already satisfied: python-dateutil>=2.8.2 in /usr/local/lib/pyt
Requirement already satisfied: pytz>=2020.1 in /usr/local/lib/python3.11/di
Requirement already satisfied: tzdata>=2022.1 in /usr/local/lib/python3.11/
Requirement already satisfied: six>=1.5 in /usr/local/lib/python3.11/dist-p
```

```
pip freeze > new_env_requirements.txt
```

```
!python --version
```

```
➞ Python 3.11.11
```

```
# Importing necessary libraries
import pandas as pd
from sklearn.model_selection import train_test_split

# Load the data from an Excel file
data = pd.read_excel('2024_corrected_global_CARDEC_3_ML_Vitor.xlsx')

# Split the dataset into training and testing sets based on a unique identifier
# This ensures that data related to the same 'IDpac' is not split across both t
unique_n_part = data['IDpac'].unique()
train_n_part, test_n_part = train_test_split(unique_n_part, test_size=0.2, rand

# Filter the original dataset to create training data that includes only the 'I
train_data = data[data['IDpac'].isin(train_n_part)]
# Similarly, filter the original dataset to create testing data that includes c
test_data = data[data['IDpac'].isin(test_n_part)]

# Separate features and target variable for training set
# 'drop' removes specified columns from the dataset, in this case removing targ
X_train = train_data.drop(['Failure', 'IDrest', 'IDpac'], axis=1)
y_train = train_data['Failure'] # Isolate the target variable for the training

# Separate features and target variable for testing set following the same proc
X_test = test_data.drop(['Failure', 'IDrest', 'IDpac'], axis=1)
y_test = test_data['Failure'] # Isolate the target variable for the testing se

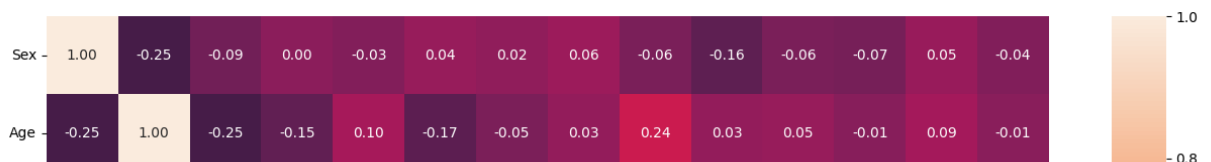
import seaborn as sns
import matplotlib.pyplot as plt

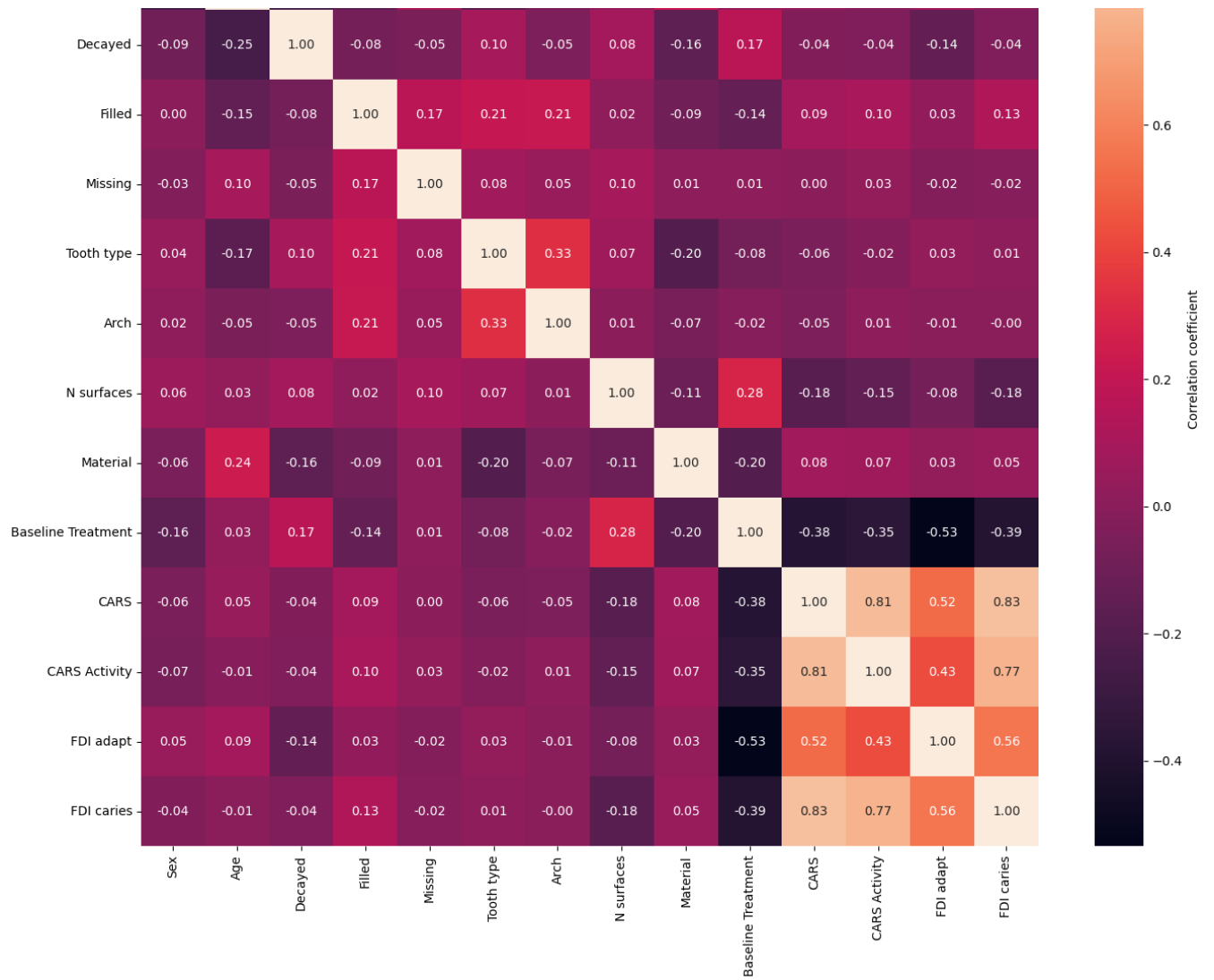
# Calculate the correlation matrix of the training data.
# The correlation matrix quantifies the linear relationships between the variabl
corr_matrix = X_train.corr()

# Initialize a matplotlib figure with a specified size (width=16 inches, height=
# This size is chosen to make the heatmap large enough to be easily readable.
plt.figure(figsize=(16, 14))

# Draw the heatmap using seaborn to visualize the correlation matrix.
sns.heatmap(corr_matrix, annot=True, annot_kws={"size": 10}, fmt=".2f", cbar_kws

# Display the plot on the screen. This command is necessary to show the figure w
plt.show()
```





```
import pandas as pd
```

```

# Define lists for each type of variable in the dataset: numeric, binary, and or
numeric_vars = ['Age', 'Decayed', 'Filled', 'Missing']
binary_vars = ['Sex', 'Tooth type', 'Arch', 'Failure', 'CARS Activity']
categorical_vars = ['N surfaces', 'Material', 'Baseline Treatment', 'CARS', 'FDI

def descriptive_statistics(train_data, test_data):
    # Print a heading for the descriptive statistics of numeric variables.
    print("Descriptive Statistics for Numeric Variables:")
    # Display descriptive statistics (like count, mean, std, min, max, etc.) for
    print("\nTraining Set:")
    print(train_data[numeric_vars].describe())
    # Repeat the process for the test set.
    print("\nTest Set:")
    print(test_data[numeric_vars].describe())

    # Initialize an empty dictionary to store statistics for binary and ordinal
    stats = {}
    # Loop through each variable in the binary and ordinal lists to calculate th
    for var in binary_vars + categorical_vars:
        stats[var] = {
            "Training Set": {
                "Count": train_data[var].value_counts().to_dict(), # Count occu
                "Percentage": (train_data[var].value_counts(normalize=True) * 10
            },
            "Test Set": {
                "Count": test_data[var].value_counts().to_dict(), # Count occur
                "Percentage": (test_data[var].value_counts(normalize=True) * 100
            }
        }

    # Loop through the stats dictionary to print the statistics for each categor
    for var, data in stats.items():
        print(f"\n{var} Statistics:") # Print the variable name.
        for dataset, values in data.items():
            print(f"\n{dataset}:") # Print which dataset (training or test) the
            for metric, metric_values in values.items():
                print(f"{metric}: {metric_values}") # Print the count and perce

# Call the function with the training and test datasets as arguments to display
descriptive_statistics(train_data, test_data)

```

➞ N surfaces Statistics:

Training Set:

Count: {1: 207, 2: 139, 3: 72, 4: 60, 5: 29}

Percentage: {1: 40.828402366863905, 2: 27.416173570019726, 3: 14.2011834319

## Test Set:

Count: {1: 56, 2: 27, 3: 20, 4: 14, 5: 13}

Percentage: {1: 43.07692307692308, 2: 20.76923076923077, 3: 15.384615384615

## Material Statistics:

## Training Set:

Count: {1: 304, 0: 189, 2: 14}

Percentage: {1: 59.96055226824457, 0: 37.278106508875744, 2: 2.761341222879

## Test Set:

Count: {1: 74, 0: 51, 2: 5}

Percentage: {1: 56.92307692307692, 0: 39.23076923076923, 2: 3.8461538461538

## Baseline Treatment Statistics:

## Training Set:

Count: {0: 292, 1: 167, 2: 48}

Percentage: {0: 57.59368836291914, 1: 32.938856015779095, 2: 9.467455621301

## Test Set:

Count: {0: 75, 1: 34, 2: 21}

Percentage: {0: 57.692307692307686, 1: 26.153846153846157, 2: 16.1538461538

## CARS Statistics:

## Training Set:

Count: {0: 399, 2: 62, 1: 46}

Percentage: {0: 78.69822485207101, 2: 12.22879684418146, 1: 9.0729783037475

## Test Set:

Count: {0: 99, 2: 20, 1: 11}

Percentage: {0: 76.15384615384615, 2: 15.384615384615385, 1: 8.461538461538

## FDI adapt Statistics:

## Training Set:

Count: {0: 333, 1: 155, 2: 19}

Percentage: {0: 65.68047337278107, 1: 30.57199211045365, 2: 3.7475345167652

## Test Set:

Count: {0: 82, 1: 43, 2: 5}

Percentage: {0: 63.07692307692307, 1: 33.07692307692307, 2: 3.8461538461538

## FDI caries Statistics:

## Training Set:

Count: {0: 401, 1: 98, 2: 8}

Percentage: {0: 79.09270216962526, 1: 19.32938856015779, 2: 1.5779092702169

## Test Set:

Count: {0: 97, 1: 30, 2: 3}

Percentage: {0: 74.61538461538461, 1: 23.076923076923077, 2: 2.307692307692

```

import pandas as pd
from sklearn.preprocessing import StandardScaler

# Convert specified categorical variables in the training data to 'category' dt
X_train['Material'] = X_train['Material'].astype('category')
X_train['Baseline Treatment'] = X_train['Baseline Treatment'].astype('category')
X_train['CARS'] = X_train['CARS'].astype('category')
X_train['FDI adapt'] = X_train['FDI adapt'].astype('category')
X_train['FDI caries'] = X_train['FDI caries'].astype('category')

# Apply one-hot encoding to the specified categorical columns in the training d
# 'prefix' argument specifies the prefix to add to the columns resulting from t
one_hot_train = pd.get_dummies(X_train[['Material', 'Baseline Treatment', 'CARS']
                                prefix=['Material', 'Baseline_Treatment', 'CARS']

# Concatenate the original training data (minus the now-encoded variables) with
X_train = pd.concat([X_train.drop(['Material', 'Baseline Treatment', 'CARS', 'F

# Initialize new one-hot encoded columns in the test data with zeros to match t
for col in one_hot_train.columns:
    X_test[col] = 0

# Convert specified categorical variables in the test data to 'category' dtype
X_test['Material'] = X_test['Material'].astype('category')
X_test['Baseline Treatment'] = X_test['Baseline Treatment'].astype('category')
X_test['CARS'] = X_test['CARS'].astype('category')
X_test['FDI adapt'] = X_test['FDI adapt'].astype('category')
X_test['FDI caries'] = X_test['FDI caries'].astype('category')

one_hot_test = pd.get_dummies(X_test[['Material', 'Baseline Treatment', 'CARS'],
                                prefix=['Material', 'Baseline_Treatment', 'CARS'],

# Update the test data with the new one-hot encoded columns.
X_test.update(one_hot_test)

# Check for any columns that are present in the training data but missing in th
# which might happen if the test data lacks certain categories.
missing_cols = set(X_train.columns) - set(X_test.columns)
for c in missing_cols:
    X_test[c] = 0 # Add these missing columns to the test data, initializing w

# Ensure the column order in the test data matches that of the training data fc
X_test = X_test[X_train.columns]

# Define a dictionary to rename the one-hot encoded columns for clarity, making
column_renaming = {'Material_0': 'Composite',
                    'Material_1': 'Glass Ionomer Cement',

```

```

'Material_2': 'Amalgam',
'Baseline_Treatment_0': 'No initial intervention',
'Baseline_Treatment_1': 'Repaired baseline',
'Baseline_Treatment_2': 'Replaced baseline',
'CARS_0': 'CARS No caries',
'CARS_1': 'CARS Initial',
'CARS_2': 'CARS Moderate/advanced',
'FDI_adapt_0': 'FDI No adaptation',
'FDI_adapt_1': 'FDI Initial adaptation',
'FDI_adapt_2': 'FDI Moderate/advanced adaptation',
'FDI_caries_0': 'FDI No caries',
'FDI_caries_1': 'FDI Initial caries',
'FDI_caries_2': 'FDI Moderate/advanced caries'}

```

```

# Rename the columns in both the training and test datasets according to the de
X_train.rename(columns=column_renaming, inplace=True)
X_test.rename(columns=column_renaming, inplace=True)

```

```


# Scale the numerical features in both training and test datasets to have mean
# This is crucial for models that are sensitive to the scale of input features.
scaler = StandardScaler()
X_train.loc[:, ['Age', 'Decayed', 'Filled', 'Missing']] = scaler.fit_transform(
X_test.loc[:, ['Age', 'Decayed', 'Filled', 'Missing']] = scaler.transform(X_tes

```

```

# Define which columns are considered categorical, excluding numerical columns
categorical_features = list(range(len(X_train.columns)))
for col in ['Age', 'Decayed', 'Filled', 'Missing']: # Assuming these are your
    categorical_features.remove(X_train.columns.get_loc(col))

```

 <ipython-input-7-1e795d60a953>:64: SettingWithCopyWarning:  
A value is trying to be set on a copy of a slice from a DataFrame

See the caveats in the documentation: <https://pandas.pydata.org/pandas-docs>  
X\_test.rename(columns=column\_renaming, inplace=True)

```
import pandas as pd
```

```

# Define lists categorizing the types of variables in the dataset.
numeric_vars = ['Age', 'Decayed', 'Filled', 'Missing'] # Numeric variables
original_categorical_vars = ['Sex', 'Tooth type', 'Arch', 'N surfaces', 'Failure
# One-hot encoded variables, representing categories as separate binary columns.
one_hot_encoded_vars = ['Composite', 'Glass Ionomer Cement', 'Amalgam', 'No init
                        'Repaired baseline', 'Replaced baseline', 'CARS No carie
                        'CARS Moderate/advanced', 'FDI No adaptation', 'FDI Init
                        'FDI Moderate/advanced adaptation', 'FDI No caries', 'FD
                        'FDI Moderate/advanced caries']

```

```

def descriptive_statistics(X_train, y_train, X_test, y_test):
    # Merge the feature DataFrame (X) and target variable Series (y) for both tr
    # This facilitates combined operations for descriptive statistics.
    train_data = pd.concat([X_train, y_train], axis=1)
    test_data = pd.concat([X_test, y_test], axis=1)

    # Print a heading and then descriptive statistics (count, mean, std, min, qu
    print("Descriptive Statistics for Numeric Variables:")
    print("\nTraining Set:")
    print(train_data[numeric_vars].describe())
    print("\nTest Set:")
    print(test_data[numeric_vars].describe())

    # Initialize a dictionary to hold statistics for categorical variables.
    stats = {}
    # Calculate and store counts and percentages for original (non-encoded) cate
    for var in original_categorical_vars:
        stats[var] = {
            "Training Set": {
                "Count": train_data[var].value_counts().to_dict(),
                "Percentage": (train_data[var].value_counts(normalize=True) * 10
            },
            "Test Set": {
                "Count": test_data[var].value_counts().to_dict(),
                "Percentage": (test_data[var].value_counts(normalize=True) * 100
            }
        }

    # Handle one-hot encoded variables by identifying all columns that match the
    # Then calculate counts and percentages for these as well.
    for var in one_hot_encoded_vars:
        encoded_columns = [col for col in train_data if col.startswith(var)]
        for col in encoded_columns:
            stats[col] = {
                "Training Set": {
                    "Count": train_data[col].value_counts().to_dict(),
                    "Percentage": (train_data[col].value_counts(normalize=True) *
                },
                "Test Set": {
                    "Count": test_data[col].value_counts().to_dict(),
                    "Percentage": (test_data[col].value_counts(normalize=True) *
                }
            }

    # Print the calculated statistics for each categorical variable, both origin
    for var, data in stats.items():
        print(f"\n{var} Statistics:")
        for dataset, values in data.items():
            print(f"\n{dataset}:")

```



```
print("\n\nDataset: ")
for metric, metric_values in values.items():
    print(f"{metric}: {metric_values}")
```

```
# Call the function, passing the training and test datasets (features and target
descriptive_statistics(X_train, y_train, X_test, y_test)
```



FDI No adaptation Statistics:

Training Set:

Count: {True: 333, False: 174}

Percentage: {True: 65.68047337278107, False: 34.319526627218934}

Test Set:

Count: {1: 82, 0: 48}

Percentage: {1: 63.07692307692307, 0: 36.92307692307693}

FDI Initial adaptation Statistics:

Training Set:

Count: {False: 352, True: 155}

Percentage: {False: 69.42800788954635, True: 30.57199211045365}

Test Set:

Count: {0: 87, 1: 43}

Percentage: {0: 66.92307692307692, 1: 33.07692307692307}

FDI Moderate/advanced adaptation Statistics:

Training Set:

Count: {False: 488, True: 19}

Percentage: {False: 96.25246548323472, True: 3.7475345167652856}

Test Set:

Count: {0: 125, 1: 5}

Percentage: {0: 96.15384615384616, 1: 3.8461538461538463}

FDI No caries Statistics:

Training Set:

Count: {True: 401, False: 106}

Percentage: {True: 79.09270216962526, False: 20.907297830374755}

Test Set:

Count: {1: 97, 0: 33}

Percentage: {1: 74.61538461538461, 0: 25.384615384615383}

FDI Initial caries Statistics:

Training Set:

Count: {False: 409, True: 98}

Percentage: {False: 80.6706114398422, True: 19.32938856015779}

```

Test Set:
Count: {0: 100, 1: 30}
Percentage: {0: 76.92307692307693, 1: 23.076923076923077}

```

FDI Moderate/advanced caries Statistics:

```

Training Set:
Count: {False: 499, True: 8}
Percentage: {False: 98.42209072978304, True: 1.5779092702169626}

```

```

Test Set:
Count: {0: 127, 1: 3}
Percentage: {0: 97.6923076923077, 1: 2.307692307692308}

```

```
# Define custom metrics
```

```
def sensitivity(y_true, y_pred):
    tn, fp, fn, tp = confusion_matrix(y_true, y_pred).ravel()
    return tp / (tp + fn)
```

```
def specificity(y_true, y_pred):
    tn, fp, fn, tp = confusion_matrix(y_true, y_pred).ravel()
    return tn / (tn + fp)
```

```

import pandas as pd
import numpy as np
import shap
import sys
import tensorflow as tf
import matplotlib.pyplot as plt
import random
import seaborn as sns
from sklearn.model_selection import cross_val_score
from sklearn.calibration import CalibratedClassifierCV
from sklearn.tree import DecisionTreeClassifier, plot_tree
from sklearn.ensemble import RandomForestClassifier
from xgboost import XGBClassifier
from sklearn.model_selection import cross_validate, StratifiedKFold, GridSearch
from sklearn.metrics import make_scorer, accuracy_score, roc_auc_score, f1_score
from sklearn.preprocessing import StandardScaler
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import Dense, Dropout, BatchNormalization
from tensorflow.keras.callbacks import EarlyStopping, ReduceLROnPlateau, LearningRateScheduler
from tensorflow.keras.regularizers import l2
from scipy import stats

```

```

def evaluate_model(model, name, grid, X_train, y_train, X_test, y_test, cv, scorer):
    print(f"\nEvaluating {name} with seed {seed}...")

```

```

inner_cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=seed)
outer_cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=seed)

clf = GridSearchCV(model, grid, cv=inner_cv, scoring='roc_auc')
nested_scores = cross_validate(clf, X=X_train, y=y_train, cv=outer_cv, scori

clf.fit(X_train, y_train)
best_model = clf.best_estimator_
best_params = clf.best_params_
print(f"Best parameters for {name}: {best_params}")

calibrated_clf = CalibratedClassifierCV(estimator=best_model, method='sigmoid')
calibrated_clf.fit(X_train, y_train)

y_probs = calibrated_clf.predict_proba(X_test)[: , 1]

# Calculate ROC curve and AUC
fpr, tpr, thresholds = roc_curve(y_test, y_probs)
roc_auc = auc(fpr, tpr)

print("\n--- ROC Data for Copying ---")
print("FPR =", fpr.tolist())
print("TPR =", tpr.tolist())
print("AUC =", roc_auc)
print("---- End of ROC Data ----\n")

# --- Calculate Training Metrics ---
y_train_pred = best_model.predict(X_train)
y_train_probs = best_model.predict_proba(X_train)[: , 1]
train_acc = accuracy_score(y_train, y_train_pred)
train_sens = sensitivity(y_train, y_train_pred)
train_spec = specificity(y_train, y_train_pred)
train_f1 = f1_score(y_train, y_train_pred)
train_roc_auc = roc_auc_score(y_train, y_train_probs)

print(f"Training - Accuracy: {train_acc:.3f}, Sensitivity: {train_sens:.3f},
      f"Specificity: {train_spec:.3f}, F1: {train_f1:.3f}, ROC AUC: {train_r

# --- Calculate Test Metrics for the manually set threshold ---
y_pred_manual = (y_probs >= manual_threshold).astype(int)
manual_acc = accuracy_score(y_test, y_pred_manual)
manual_sens = sensitivity(y_test, y_pred_manual)
manual_spec = specificity(y_test, y_pred_manual)
manual_f1 = f1_score(y_test, y_pred_manual)
manual_roc_auc = roc_auc_score(y_test, y_probs)

print(f"\nTest Metrics for manual threshold {manual_threshold}:")
print(f"Accuracy: {manual_acc:.3f}, Sensitivity: {manual_sens:.3f}, "

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        f"Specificity: {manual_spec:.3f}, F1: {manual_f1:.3f}, ROC AUC: {manua

# --- Evaluate metrics across a range of thresholds ---
threshold_metrics = {}
for threshold in threshold_list:
    y_pred_threshold = (y_probs >= threshold).astype(int)
    threshold_acc = accuracy_score(y_test, y_pred_threshold)
    threshold_sens = sensitivity(y_test, y_pred_threshold)
    threshold_spec = specificity(y_test, y_pred_threshold)
    threshold_f1 = f1_score(y_test, y_pred_threshold)
    threshold_metrics[threshold] = {
        'Accuracy': threshold_acc,
        'Sensitivity': threshold_sens,
        'Specificity': threshold_spec,
        'F1': threshold_f1,
        'ROC AUC': manual_roc_auc # Same ROC AUC regardless of threshold
    }
for threshold, metrics in threshold_metrics.items():
    print(f"Threshold: {threshold:.2f}, Metrics: {metrics}")

calculate_and_plot_shap(best_model, X_train, X_test, name)

# Prepare dictionary of test metrics for aggregation
test_metrics = {
    "accuracy": manual_acc,
    "sensitivity": manual_sens,
    "specificity": manual_spec,
    "f1": manual_f1,
    "roc_auc": manual_roc_auc
}

return best_model, manual_threshold, best_params, nested_scores, calibrated_

def calculate_and_plot_shap(model, X_train, X_test, model_name):
    if isinstance(model, DecisionTreeClassifier):
        explainer = shap.TreeExplainer(model)
    else:
        explainer = shap.KernelExplainer(model.predict_proba, X_train.sample(100))
    shap_values = explainer.shap_values(X_test)
    print(f"SHAP Summary for {model_name}")
    shap.summary_plot(shap_values, X_test, max_display=10)

def plot_confusion_matrix(y_true, y_pred):
    matrix = confusion_matrix(y_true, y_pred)
    sns.heatmap(matrix, annot=True, fmt='d', cmap='Blues',
                xticklabels=['Predicted Success', 'Predicted Failure'],
                yticklabels=['Actual Success', 'Actual Failure'])
    plt.title('Confusion Matrix')

```

```

plt.show()

def plot_roc_curve(y_true, y_probs):
    fpr, tpr, thresholds = roc_curve(y_true, y_probs)
    roc_auc = auc(fpr, tpr)
    plt.figure()
    plt.plot(fpr, tpr, color='darkorange', lw=2, label=f'ROC curve (area = {roc_auc})')
    plt.plot([0, 1], [0, 1], color='navy', lw=2, linestyle='--')
    plt.xlim([0.0, 1.0])
    plt.ylim([0.0, 1.05])
    plt.xlabel('False Positive Rate')
    plt.ylabel('True Positive Rate')
    plt.title('Receiver Operating Characteristic')
    plt.legend(loc="lower right")
    plt.show()

def evaluate_decision_tree(X_train, y_train, X_test, y_test, cv, scoring, manual_threshold):
    model = DecisionTreeClassifier(random_state=seed)
    grid = {
        'max_depth': [6],
        'criterion': ['gini'],
        'min_samples_split': [4],
        'min_samples_leaf': [8],
        'ccp_alpha': [0.001]
    }
    return evaluate_model(model, "Decision Tree", grid, X_train, y_train, X_test, y_test, cv, scoring, manual_threshold)

def main(X_train, y_train, X_test, y_test):
    cv = RepeatedStratifiedKFold(n_splits=10, n_repeats=10, random_state=42)
    scoring = {
        'accuracy': make_scorer(accuracy_score),
        'sensitivity': make_scorer(sensitivity),
        'specificity': make_scorer(specificity),
        'f1': make_scorer(f1_score),
        'roc_auc': make_scorer(roc_auc_score)
    }
    manual_threshold = 0.5
    threshold_list = np.arange(0.1, 1.05, 0.05)

    aggregated_metrics = []

    # Loop over seeds
    for seed in range(40, 50):
        print(f"\nRunning evaluation with seed {seed}")
        (best_model, manual_threshold, best_params, nested_scores,
         calibrated_clf, threshold_metrics, test_metrics) = evaluate_decision_tree(
            X_train, y_train, X_test, y_test, cv, scoring, manual_threshold, threshold_list
        )

```

```

# Use calibrated classifier for plotting
y_probs = calibrated_clf.predict_proba(X_test)[: , 1]
y_pred_manual = (y_probs >= manual_threshold).astype(int)

plot_confusion_matrix(y_test, y_pred_manual)
plot_roc_curve(y_test, y_probs)

aggregated_metrics.append(test_metrics)

# Aggregate results across seeds
results_df = pd.DataFrame(aggregated_metrics)
n = len(results_df)
print("\nAggregated Test Set Metrics Across Seeds:")
print(results_df)

# Compute mean, standard error, and 95% confidence interval for each metric
def summarize_metric(metric_values):
    mean_val = metric_values.mean()
    std_val = metric_values.std(ddof=1)
    se = std_val / np.sqrt(n)
    t_crit = stats.t.ppf(0.975, df=n - 1)
    ci_lower = mean_val - t_crit * se
    ci_upper = mean_val + t_crit * se
    return mean_val, se, (ci_lower, ci_upper)

metrics_summary = {}
for metric in results_df.columns:
    mean_val, se, ci = summarize_metric(results_df[metric])
    metrics_summary[metric] = {
        "Mean": mean_val,
        "Standard Error": se,
        "95% CI": ci
    }

print("\nSummary of Test Set Metrics (Mean, Standard Error, 95% Confidence I
for metric, summary in metrics_summary.items():
    print(f"{metric.capitalize()}: Mean = {summary['Mean']:.3f}, SE = {summa
          f"95% CI = [{summary['95% CI'][0]:.3f}, {summary['95% CI'][1]:.3f}

# RUN THE MAIN FUNCTION (Ensure X_train, y_train, X_test, y_test are defined)
if __name__ == '__main__':
    main(X_train, y_train, X_test, y_test)

```



Running evaluation with seed 40

Evaluating Decision Tree with seed 40...

Best parameters for Decision Tree: {'ccp\_alpha': 0.001, 'criterion': 'gini'

--- ROC Data for Copying ---

FPR = [0.0, 0.0, 0.0, 0.02857142857142857, 0.02857142857142857, 0.028571428

TPR = [0.0, 0.016666666666666666, 0.03333333333333333, 0.06666666666666667,

AUC = 0.7550000000000001

--- End of ROC Data ---

Training - Accuracy: 0.728, Sensitivity: 0.805, Specificity: 0.652, F1: 0.7

Test Metrics for manual threshold 0.5:

Accuracy: 0.723, Sensitivity: 0.833, Specificity: 0.629, F1: 0.735, ROC AUC

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.30, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.35, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.40, Metrics: {'Accuracy': 0.49230769230769234, 'Sensitivity':

Threshold: 0.45, Metrics: {'Accuracy': 0.5538461538461539, 'Sensitivity': 0

Threshold: 0.50, Metrics: {'Accuracy': 0.7230769230769231, 'Sensitivity': 0

Threshold: 0.55, Metrics: {'Accuracy': 0.7230769230769231, 'Sensitivity': 0

Threshold: 0.60, Metrics: {'Accuracy': 0.5538461538461539, 'Sensitivity': 0

Threshold: 0.65, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

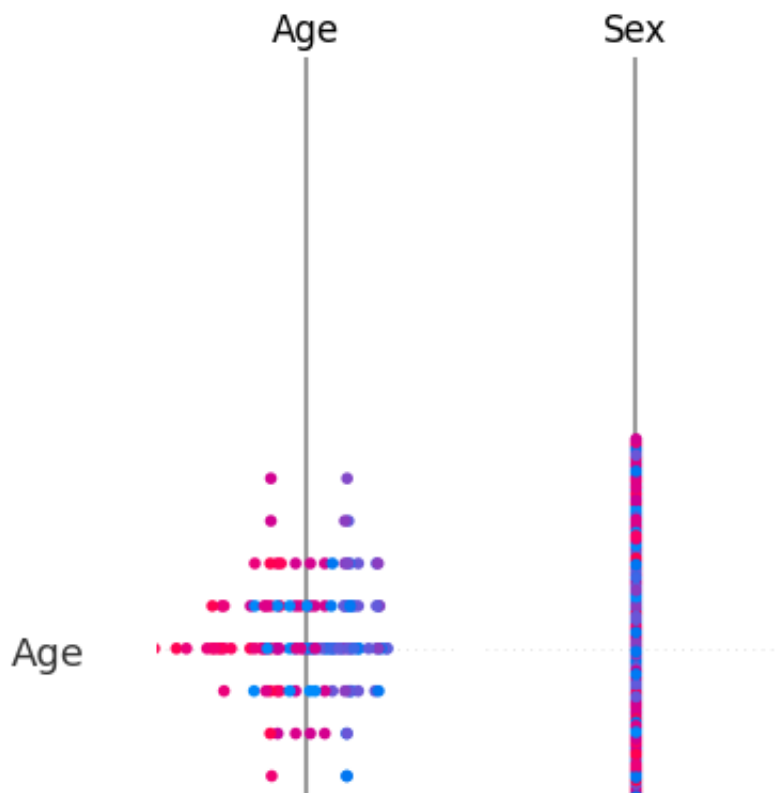
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

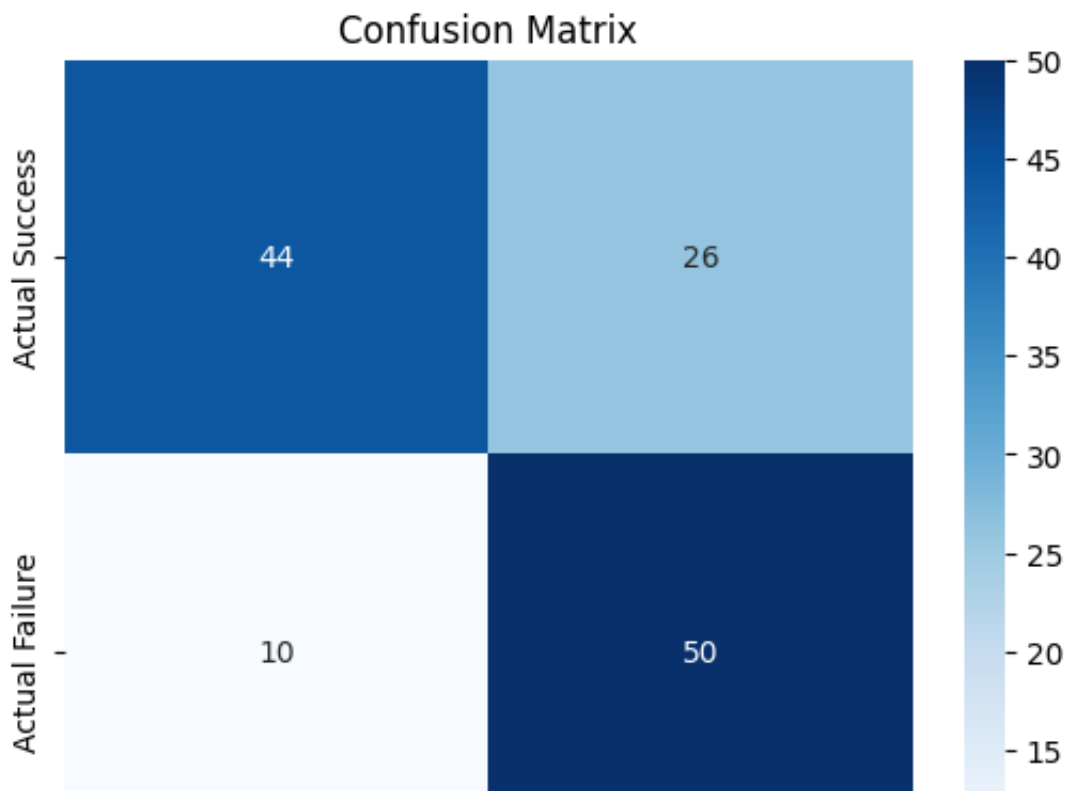
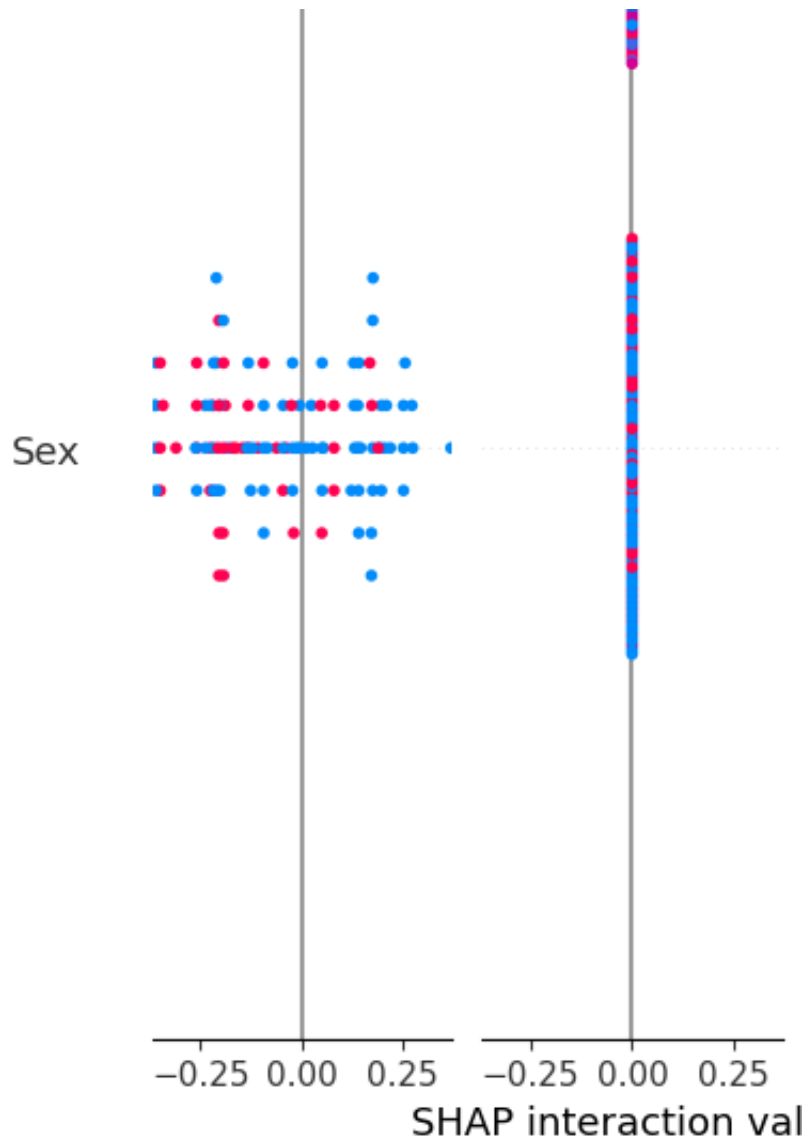
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

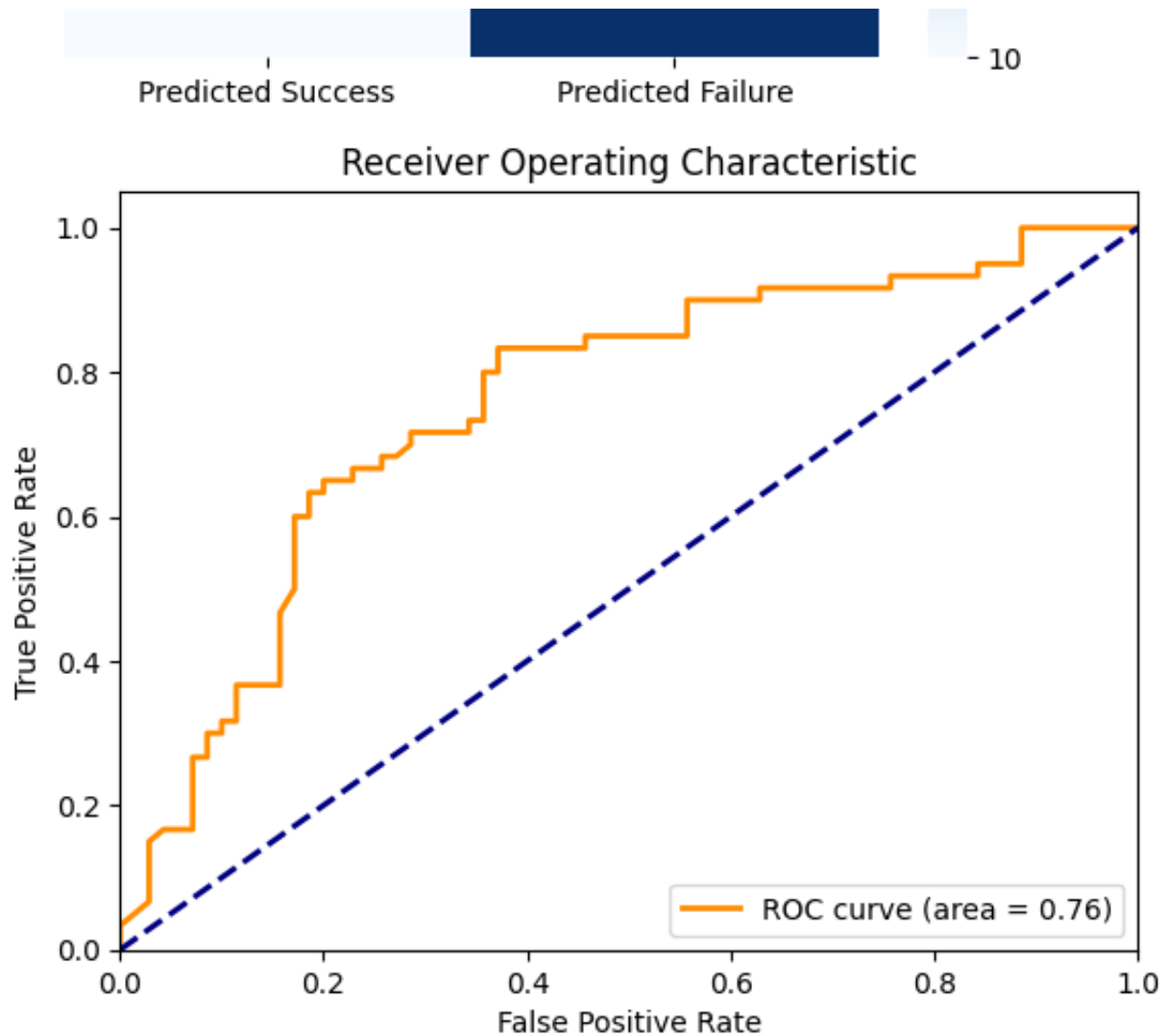
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

SHAP Summary for Decision Tree









Running evaluation with seed 41

Evaluating Decision Tree with seed 41...

Best parameters for Decision Tree: {'ccp\_alpha': 0.001, 'criterion': 'gini'}

--- ROC Data for Copying ---

FPR = [0.0, 0.0, 0.0, 0.02857142857142857, 0.02857142857142857, 0.028571428

TPR = [0.0, 0.016666666666666666, 0.03333333333333333, 0.06666666666666667,

AUC = 0.7557142857142857

--- End of ROC Data ---

Training - Accuracy: 0.728, Sensitivity: 0.805, Specificity: 0.652, F1: 0.7

Test Metrics for manual threshold 0.5:

Accuracy: 0.723, Sensitivity: 0.833, Specificity: 0.629, F1: 0.735, ROC AUC

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

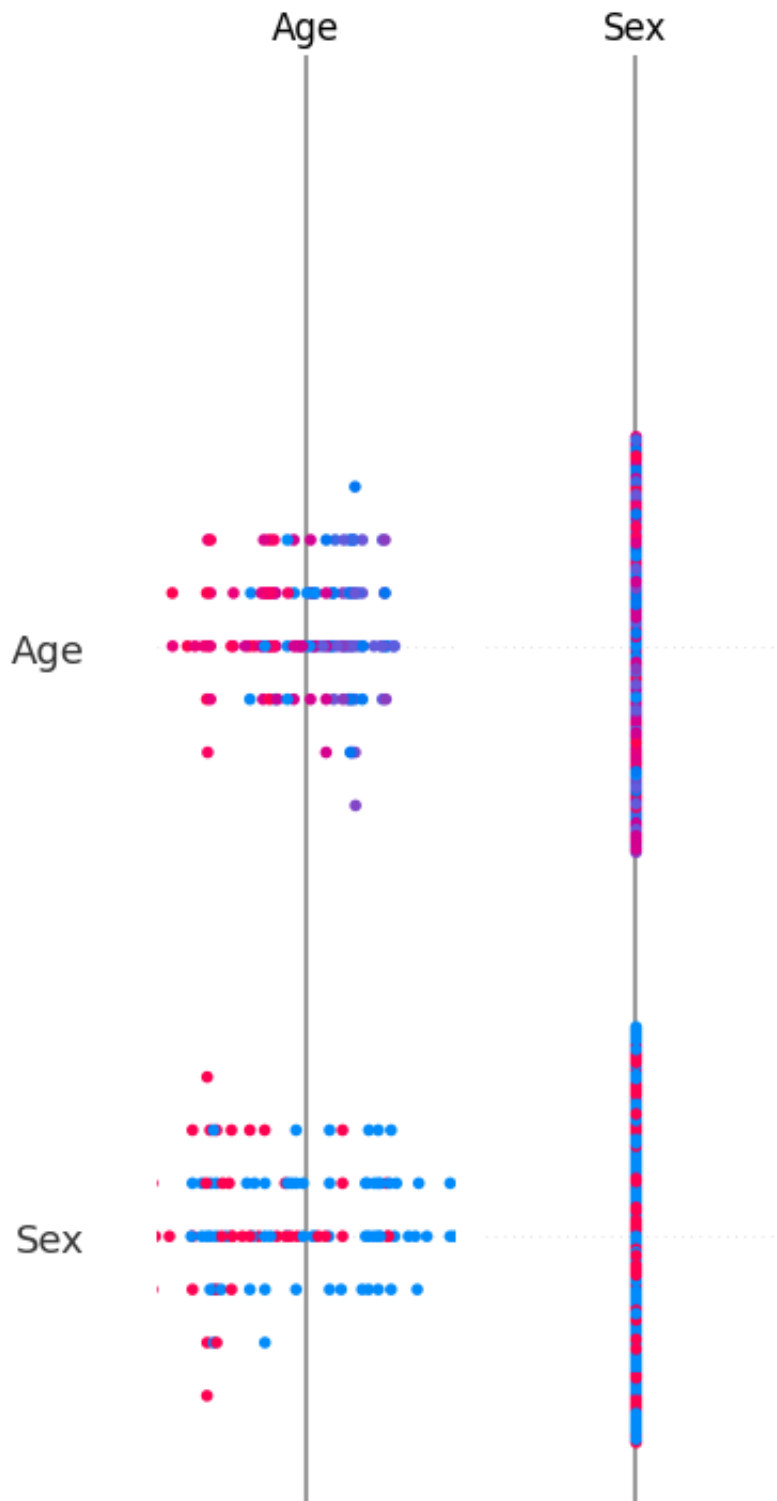
Threshold: 0.30, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

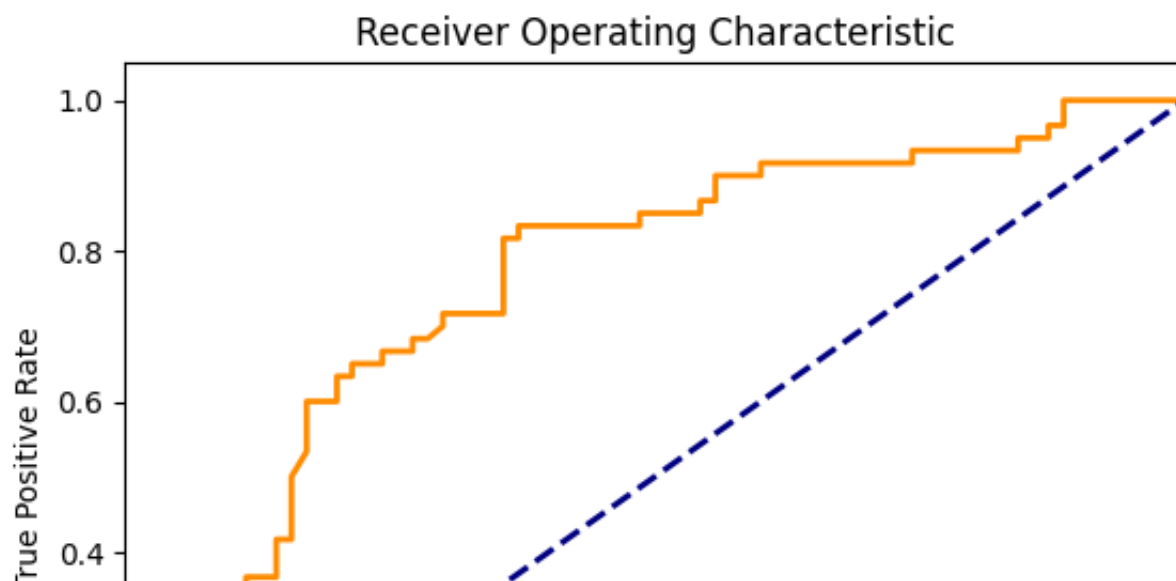
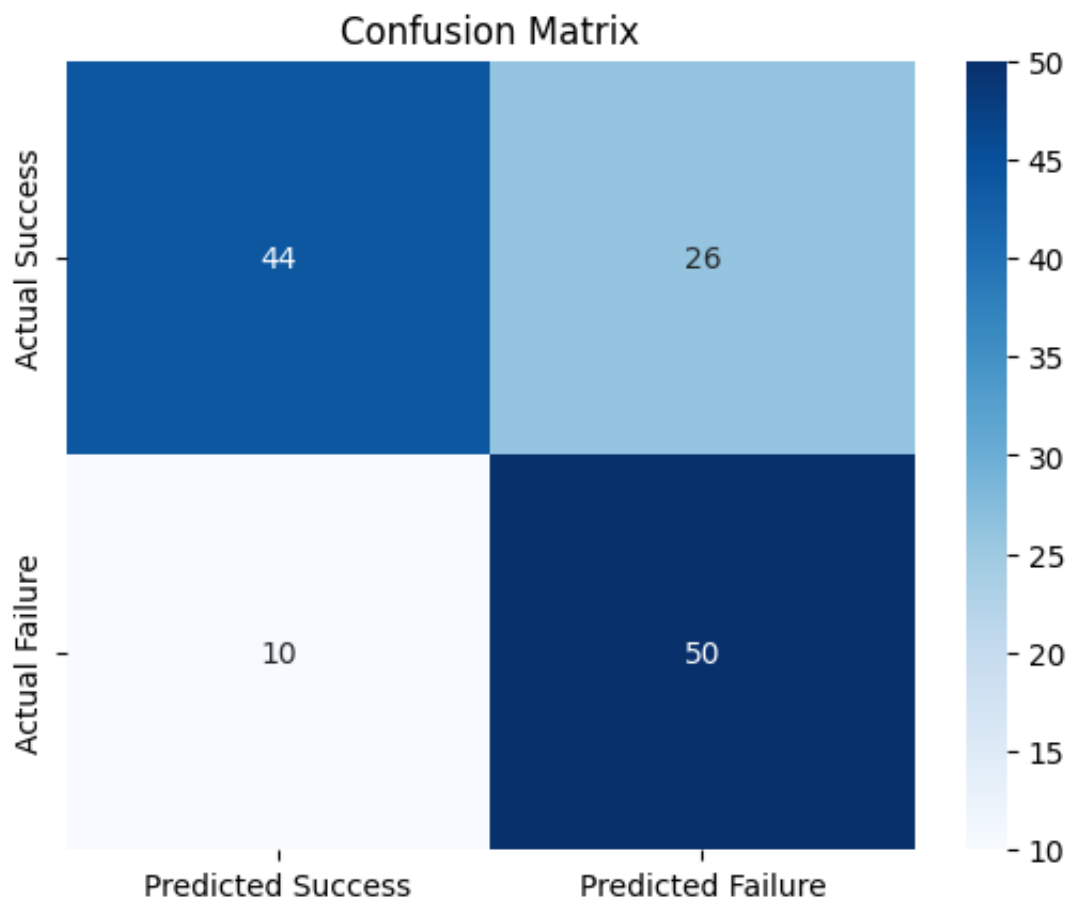
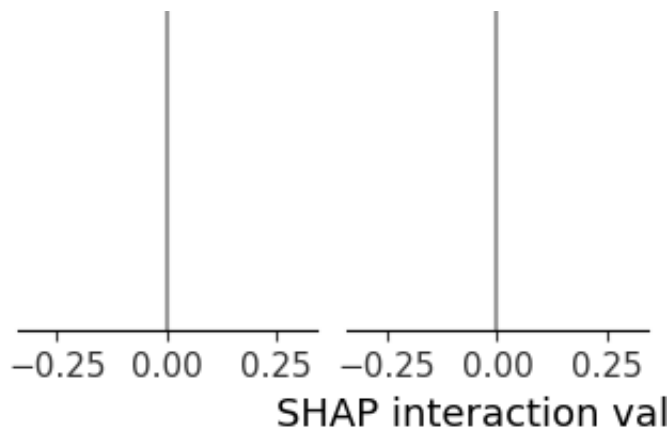
Threshold: 0.35, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

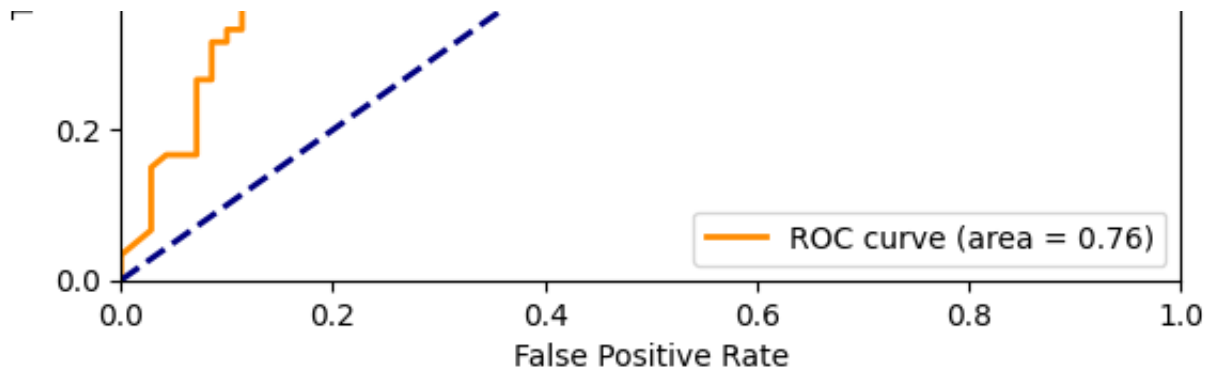
Threshold: 0.40, Metrics: {'Accuracy': 0.49230769230769234, 'Sensitivity':

Threshold: 0.45, Metrics: {'Accuracy': 0.5615384615384615, 'Sensitivity': 0

```
Threshold: 0.50, Metrics: {'Accuracy': 0.7230769230769231, 'Sensitivity': 0
Threshold: 0.55, Metrics: {'Accuracy': 0.7076923076923077, 'Sensitivity': 0
Threshold: 0.60, Metrics: {'Accuracy': 0.5538461538461539, 'Sensitivity': 0
Threshold: 0.65, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
SHAP Summary for Decision Tree
```







Running evaluation with seed 42

Evaluating Decision Tree with seed 42...

Best parameters for Decision Tree: {'ccp\_alpha': 0.001, 'criterion': 'gini'}

--- ROC Data for Copying ---

FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.0285714

TPR = [0.0, 0.016666666666666666, 0.05, 0.066666666666666667, 0.1, 0.1166666

AUC = 0.7501190476190476

--- End of ROC Data ---

Training - Accuracy: 0.728, Sensitivity: 0.805, Specificity: 0.652, F1: 0.7

Test Metrics for manual threshold 0.5:

Accuracy: 0.715, Sensitivity: 0.817, Specificity: 0.629, F1: 0.726, ROC AUC

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.30, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.35, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.40, Metrics: {'Accuracy': 0.49230769230769234, 'Sensitivity':

Threshold: 0.45, Metrics: {'Accuracy': 0.5538461538461539, 'Sensitivity': 0

Threshold: 0.50, Metrics: {'Accuracy': 0.7153846153846154, 'Sensitivity': 0

Threshold: 0.55, Metrics: {'Accuracy': 0.6692307692307692, 'Sensitivity': 0

Threshold: 0.60, Metrics: {'Accuracy': 0.5461538461538461, 'Sensitivity': 0

Threshold: 0.65, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

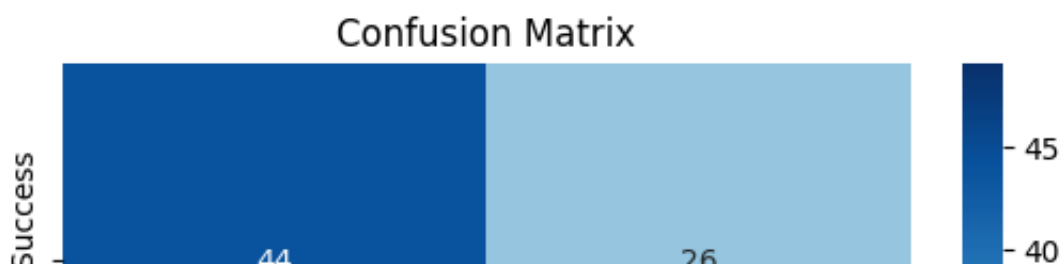
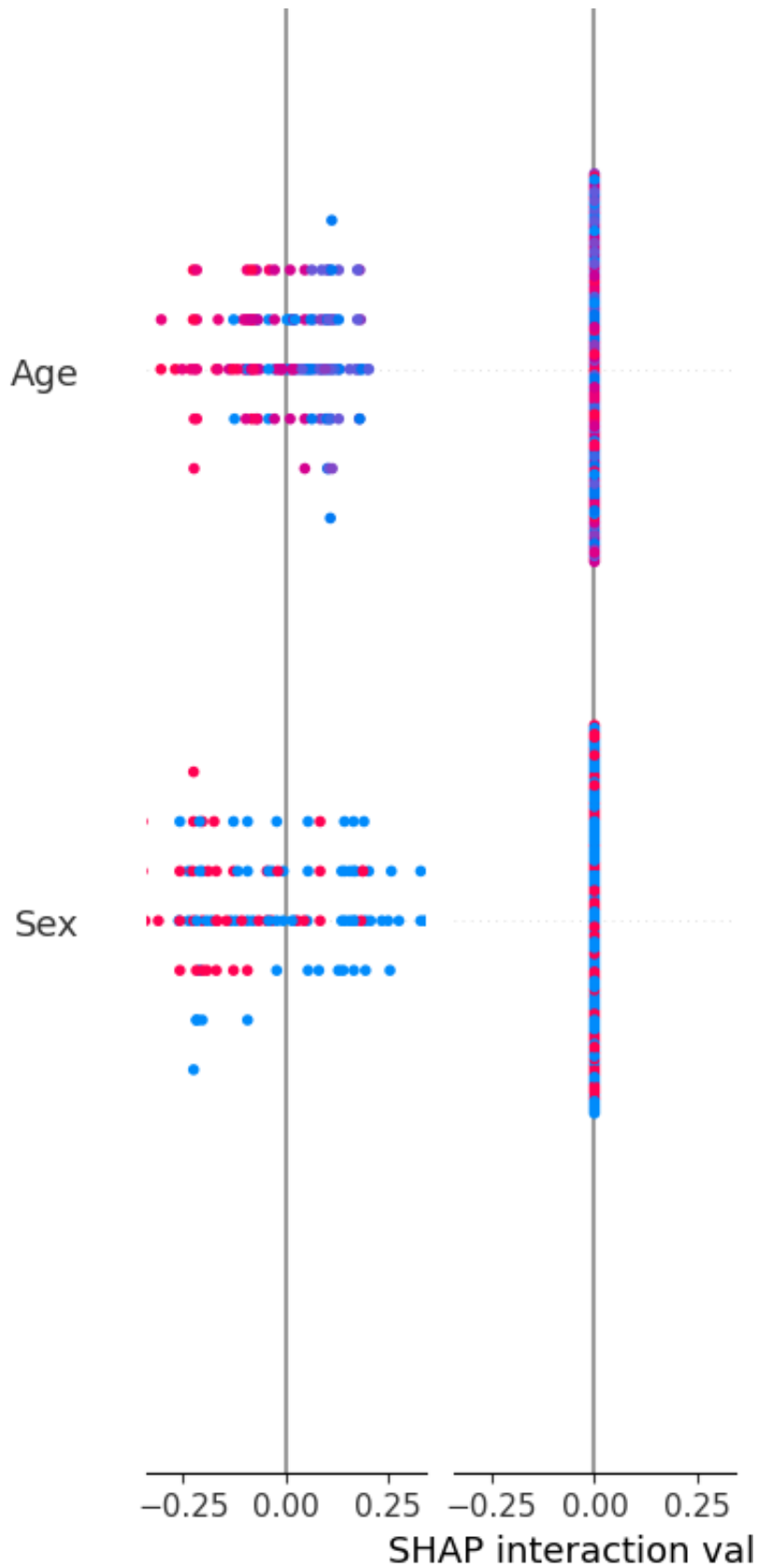
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

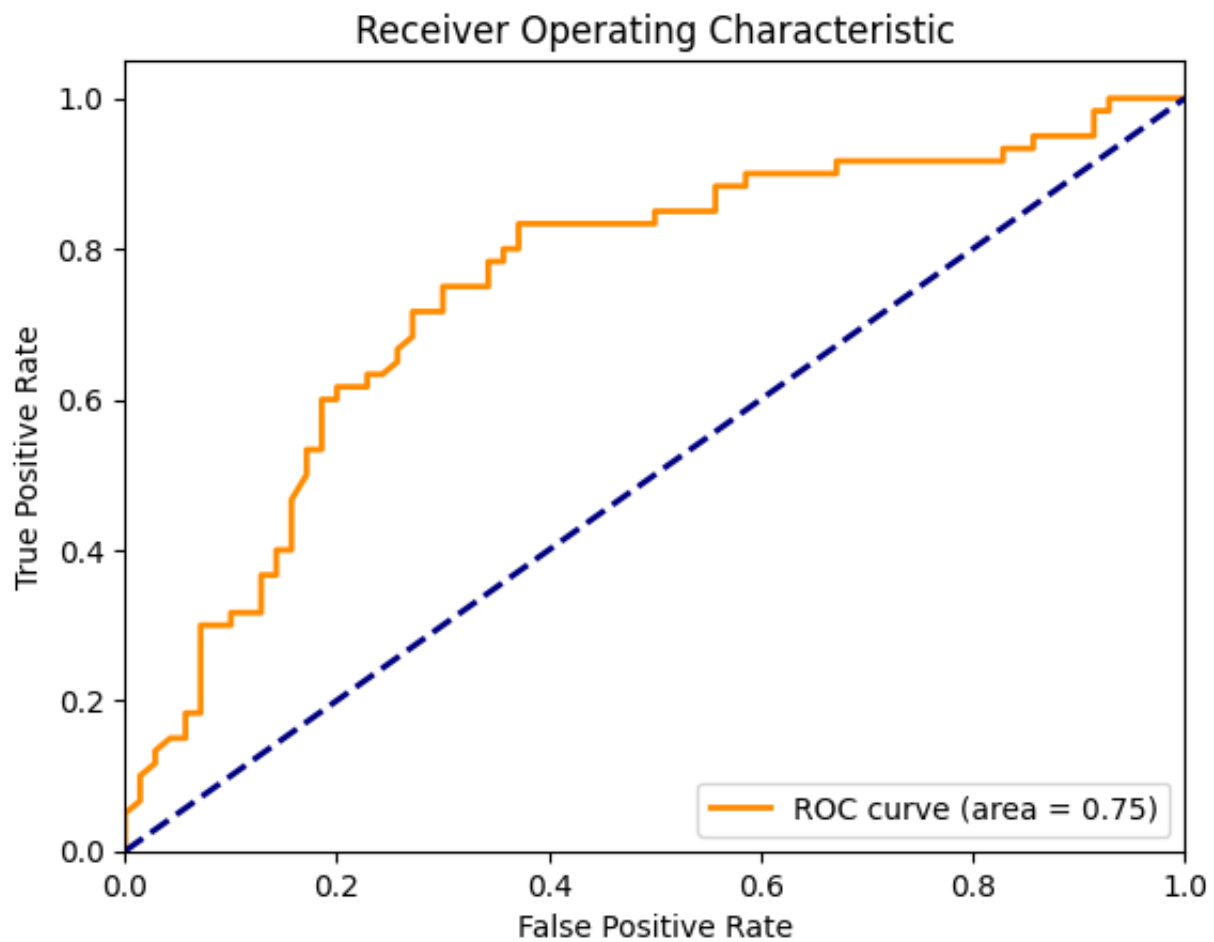
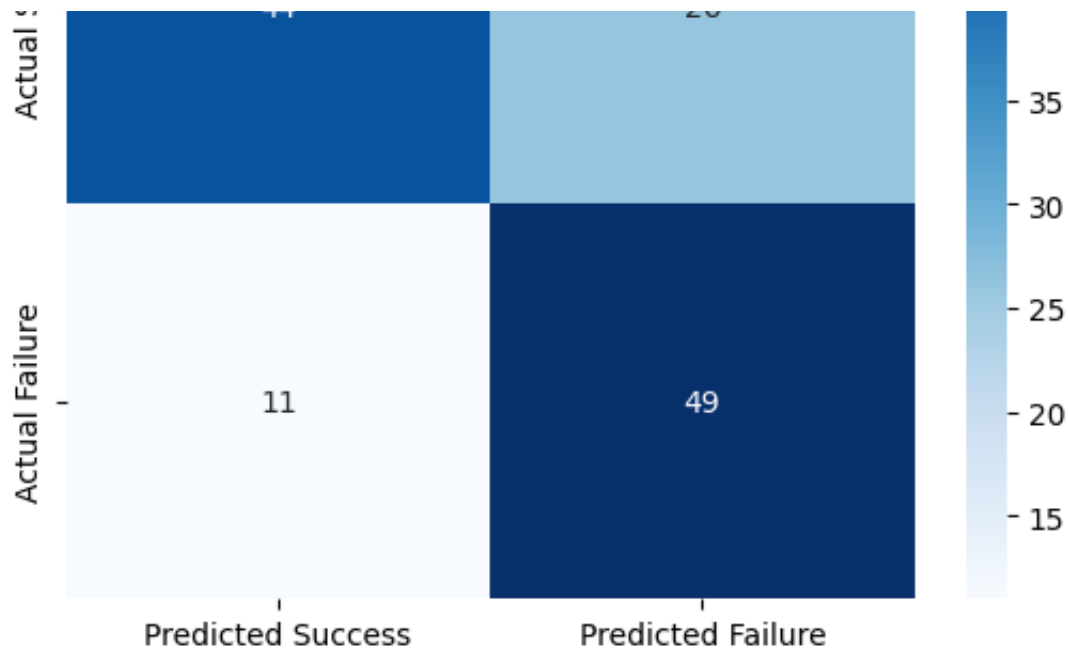
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

SHAP Summary for Decision Tree

Age

Sex





Running evaluation with seed 43

Evaluating Decision Tree with seed 43...

Best parameters for Decision Tree: {'ccp\_alpha': 0.001, 'criterion': 'gini'}

--- ROC Data for Copying ---

FPR = [0.0, 0.0, 0.0, 0.02857142857142857, 0.02857142857142857, 0.028571428

TPR = [0.0, 0.016666666666666666, 0.03333333333333333, 0.06666666666666667,

AUC = 0.7533333333333333

--- End of ROC Data ---

Training - Accuracy: 0.728, Sensitivity: 0.805, Specificity: 0.652, F1: 0.7

Test Metrics for manual threshold 0.5:

Accuracy: 0.723, Sensitivity: 0.833, Specificity: 0.629, F1: 0.735, ROC AUC

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.30, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.35, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.40, Metrics: {'Accuracy': 0.4846153846153846, 'Sensitivity': 0

Threshold: 0.45, Metrics: {'Accuracy': 0.5769230769230769, 'Sensitivity': 0

Threshold: 0.50, Metrics: {'Accuracy': 0.7230769230769231, 'Sensitivity': 0

Threshold: 0.55, Metrics: {'Accuracy': 0.7230769230769231, 'Sensitivity': 0

Threshold: 0.60, Metrics: {'Accuracy': 0.5538461538461539, 'Sensitivity': 0

Threshold: 0.65, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

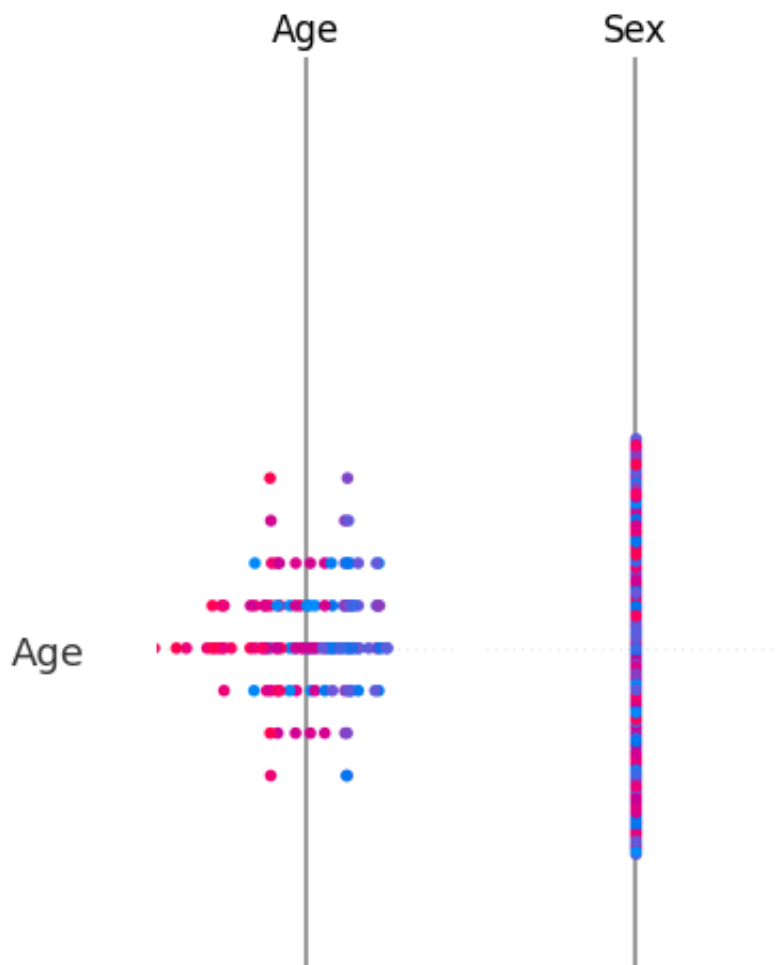
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

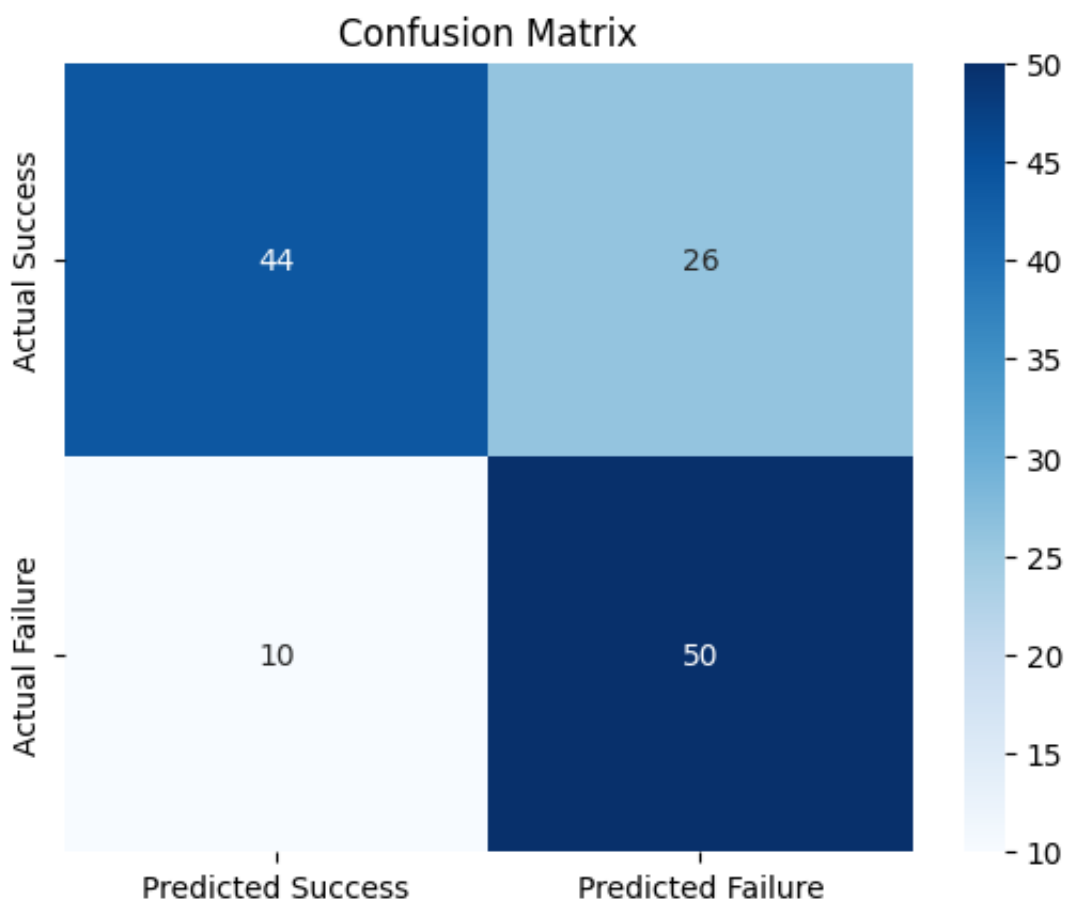
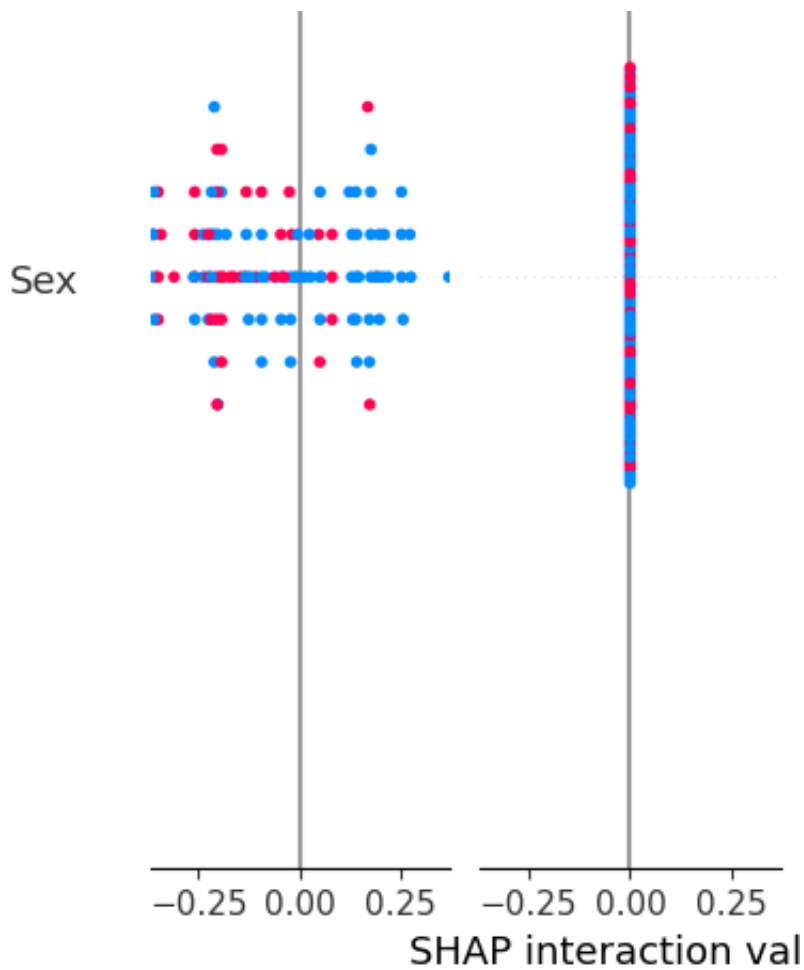
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

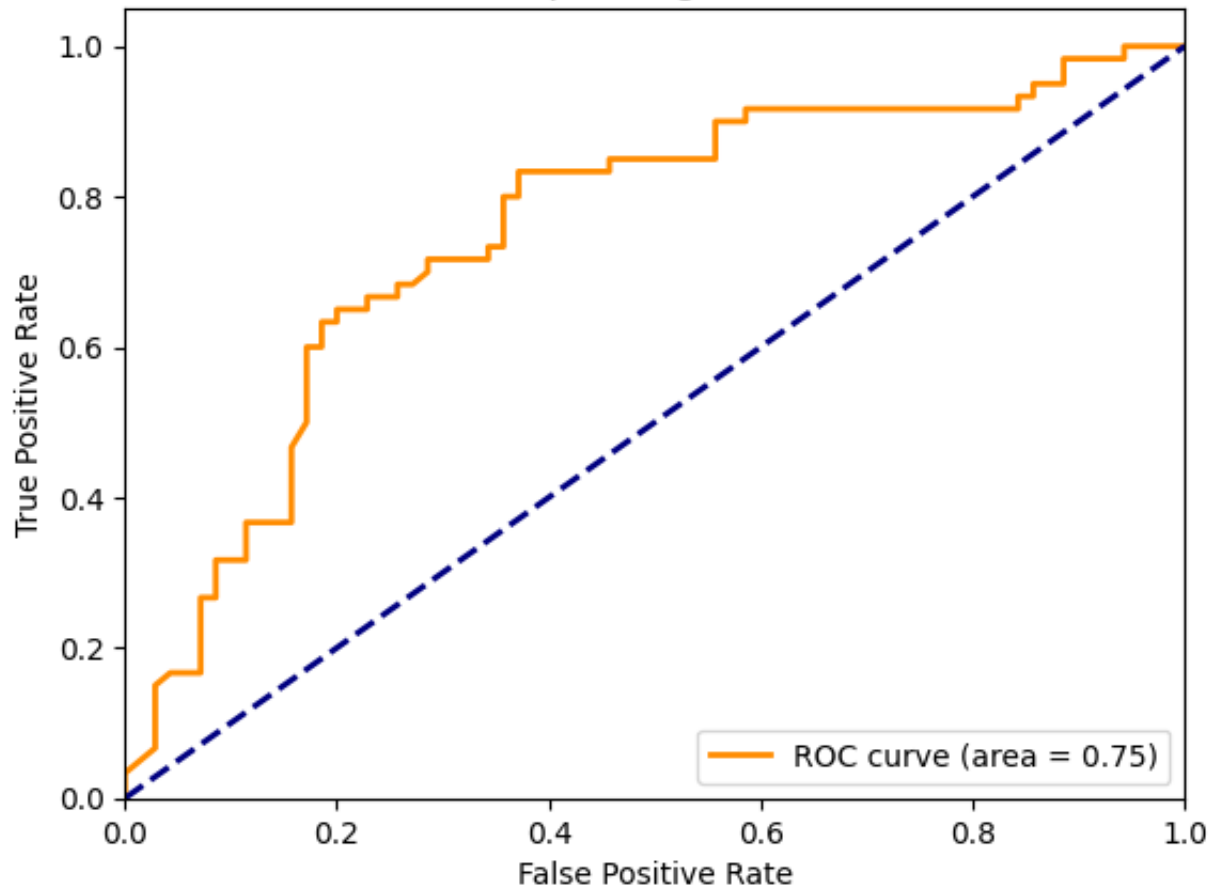
SHAP Summary for Decision Tree





Receiver Operating Characteristic





Running evaluation with seed 44

Evaluating Decision Tree with seed 44...

Best parameters for Decision Tree: {'ccp\_alpha': 0.001, 'criterion': 'gini'

--- ROC Data for Copying ---

FPR = [0.0, 0.0, 0.0, 0.02857142857142857, 0.02857142857142857, 0.028571428

TPR = [0.0, 0.016666666666666666, 0.03333333333333333, 0.06666666666666667,

AUC = 0.7533333333333332

--- End of ROC Data ---

Training - Accuracy: 0.728, Sensitivity: 0.805, Specificity: 0.652, F1: 0.7

Test Metrics for manual threshold 0.5:

Accuracy: 0.723, Sensitivity: 0.833, Specificity: 0.629, F1: 0.735, ROC AUC

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.30, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.35, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.40, Metrics: {'Accuracy': 0.49230769230769234, 'Sensitivity':

Threshold: 0.45, Metrics: {'Accuracy': 0.5769230769230769, 'Sensitivity': 0

Threshold: 0.50, Metrics: {'Accuracy': 0.7230769230769231, 'Sensitivity': 0

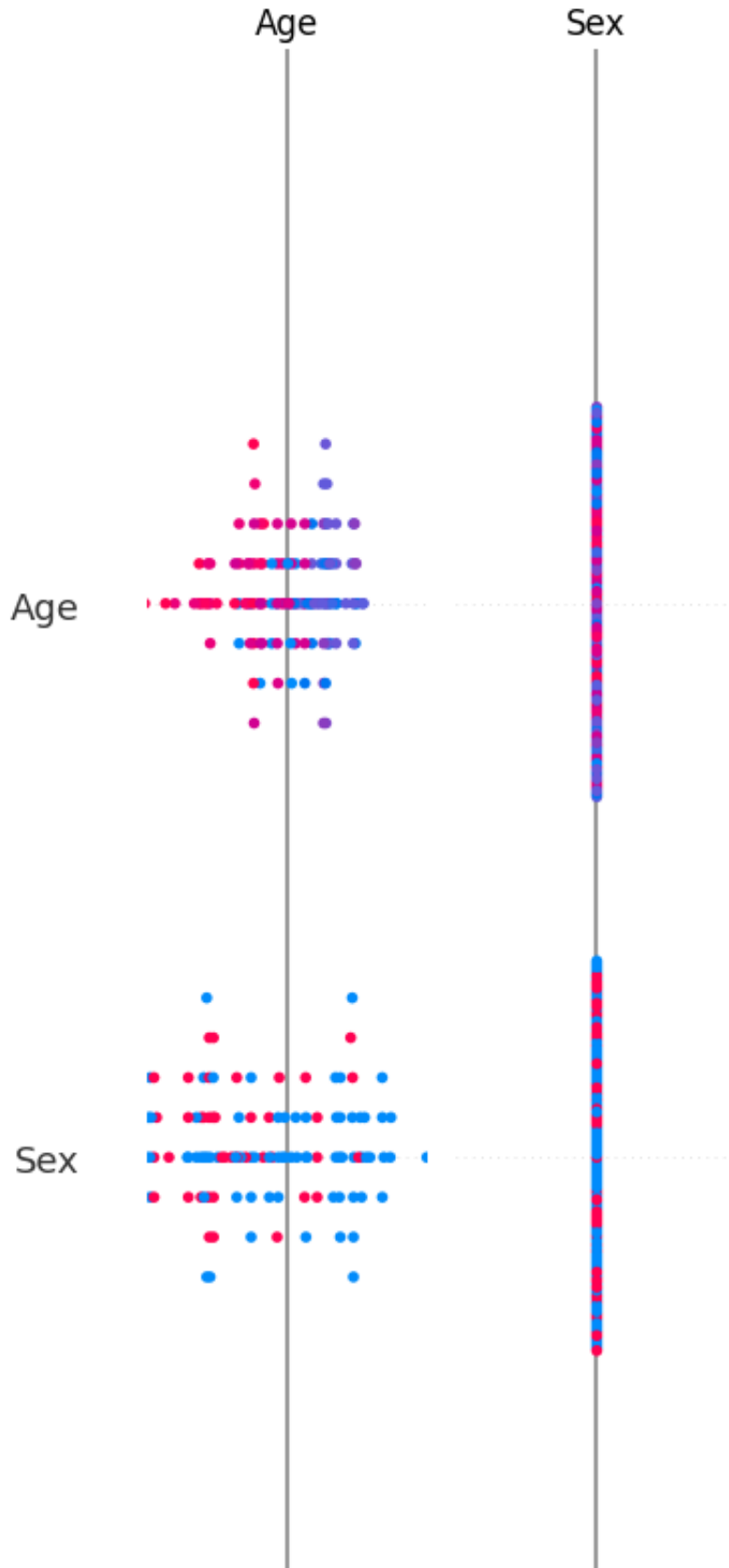
Threshold: 0.55, Metrics: {'Accuracy': 0.7307692307692307, 'Sensitivity': 0

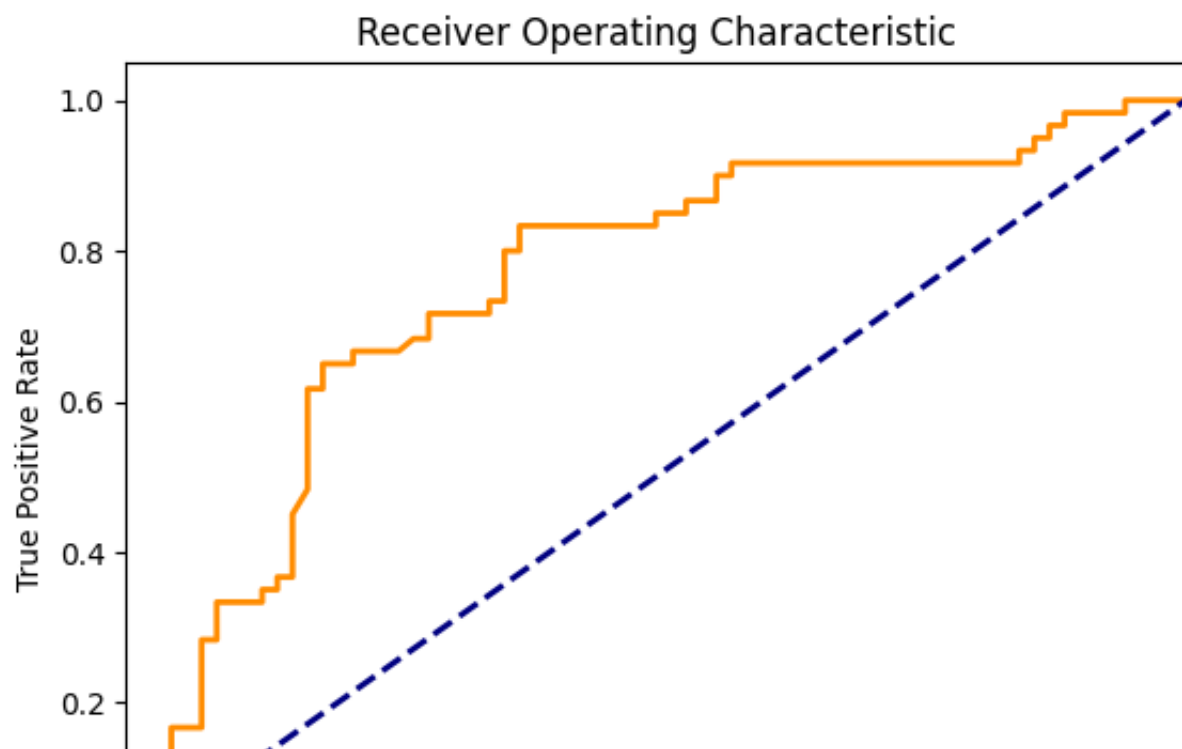
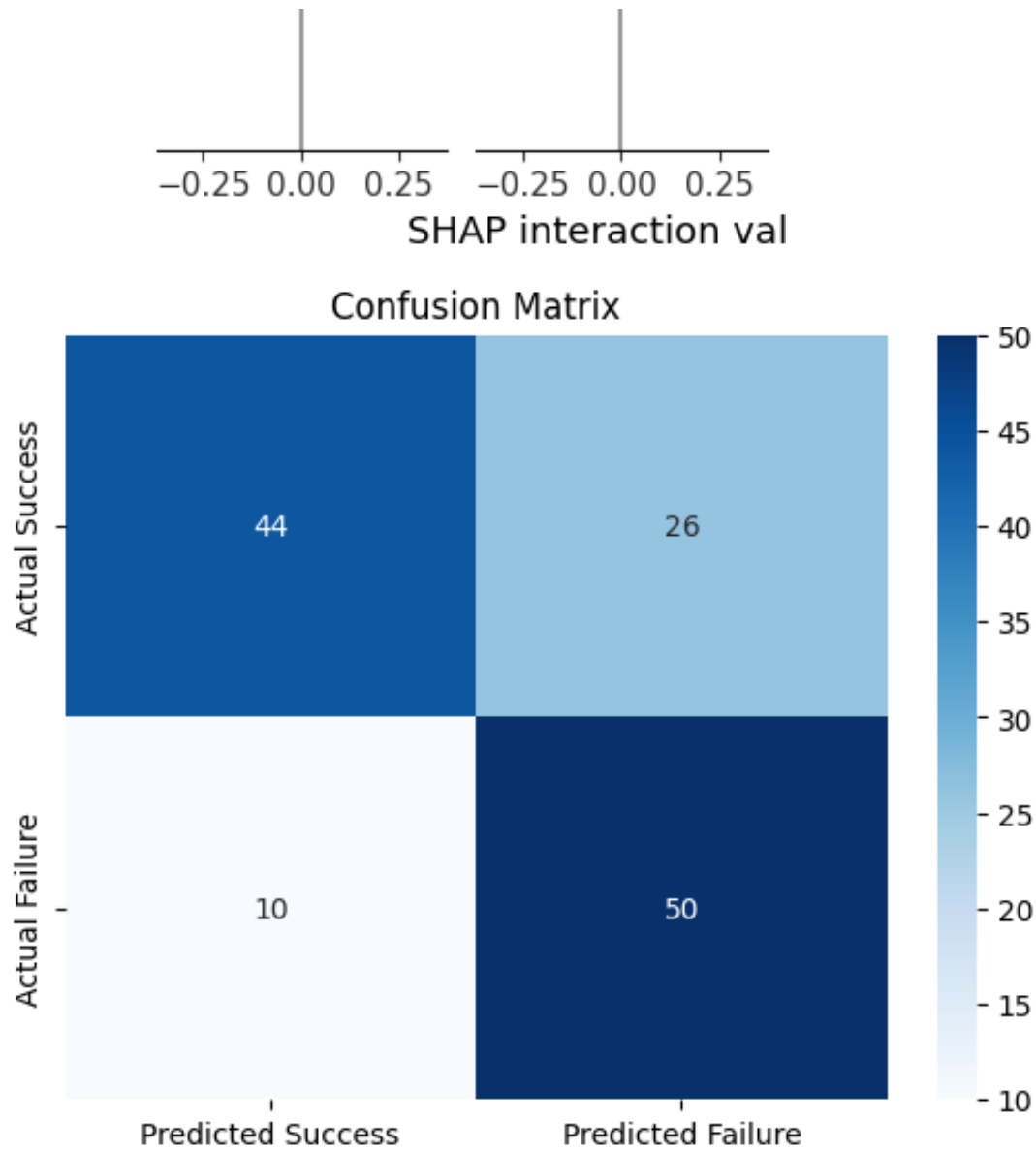
Threshold: 0.60, Metrics: {'Accuracy': 0.5538461538461539, 'Sensitivity': 0

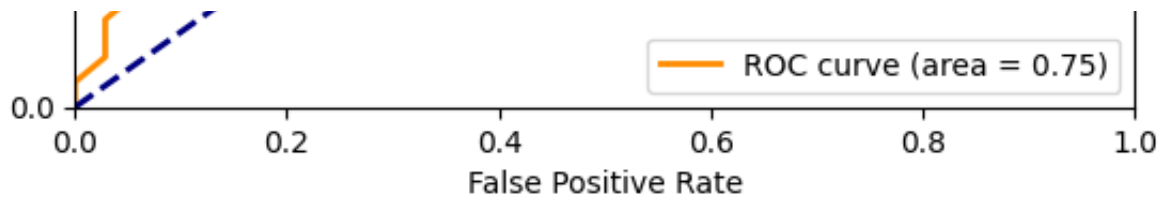
Threshold: 0.65, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

```
Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
SHAP Summary for Decision Tree
```







Running evaluation with seed 45

Evaluating Decision Tree with seed 45...

Best parameters for Decision Tree: {'ccp\_alpha': 0.001, 'criterion': 'gini'}

--- ROC Data for Copying ---

FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.0285714

TPR = [0.0, 0.016666666666666666, 0.05, 0.06666666666666667, 0.1, 0.1166666

AUC = 0.7505952380952381

--- End of ROC Data ---

Training - Accuracy: 0.728, Sensitivity: 0.805, Specificity: 0.652, F1: 0.7

Test Metrics for manual threshold 0.5:

Accuracy: 0.715, Sensitivity: 0.817, Specificity: 0.629, F1: 0.726, ROC AUC

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.30, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.35, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.40, Metrics: {'Accuracy': 0.4846153846153846, 'Sensitivity': 0

Threshold: 0.45, Metrics: {'Accuracy': 0.5615384615384615, 'Sensitivity': 0

Threshold: 0.50, Metrics: {'Accuracy': 0.7153846153846154, 'Sensitivity': 0

Threshold: 0.55, Metrics: {'Accuracy': 0.6846153846153846, 'Sensitivity': 0

Threshold: 0.60, Metrics: {'Accuracy': 0.5461538461538461, 'Sensitivity': 0

Threshold: 0.65, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

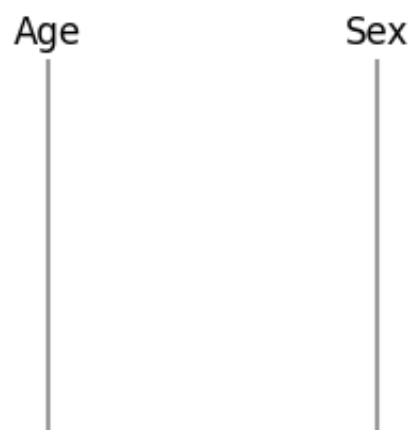
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

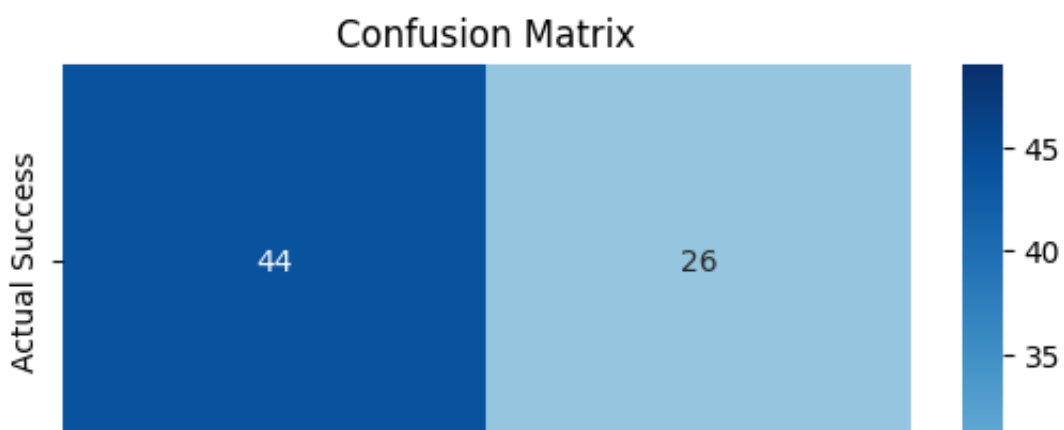
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

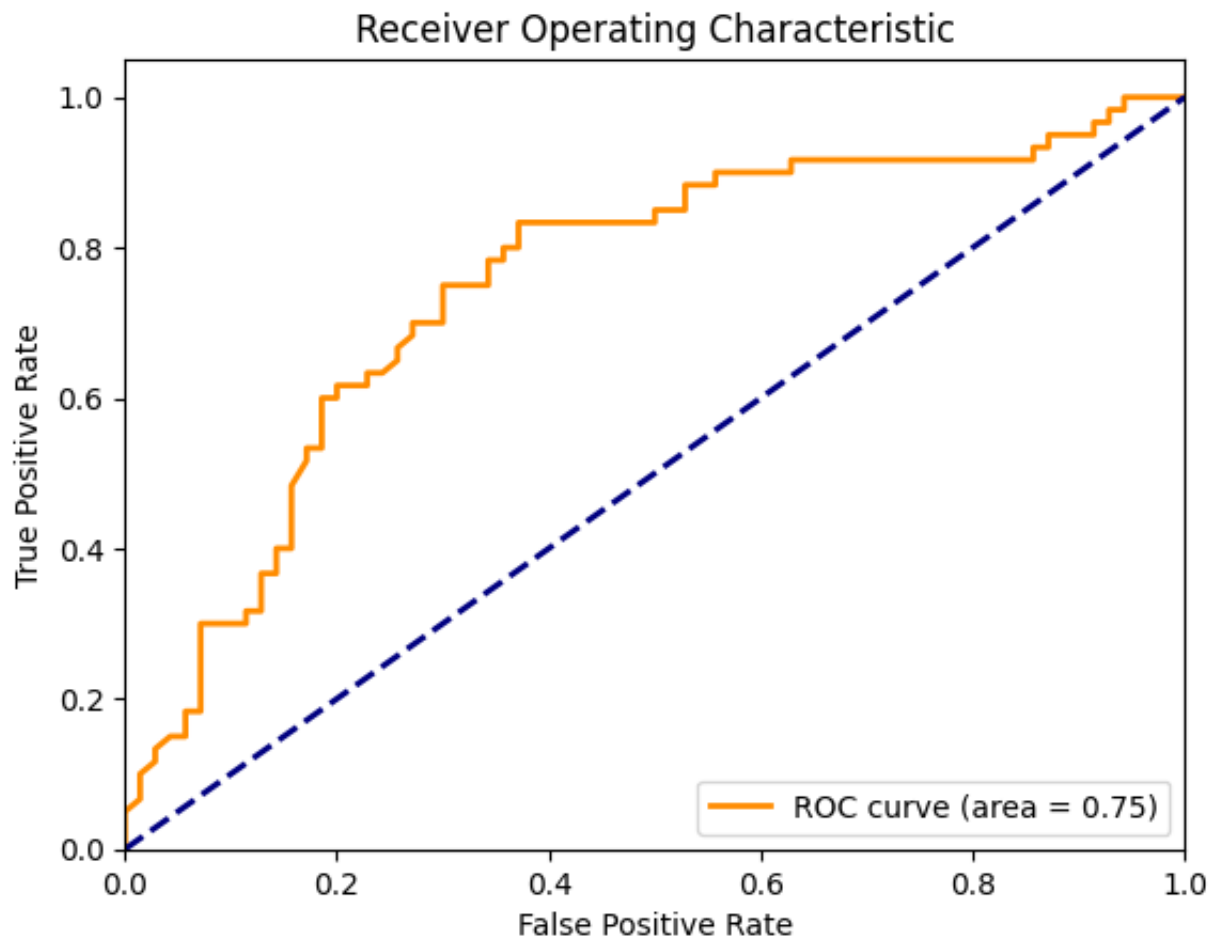
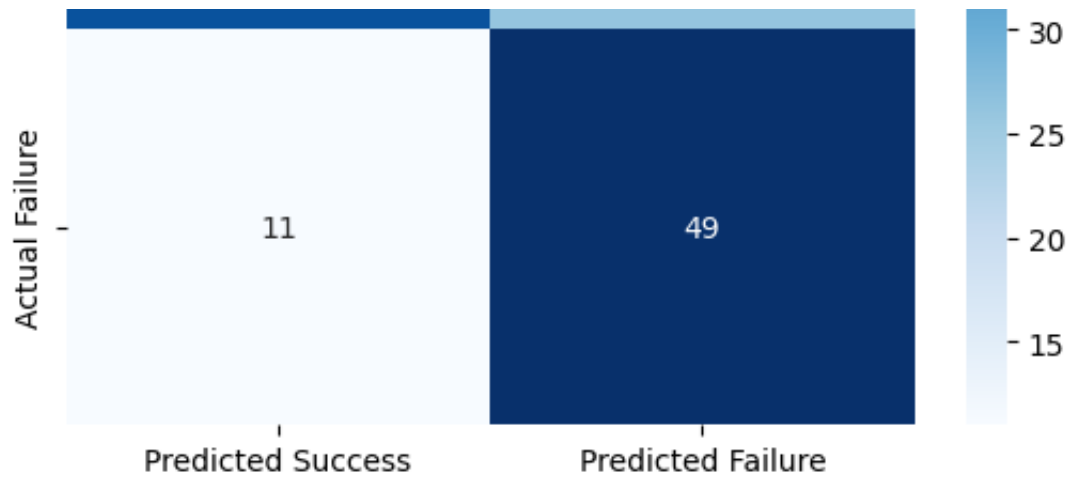
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

SHAP Summary for Decision Tree







Running evaluation with seed 46

Evaluating Decision Tree with seed 46...

Best parameters for Decision Tree: {'ccp\_alpha': 0.001, 'criterion': 'gini'}

--- ROC Data for Copying ---

FPR = [0.0, 0.0, 0.0, 0.02857142857142857, 0.02857142857142857, 0.028571428

TPR = [0.0, 0.016666666666666666, 0.03333333333333333, 0.06666666666666667,

AUC = 0.7573809523809523

--- End of ROC Data ---

Training - Accuracy: 0.728, Sensitivity: 0.805, Specificity: 0.652, F1: 0.7

Test Metrics for manual threshold 0.5:

Accuracy: 0.723, Sensitivity: 0.833, Specificity: 0.629, F1: 0.735, ROC AUC

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.30, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.35, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.40, Metrics: {'Accuracy': 0.49230769230769234, 'Sensitivity':

Threshold: 0.45, Metrics: {'Accuracy': 0.5615384615384615, 'Sensitivity': 0

Threshold: 0.50, Metrics: {'Accuracy': 0.7230769230769231, 'Sensitivity': 0

Threshold: 0.55, Metrics: {'Accuracy': 0.7153846153846154, 'Sensitivity': 0

Threshold: 0.60, Metrics: {'Accuracy': 0.5538461538461539, 'Sensitivity': 0

Threshold: 0.65, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

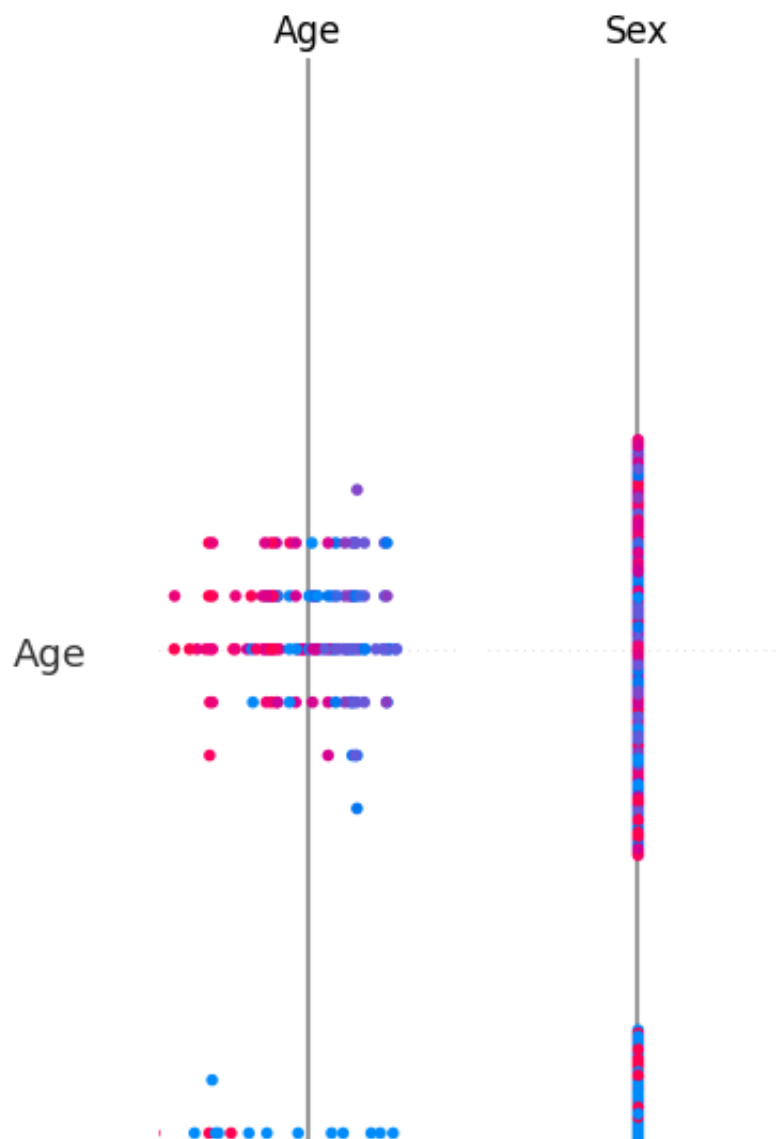
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

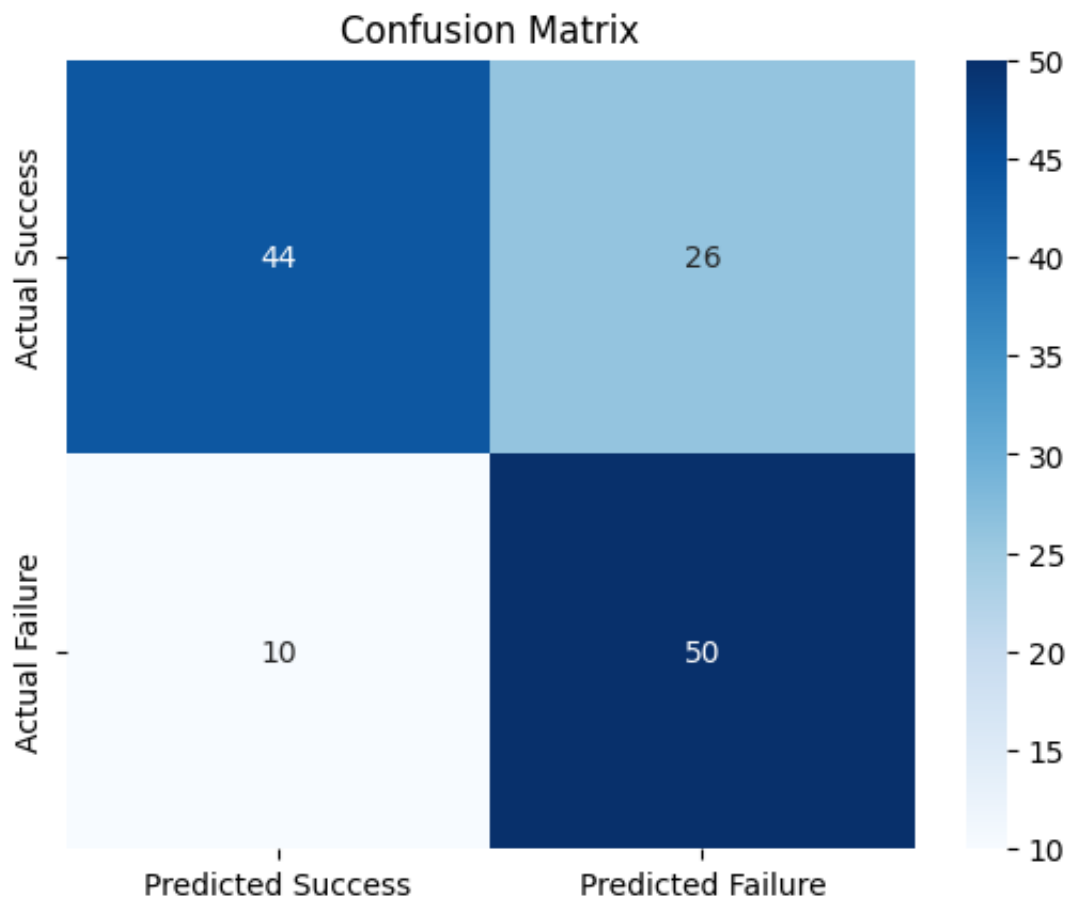
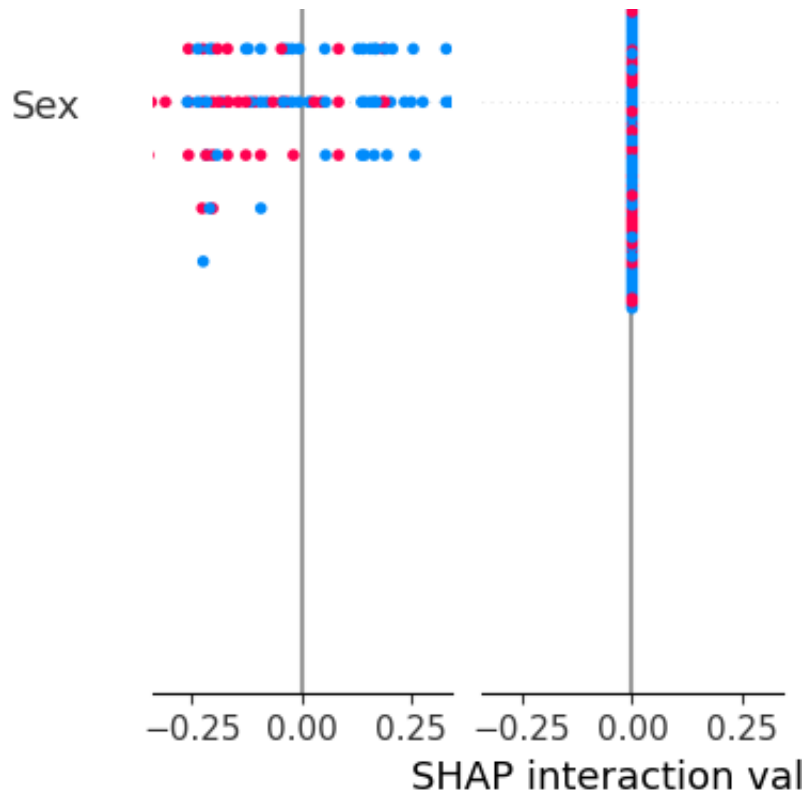
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

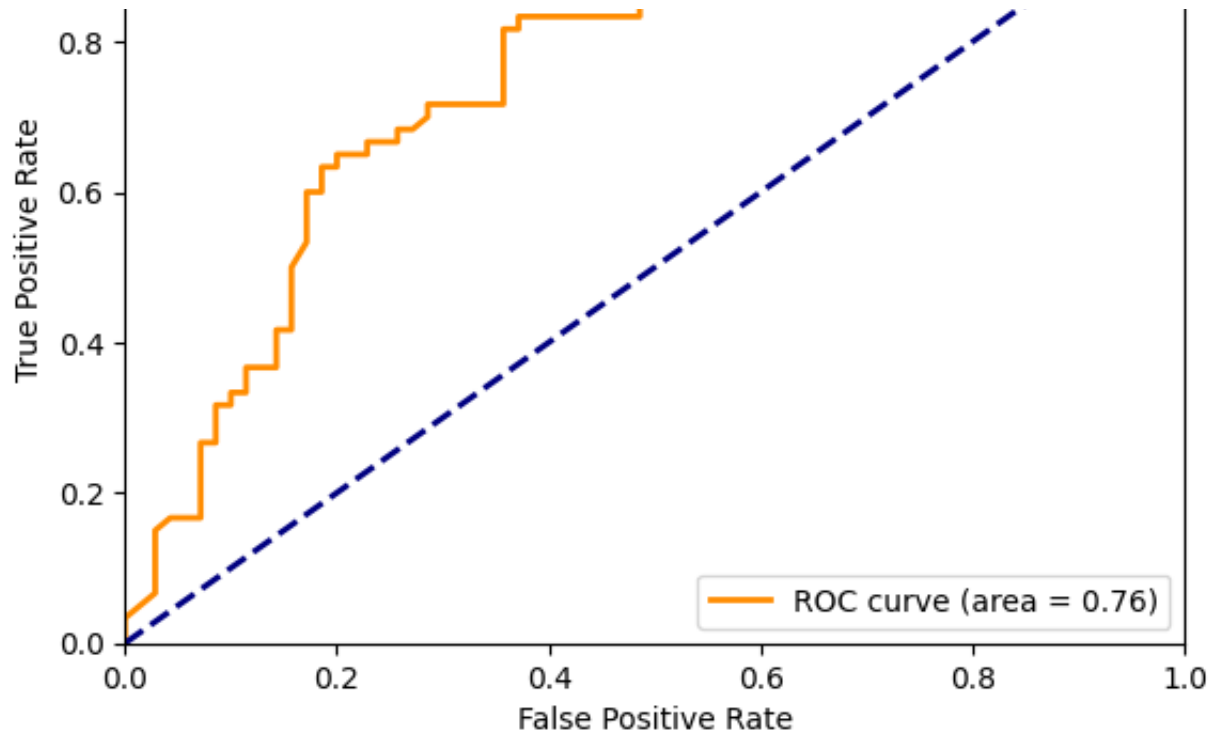
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

SHAP Summary for Decision Tree









Running evaluation with seed 47

Evaluating Decision Tree with seed 47...

Best parameters for Decision Tree: {'ccp\_alpha': 0.001, 'criterion': 'gini'

--- ROC Data for Copying ---

FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.0285714

TPR = [0.0, 0.016666666666666666, 0.05, 0.06666666666666667, 0.1, 0.1166666

AUC = 0.7477380952380953

--- End of ROC Data ---

Training - Accuracy: 0.728, Sensitivity: 0.805, Specificity: 0.652, F1: 0.7

Test Metrics for manual threshold 0.5:

Accuracy: 0.715, Sensitivity: 0.817, Specificity: 0.629, F1: 0.726, ROC AUC

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.30, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.35, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.40, Metrics: {'Accuracy': 0.4846153846153846, 'Sensitivity': 0

Threshold: 0.45, Metrics: {'Accuracy': 0.5615384615384615, 'Sensitivity': 0

Threshold: 0.50, Metrics: {'Accuracy': 0.7153846153846154, 'Sensitivity': 0

Threshold: 0.55, Metrics: {'Accuracy': 0.6846153846153846, 'Sensitivity': 0

Threshold: 0.60, Metrics: {'Accuracy': 0.5461538461538461, 'Sensitivity': 0

Threshold: 0.65, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

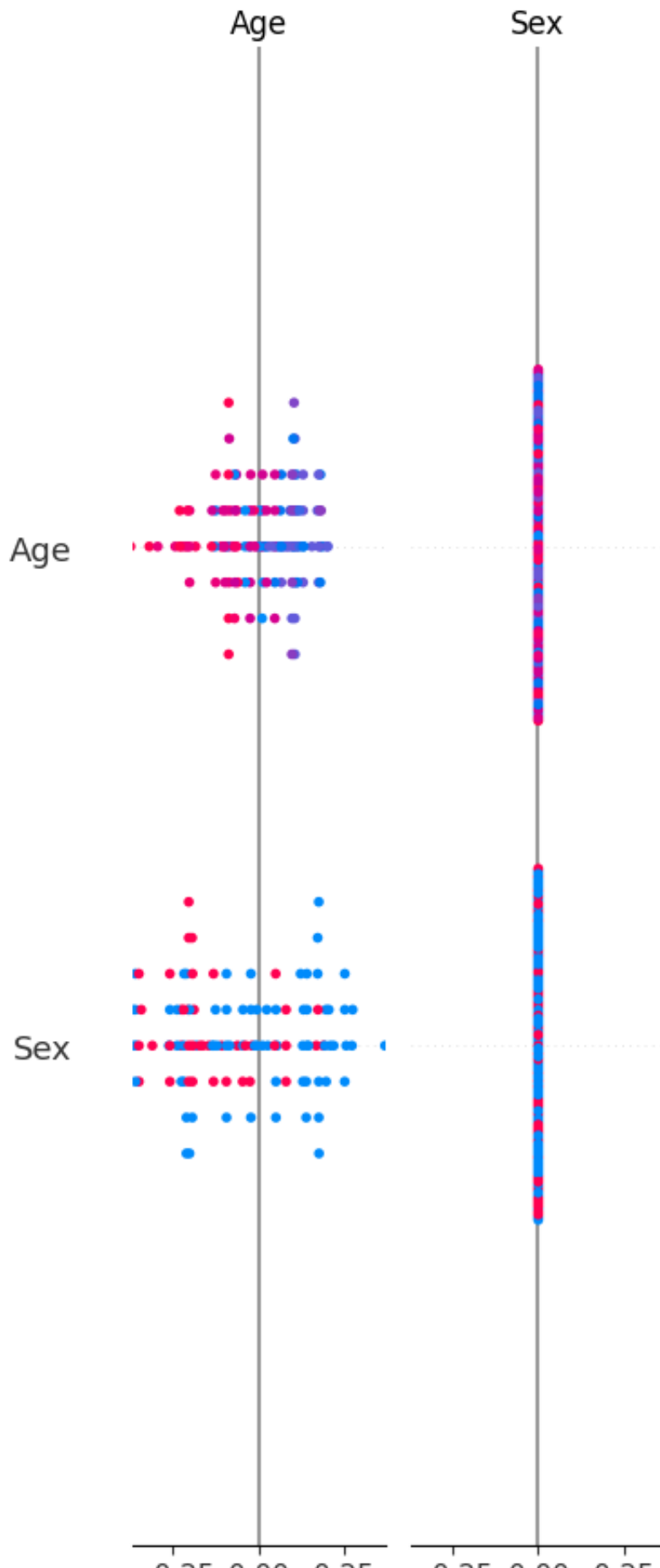
Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

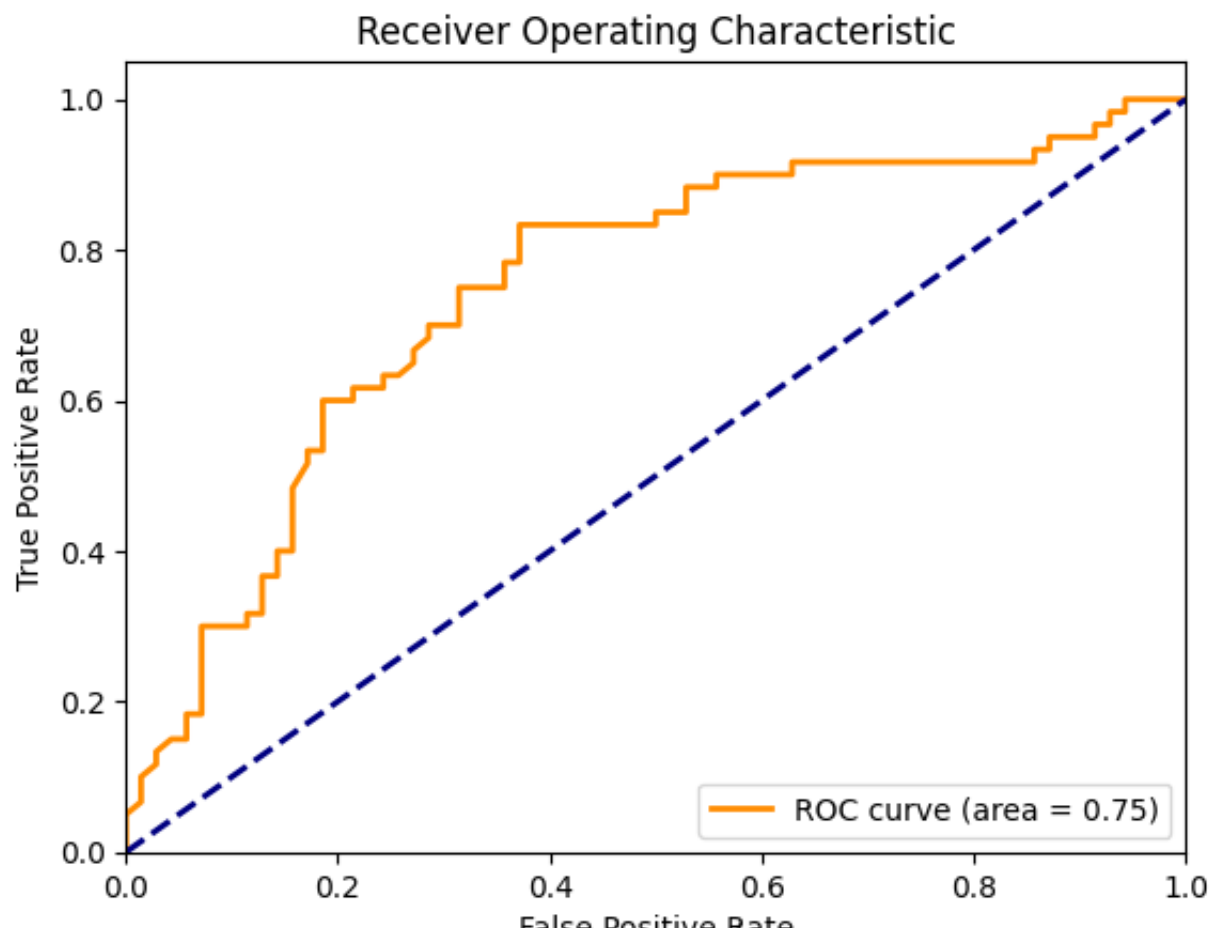
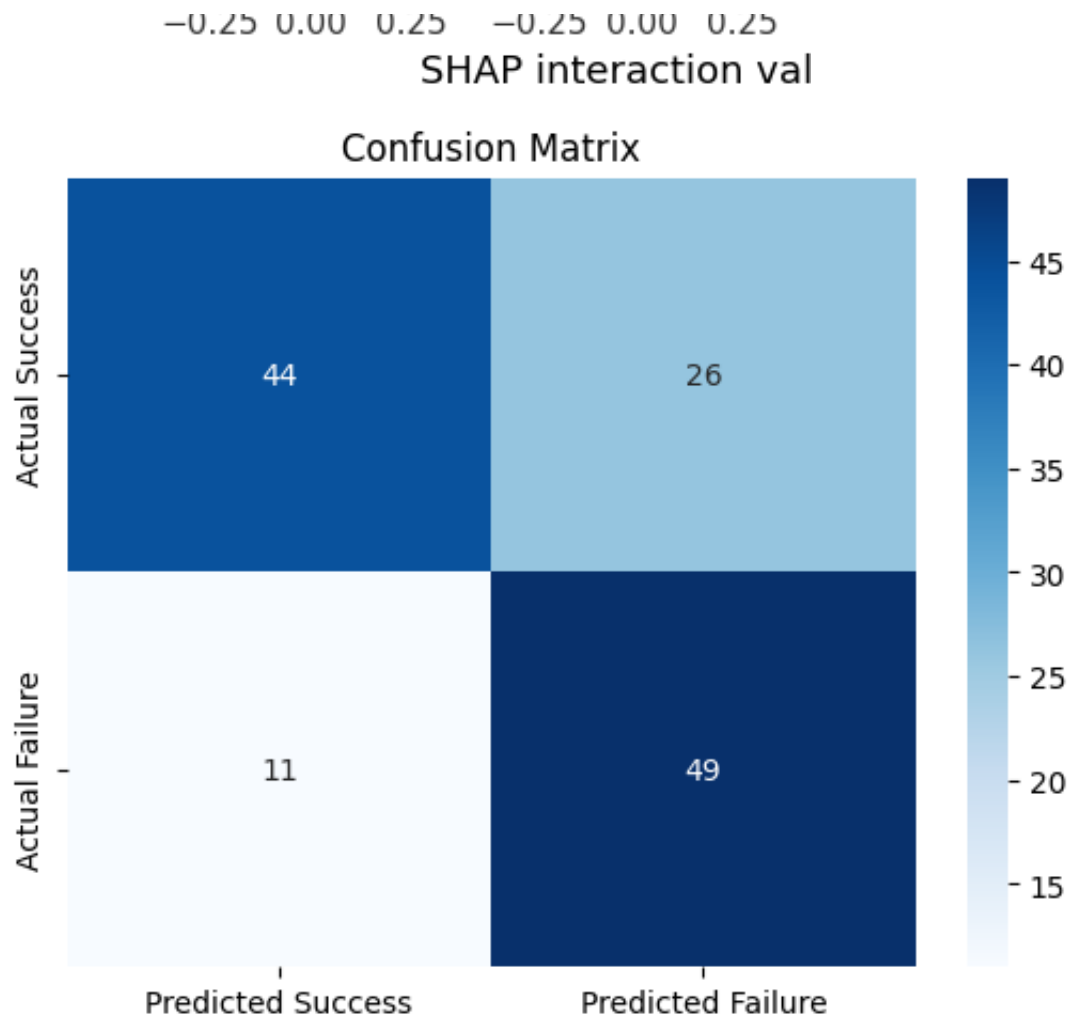
Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

```
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
SHAP Summary for Decision Tree
```





## FALSE POSITIVE RATE

Running evaluation with seed 48

Evaluating Decision Tree with seed 48...

Best parameters for Decision Tree: {'ccp\_alpha': 0.001, 'criterion': 'gini'}

--- ROC Data for Copying ---

FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.0285714

TPR = [0.0, 0.016666666666666666, 0.05, 0.06666666666666667, 0.1, 0.1166666

AUC = 0.7505952380952381

--- End of ROC Data ---

Training - Accuracy: 0.728, Sensitivity: 0.805, Specificity: 0.652, F1: 0.7

Test Metrics for manual threshold 0.5:

Accuracy: 0.715, Sensitivity: 0.817, Specificity: 0.629, F1: 0.726, ROC AUC

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.30, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.35, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.40, Metrics: {'Accuracy': 0.4846153846153846, 'Sensitivity': 0

Threshold: 0.45, Metrics: {'Accuracy': 0.5615384615384615, 'Sensitivity': 0

Threshold: 0.50, Metrics: {'Accuracy': 0.7153846153846154, 'Sensitivity': 0

Threshold: 0.55, Metrics: {'Accuracy': 0.6846153846153846, 'Sensitivity': 0

Threshold: 0.60, Metrics: {'Accuracy': 0.5461538461538461, 'Sensitivity': 0

Threshold: 0.65, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

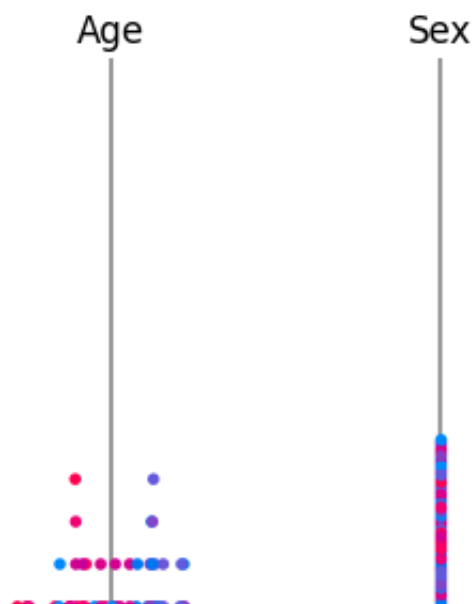
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

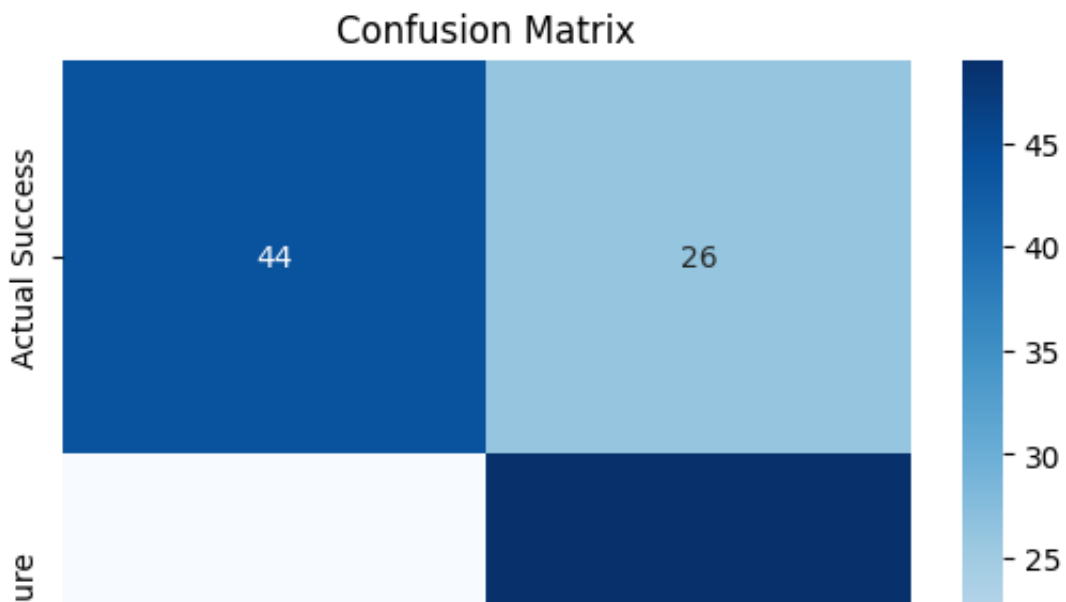
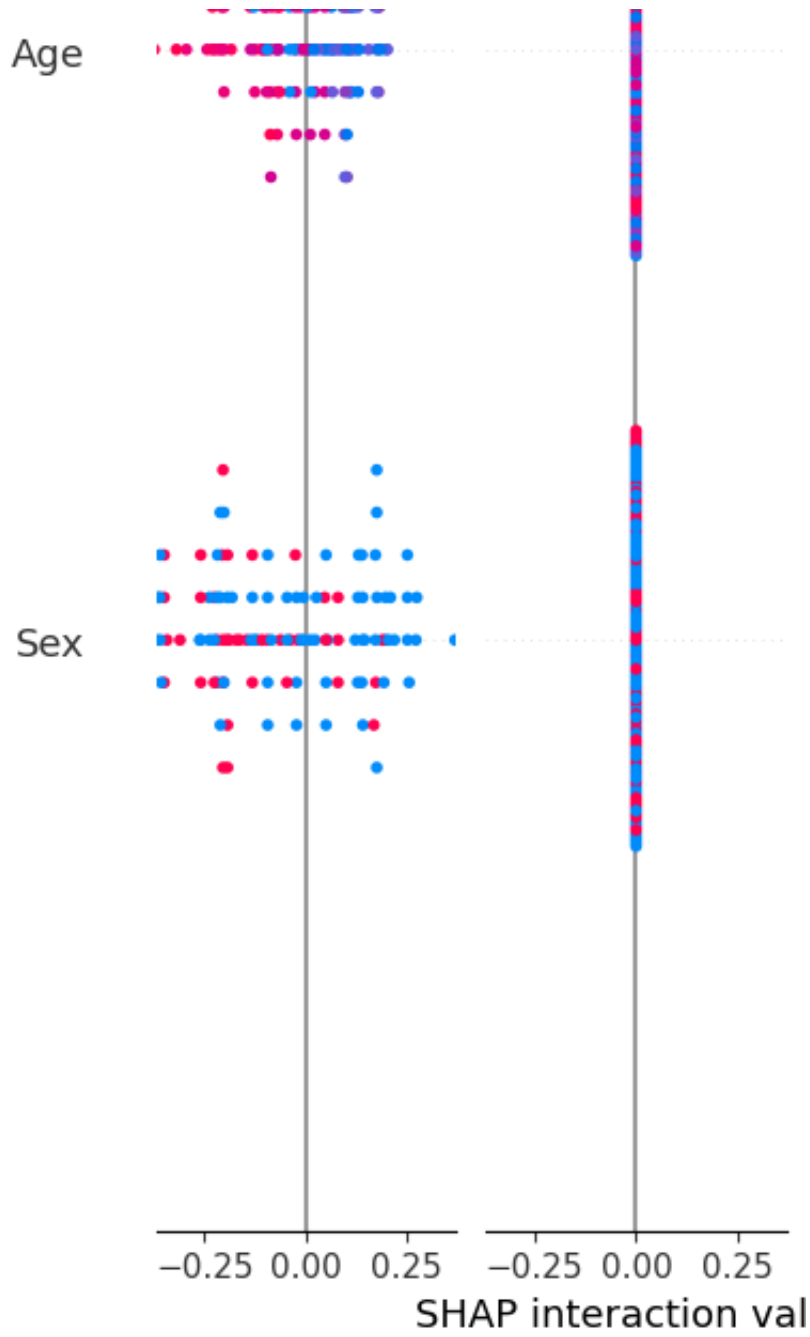
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

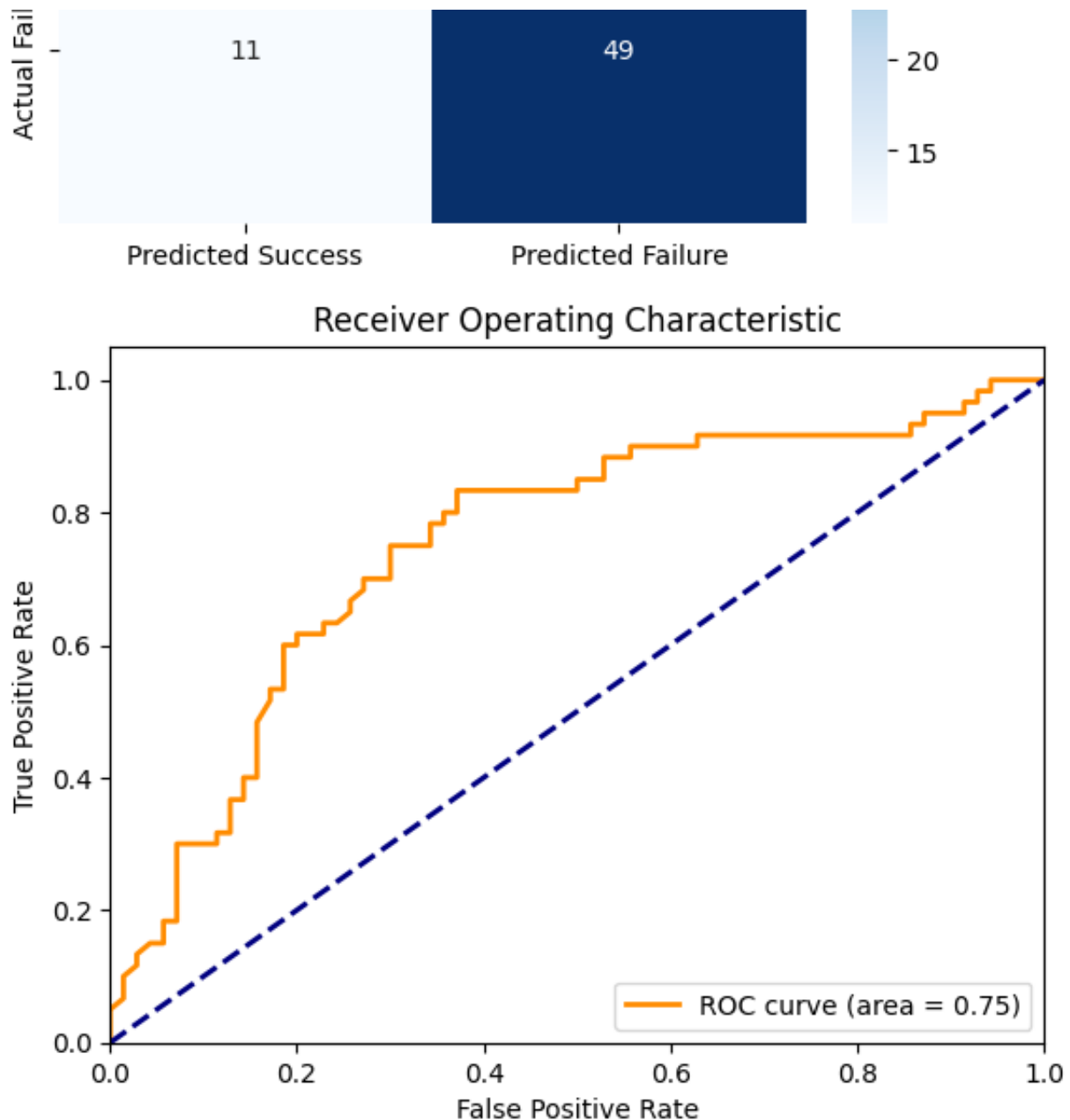
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

SHAP Summary for Decision Tree







Running evaluation with seed 49

Evaluating Decision Tree with seed 49...

Best parameters for Decision Tree: {'ccp\_alpha': 0.001, 'criterion': 'gini'}

--- ROC Data for Copying ---

FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.0285714

TPR = [0.0, 0.016666666666666666, 0.05, 0.06666666666666667, 0.1, 0.1166666

AUC = 0.7472619047619048

--- End of ROC Data ---

Training - Accuracy: 0.728, Sensitivity: 0.805, Specificity: 0.652, F1: 0.7

Test Metrics for manual threshold 0.5:

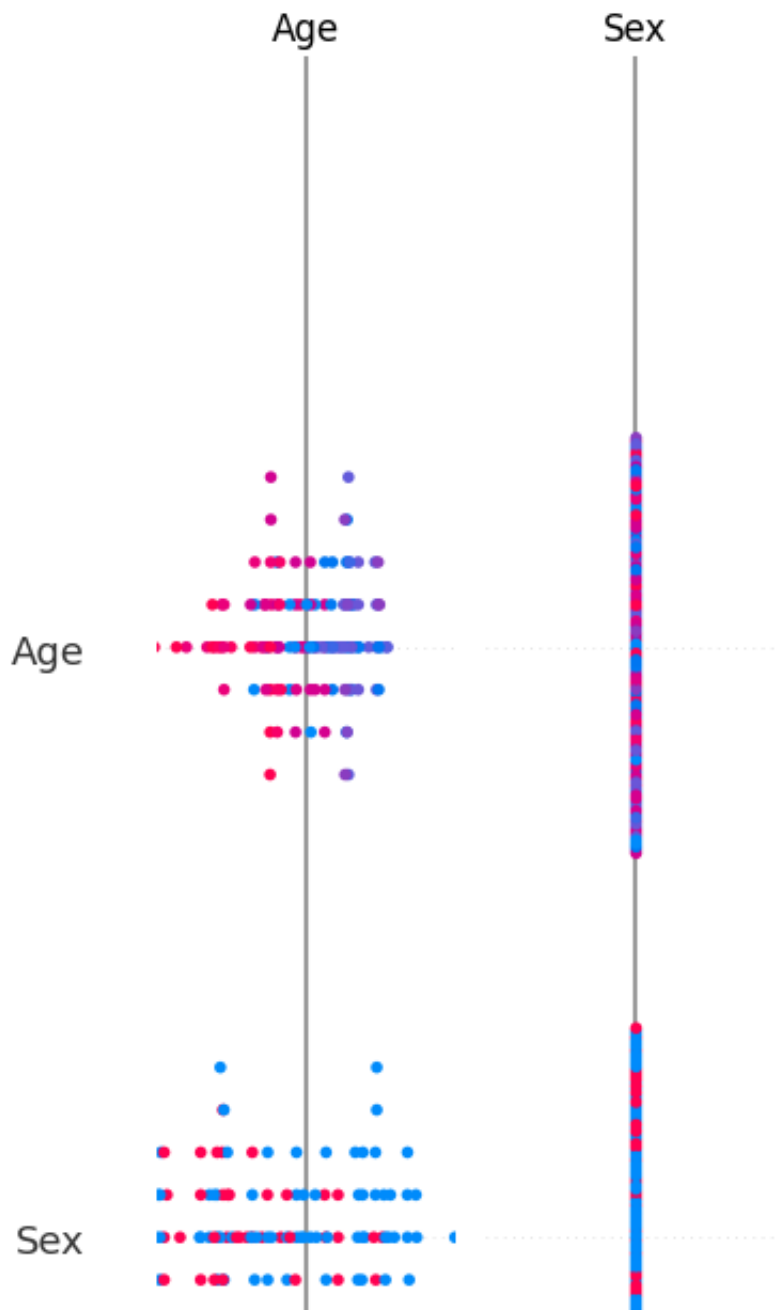
Accuracy: 0.715, Sensitivity: 0.817, Specificity: 0.629, F1: 0.726, ROC AUC

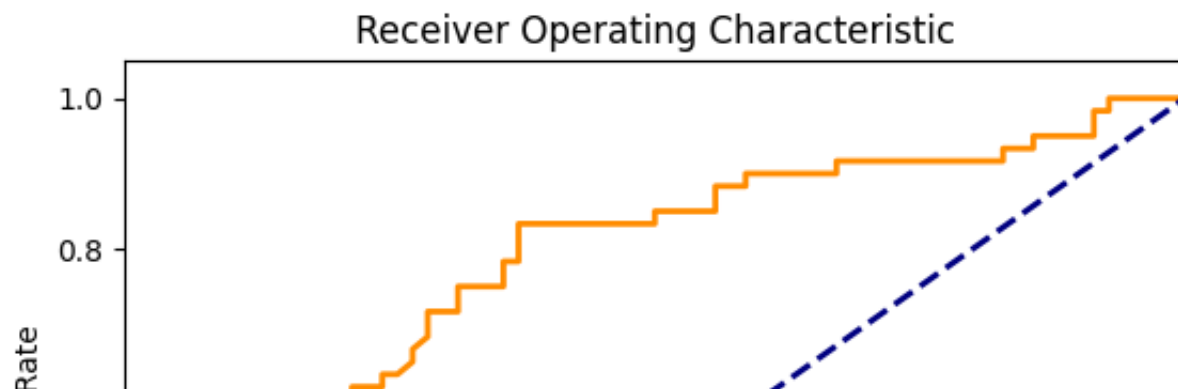
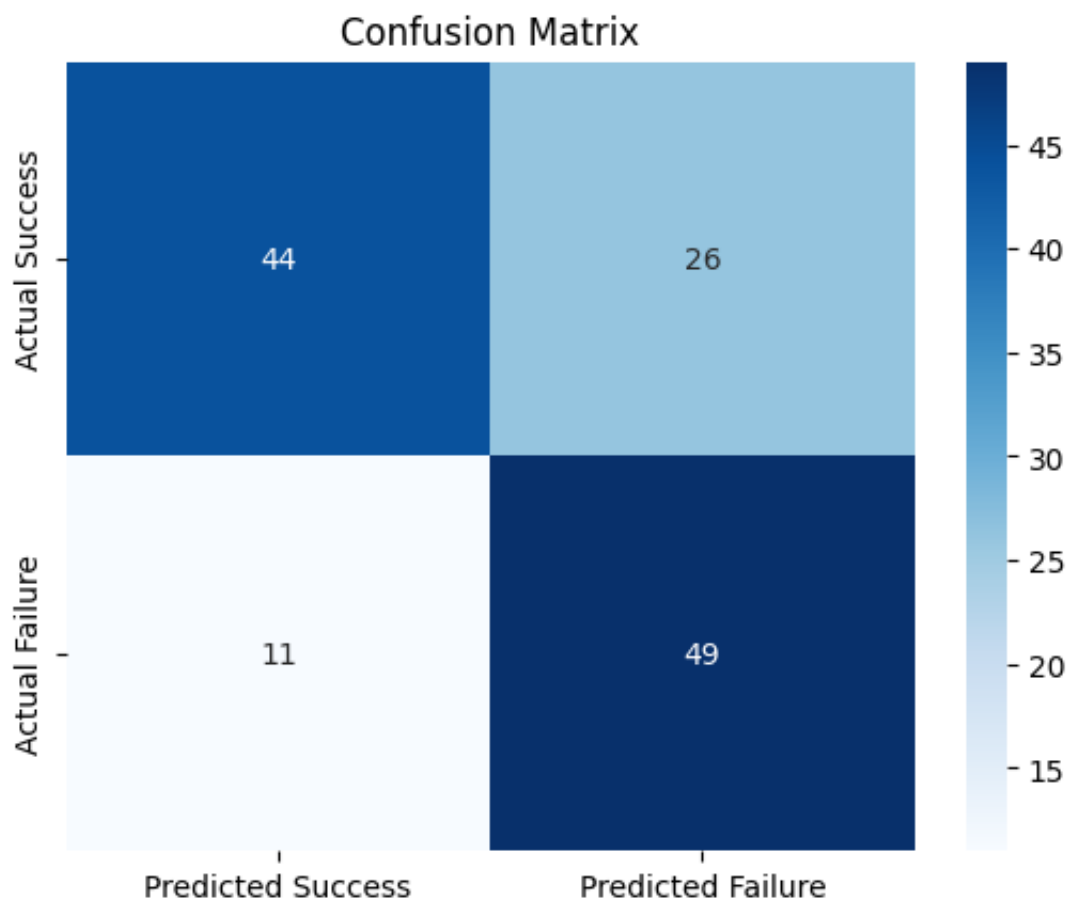
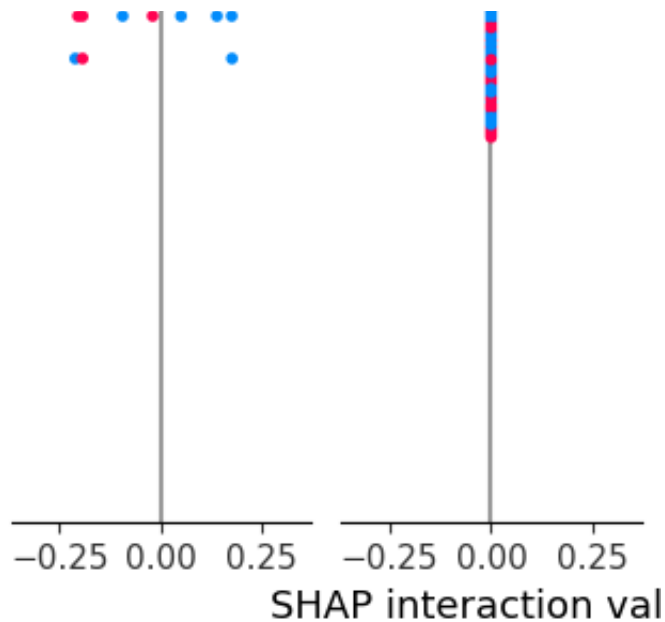
Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

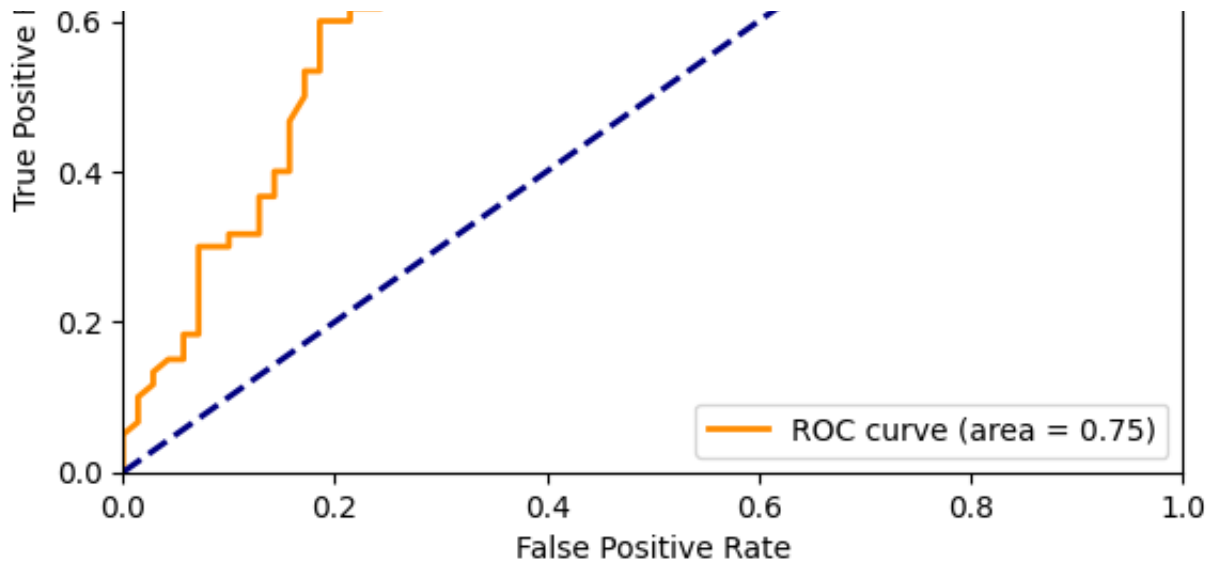
Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

```
Threshold: 0.20, Metrics: {'Accuracy': 0.4015384615384615, 'Sensitivity': 0.4015384615384615}
Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156}
Threshold: 0.30, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156}
Threshold: 0.35, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156}
Threshold: 0.40, Metrics: {'Accuracy': 0.49230769230769234, 'Sensitivity': 0.49230769230769234}
Threshold: 0.45, Metrics: {'Accuracy': 0.5538461538461539, 'Sensitivity': 0.5538461538461539}
Threshold: 0.50, Metrics: {'Accuracy': 0.7153846153846154, 'Sensitivity': 0.7153846153846154}
Threshold: 0.55, Metrics: {'Accuracy': 0.6692307692307692, 'Sensitivity': 0.6692307692307692}
Threshold: 0.60, Metrics: {'Accuracy': 0.5461538461538461, 'Sensitivity': 0.5461538461538461}
Threshold: 0.65, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384}
Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384}
Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384}
Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384}
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384}
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384}
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384}
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384}
SHAP Summary for Decision Tree
```









#### Aggregated Test Set Metrics Across Seeds:

	accuracy	sensitivity	specificity	f1	roc_auc
0	0.723077	0.833333	0.628571	0.735294	0.755000
1	0.723077	0.833333	0.628571	0.735294	0.755714
2	0.715385	0.816667	0.628571	0.725926	0.750119
3	0.723077	0.833333	0.628571	0.735294	0.753333
4	0.723077	0.833333	0.628571	0.735294	0.753333
5	0.715385	0.816667	0.628571	0.725926	0.750595
6	0.723077	0.833333	0.628571	0.735294	0.757381
7	0.715385	0.816667	0.628571	0.725926	0.747738
8	0.715385	0.816667	0.628571	0.725926	0.750595
9	0.715385	0.816667	0.628571	0.725926	0.747262

#### Summary of Test Set Metrics (Mean, Standard Error, 95% Confidence Interval)

Accuracy: Mean = 0.719, SE = 0.001, 95% CI = [0.716, 0.722]

Sensitivity: Mean = 0.825, SE = 0.003, 95% CI = [0.819, 0.831]

Specificity: Mean = 0.629, SE = 0.000, 95% CI = [0.629, 0.629]

F1: Mean = 0.731, SE = 0.002, 95% CI = [0.727, 0.734]

Roc\_auc: Mean = 0.752, SE = 0.001, 95% CI = [0.750, 0.755]

```
def evaluate_model(model, name, grid, X_train, y_train, X_test, y_test, cv, scor
    print(f"Evaluating {name} with seed {seed}...")
```

```
    inner_cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=seed)
    outer_cv = StratifiedKFold(n_splits=5, shuffle=True, random_state=seed)
```

```
    clf = GridSearchCV(model, grid, cv=inner_cv, scoring='roc_auc')
    nested_scores = cross_validate(clf, X=X_train, y=y_train, cv=outer_cv, scori
```

```
    clf.fit(X_train, y_train)
    best_model = clf.best_estimator_
    best_params = clf.best_params_
```

```
    calibrated_clf = CalibratedClassifierCV(estimator=best_model, method='sigmoid')
```

```

calibrated_clf = CalibratedClassifierCV(estimator=best_model, method='sigmoid')
calibrated_clf.fit(X_train, y_train)

y_probs = calibrated_clf.predict_proba(X_test)[:, 1]

# Calcular FPR, TPR e AUC
fpr, tpr, thresholds = roc_curve(y_test, y_probs)
roc_auc = auc(fpr, tpr)

# Imprimir os valores de FPR, TPR e AUC de forma fácil de copiar
print("\n--- Dados ROC para copiar ---")
print("FPR =", fpr.tolist())
print("TPR =", tpr.tolist())
print("AUC =", roc_auc)
print("--- Fim dos Dados ROC ---\n")

# Calculate metrics for the training set
y_train_pred = best_model.predict(X_train)
y_train_probs = best_model.predict_proba(X_train)[:, 1]
train_acc = accuracy_score(y_train, y_train_pred)
train_sens = sensitivity(y_train, y_train_pred)
train_spec = specificity(y_train, y_train_pred)
train_f1 = f1_score(y_train, y_train_pred)
train_roc_auc = roc_auc_score(y_train, y_train_probs)

print(f"Training - Accuracy: {train_acc}, Sensitivity: {train_sens}, Specifici

# Metrics for the manually set threshold
y_pred_manual = (y_probs >= manual_threshold).astype(int)
manual_acc = accuracy_score(y_test, y_pred_manual)
manual_sens = sensitivity(y_test, y_pred_manual)
manual_spec = specificity(y_test, y_pred_manual)
manual_f1 = f1_score(y_test, y_pred_manual)
manual_roc_auc = roc_auc_score(y_test, y_probs)

print(f"Metrics for manual threshold {manual_threshold}:")
print(f"Accuracy: {manual_acc}, Sensitivity: {manual_sens}, Specificity: {ma

threshold_metrics = {}
for threshold in threshold_list:
    y_pred_threshold = (y_probs >= threshold).astype(int)
    threshold_acc = accuracy_score(y_test, y_pred_threshold)
    threshold_sens = sensitivity(y_test, y_pred_threshold)
    threshold_spec = specificity(y_test, y_pred_threshold)
    threshold_f1 = f1_score(y_test, y_pred_threshold)
    threshold_metrics[threshold] = {
        'Accuracy': threshold_acc,
        'Sensitivity': threshold_sens,
        'Specificity': threshold_spec,

```

```

        'F1': threshold_f1,
        'ROC AUC': manual_roc_auc
    }

    for threshold, metrics in threshold_metrics.items():
        print(f"Threshold: {threshold:.2f}, Metrics: {metrics}")

    calculate_and_plot_shap(best_model, X_train, X_test, name)

    # Prepare dictionary of test metrics for aggregation
    test_metrics = {
        "accuracy": manual_acc,
        "sensitivity": manual_sens,
        "specificity": manual_spec,
        "f1": manual_f1,
        "roc_auc": manual_roc_auc
    }

    return best_model, manual_threshold, best_params, nested_scores, calibrated_

def calculate_and_plot_shap(model, X_train, X_test, model_name):
    if isinstance(model, (RandomForestClassifier)):
        explainer = shap.TreeExplainer(model)
    else:
        explainer = shap.KernelExplainer(model.predict_proba, X_train.sample(100))
    shap_values = explainer.shap_values(X_test)
    print(f"SHAP Summary for {model_name}")
    shap.summary_plot(shap_values, X_test, max_display=10)

def plot_confusion_matrix(y_true, y_pred):
    matrix = confusion_matrix(y_true, y_pred)
    sns.heatmap(matrix, annot=True, fmt='d', cmap='Blues',
                xticklabels=['Predicted Success', 'Predicted Failure'],
                yticklabels=['Actual Success', 'Actual Failure'])
    plt.title('Confusion Matrix Random Forest')
    plt.show()

def plot_roc_curve(y_true, y_probs):
    fpr, tpr, thresholds = roc_curve(y_true, y_probs)
    roc_auc = auc(fpr, tpr)

    plt.figure()
    plt.plot(fpr, tpr, color='darkorange', lw=2, label=f'ROC curve (area = {roc_auc:.2f})')
    plt.plot([0, 1], [0, 1], color='navy', lw=2, linestyle='--')
    plt.xlim([0.0, 1.0])
    plt.ylim([0.0, 1.05])
    plt.xlabel('False Positive Rate')
    plt.ylabel('True Positive Rate')

```

```

plt.title('Receiver Operating Characteristic Random Forest')
plt.legend(loc="lower right")
plt.show()

def evaluate_random_forest(X_train, y_train, X_test, y_test, cv, scoring, manual_model = RandomForestClassifier(n_jobs=-1, random_state=seed)
grid = {
    'n_estimators': [500],
    'max_depth': [5],
    'min_samples_split': [2],
    'min_samples_leaf': [6],
    'max_features': ['sqrt'],
}
return evaluate_model(model, "Random Forest", grid, X_train, y_train, X_test

def main(X_train, y_train, X_test, y_test):
cv = RepeatedStratifiedKFold(n_splits=10, n_repeats=10, random_state=42)
scoring = {
    'accuracy': make_scorer(accuracy_score),
    'sensitivity': make_scorer(sensitivity),
    'specificity': make_scorer(specificity),
    'f1': make_scorer(f1_score),
    'roc_auc': make_scorer(roc_auc_score)
}
manual_threshold = 0.55
threshold_list = np.arange(0.1, 1.05, 0.05)

aggregated_metrics = []

for seed in range(40, 50):
    print(f"Running evaluation with seed {seed}")
    best_model, manual_threshold, best_params, nested_scores, calibrated_clf,
        X_train, y_train, X_test, y_test, cv, scoring, manual_threshold, thr
    )

    # Use calibrated_clf for prediction probabilities
    y_probs = calibrated_clf.predict_proba(X_test)[: , 1]
    y_pred_manual = (y_probs >= manual_threshold).astype(int)

    plot_confusion_matrix(y_test, y_pred_manual)
    plot_roc_curve(y_test, y_probs)

    aggregated_metrics.append(test_metrics)

# Aggregate results across seeds
results_df = pd.DataFrame(aggregated_metrics)
n = len(results_df)
print("\nAggregated Test Set Metrics Across Seeds:")
print(results_df)

```

```

print(results_df)

# Compute mean, standard error, and 95% confidence interval for each metric
def summarize_metric(metric_values):
    mean_val = metric_values.mean()
    std_val = metric_values.std(ddof=1)
    se = std_val / np.sqrt(n)
    t_crit = stats.t.ppf(0.975, df=n - 1)
    ci_lower = mean_val - t_crit * se
    ci_upper = mean_val + t_crit * se
    return mean_val, se, (ci_lower, ci_upper)

metrics_summary = {}
for metric in results_df.columns:
    mean_val, se, ci = summarize_metric(results_df[metric])
    metrics_summary[metric] = {
        "Mean": mean_val,
        "Standard Error": se,
        "95% CI": ci
    }

print("\nSummary of Test Set Metrics (Mean, Standard Error, 95% Confidence I
for metric, summary in metrics_summary.items():
    print(f"{metric.capitalize()}: Mean = {summary['Mean']:.3f}, SE = {summa
          f"95% CI = [{summary['95% CI'][0]:.3f}, {summary['95% CI'][1]:.3f}

if __name__ == '__main__':
    main(X_train, y_train, X_test, y_test)

```



Running evaluation with seed 40  
Evaluating Random Forest with seed 40...

--- Dados ROC para copiar ---

FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.02857142857142857, 0.02857142

TPR = [0.0, 0.016666666666666666, 0.03333333333333333, 0.05, 0.05, 0.1, 0.1

AUC = 0.7471428571428571

--- Fim dos Dados ROC ---

Training - Accuracy: 0.7238658777120316, Sensitivity: 0.7529880478087649, S  
Metrics for manual threshold 0.55:

Accuracy: 0.6923076923076923, Sensitivity: 0.6166666666666667, Specificity:

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.25, Metrics: {'Accuracy': 0.46923076923076923, 'Sensitivity':

Threshold: 0.30, Metrics: {'Accuracy': 0.5, 'Sensitivity': 1.0, 'Specificit

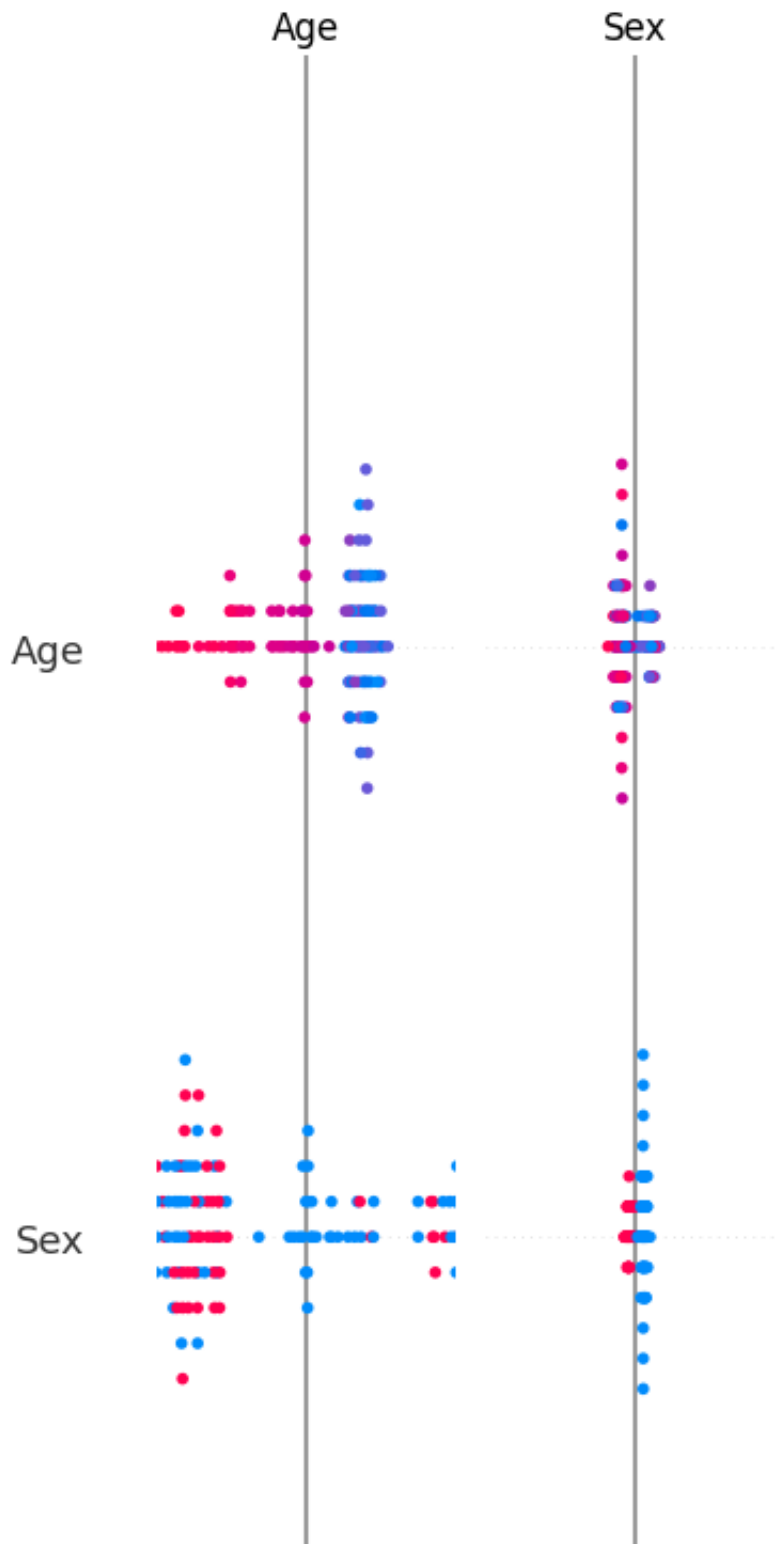
Threshold: 0.35, Metrics: {'Accuracy': 0.5538461538461539, 'Sensitivity': 0

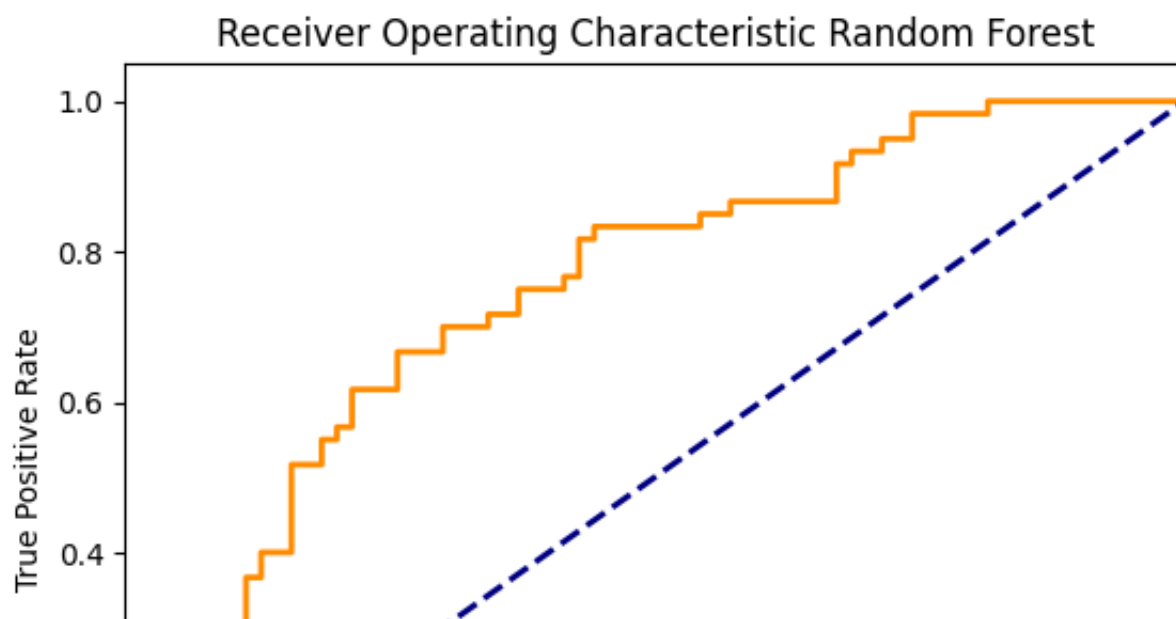
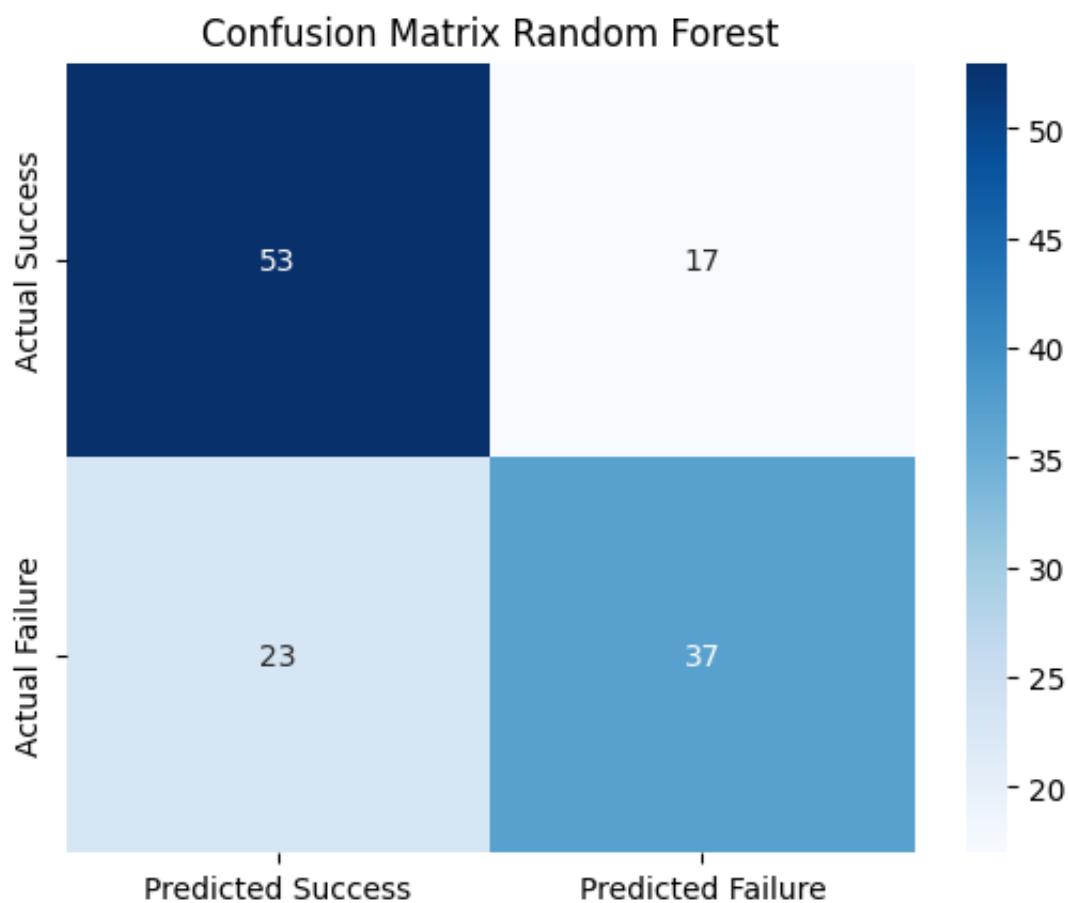
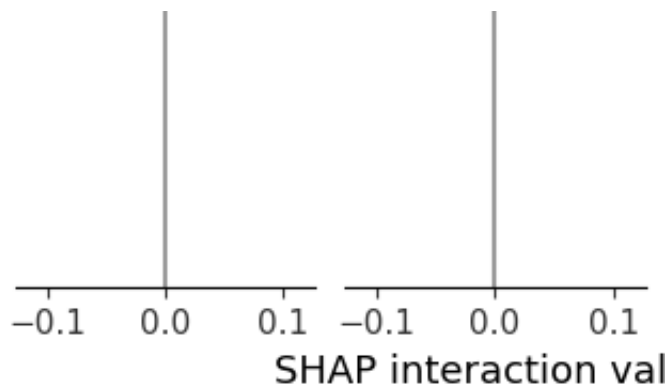
Threshold: 0.40, Metrics: {'Accuracy': 0.5923076923076923, 'Sensitivity': 0

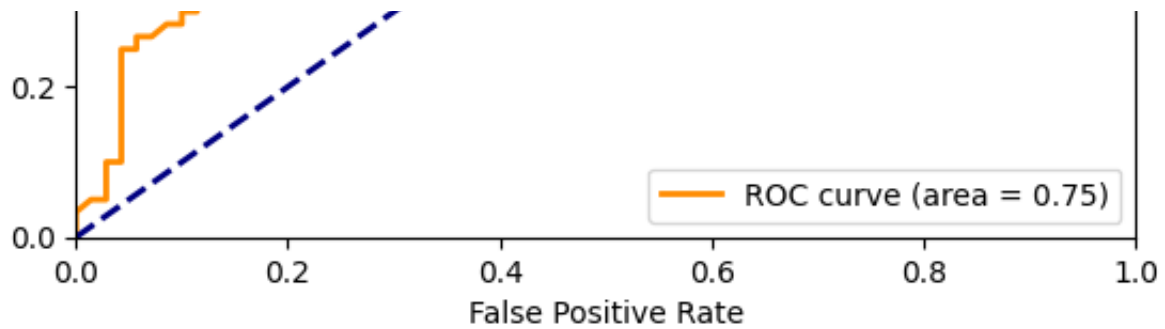
Threshold: 0.45, Metrics: {'Accuracy': 0.6384615384615384, 'Sensitivity': 0

Threshold: 0.50, Metrics: {'Accuracy': 0.676923076923077, 'Sensitivity': 0.

```
Threshold: 0.55, Metrics: {'Accuracy': 0.6923076923076923, 'Sensitivity': 0
Threshold: 0.60, Metrics: {'Accuracy': 0.6538461538461539, 'Sensitivity': 0
Threshold: 0.65, Metrics: {'Accuracy': 0.6307692307692307, 'Sensitivity': 0
Threshold: 0.70, Metrics: {'Accuracy': 0.5692307692307692, 'Sensitivity': 0
Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
SHAP Summary for Random Forest
```







Running evaluation with seed 41

Evaluating Random Forest with seed 41...

--- Dados ROC para copiar ---

FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.0285714

TPR = [0.0, 0.016666666666666666, 0.033333333333333333, 0.05, 0.06666666666666666

AUC = 0.7457142857142857

--- Fim dos Dados ROC ---

Training - Accuracy: 0.7218934911242604, Sensitivity: 0.7569721115537849, S  
Metrics for manual threshold 0.55:

Accuracy: 0.7076923076923077, Sensitivity: 0.6333333333333333, Specificity:

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.25, Metrics: {'Accuracy': 0.46923076923076923, 'Sensitivity':

Threshold: 0.30, Metrics: {'Accuracy': 0.5153846153846153, 'Sensitivity': 1

Threshold: 0.35, Metrics: {'Accuracy': 0.5538461538461539, 'Sensitivity': 0

Threshold: 0.40, Metrics: {'Accuracy': 0.6, 'Sensitivity': 0.9333333333333333

Threshold: 0.45, Metrics: {'Accuracy': 0.6153846153846154, 'Sensitivity': 0

Threshold: 0.50, Metrics: {'Accuracy': 0.6615384615384615, 'Sensitivity': 0

Threshold: 0.55, Metrics: {'Accuracy': 0.7076923076923077, 'Sensitivity': 0

Threshold: 0.60, Metrics: {'Accuracy': 0.6538461538461539, 'Sensitivity': 0

Threshold: 0.65, Metrics: {'Accuracy': 0.6230769230769231, 'Sensitivity': 0

Threshold: 0.70, Metrics: {'Accuracy': 0.5692307692307692, 'Sensitivity': 0

Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

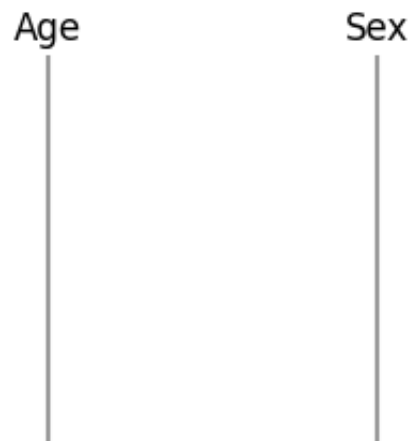
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

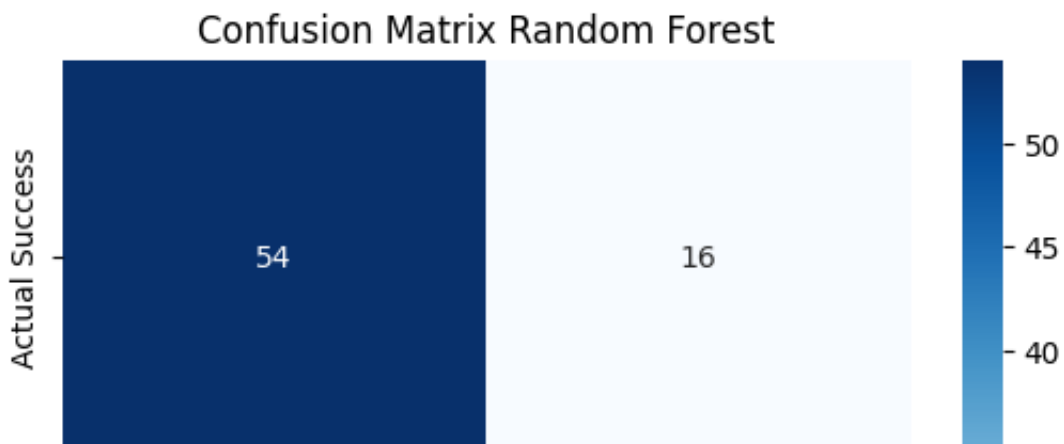
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

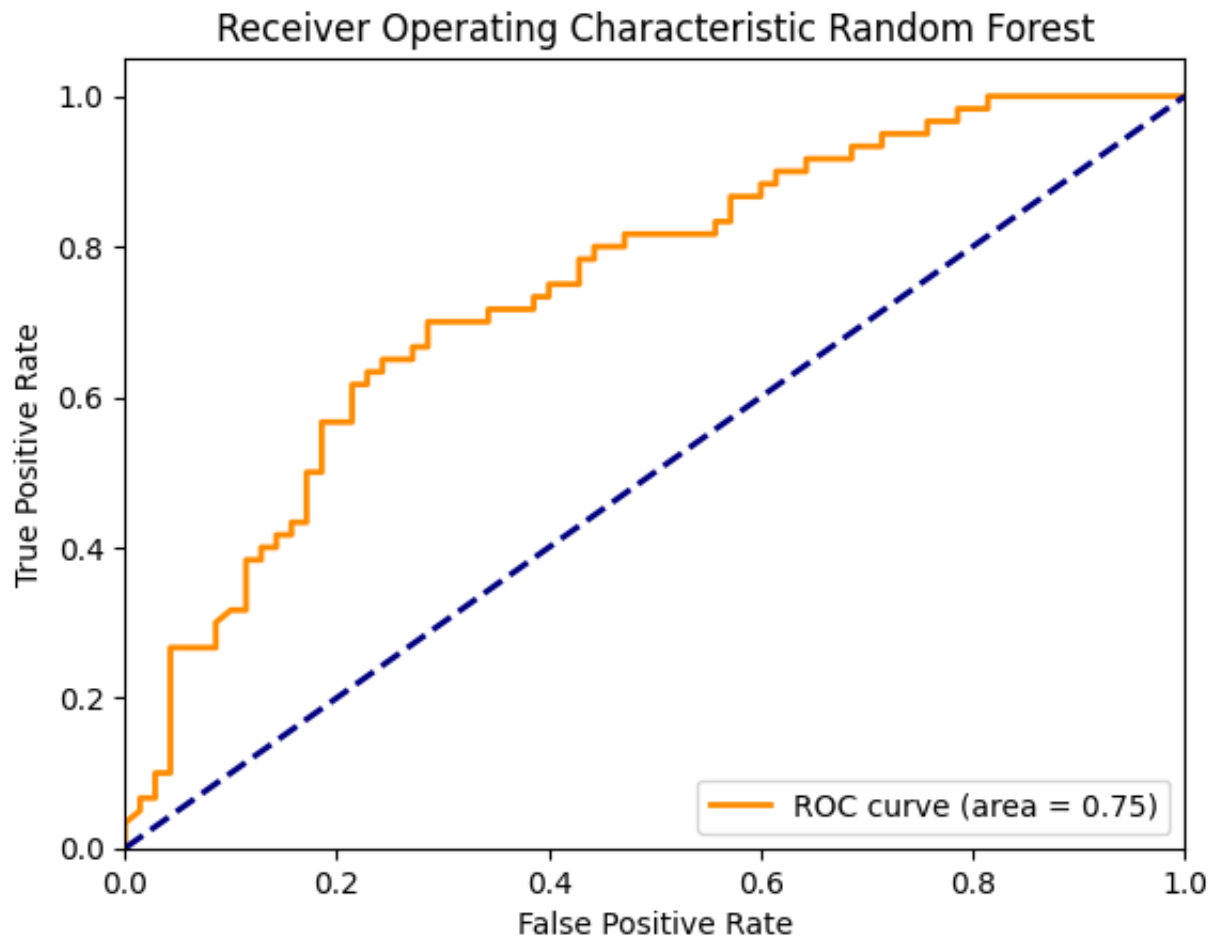
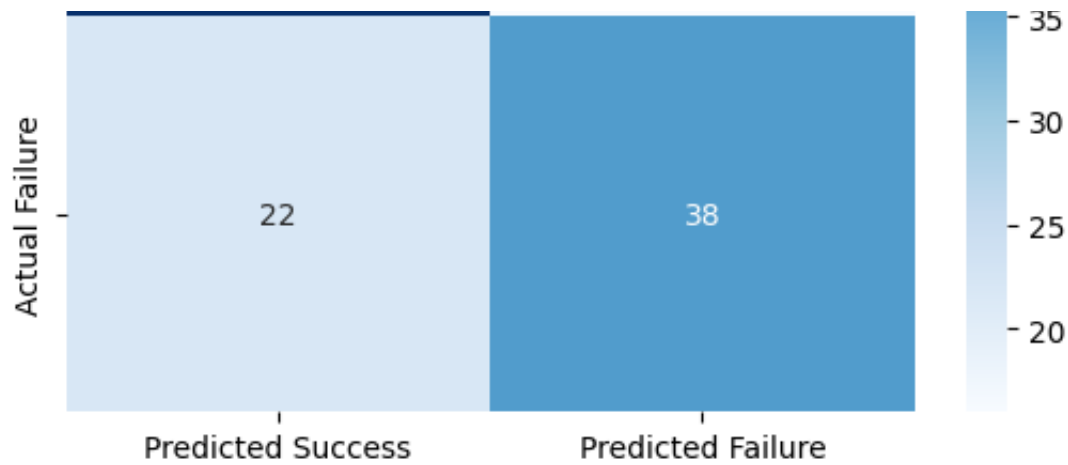
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

SHAP Summary for Random Forest









Running evaluation with seed 42

Evaluating Random Forest with seed 42...

--- Dados ROC para copiar ---

FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.0285714

TPR = [0.0, 0.016666666666666666, 0.03333333333333333, 0.05, 0.06666666666666666

AUC = 0.75

--- Fim dos Dados ROC ---

Training - Accuracy: 0.7140039447731755, Sensitivity: 0.7569721115537849, S  
Metrics for manual threshold 0.55:

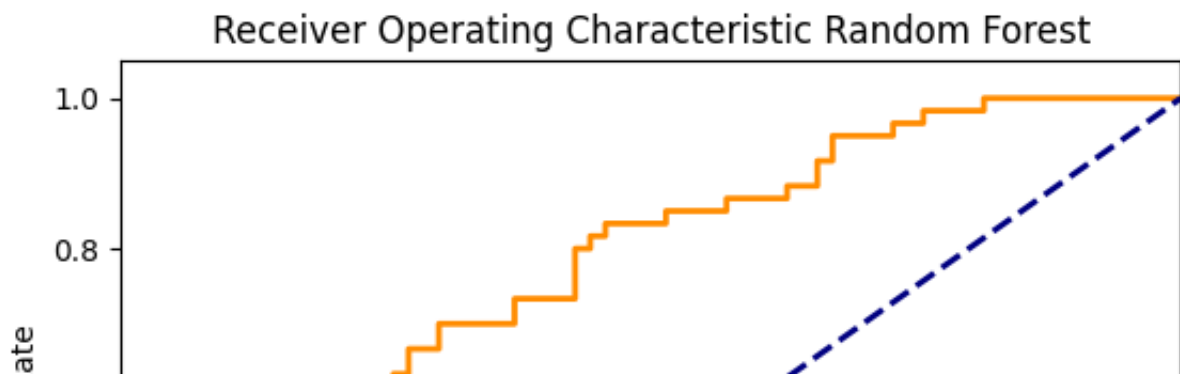
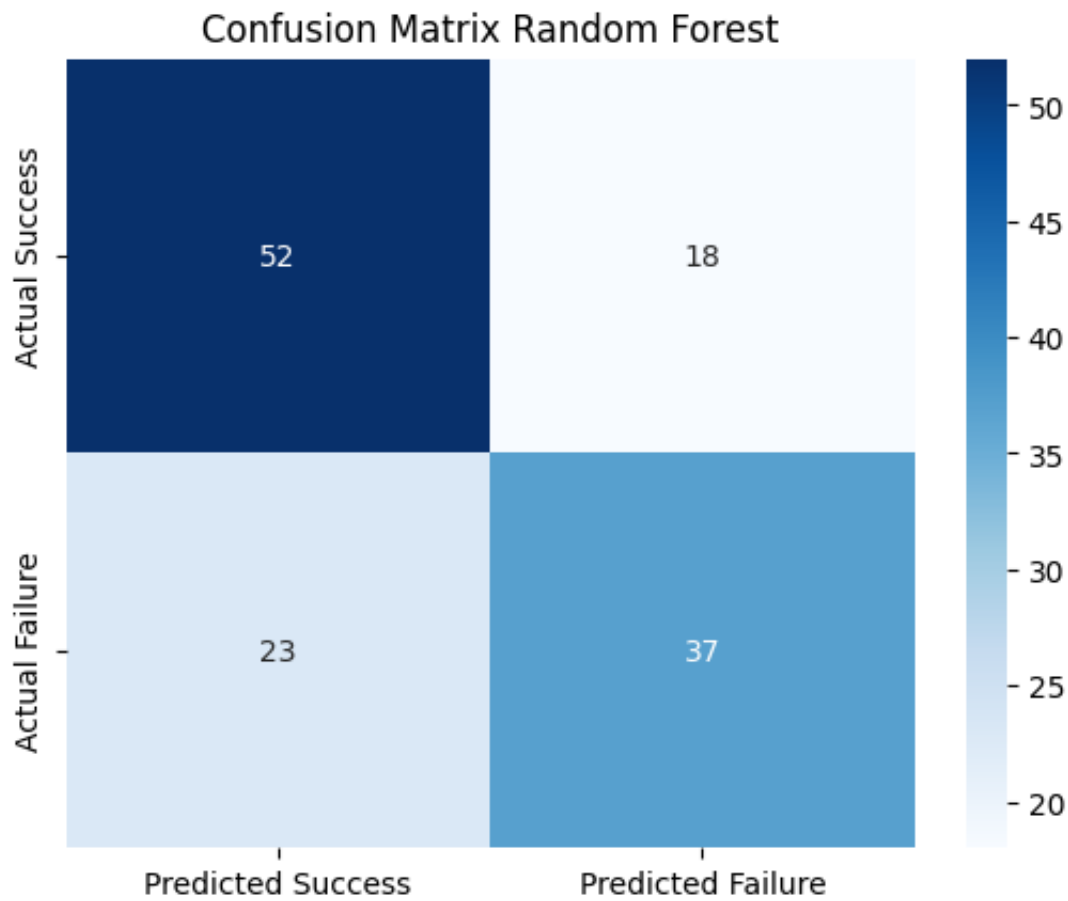
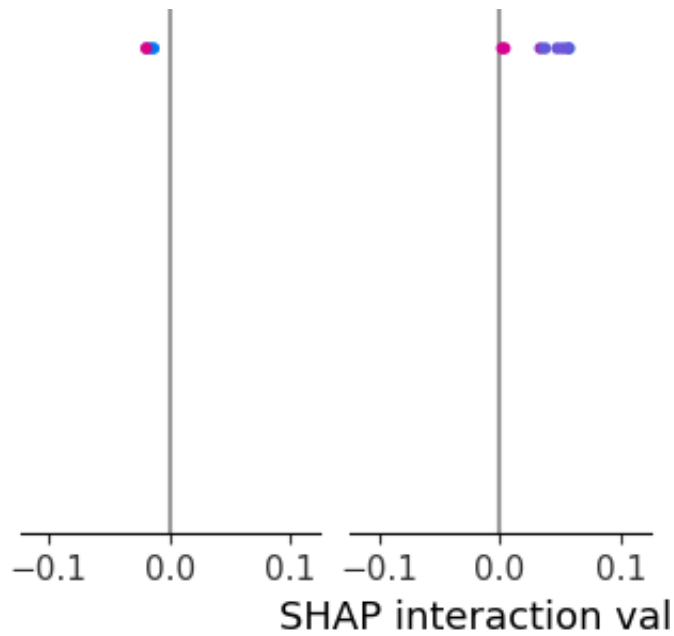
Accuracy: 0.6846153846153846, Sensitivity: 0.6166666666666667, Specificity:

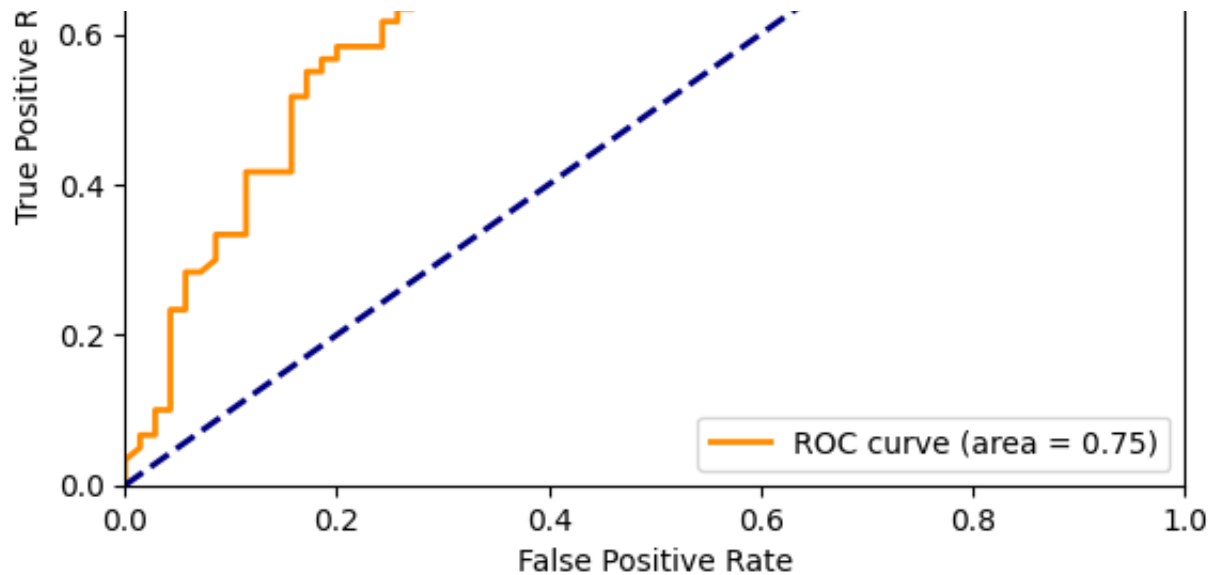
Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

```
Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':  
Threshold: 0.25, Metrics: {'Accuracy': 0.46923076923076923, 'Sensitivity':  
Threshold: 0.30, Metrics: {'Accuracy': 0.5, 'Sensitivity': 1.0, 'Specificit  
Threshold: 0.35, Metrics: {'Accuracy': 0.5615384615384615, 'Sensitivity': 0  
Threshold: 0.40, Metrics: {'Accuracy': 0.6076923076923076, 'Sensitivity': 0  
Threshold: 0.45, Metrics: {'Accuracy': 0.6461538461538462, 'Sensitivity': 0  
Threshold: 0.50, Metrics: {'Accuracy': 0.6461538461538462, 'Sensitivity': 0  
Threshold: 0.55, Metrics: {'Accuracy': 0.6846153846153846, 'Sensitivity': 0  
Threshold: 0.60, Metrics: {'Accuracy': 0.6615384615384615, 'Sensitivity': 0  
Threshold: 0.65, Metrics: {'Accuracy': 0.6153846153846154, 'Sensitivity': 0  
Threshold: 0.70, Metrics: {'Accuracy': 0.5692307692307692, 'Sensitivity': 0  
Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
SHAP Summary for Random Forest
```







Running evaluation with seed 43

Evaluating Random Forest with seed 43...

--- Dados ROC para copiar ---

FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.0285714

TPR = [0.0, 0.016666666666666666, 0.033333333333333333, 0.05, 0.06666666666666666

AUC = 0.7492857142857143

--- Fim dos Dados ROC ---

Training - Accuracy: 0.7199211045364892, Sensitivity: 0.7529880478087649, S  
Metrics for manual threshold 0.55:

Accuracy: 0.7076923076923077, Sensitivity: 0.6333333333333333, Specificity:

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.25, Metrics: {'Accuracy': 0.46923076923076923, 'Sensitivity':

Threshold: 0.30, Metrics: {'Accuracy': 0.5153846153846153, 'Sensitivity': 1

Threshold: 0.35, Metrics: {'Accuracy': 0.5769230769230769, 'Sensitivity': 0

Threshold: 0.40, Metrics: {'Accuracy': 0.5846153846153846, 'Sensitivity': 0

Threshold: 0.45, Metrics: {'Accuracy': 0.6384615384615384, 'Sensitivity': 0

Threshold: 0.50, Metrics: {'Accuracy': 0.6692307692307692, 'Sensitivity': 0

Threshold: 0.55, Metrics: {'Accuracy': 0.7076923076923077, 'Sensitivity': 0

Threshold: 0.60, Metrics: {'Accuracy': 0.6615384615384615, 'Sensitivity': 0

Threshold: 0.65, Metrics: {'Accuracy': 0.6384615384615384, 'Sensitivity': 0

Threshold: 0.70, Metrics: {'Accuracy': 0.5692307692307692, 'Sensitivity': 0

Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

SHAP Summary for Random Forest

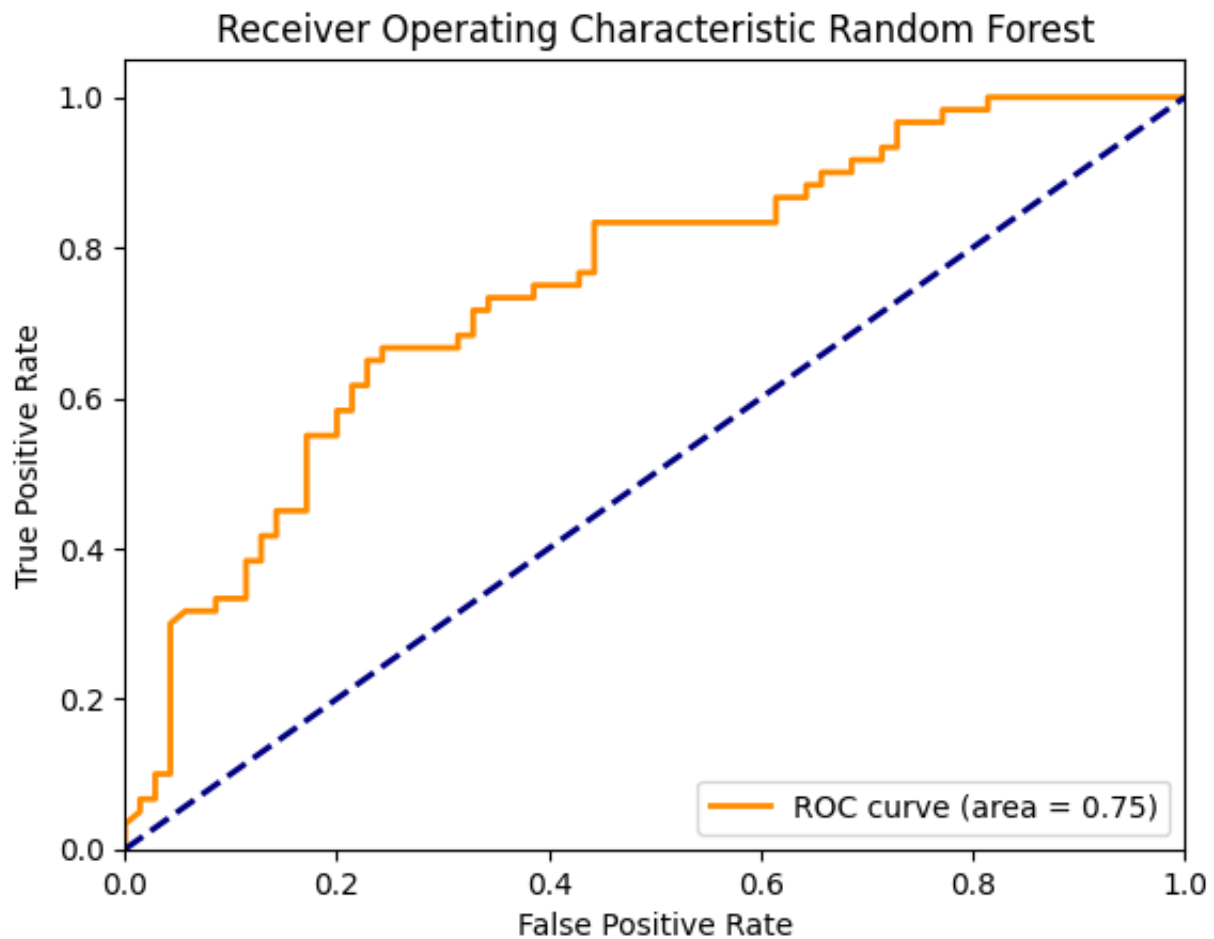
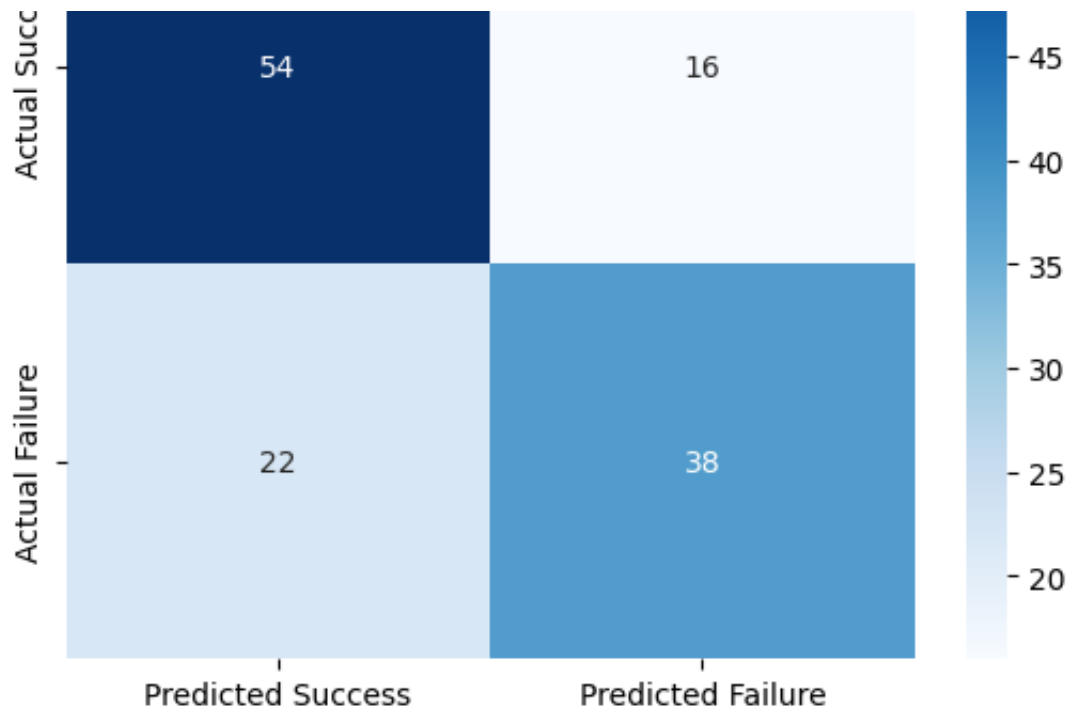
Age

Sex



Confusion Matrix Random Forest





Running evaluation with seed 44  
Evaluating Random Forest with seed 44...

--- Dados ROC para copiar ---

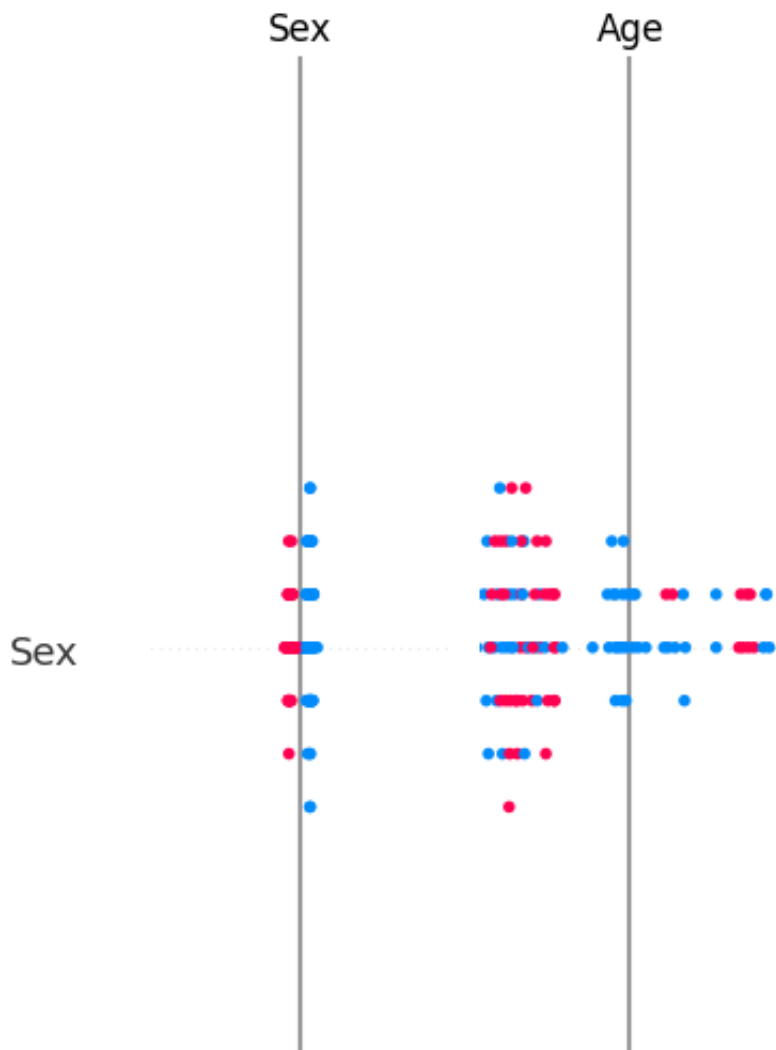
```
FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.02857142857142857, 0.04285714285714285, 0.05714285714285714, 0.07142857142857142, 0.08571428571428571, 0.1, 0.11428571428571428, 0.12857142857142857, 0.14285714285714285, 0.15714285714285714, 0.17142857142857142, 0.18571428571428571, 0.2, 0.21428571428571428, 0.22857142857142857, 0.24285714285714285, 0.25714285714285714, 0.27142857142857142, 0.28571428571428571, 0.3, 0.31428571428571428, 0.32857142857142857, 0.34285714285714285, 0.35714285714285714, 0.37142857142857142, 0.38571428571428571, 0.4, 0.41428571428571428, 0.42857142857142857, 0.44285714285714285, 0.45714285714285714, 0.47142857142857142, 0.48571428571428571, 0.5, 0.51428571428571428, 0.52857142857142857, 0.54285714285714285, 0.55714285714285714, 0.57142857142857142, 0.58571428571428571, 0.6, 0.61428571428571428, 0.62857142857142857, 0.64285714285714285, 0.65714285714285714, 0.67142857142857142, 0.68571428571428571, 0.7, 0.71428571428571428, 0.72857142857142857, 0.74285714285714285, 0.75714285714285714, 0.77142857142857142, 0.78571428571428571, 0.8, 0.81428571428571428, 0.82857142857142857, 0.84285714285714285, 0.85714285714285714, 0.87142857142857142, 0.88571428571428571, 0.9, 0.91428571428571428, 0.92857142857142857, 0.94285714285714285, 0.95714285714285714, 0.97142857142857142, 0.98571428571428571, 1.0]
TPR = [0.0, 0.016666666666666666, 0.033333333333333333, 0.05, 0.06666666666666666, 0.08333333333333333, 0.1, 0.11666666666666666, 0.13333333333333333, 0.15, 0.16666666666666666, 0.18333333333333333, 0.2, 0.21666666666666666, 0.23333333333333333, 0.25, 0.26666666666666666, 0.28333333333333333, 0.3, 0.31666666666666666, 0.33333333333333333, 0.35, 0.36666666666666666, 0.38333333333333333, 0.4, 0.41666666666666666, 0.43333333333333333, 0.45, 0.46666666666666666, 0.48333333333333333, 0.5, 0.51666666666666666, 0.53333333333333333, 0.55, 0.56666666666666666, 0.58333333333333333, 0.6, 0.61666666666666666, 0.63333333333333333, 0.65, 0.66666666666666666, 0.68333333333333333, 0.7, 0.71666666666666666, 0.73333333333333333, 0.75, 0.76666666666666666, 0.78333333333333333, 0.8, 0.81666666666666666, 0.83333333333333333, 0.85, 0.86666666666666666, 0.88333333333333333, 0.9, 0.91666666666666666, 0.93333333333333333, 0.95, 0.96666666666666666, 0.98333333333333333, 1.0]
AUC = 0.7473809523809524
```

--- Film dos Dados ROC ---

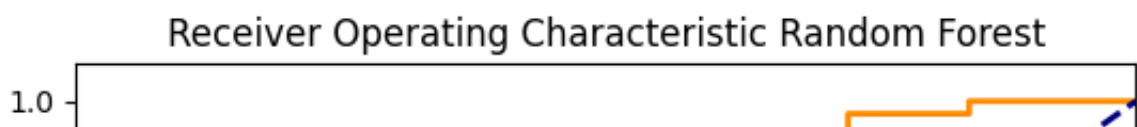
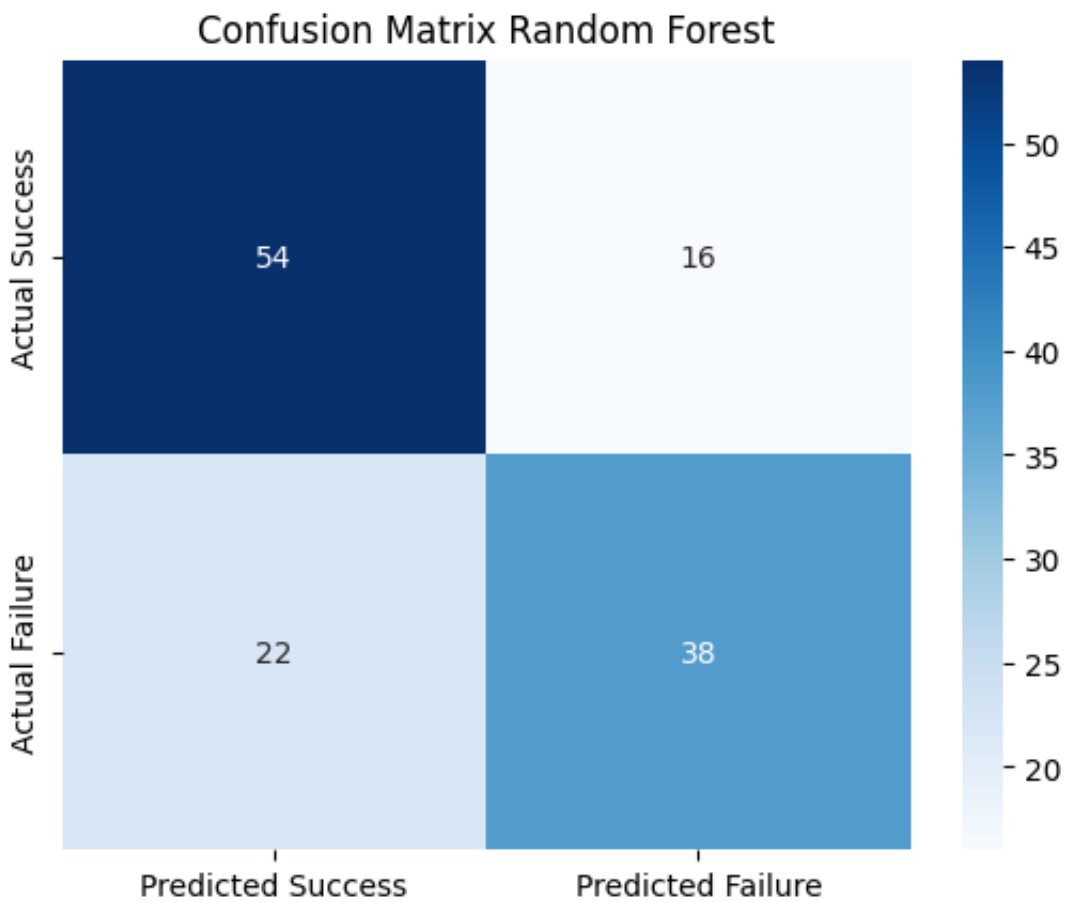
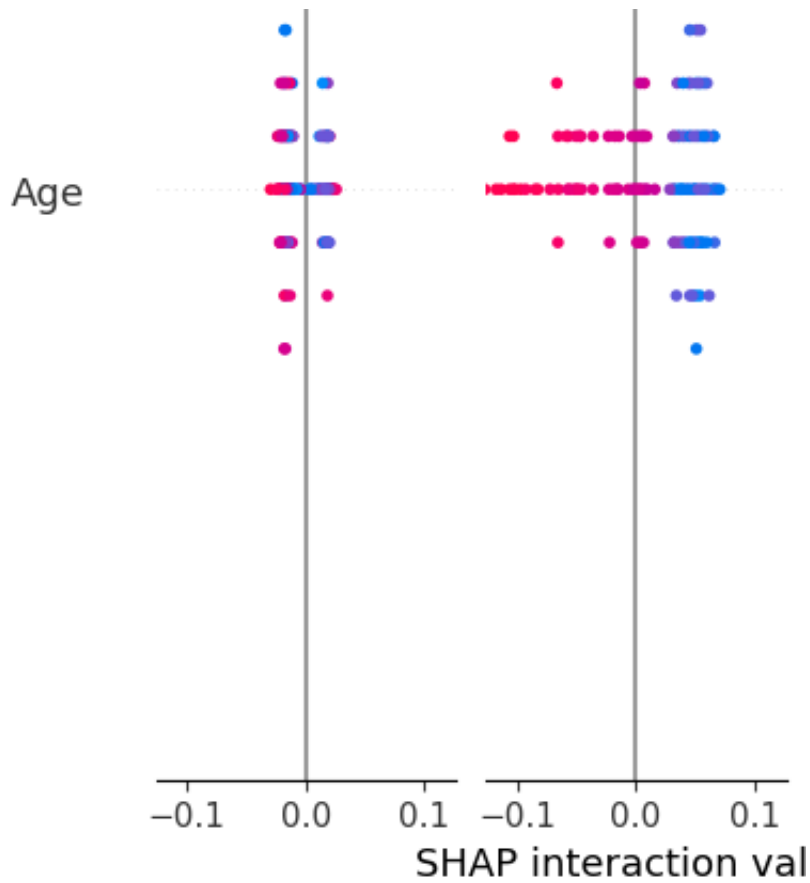
Training - Accuracy: 0.717948717948718, Sensitivity: 0.7569721115537849, Sp  
Metrics for manual threshold 0.55:

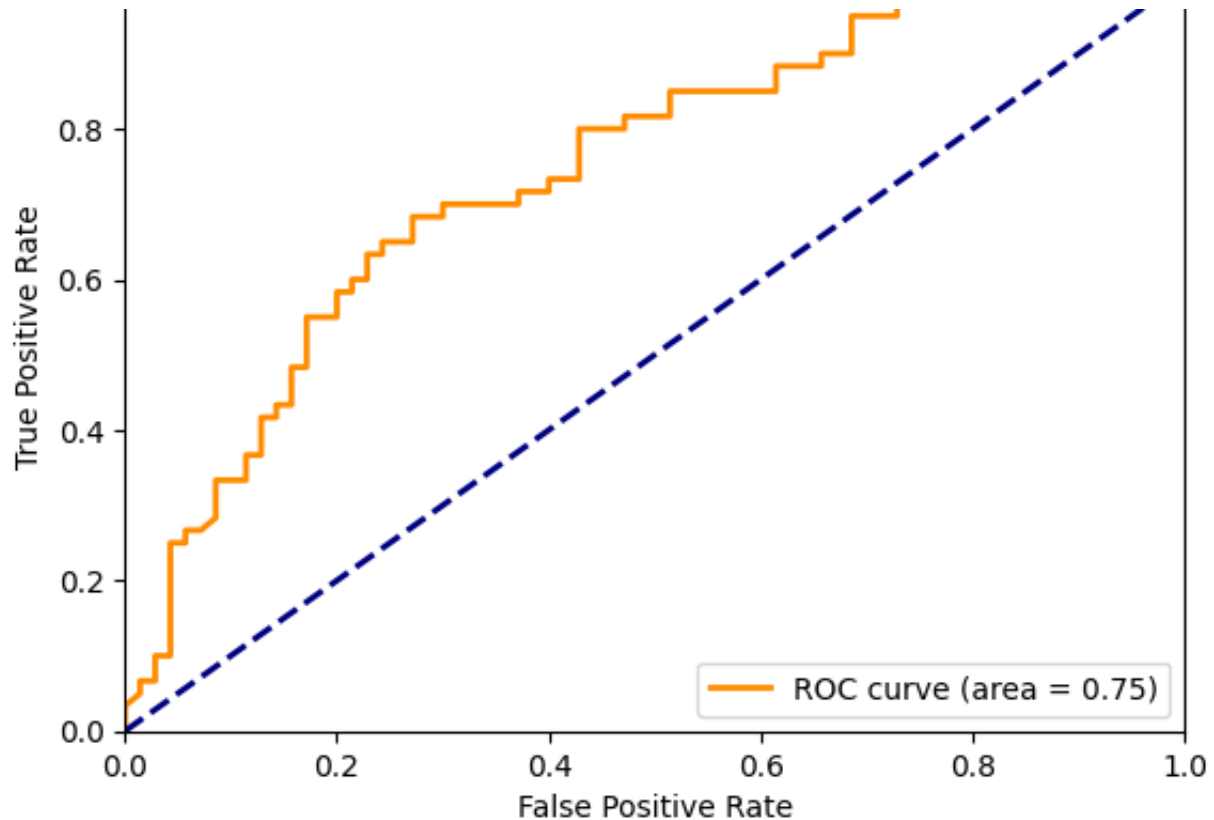
Accuracy: 0.7076923076923077, Sensitivity: 0.6333333333333333, Specificity:  
Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':  
Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':  
Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':  
Threshold: 0.25, Metrics: {'Accuracy': 0.46923076923076923, 'Sensitivity':  
Threshold: 0.30, Metrics: {'Accuracy': 0.5, 'Sensitivity': 1.0, 'Specificit  
Threshold: 0.35, Metrics: {'Accuracy': 0.5769230769230769, 'Sensitivity': 0  
Threshold: 0.40, Metrics: {'Accuracy': 0.6076923076923076, 'Sensitivity': 0  
Threshold: 0.45, Metrics: {'Accuracy': 0.6461538461538462, 'Sensitivity': 0  
Threshold: 0.50, Metrics: {'Accuracy': 0.6461538461538462, 'Sensitivity': 0  
Threshold: 0.55, Metrics: {'Accuracy': 0.7076923076923077, 'Sensitivity': 0  
Threshold: 0.60, Metrics: {'Accuracy': 0.6615384615384615, 'Sensitivity': 0  
Threshold: 0.65, Metrics: {'Accuracy': 0.6230769230769231, 'Sensitivity': 0  
Threshold: 0.70, Metrics: {'Accuracy': 0.5692307692307692, 'Sensitivity': 0  
Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

SHAP Summary for Random Forest









Running evaluation with seed 45  
Evaluating Random Forest with seed 45...

--- Dados ROC para copiar ---

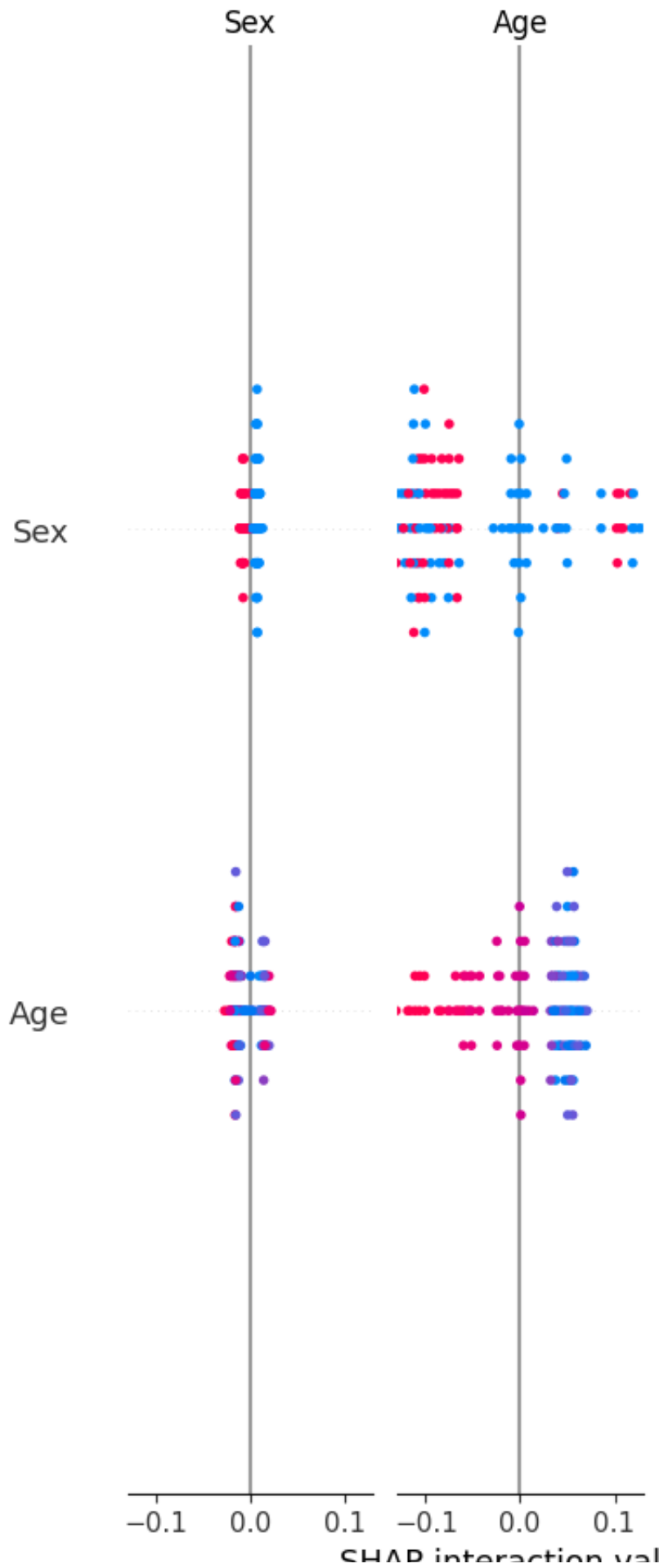
```
FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.02857142857142857, 0.02857142
TPR = [0.0, 0.016666666666666666, 0.05, 0.06666666666666667, 0.066666666666
AUC = 0.7440476190476191
```

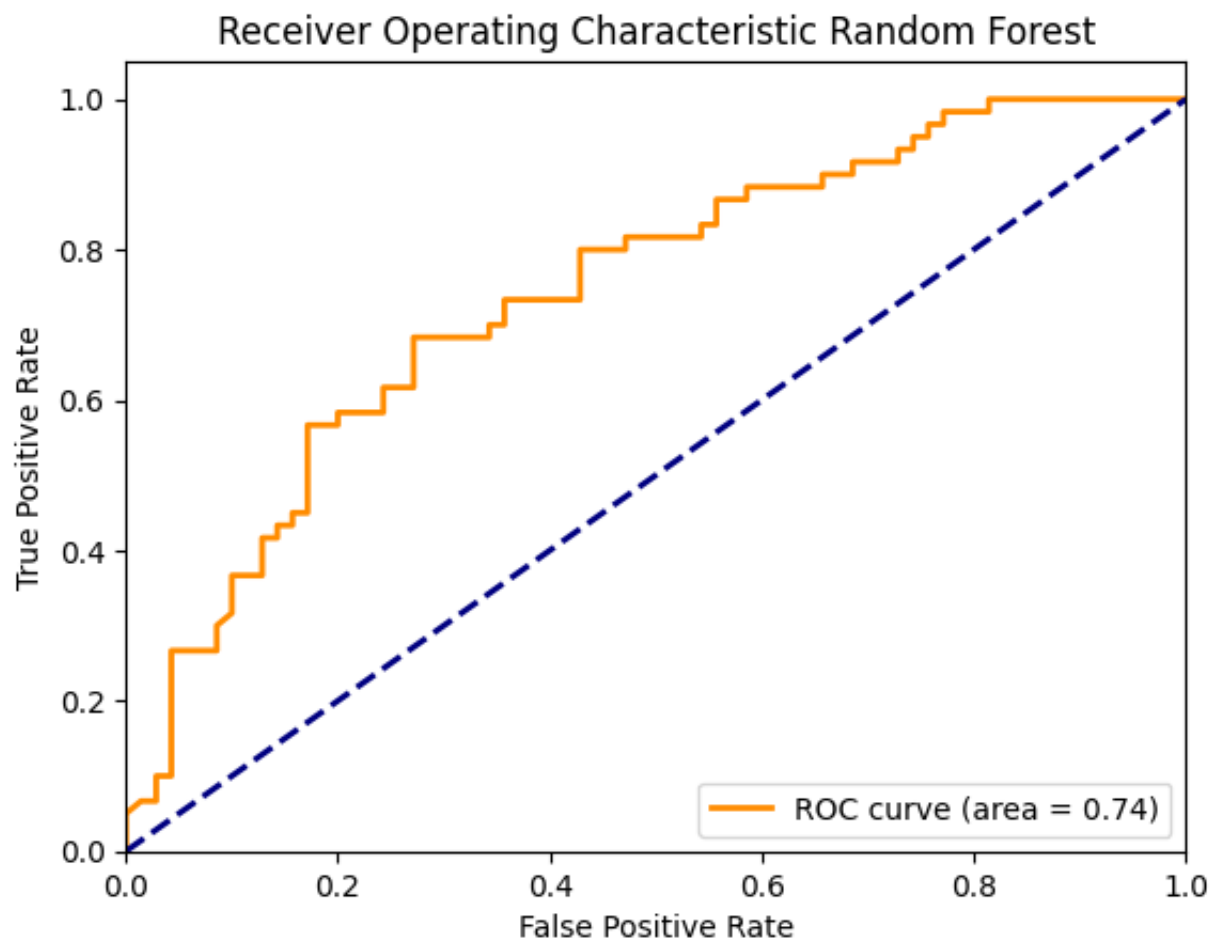
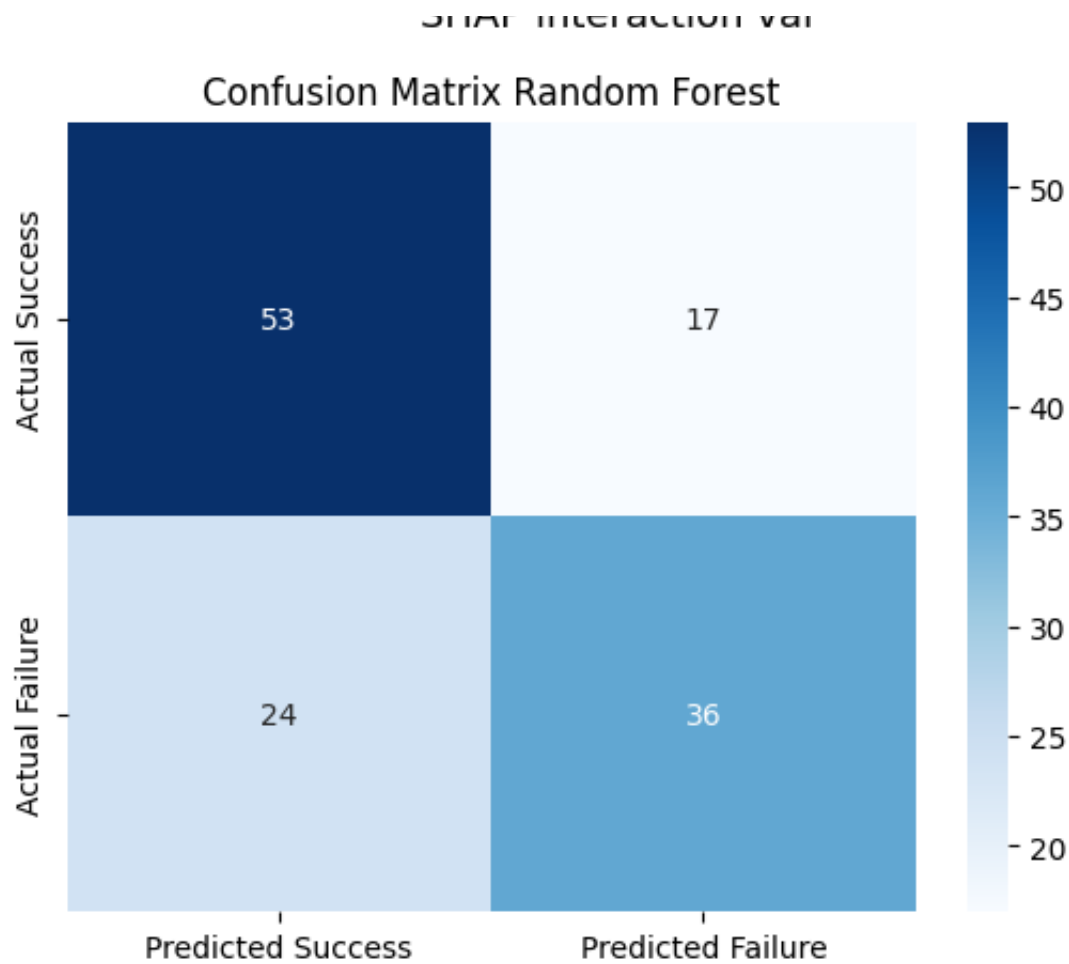
--- Fim dos Dados ROC ---

Training - Accuracy: 0.7238658777120316, Sensitivity: 0.7569721115537849, S  
Metrics for manual threshold 0.55:

```
Accuracy: 0.6846153846153846, Sensitivity: 0.6, Specificity: 0.757142857142
Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':
Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':
Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':
Threshold: 0.25, Metrics: {'Accuracy': 0.46923076923076923, 'Sensitivity':
Threshold: 0.30, Metrics: {'Accuracy': 0.5076923076923077, 'Sensitivity': 1
Threshold: 0.35, Metrics: {'Accuracy': 0.5538461538461539, 'Sensitivity': 0
Threshold: 0.40, Metrics: {'Accuracy': 0.5923076923076923, 'Sensitivity': 0
Threshold: 0.45, Metrics: {'Accuracy': 0.6230769230769231, 'Sensitivity': 0
Threshold: 0.50, Metrics: {'Accuracy': 0.6538461538461539, 'Sensitivity': 0
Threshold: 0.55, Metrics: {'Accuracy': 0.6846153846153846, 'Sensitivity': 0
Threshold: 0.60, Metrics: {'Accuracy': 0.6615384615384615, 'Sensitivity': 0
Threshold: 0.65, Metrics: {'Accuracy': 0.6384615384615384, 'Sensitivity': 0
Threshold: 0.70, Metrics: {'Accuracy': 0.5692307692307692, 'Sensitivity': 0
Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
```

# SHAP Summary for Random Forest





Running evaluation with seed 46

Running evaluation with seed 46  
Evaluating Random Forest with seed 46...

--- Dados ROC para copiar ---

FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.02857142857142857, 0.02857142

TPR = [0.0, 0.016666666666666666, 0.05, 0.06666666666666667, 0.06666666666666

AUC = 0.7428571428571429

--- Fim dos Dados ROC ---

Training - Accuracy: 0.727810650887574, Sensitivity: 0.7729083665338645, Sp  
Metrics for manual threshold 0.55:

Accuracy: 0.6923076923076923, Sensitivity: 0.6333333333333333, Specificity:

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.25, Metrics: {'Accuracy': 0.4846153846153846, 'Sensitivity': 1

Threshold: 0.30, Metrics: {'Accuracy': 0.5153846153846153, 'Sensitivity': 1

Threshold: 0.35, Metrics: {'Accuracy': 0.5692307692307692, 'Sensitivity': 0

Threshold: 0.40, Metrics: {'Accuracy': 0.6, 'Sensitivity': 0.9333333333333333

Threshold: 0.45, Metrics: {'Accuracy': 0.6307692307692307, 'Sensitivity': 0

Threshold: 0.50, Metrics: {'Accuracy': 0.6615384615384615, 'Sensitivity': 0

Threshold: 0.55, Metrics: {'Accuracy': 0.6923076923076923, 'Sensitivity': 0

Threshold: 0.60, Metrics: {'Accuracy': 0.6538461538461539, 'Sensitivity': 0

Threshold: 0.65, Metrics: {'Accuracy': 0.6230769230769231, 'Sensitivity': 0

Threshold: 0.70, Metrics: {'Accuracy': 0.5692307692307692, 'Sensitivity': 0

Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

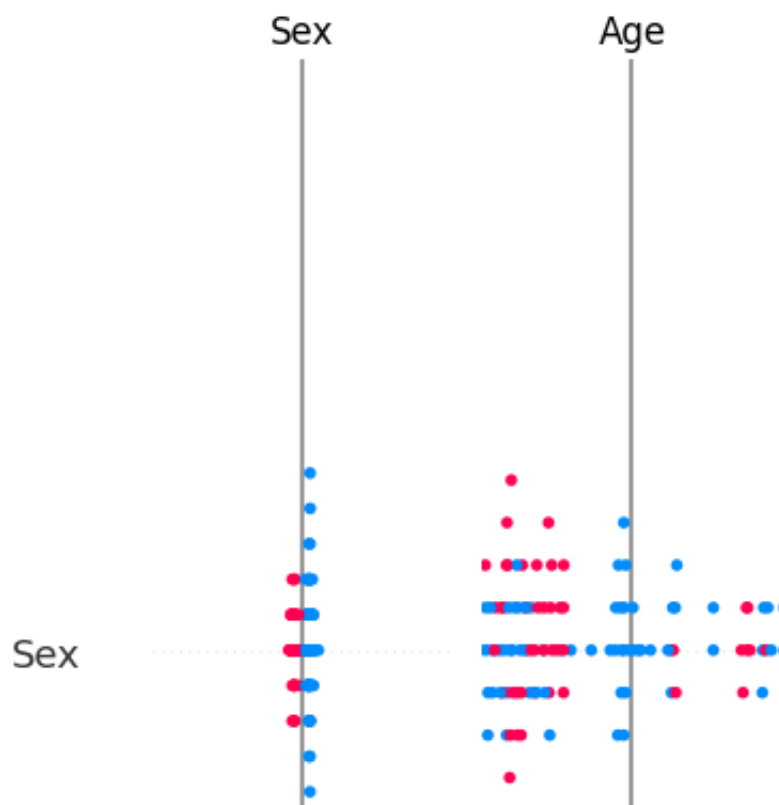
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

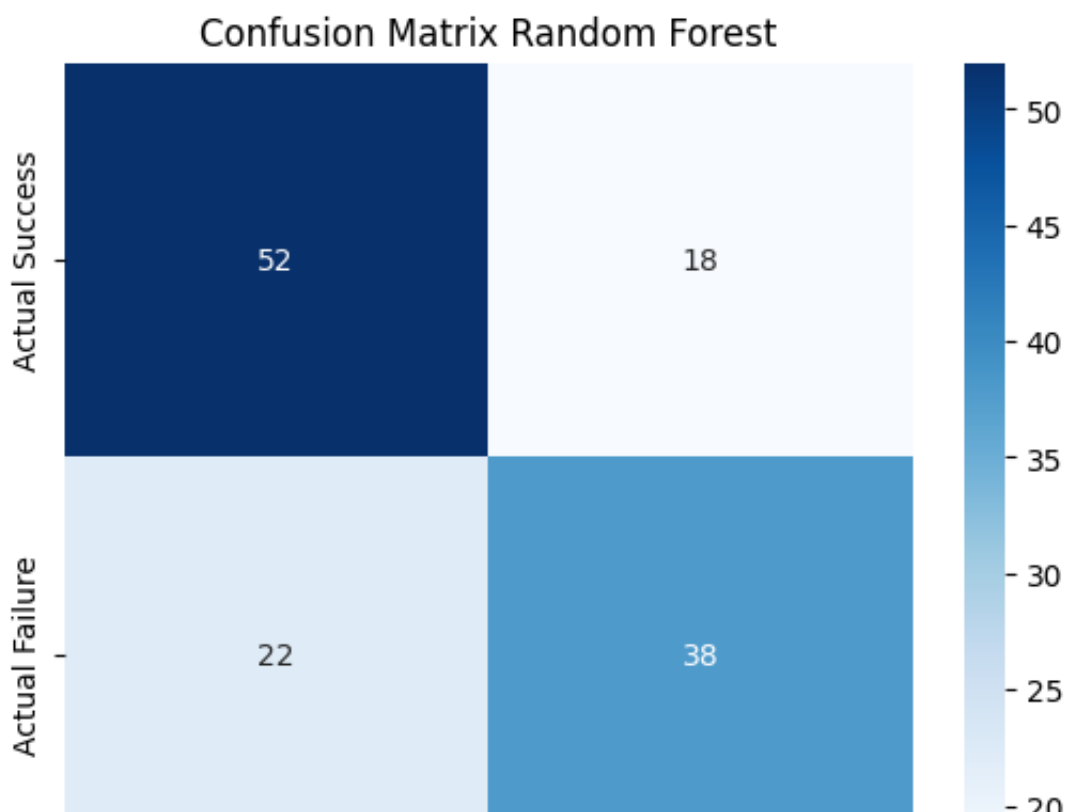
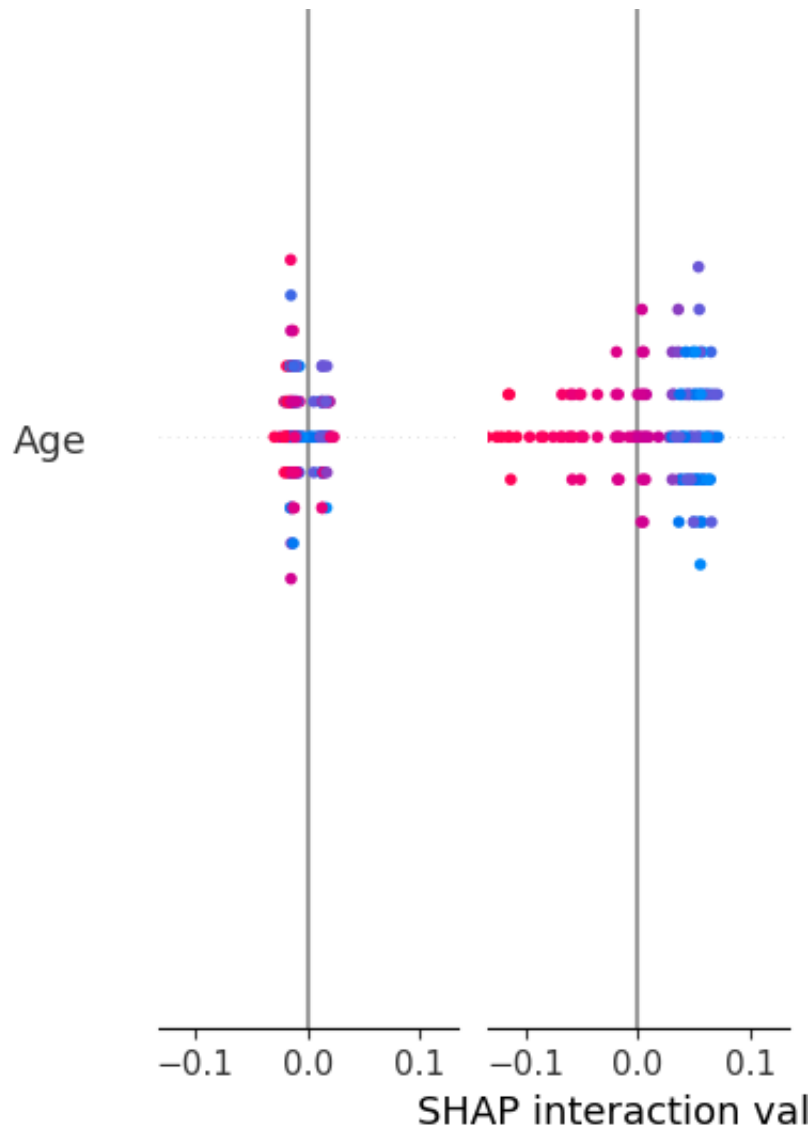
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

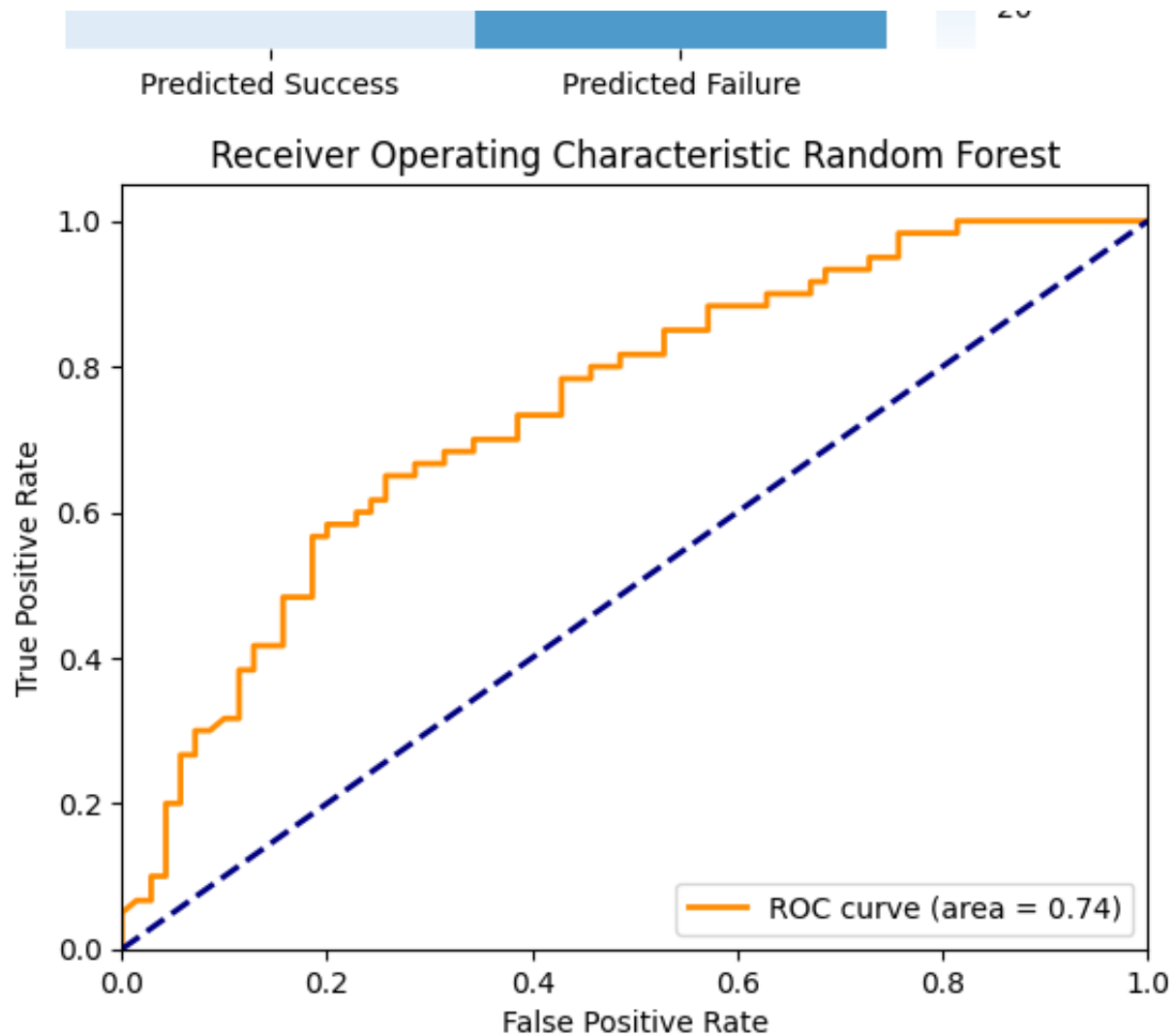
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

SHAP Summary for Random Forest







Running evaluation with seed 47

Evaluating Random Forest with seed 47...

--- Dados ROC para copiar ---

FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.02857142857142857, 0.02857142

TPR = [0.0, 0.016666666666666666, 0.05, 0.06666666666666667, 0.06666666666666

AUC = 0.7454761904761905

--- Fim dos Dados ROC ---

Training - Accuracy: 0.7140039447731755, Sensitivity: 0.749003984063745, Sp  
Metrics for manual threshold 0.55:

Accuracy: 0.6846153846153846, Sensitivity: 0.6, Specificity: 0.757142857142

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.25, Metrics: {'Accuracy': 0.46923076923076923, 'Sensitivity':

Threshold: 0.30, Metrics: {'Accuracy': 0.5153846153846153, 'Sensitivity': 1

Threshold: 0.35, Metrics: {'Accuracy': 0.5692307692307692, 'Sensitivity': 0

Threshold: 0.40, Metrics: {'Accuracy': 0.5846153846153846, 'Sensitivity': 0

Threshold: 0.45, Metrics: {'Accuracy': 0.6384615384615384, 'Sensitivity': 0

Threshold: 0.50, Metrics: {'Accuracy': 0.676923076923077, 'Sensitivity': 0.

Threshold: 0.55, Metrics: {'Accuracy': 0.6846153846153846, 'Sensitivity': 0

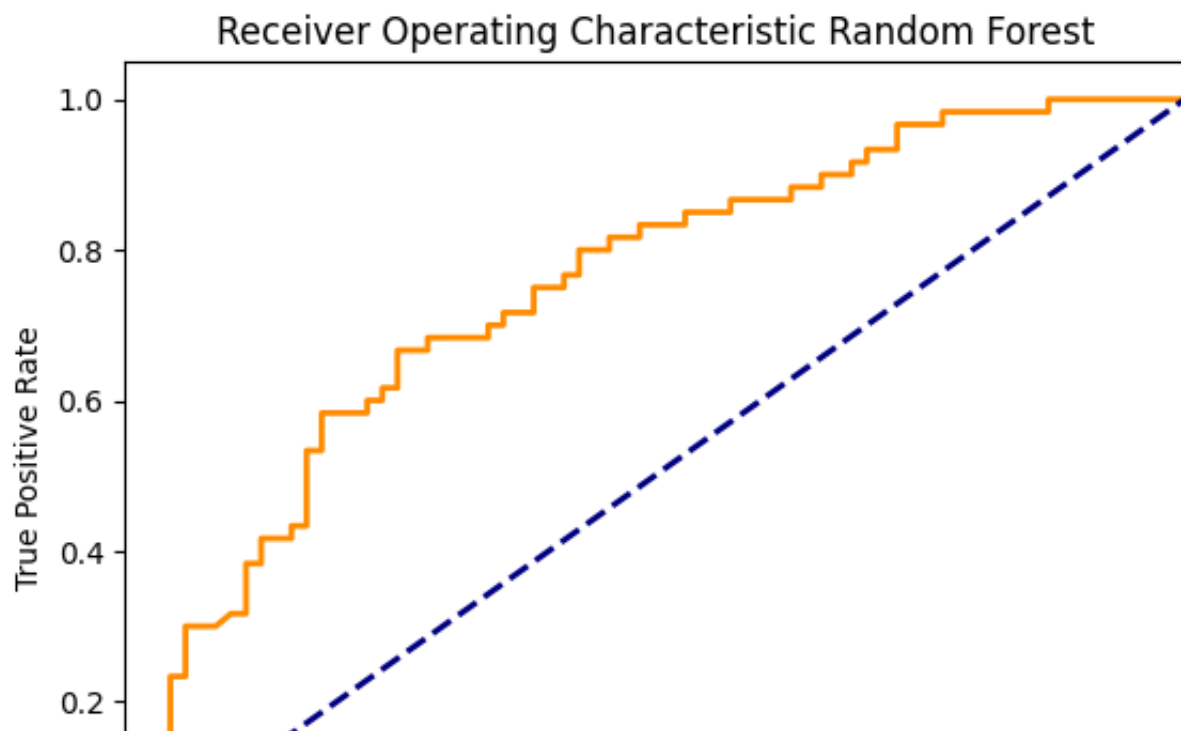
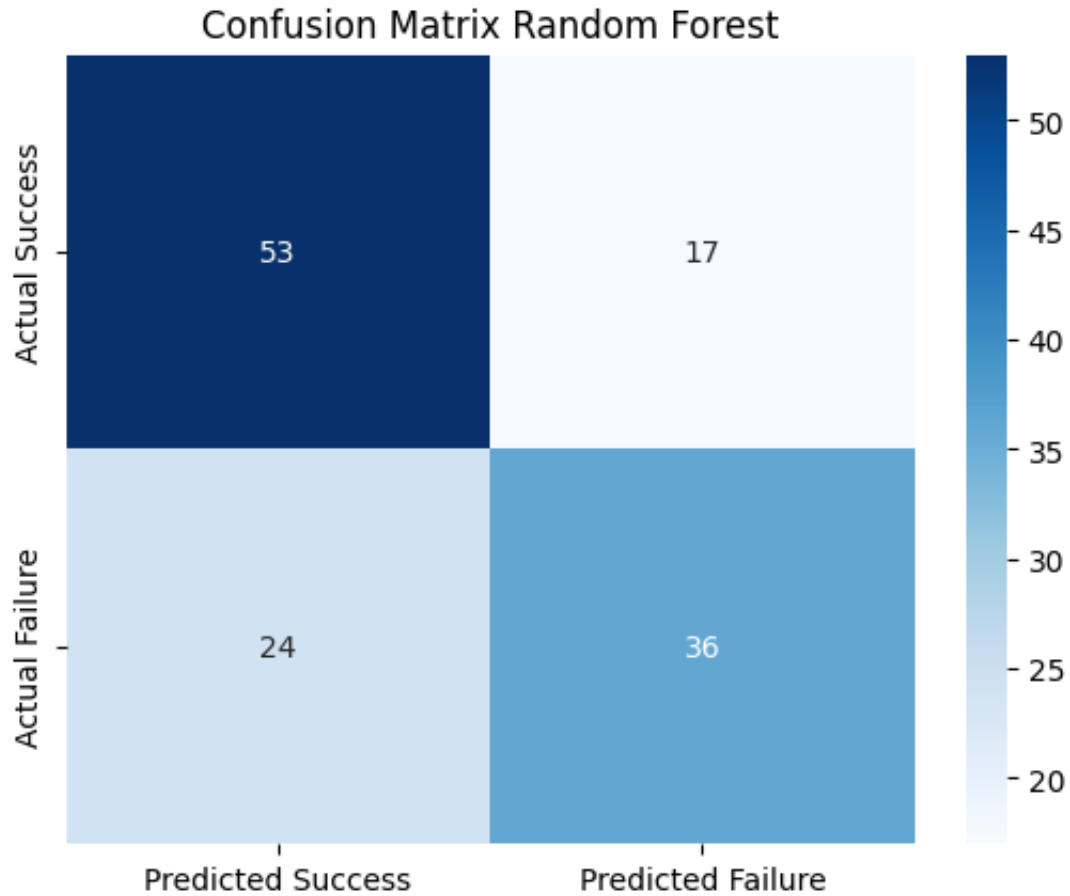
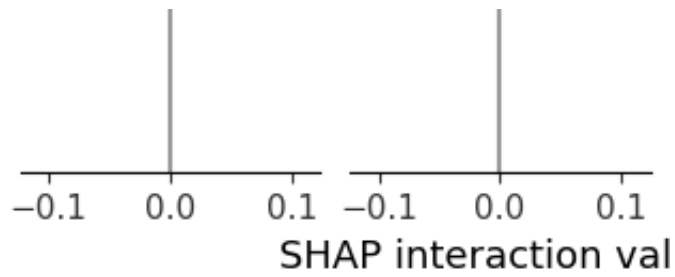
Threshold: 0.60, Metrics: {'Accuracy': 0.6538461538461539, 'Sensitivity': 0

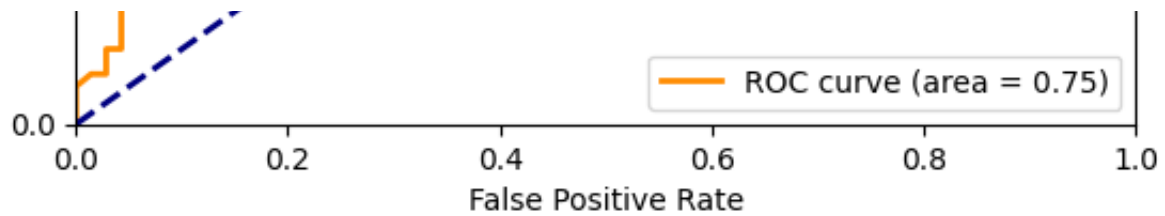
Threshold: 0.65, Metrics: {'Accuracy': 0.6307692307692307, 'Sensitivity': 0

```
Threshold: 0.70, Metrics: {'Accuracy': 0.5692307692307692, 'Sensitivity': 0
Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
SHAP Summary for Random Forest
```









Running evaluation with seed 48

Evaluating Random Forest with seed 48...

--- Dados ROC para copiar ---

FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.02857142857142857, 0.02857142

TPR = [0.0, 0.016666666666666666, 0.05, 0.06666666666666667, 0.06666666666666

AUC = 0.745

--- Fim dos Dados ROC ---

Training - Accuracy: 0.7199211045364892, Sensitivity: 0.749003984063745, Sp  
Metrics for manual threshold 0.55:

Accuracy: 0.676923076923077, Sensitivity: 0.6, Specificity: 0.7428571428571

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.25, Metrics: {'Accuracy': 0.46923076923076923, 'Sensitivity':

Threshold: 0.30, Metrics: {'Accuracy': 0.5153846153846153, 'Sensitivity': 1

Threshold: 0.35, Metrics: {'Accuracy': 0.5615384615384615, 'Sensitivity': 0

Threshold: 0.40, Metrics: {'Accuracy': 0.5923076923076923, 'Sensitivity': 0

Threshold: 0.45, Metrics: {'Accuracy': 0.6384615384615384, 'Sensitivity': 0

Threshold: 0.50, Metrics: {'Accuracy': 0.6692307692307692, 'Sensitivity': 0

Threshold: 0.55, Metrics: {'Accuracy': 0.676923076923077, 'Sensitivity': 0.

Threshold: 0.60, Metrics: {'Accuracy': 0.6461538461538462, 'Sensitivity': 0

Threshold: 0.65, Metrics: {'Accuracy': 0.6230769230769231, 'Sensitivity': 0

Threshold: 0.70, Metrics: {'Accuracy': 0.5692307692307692, 'Sensitivity': 0

Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

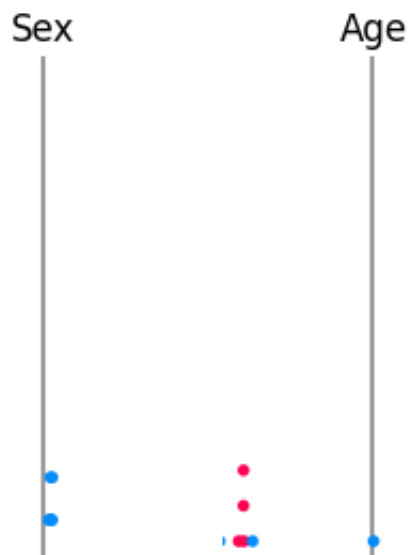
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

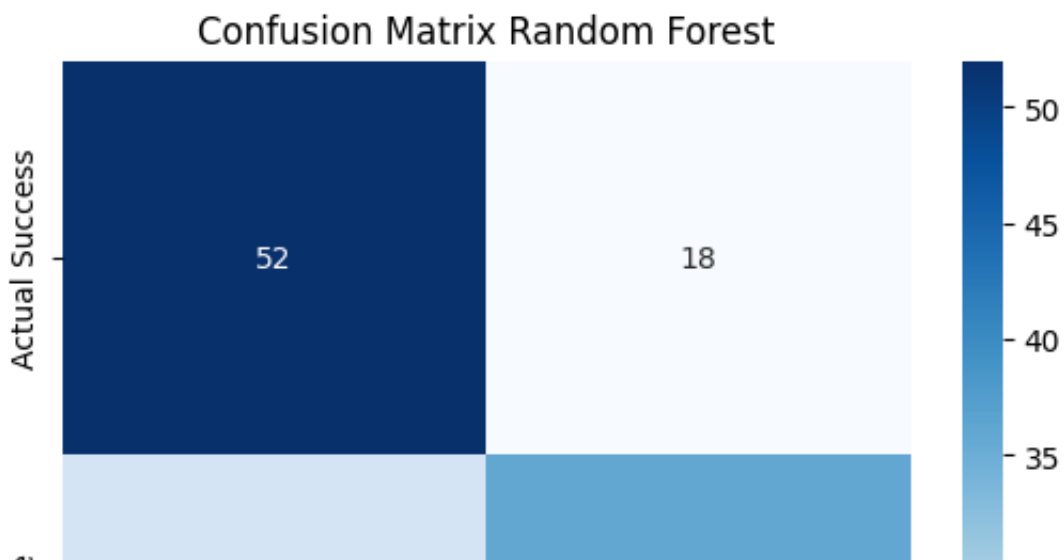
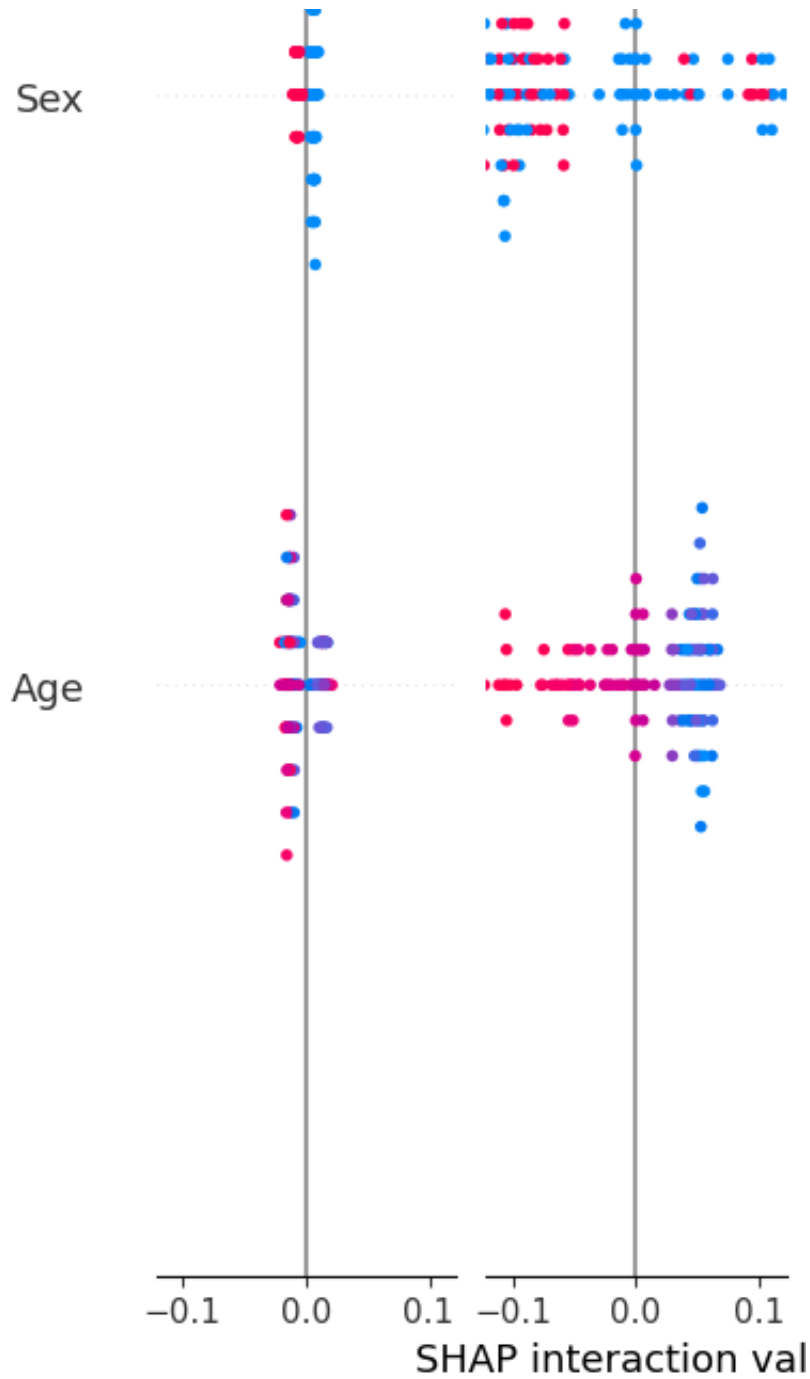
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

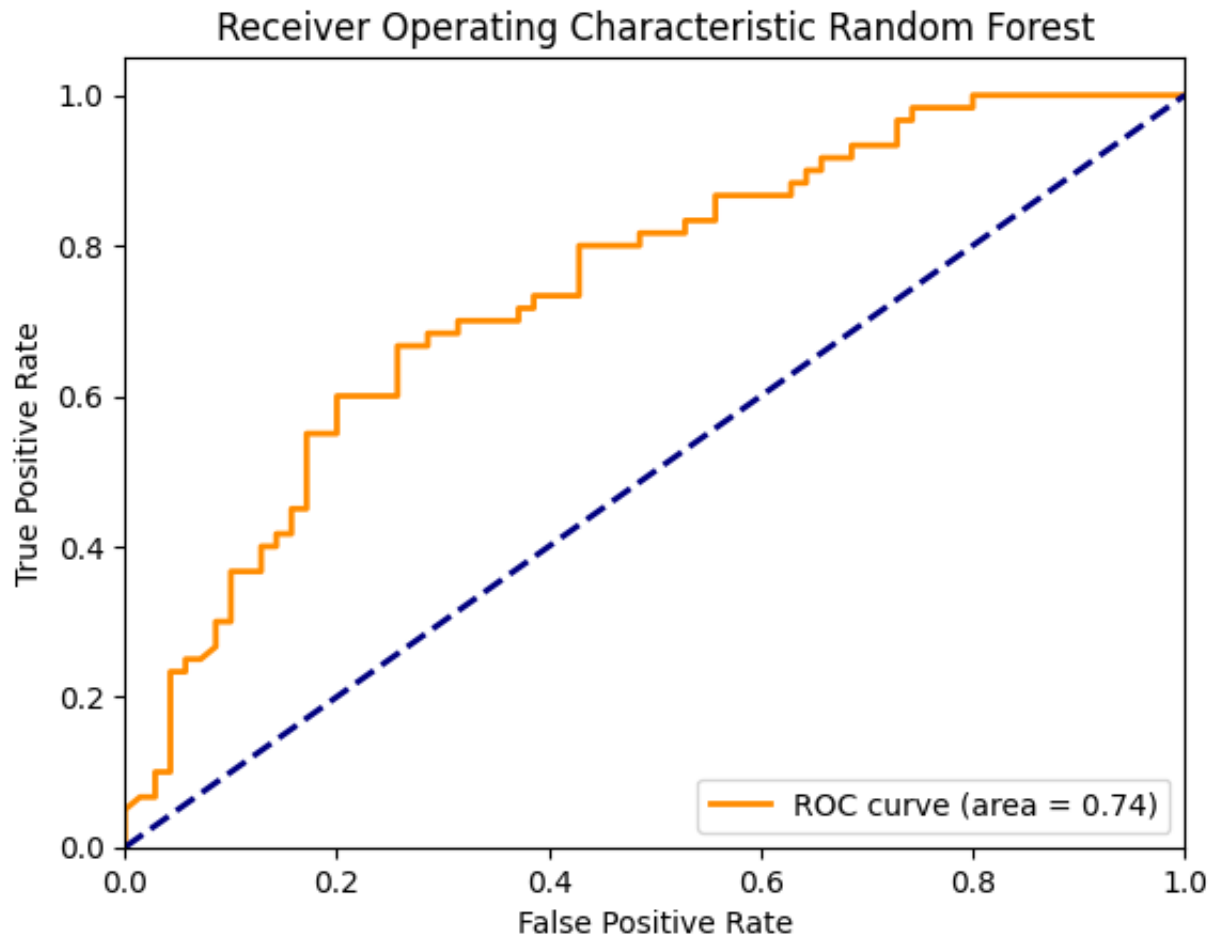
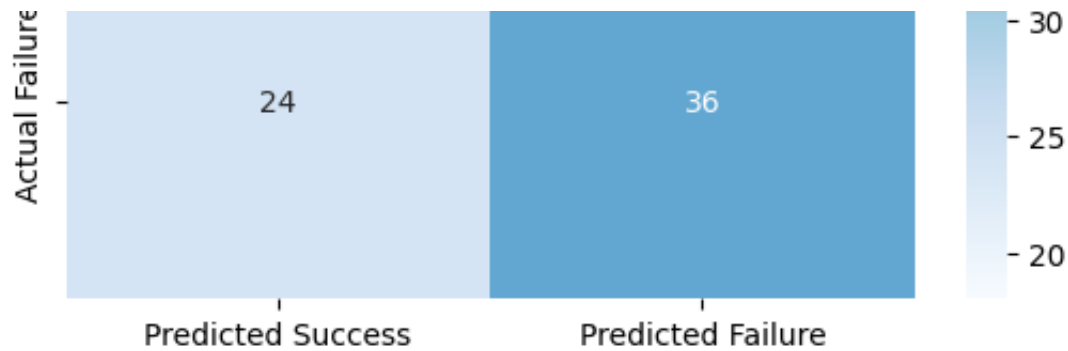
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

SHAP Summary for Random Forest







Running evaluation with seed 49

Evaluating Random Forest with seed 49...

--- Dados ROC para copiar ---

FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.0285714

TPR = [0.0, 0.016666666666666666, 0.033333333333333333, 0.05, 0.0666666666666

AUC = 0.7402380952380953

--- Fim dos Dados ROC ---

Training - Accuracy: 0.7159763313609467, Sensitivity: 0.7450199203187251, S  
Metrics for manual threshold 0.55:

Accuracy: 0.7, Sensitivity: 0.6333333333333333, Specificity: 0.757142857142

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

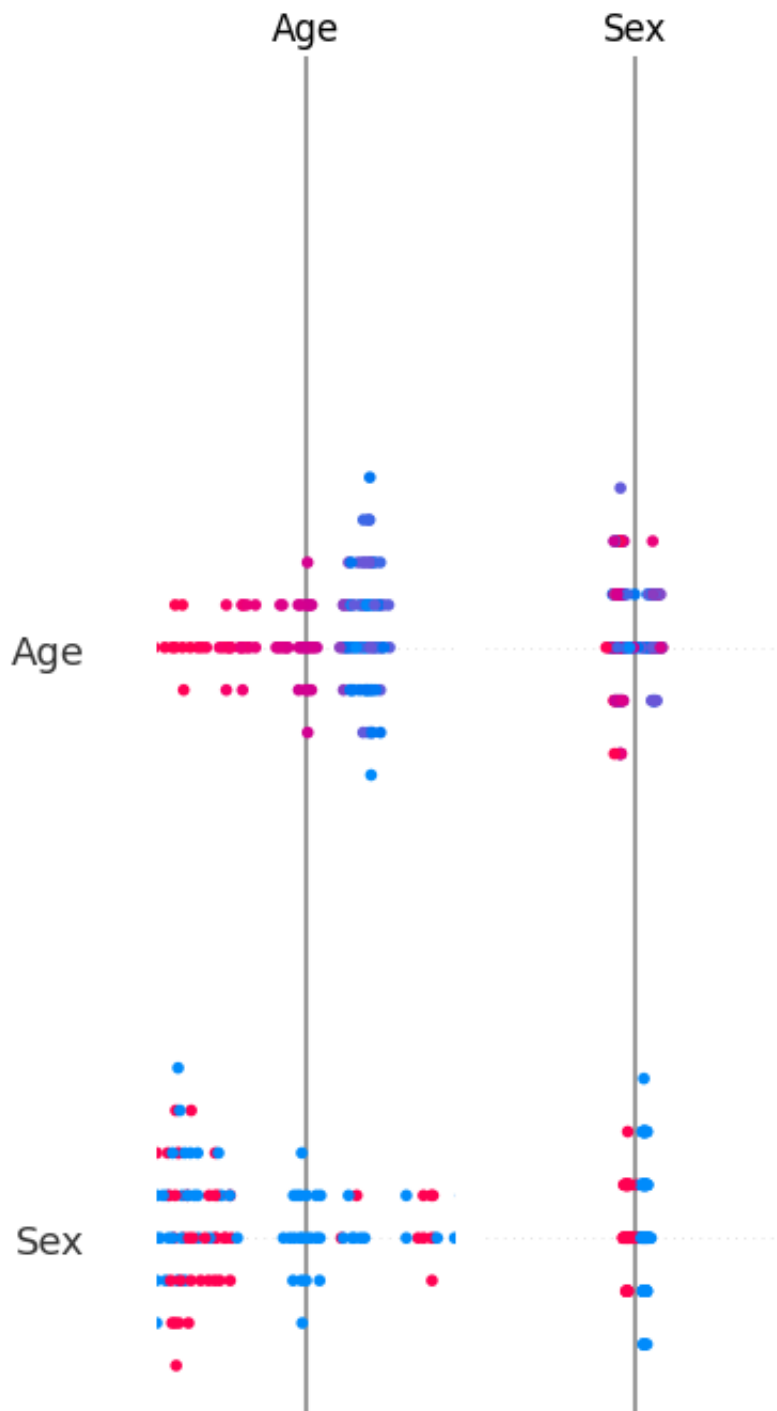
Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

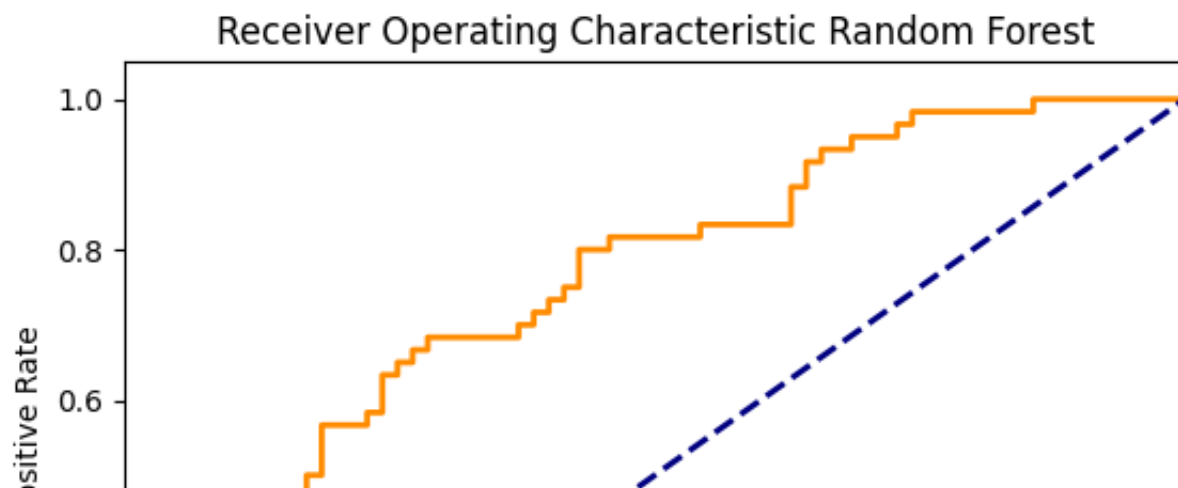
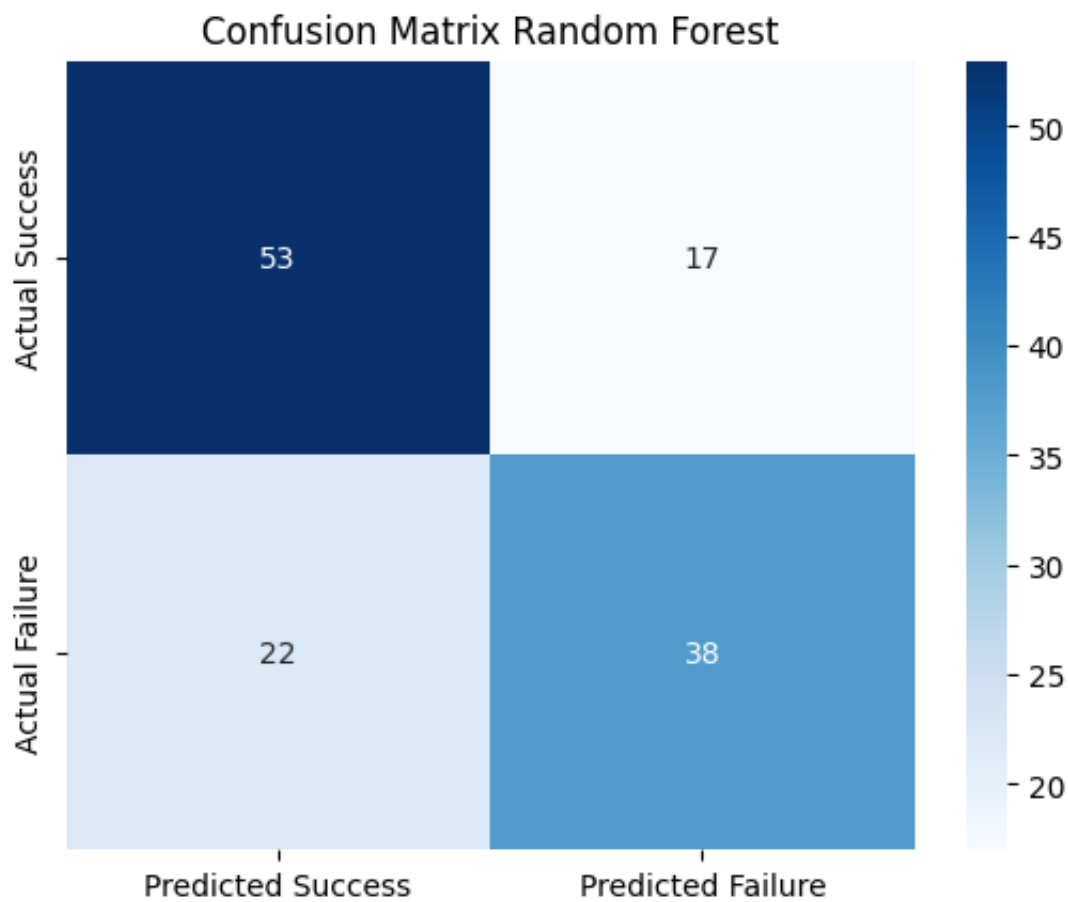
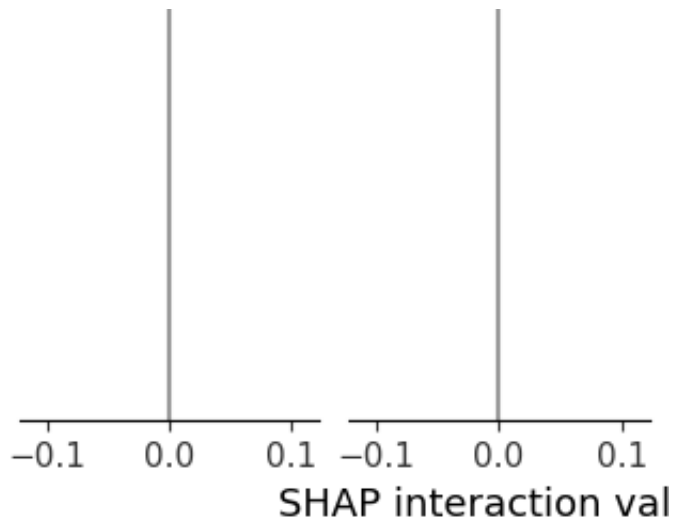
Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

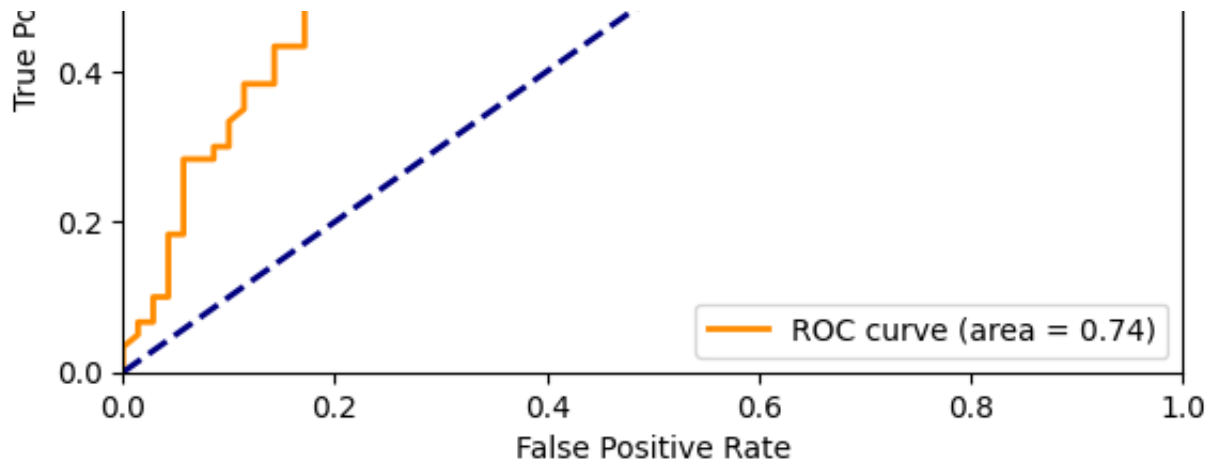
Threshold: 0.25, Metrics: {'Accuracy': 0.4846153846153846, 'Sensitivity': 1

Threshold: 0.30, Metrics: {'Accuracy': 0.5153846153846153, 'Sensitivity': 1

```
Threshold: 0.35, Metrics: {'Accuracy': 0.5692307692307692, 'Sensitivity': 0
Threshold: 0.40, Metrics: {'Accuracy': 0.6, 'Sensitivity': 0.9333333333333333
Threshold: 0.45, Metrics: {'Accuracy': 0.6461538461538462, 'Sensitivity': 0
Threshold: 0.50, Metrics: {'Accuracy': 0.6538461538461539, 'Sensitivity': 0
Threshold: 0.55, Metrics: {'Accuracy': 0.7, 'Sensitivity': 0.6333333333333333
Threshold: 0.60, Metrics: {'Accuracy': 0.6615384615384615, 'Sensitivity': 0
Threshold: 0.65, Metrics: {'Accuracy': 0.6307692307692307, 'Sensitivity': 0
Threshold: 0.70, Metrics: {'Accuracy': 0.5692307692307692, 'Sensitivity': 0
Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
SHAP Summary for Random Forest
```







Aggregated Test Set Metrics Across Seeds:

	accuracy	sensitivity	specificity	f1	roc_auc
0	0.692308	0.616667	0.757143	0.649123	0.747143
1	0.707692	0.633333	0.771429	0.666667	0.745714
2	0.684615	0.616667	0.742857	0.643478	0.750000
3	0.707692	0.633333	0.771429	0.666667	0.749286
4	0.707692	0.633333	0.771429	0.666667	0.747381
5	0.684615	0.600000	0.757143	0.637168	0.744048
6	0.692308	0.633333	0.742857	0.655172	0.742857
7	0.684615	0.600000	0.757143	0.637168	0.745476
8	0.676923	0.600000	0.742857	0.631579	0.745000
9	0.700000	0.633333	0.757143	0.660870	0.740238

Summary of Test Set Metrics (Mean, Standard Error, 95% Confidence Interval)

Accuracy: Mean = 0.694, SE = 0.004, 95% CI = [0.686, 0.702]

Sensitivity: Mean = 0.620, SE = 0.005, 95% CI = [0.609, 0.631]

Specificity: Mean = 0.757, SE = 0.004, 95% CI = [0.749, 0.765]

F1: Mean = 0.651, SE = 0.004, 95% CI = [0.642, 0.661]

Roc\_auc: Mean = 0.746, SE = 0.001, 95% CI = [0.744, 0.748]

```
def evaluate_model(model, name, grid, X_train, y_train, X_test, y_test, cv, scc
    print(f"Evaluating {name}...")

    inner_cv = StratifiedKfold(n_splits=5, shuffle=True, random_state=seed)
    outer_cv = StratifiedKfold(n_splits=5, shuffle=True, random_state=seed)

    clf = GridSearchCV(model, grid, cv=inner_cv, scoring='roc_auc')
    nested_scores = cross_validate(clf, X=X_train, y=y_train, cv=outer_cv, scor

    clf.fit(X_train, y_train)
    best_model = clf.best_estimator_
    best_params = clf.best_params_

    print(f"Best parameters for {name}: {best_params}") # Print the best param

    calibrated_clf = CalibratedClassifierCV(estimator=best_model, method='sigmc
```

```

calibrated_clf.fit(X_train, y_train)

y_probs = calibrated_clf.predict_proba(X_test)[:, 1]

# Calcular FPR, TPR e AUC
fpr, tpr, thresholds = roc_curve(y_test, y_probs)
roc_auc = auc(fpr, tpr)

# Imprimir os valores de FPR, TPR e AUC de forma fácil de copiar
print("\n--- Dados ROC para copiar ---")
print("FPR =", fpr.tolist())
print("TPR =", tpr.tolist())
print("AUC =", roc_auc)
print("--- Fim dos Dados ROC ---\n")

# Calculate metrics for the training set
y_train_pred = best_model.predict(X_train)
y_train_probs = best_model.predict_proba(X_train)[:, 1]
train_acc = accuracy_score(y_train, y_train_pred)
train_sens = sensitivity(y_train, y_train_pred)
train_spec = specificity(y_train, y_train_pred)
train_f1 = f1_score(y_train, y_train_pred)
train_roc_auc = roc_auc_score(y_train, y_train_probs)

# Print training set metrics
print(f"Training - Accuracy: {train_acc}, Sensitivity: {train_sens}, Specif

# Metrics for the manually set threshold
y_pred_manual = (y_probs >= manual_threshold).astype(int)
manual_acc = accuracy_score(y_test, y_pred_manual)
manual_sens = sensitivity(y_test, y_pred_manual)
manual_spec = specificity(y_test, y_pred_manual)
manual_f1 = f1_score(y_test, y_pred_manual)
manual_roc_auc = roc_auc_score(y_test, y_probs)

print(f"Metrics for manual threshold {manual_threshold}:")
print(f"Accuracy: {manual_acc}, Sensitivity: {manual_sens}, Specificity: {r

threshold_metrics = {}
for threshold in threshold_list:
    y_pred_threshold = (y_probs >= threshold).astype(int)
    threshold_acc = accuracy_score(y_test, y_pred_threshold)
    threshold_sens = sensitivity(y_test, y_pred_threshold)
    threshold_spec = specificity(y_test, y_pred_threshold)
    threshold_f1 = f1_score(y_test, y_pred_threshold)
    threshold_metrics[threshold] = {'Accuracy': threshold_acc, 'Sensitivity

for threshold, metrics in threshold_metrics.items():

```



```

    print(f"Threshold: {threshold:.2f}, Metrics: {metrics}")

calculate_and_plot_shap(best_model, X_train, X_test, name)

# Prepare dictionary of test metrics for aggregation
test_metrics = {
    "accuracy": manual_acc,
    "sensitivity": manual_sens,
    "specificity": manual_spec,
    "f1": manual_f1,
    "roc_auc": manual_roc_auc
}

return best_model, manual_threshold, best_params, nested_scores, calibrated

def calculate_and_plot_shap(model, X_train, X_test, model_name):
    if isinstance(model, (XGBClassifier)):
        explainer = shap.TreeExplainer(model)
    else:
        explainer = shap.KernelExplainer(model.predict_proba, X_train.sample(10))
    shap_values = explainer.shap_values(X_test)
    print(f"SHAP Summary for {model_name}")
    shap.summary_plot(shap_values, X_test, max_display=10)

# Plotting functions for confusion matrix and ROC curve visualization.
def plot_confusion_matrix(y_true, y_pred):
    matrix = confusion_matrix(y_true, y_pred)
    sns.heatmap(matrix, annot=True, fmt='d', cmap='Blues', xticklabels=['Predic
plt.title('Confusion Matrix XGBoosting')
plt.show()

def plot_roc_curve(y_true, y_probs):
    fpr, tpr, thresholds = roc_curve(y_true, y_probs)
    roc_auc = auc(fpr, tpr)

    plt.figure()
    plt.plot(fpr, tpr, color='darkorange', lw=2, label=f'ROC curve (area = {roc
    plt.plot([0, 1], [0, 1], color='navy', lw=2, linestyle='--')
    plt.xlim([0.0, 1.0])
    plt.ylim([0.0, 1.05])
    plt.xlabel('False Positive Rate')
    plt.ylabel('True Positive Rate')
    plt.title('Receiver Operating Characteristic XGBoosting')
    plt.legend(loc="lower right")
    plt.show()

def evaluate_xgboost(X_train, y_train, X_test, y_test, cv, scoring, manual_thre
    print("Inside evaluate_xgboost function")

```

```

model = XGBClassifier(eval_metric='logloss', random_state=seed)
grid = {
    'max_depth': [6],
    'gamma': [0.1],
    'learning_rate': [0.01],
    'subsample': [0.8],
    'colsample_bytree': [1],
    'reg_alpha': [0],
    'reg_lambda': [1],
    'n_estimators': [300]
}

return evaluate_model(model, "XGBoost", grid, X_train, y_train, X_test, y_t

def main(X_train, y_train, X_test, y_test):
    cv = RepeatedStratifiedKFold(n_splits=10, n_repeats=10, random_state=42)
    scoring = {
        'accuracy': make_scorer(accuracy_score),
        'sensitivity': make_scorer(sensitivity),
        'specificity': make_scorer(specificity),
        'f1': make_scorer(f1_score),
        'roc_auc': make_scorer(roc_auc_score)
    }
    manual_threshold = 0.5
    threshold_list = np.arange(0.1, 1.05, 0.05)

    aggregated_metrics = []

    for seed in range(40, 50):
        print(f"Running evaluation with seed {seed}")
        best_model, manual_threshold, best_params, nested_scores, calibrated_clf,
        X_train, y_train, X_test, y_test, cv, scoring, manual_threshold, th
        )

        # Use calibrated_clf for prediction probabilities
        y_probs = calibrated_clf.predict_proba(X_test)[: , 1]
        y_pred_manual = (y_probs >= manual_threshold).astype(int)

        # Plotting functions assuming they are imported or defined elsewhere
        plot_confusion_matrix(y_test, y_pred_manual)
        plot_roc_curve(y_test, y_probs)

        aggregated_metrics.append(test_metrics)

    # Aggregate results across seeds
    results_df = pd.DataFrame(aggregated_metrics)
    n = len(results_df)
    print("\nAggregated Test Set Metrics Across Seeds:")

```

```

print(results_df)

# Compute mean, standard error, and 95% confidence interval for each metric
def summarize_metric(metric_values):
    mean_val = metric_values.mean()
    std_val = metric_values.std(ddof=1)
    se = std_val / np.sqrt(n)
    t_crit = stats.t.ppf(0.975, df=n - 1)
    ci_lower = mean_val - t_crit * se
    ci_upper = mean_val + t_crit * se
    return mean_val, se, (ci_lower, ci_upper)

metrics_summary = {}
for metric in results_df.columns:
    mean_val, se, ci = summarize_metric(results_df[metric])
    metrics_summary[metric] = {
        "Mean": mean_val,
        "Standard Error": se,
        "95% CI": ci
    }

print("\nSummary of Test Set Metrics (Mean, Standard Error, 95% Confidence
for metric, summary in metrics_summary.items():
    print(f"{metric.capitalize()}: Mean = {summary['Mean']:.3f}, SE = {sumr
          f"95% CI = [{summary['95% CI'][0]:.3f}, {summary['95% CI'][1]:.3f

if __name__ == '__main__':
    main(X_train, y_train, X_test, y_test)

```



```

Running evaluation with seed 40
Inside evaluate_xgboost function
Evaluating XGBoost...
Best parameters for XGBoost: {'colsample_bytree': 1, 'gamma': 0.1, 'learning_rate': 0.1}

--- Dados ROC para copiar ---
FPR = [0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.028571428571428571, 0.04285714285714285, 0.05714285714285714, 0.07142857142857143, 0.08571428571428571, 0.1, 0.11428571428571429, 0.12857142857142858, 0.14285714285714287, 0.15714285714285715, 0.17142857142857143, 0.1857142857142857, 0.2, 0.21428571428571429, 0.22857142857142858, 0.24285714285714287, 0.25714285714285715, 0.27142857142857143, 0.2857142857142857, 0.3, 0.31428571428571429, 0.32857142857142858, 0.34285714285714287, 0.35714285714285715, 0.37142857142857143, 0.3857142857142857, 0.4, 0.41428571428571429, 0.42857142857142858, 0.44285714285714287, 0.45714285714285715, 0.47142857142857143, 0.4857142857142857, 0.5, 0.51428571428571429, 0.52857142857142858, 0.54285714285714287, 0.55714285714285715, 0.57142857142857143, 0.5857142857142857, 0.6, 0.61428571428571429, 0.62857142857142858, 0.64285714285714287, 0.65714285714285715, 0.67142857142857143, 0.6857142857142857, 0.7, 0.71428571428571429, 0.72857142857142858, 0.74285714285714287, 0.75714285714285715, 0.77142857142857143, 0.7857142857142857, 0.8, 0.81428571428571429, 0.82857142857142858, 0.84285714285714287, 0.85714285714285715, 0.87142857142857143, 0.8857142857142857, 0.9, 0.91428571428571429, 0.92857142857142858, 0.94285714285714287, 0.95714285714285715, 0.97142857142857143, 0.9857142857142857, 1.0]
TPR = [0.0, 0.016666666666666666, 0.03333333333333333, 0.05, 0.06666666666666666, 0.08333333333333333, 0.1, 0.11666666666666666, 0.13333333333333333, 0.15, 0.16666666666666666, 0.18333333333333333, 0.2, 0.21666666666666666, 0.23333333333333333, 0.25, 0.26666666666666666, 0.28333333333333333, 0.3, 0.31666666666666666, 0.33333333333333333, 0.35, 0.36666666666666666, 0.38333333333333333, 0.4, 0.41666666666666666, 0.43333333333333333, 0.45, 0.46666666666666666, 0.48333333333333333, 0.5, 0.51666666666666666, 0.53333333333333333, 0.55, 0.56666666666666666, 0.58333333333333333, 0.6, 0.61666666666666666, 0.63333333333333333, 0.65, 0.66666666666666666, 0.68333333333333333, 0.7, 0.71666666666666666, 0.73333333333333333, 0.75, 0.76666666666666666, 0.78333333333333333, 0.8, 0.81666666666666666, 0.83333333333333333, 0.85, 0.86666666666666666, 0.88333333333333333, 0.9, 0.91666666666666666, 0.93333333333333333, 0.95, 0.96666666666666666, 0.98333333333333333, 1.0]
AUC = 0.7540476190476191

--- Fim dos Dados ROC ---

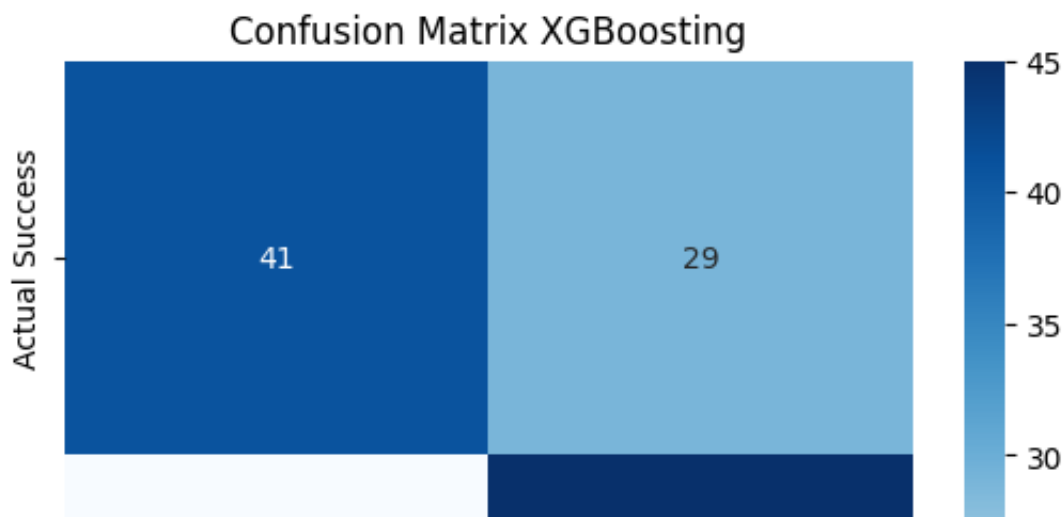
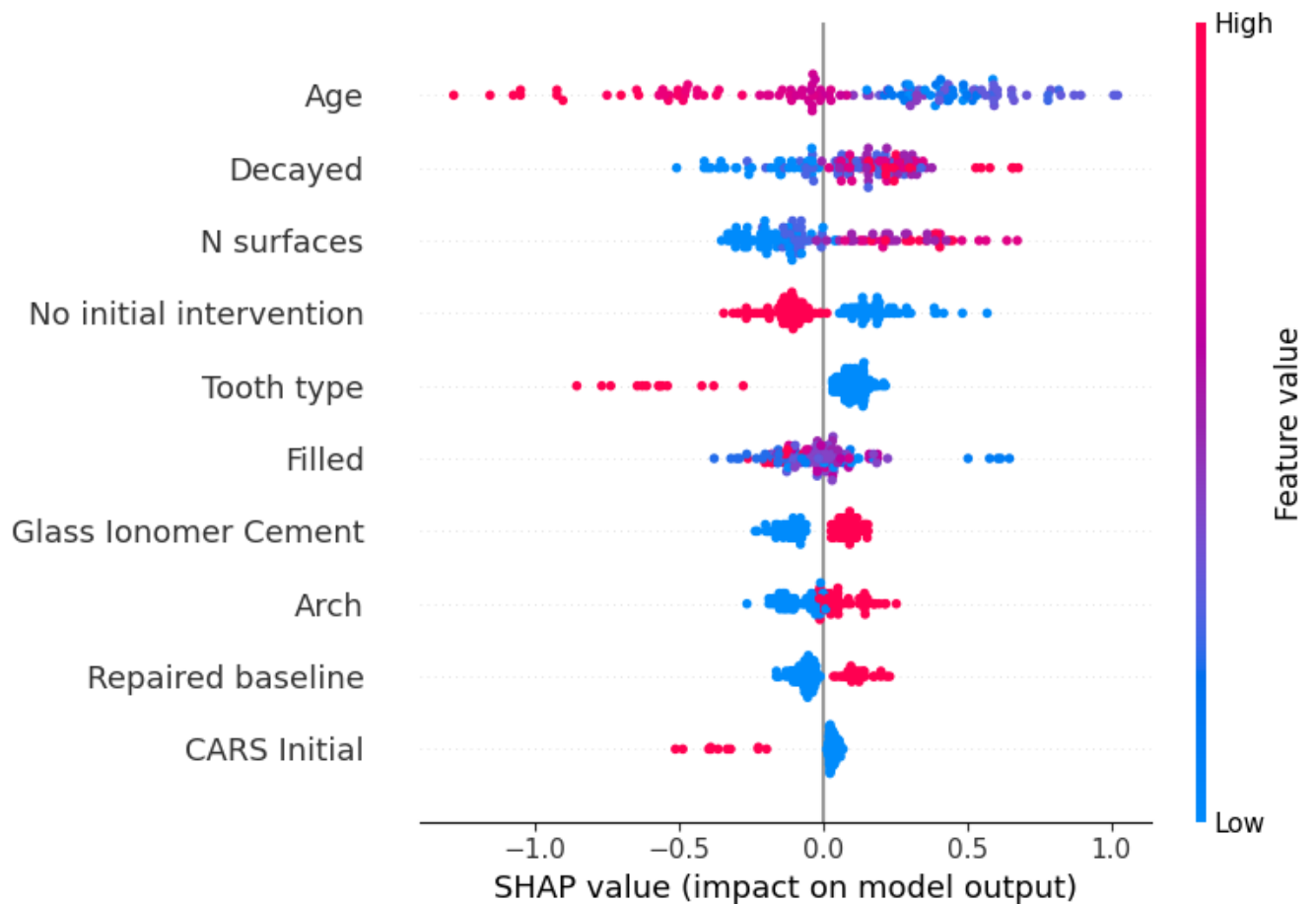
Training - Accuracy: 0.8678500986193294, Sensitivity: 0.8804780876494024, Specificity: 0.5857142857142857
Metrics for manual threshold 0.5:
Accuracy: 0.6615384615384615, Sensitivity: 0.75, Specificity: 0.5857142857142857
Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.0, 'Specificity': 1.0}
Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.0, 'Specificity': 1.0}
Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.0, 'Specificity': 1.0}
Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.0, 'Specificity': 1.0}
Threshold: 0.30, Metrics: {'Accuracy': 0.46923076923076923, 'Sensitivity': 0.0, 'Specificity': 1.0}
Threshold: 0.35, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.0, 'Specificity': 1.0}
Threshold: 0.40, Metrics: {'Accuracy': 0.5822076923076923, 'Sensitivity': 0.0, 'Specificity': 1.0}
Threshold: 0.45, Metrics: {'Accuracy': 0.6153846153846154, 'Sensitivity': 0.0, 'Specificity': 1.0}
Threshold: 0.50, Metrics: {'Accuracy': 0.6615384615384615, 'Sensitivity': 0.75, 'Specificity': 0.5857142857142857}
Threshold: 0.55, Metrics: {'Accuracy': 0.7142857142857143, 'Sensitivity': 0.8804780876494024, 'Specificity': 0.5857142857142857}
Threshold: 0.60, Metrics: {'Accuracy': 0.7692307692307692, 'Sensitivity': 0.9166666666666666, 'Specificity': 0.5857142857142857}
Threshold: 0.65, Metrics: {'Accuracy': 0.8153846153846154, 'Sensitivity': 0.95, 'Specificity': 0.5857142857142857}
Threshold: 0.70, Metrics: {'Accuracy': 0.8615384615384615, 'Sensitivity': 0.9833333333333333, 'Specificity': 0.5857142857142857}
Threshold: 0.75, Metrics: {'Accuracy': 0.9, 'Sensitivity': 1.0, 'Specificity': 0.5857142857142857}
Threshold: 0.80, Metrics: {'Accuracy': 0.9384615384615384, 'Sensitivity': 1.0, 'Specificity': 0.5857142857142857}
Threshold: 0.85, Metrics: {'Accuracy': 0.9769230769230769, 'Sensitivity': 1.0, 'Specificity': 0.5857142857142857}
Threshold: 0.90, Metrics: {'Accuracy': 1.0, 'Sensitivity': 1.0, 'Specificity': 0.5857142857142857}
Threshold: 0.95, Metrics: {'Accuracy': 1.0, 'Sensitivity': 1.0, 'Specificity': 0.5857142857142857}
Threshold: 1.0, Metrics: {'Accuracy': 1.0, 'Sensitivity': 1.0, 'Specificity': 0.5857142857142857}

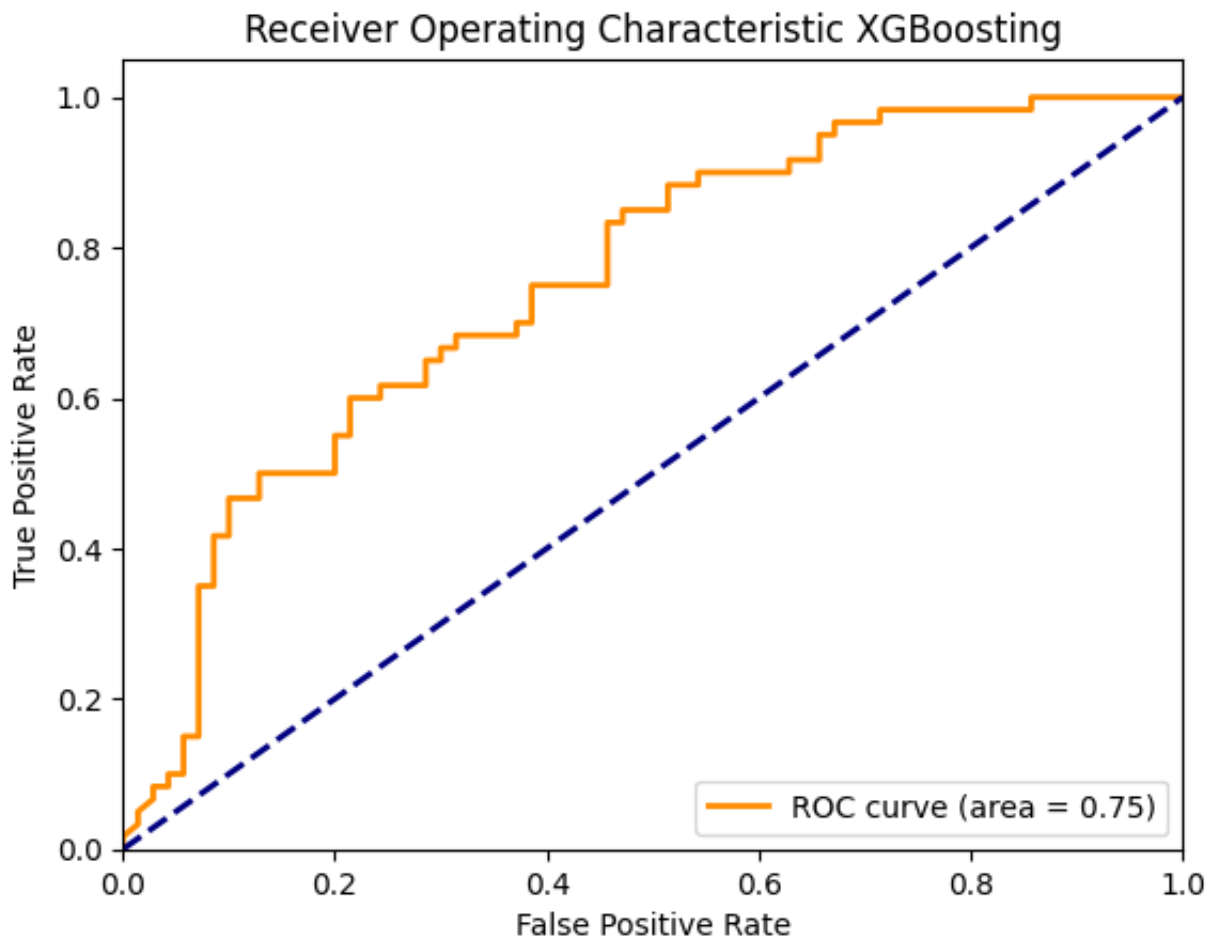
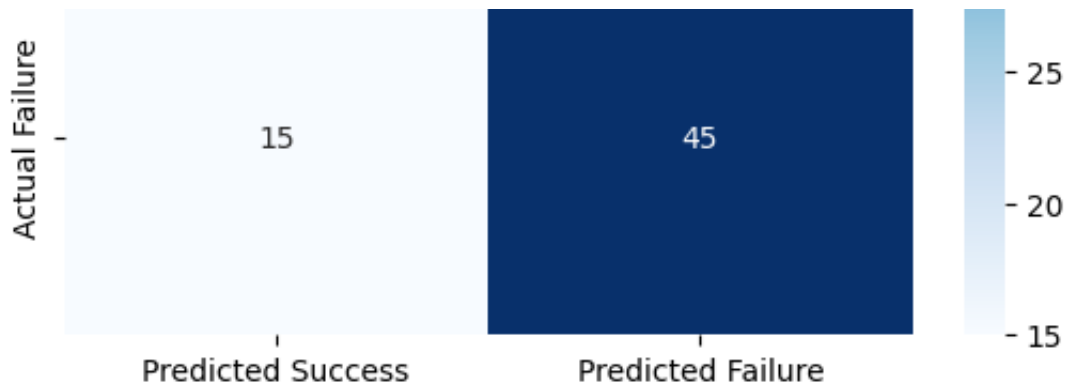
```

```

Threshold: 0.40, Metrics: {'Accuracy': 0.5923076923076923, 'Sensitivity': 0
Threshold: 0.45, Metrics: {'Accuracy': 0.6692307692307692, 'Sensitivity': 0
Threshold: 0.50, Metrics: {'Accuracy': 0.6615384615384615, 'Sensitivity': 0
Threshold: 0.55, Metrics: {'Accuracy': 0.6692307692307692, 'Sensitivity': 0
Threshold: 0.60, Metrics: {'Accuracy': 0.676923076923077, 'Sensitivity': 0.
Threshold: 0.65, Metrics: {'Accuracy': 0.5846153846153846, 'Sensitivity': 0
Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
SHAP Summary for XGBoost

```





Running evaluation with seed 41

Inside evaluate\_xgboost function

Evaluating XGBoost...

Best parameters for XGBoost: {'colsample\_bytree': 1, 'gamma': 0.1, 'learning\_rate': 0.1}

--- Dados ROC para copiar ---

FPR = [0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.028571428571428571,

TPR = [0.0, 0.016666666666666666, 0.03333333333333333, 0.06666666666666667,

AUC = 0.7526190476190475

--- Fim dos Dados ROC ---

Training - Accuracy: 0.8757396449704142, Sensitivity: 0.8804780876494024, Specificity: 0.5857142857142857  
Metrics for manual threshold 0.5:

Accuracy: 0.6615384615384615, Sensitivity: 0.75, Specificity: 0.5857142857142857

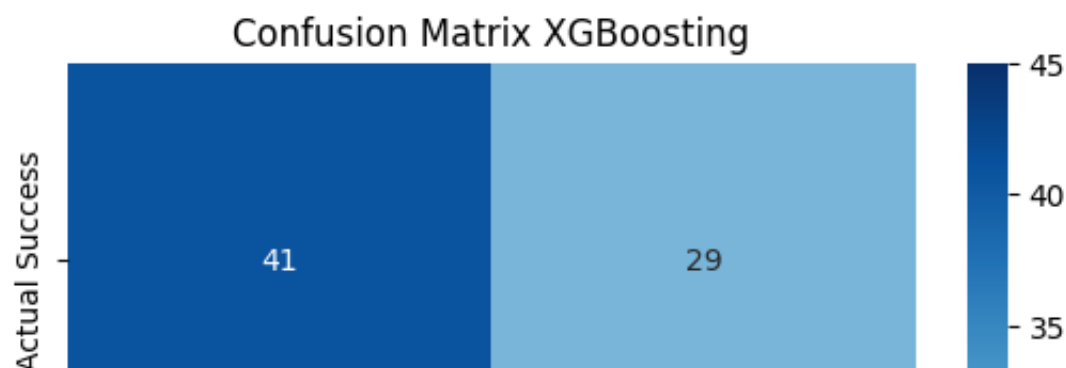
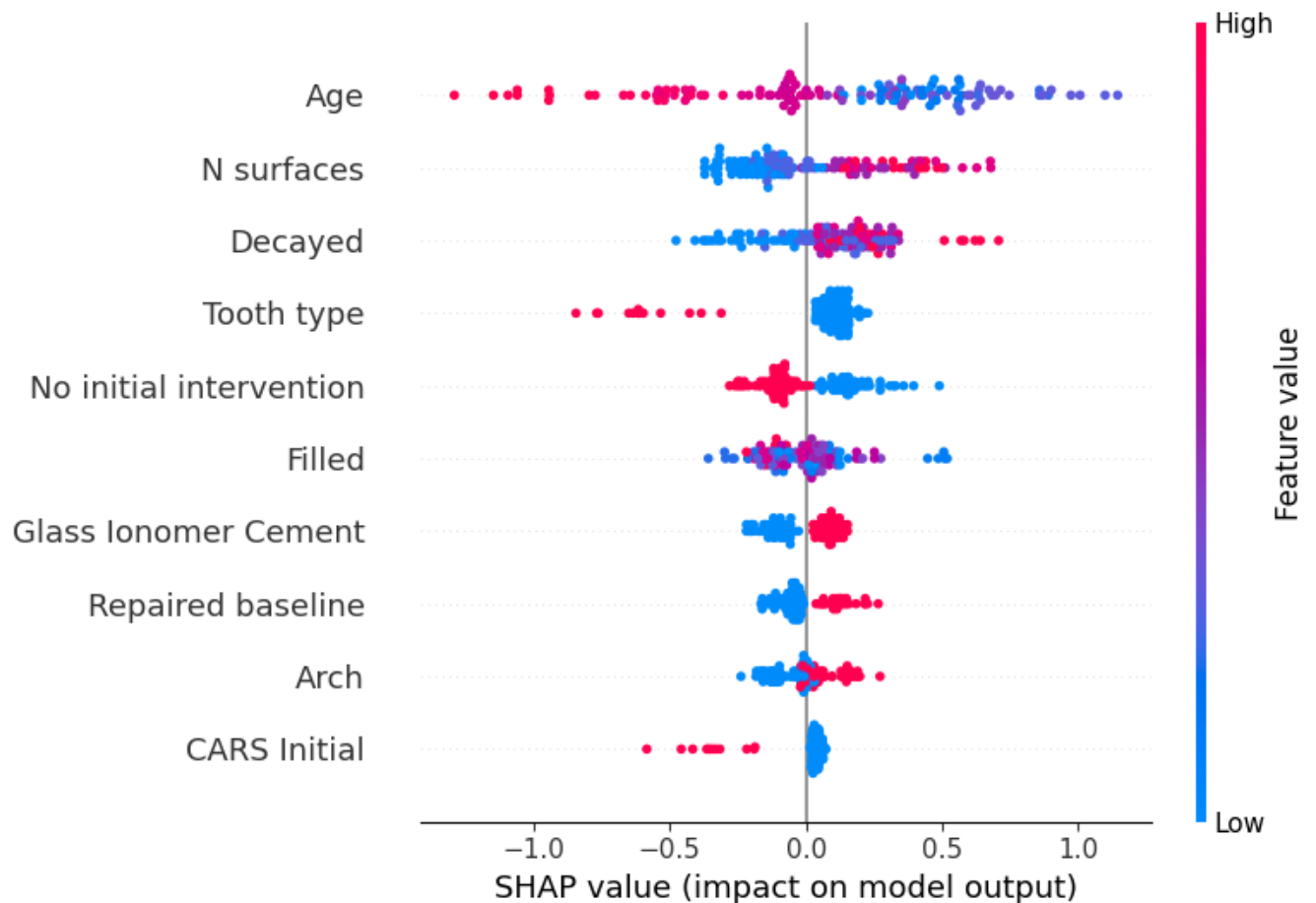
Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.5857142857142857,

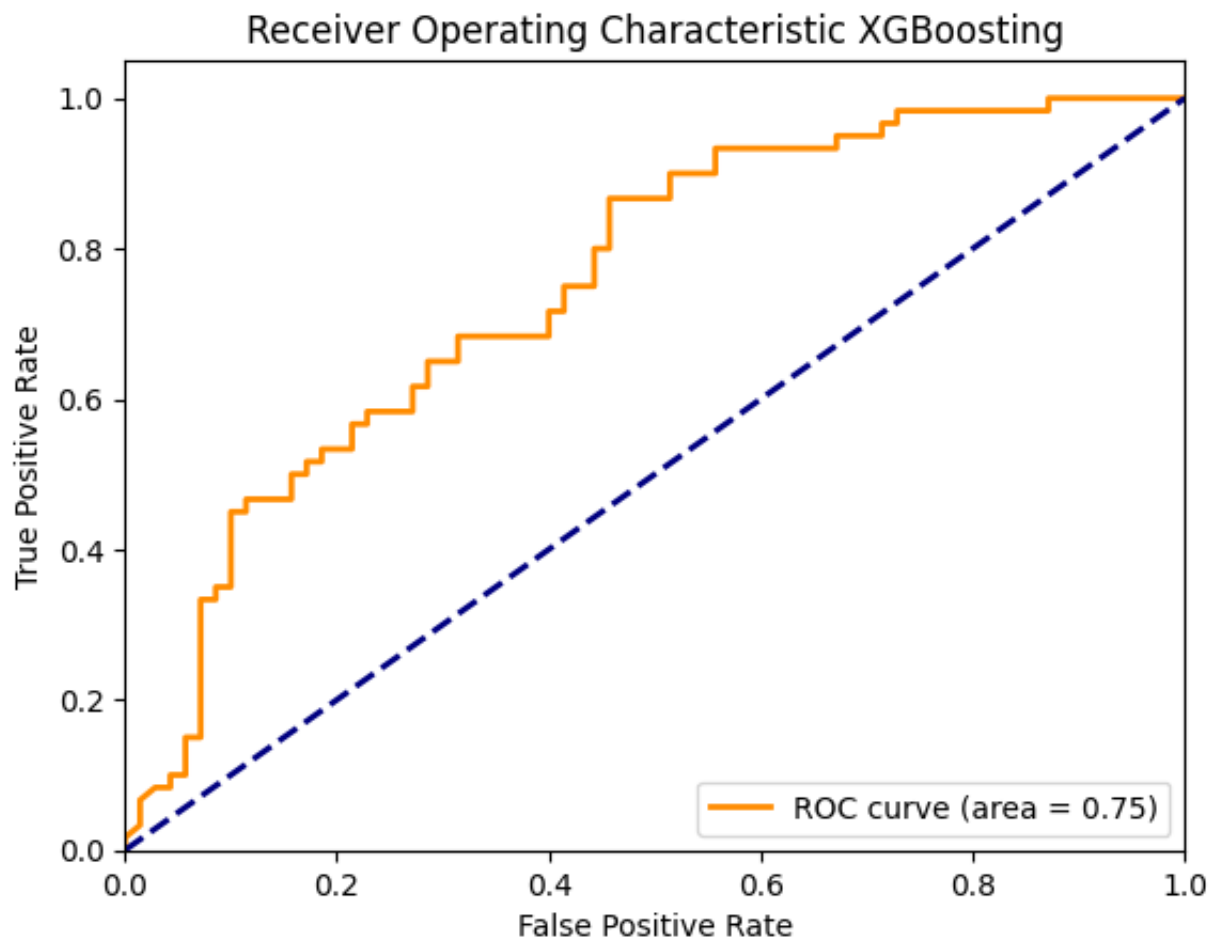
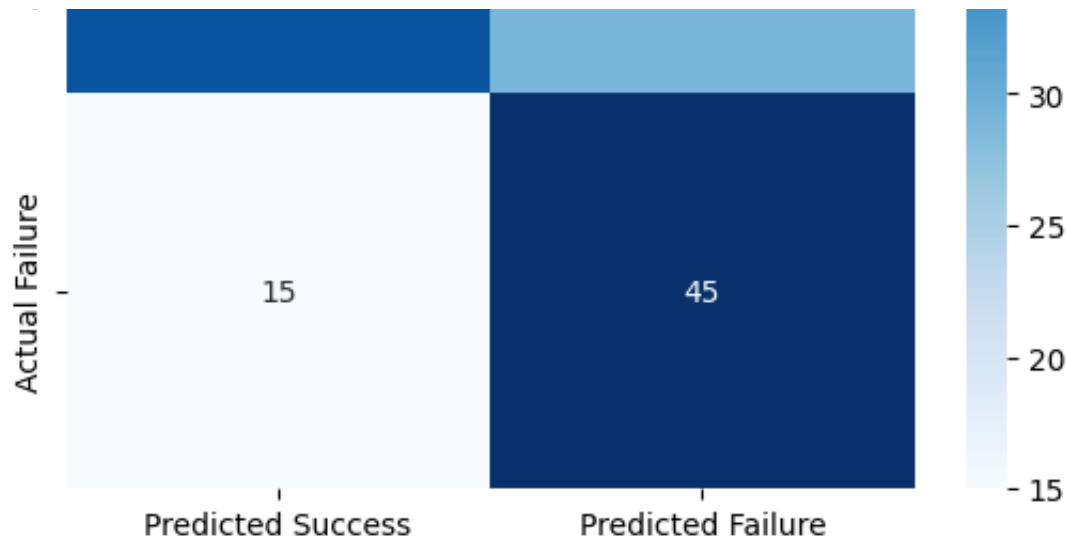
Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.5857142857142857,

```

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':
Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':
Threshold: 0.30, Metrics: {'Accuracy': 0.47692307692307695, 'Sensitivity':
Threshold: 0.35, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.40, Metrics: {'Accuracy': 0.5923076923076923, 'Sensitivity': 0
Threshold: 0.45, Metrics: {'Accuracy': 0.6615384615384615, 'Sensitivity': 0
Threshold: 0.50, Metrics: {'Accuracy': 0.6615384615384615, 'Sensitivity': 0
Threshold: 0.55, Metrics: {'Accuracy': 0.676923076923077, 'Sensitivity': 0.
Threshold: 0.60, Metrics: {'Accuracy': 0.676923076923077, 'Sensitivity': 0.
Threshold: 0.65, Metrics: {'Accuracy': 0.5769230769230769, 'Sensitivity': 0
Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
SHAP Summary for XGBoost

```





Running evaluation with seed 42

Inside evaluate\_xgboost function

Evaluating XGBoost...

Best parameters for XGBoost: {'colsample\_bytree': 1, 'gamma': 0.1, 'learning\_rate': 0.1, 'max\_depth': 6, 'min\_child\_weight': 1, 'n\_estimators': 100, 'objective': 'binary:logistic', 'random\_state': 42, 'subsample': 0.8}

--- Dados ROC para copiar ---

FPR = [0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.02857142857142857, 0.04285714285714285, 0.05714285714285714, 0.07142857142857143, 0.08571428571428571, 0.1, 0.11428571428571428, 0.12857142857142858, 0.14285714285714287, 0.15714285714285715, 0.17142857142857143, 0.1857142857142857, 0.2, 0.21428571428571428, 0.22857142857142858, 0.24285714285714287, 0.25714285714285715, 0.27142857142857143, 0.2857142857142857, 0.3, 0.31428571428571428, 0.32857142857142858, 0.34285714285714287, 0.35714285714285715, 0.37142857142857143, 0.3857142857142857, 0.4, 0.41428571428571428, 0.42857142857142858, 0.44285714285714287, 0.45714285714285715, 0.47142857142857143, 0.4857142857142857, 0.5, 0.51428571428571428, 0.52857142857142858, 0.54285714285714287, 0.55714285714285715, 0.57142857142857143, 0.5857142857142857, 0.6, 0.61428571428571428, 0.62857142857142858, 0.64285714285714287, 0.65714285714285715, 0.67142857142857143, 0.6857142857142857, 0.7, 0.71428571428571428, 0.72857142857142858, 0.74285714285714287, 0.75714285714285715, 0.77142857142857143, 0.7857142857142857, 0.8, 0.81428571428571428, 0.82857142857142858, 0.84285714285714287, 0.85714285714285715, 0.87142857142857143, 0.8857142857142857, 0.9, 0.91428571428571428, 0.92857142857142858, 0.94285714285714287, 0.95714285714285715, 0.97142857142857143, 0.9857142857142857, 1.0]

TPR = [0.0, 0.016666666666666666, 0.03333333333333333, 0.05, 0.06666666666666666, 0.08333333333333333, 0.1, 0.11666666666666666, 0.13333333333333333, 0.15, 0.16666666666666666, 0.18333333333333333, 0.2, 0.21666666666666666, 0.23333333333333333, 0.25, 0.26666666666666666, 0.28333333333333333, 0.3, 0.31666666666666666, 0.33333333333333333, 0.35, 0.36666666666666666, 0.38333333333333333, 0.4, 0.41666666666666666, 0.43333333333333333, 0.45, 0.46666666666666666, 0.48333333333333333, 0.5, 0.51666666666666666, 0.53333333333333333, 0.55, 0.56666666666666666, 0.58333333333333333, 0.6, 0.61666666666666666, 0.63333333333333333, 0.65, 0.66666666666666666, 0.68333333333333333, 0.7, 0.71666666666666666, 0.73333333333333333, 0.75, 0.76666666666666666, 0.78333333333333333, 0.8, 0.81666666666666666, 0.83333333333333333, 0.85, 0.86666666666666666, 0.88333333333333333, 0.9, 0.91666666666666666, 0.93333333333333333, 0.95, 0.96666666666666666, 0.98333333333333333, 1.0]

AUC = 0.7609523809523809

--- Fim dos Dados ROC ---

Training - Accuracy: 0.8658777120315582, Sensitivity: 0.8804780876494024, Specificity: 0.8804780876494024

Metrics for manual threshold 0.5:

Accuracy: 0.6615384615384615, Sensitivity: 0.7333333333333333, Specificity:

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':

Threshold: 0.30, Metrics: {'Accuracy': 0.46923076923076923, 'Sensitivity':

Threshold: 0.35, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.40, Metrics: {'Accuracy': 0.5923076923076923, 'Sensitivity': 0

Threshold: 0.45, Metrics: {'Accuracy': 0.676923076923077, 'Sensitivity': 0.

Threshold: 0.50, Metrics: {'Accuracy': 0.6615384615384615, 'Sensitivity': 0

Threshold: 0.55, Metrics: {'Accuracy': 0.6692307692307692, 'Sensitivity': 0

Threshold: 0.60, Metrics: {'Accuracy': 0.676923076923077, 'Sensitivity': 0.

Threshold: 0.65, Metrics: {'Accuracy': 0.5769230769230769, 'Sensitivity': 0

Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

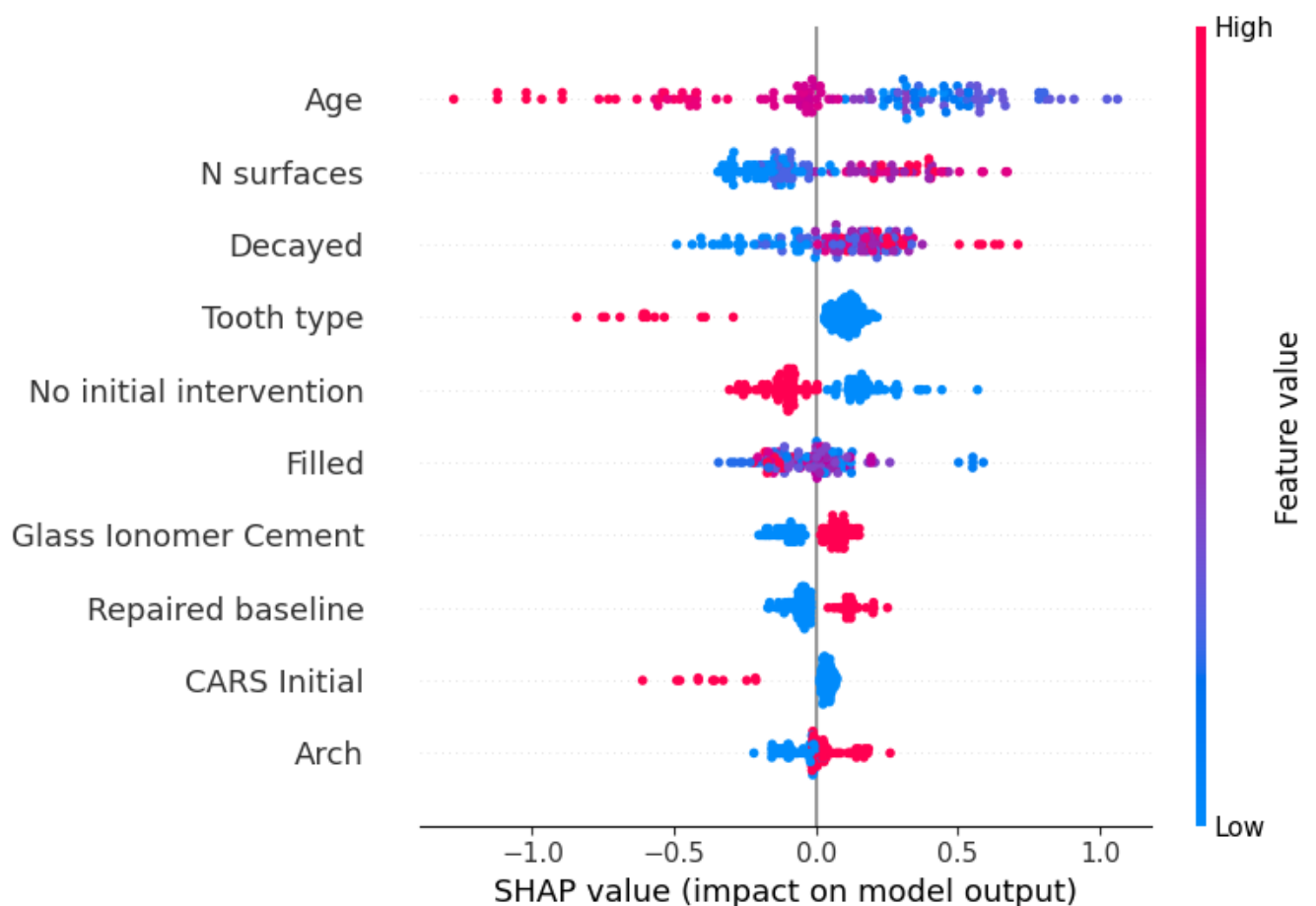
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

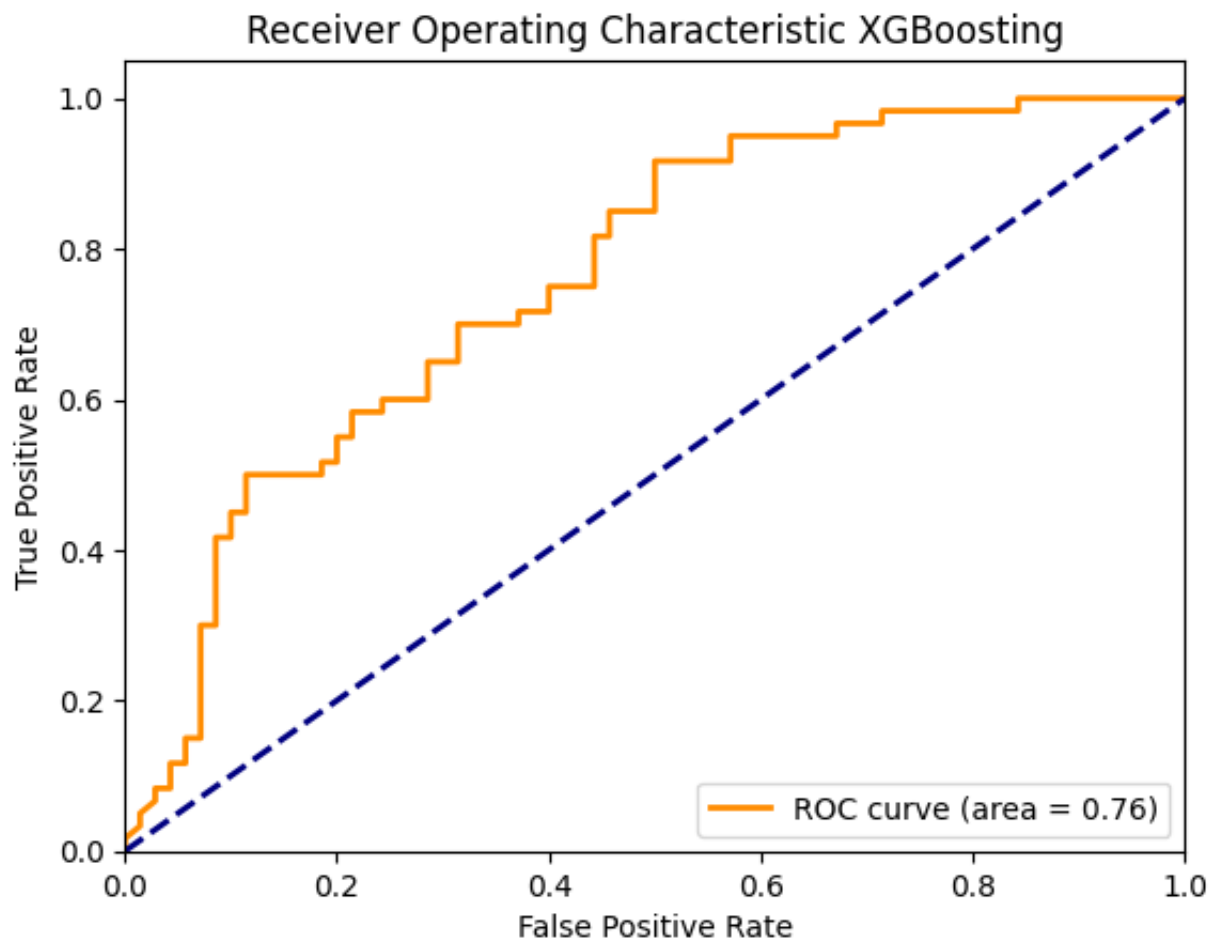
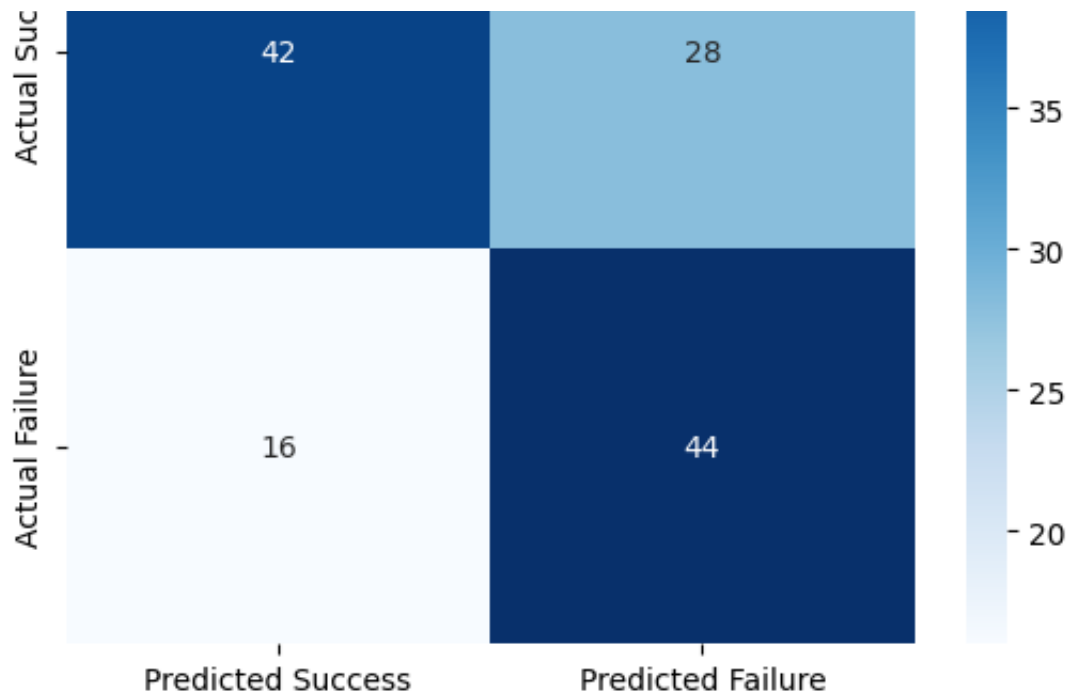
SHAP Summary for XGBoost



Confusion Matrix XGBoosting







Running evaluation with seed 43

Inside evaluate\_xgboost function

Evaluating XGBoost...

Best parameters for XGBoost: {'colsample\_bytree': 1, 'gamma': 0.1, 'learning\_rate': 0.1, 'max\_depth': 6, 'min\_child\_weight': 1, 'n\_estimators': 100, 'objective': 'binary:logistic', 'random\_state': 43, 'subsample': 0.8}

--- Dados ROC para copiar ---

FPR = [0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.02857142857142857, 0.04285714285714285, 0.05714285714285714, 0.07142857142857143, 0.08571428571428571, 0.1, 0.11428571428571428, 0.12857142857142858, 0.14285714285714285, 0.15714285714285715, 0.17142857142857143, 0.1857142857142857, 0.2, 0.21428571428571428, 0.22857142857142858, 0.24285714285714285, 0.25714285714285715, 0.27142857142857143, 0.2857142857142857, 0.3, 0.31428571428571428, 0.32857142857142858, 0.34285714285714285, 0.35714285714285715, 0.37142857142857143, 0.3857142857142857, 0.4, 0.41428571428571428, 0.42857142857142858, 0.44285714285714285, 0.45714285714285715, 0.47142857142857143, 0.4857142857142857, 0.5, 0.51428571428571428, 0.52857142857142858, 0.54285714285714285, 0.55714285714285715, 0.57142857142857143, 0.5857142857142857, 0.6, 0.61428571428571428, 0.62857142857142858, 0.64285714285714285, 0.65714285714285715, 0.67142857142857143, 0.6857142857142857, 0.7, 0.71428571428571428, 0.72857142857142858, 0.74285714285714285, 0.75714285714285715, 0.77142857142857143, 0.7857142857142857, 0.8, 0.81428571428571428, 0.82857142857142858, 0.84285714285714285, 0.85714285714285715, 0.87142857142857143, 0.8857142857142857, 0.9, 0.91428571428571428, 0.92857142857142858, 0.94285714285714285, 0.95714285714285715, 0.97142857142857143, 0.9857142857142857, 1.0]

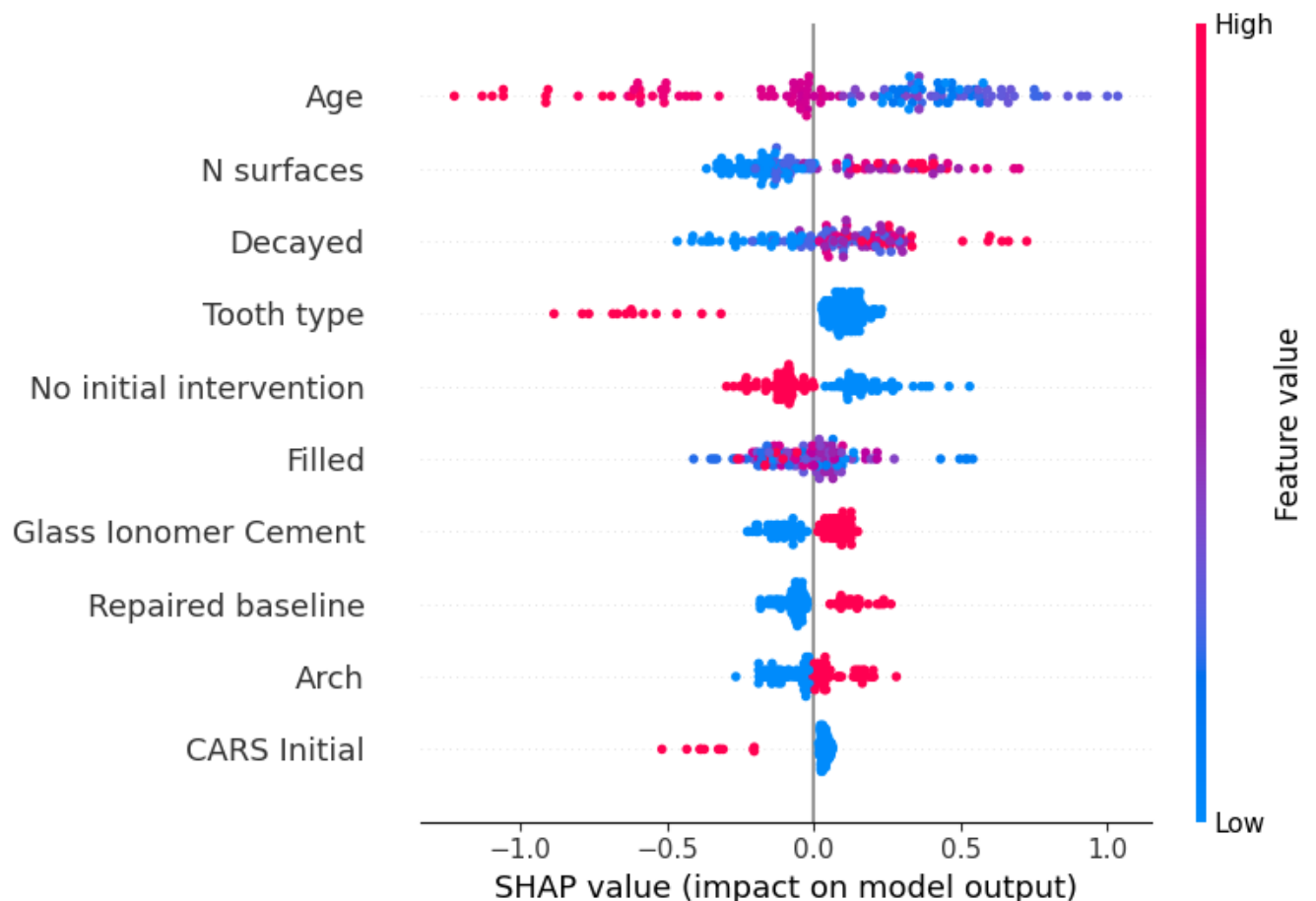
TPR = [0.0, 0.016666666666666666, 0.03333333333333333, 0.05, 0.06666666666666666, 0.08333333333333333, 0.1, 0.11666666666666666, 0.13333333333333333, 0.15, 0.16666666666666666, 0.18333333333333333, 0.2, 0.21666666666666666, 0.23333333333333333, 0.25, 0.26666666666666666, 0.28333333333333333, 0.3, 0.31666666666666666, 0.33333333333333333, 0.35, 0.36666666666666666, 0.38333333333333333, 0.4, 0.41666666666666666, 0.43333333333333333, 0.45, 0.46666666666666666, 0.48333333333333333, 0.5, 0.51666666666666666, 0.53333333333333333, 0.55, 0.56666666666666666, 0.58333333333333333, 0.6, 0.61666666666666666, 0.63333333333333333, 0.65, 0.66666666666666666, 0.68333333333333333, 0.7, 0.71666666666666666, 0.73333333333333333, 0.75, 0.76666666666666666, 0.78333333333333333, 0.8, 0.81666666666666666, 0.83333333333333333, 0.85, 0.86666666666666666, 0.88333333333333333, 0.9, 0.91666666666666666, 0.93333333333333333, 0.95, 0.96666666666666666, 0.98333333333333333, 1.0]

AUC = 0.7635714285714285  
 --- Fim dos Dados ROC ---

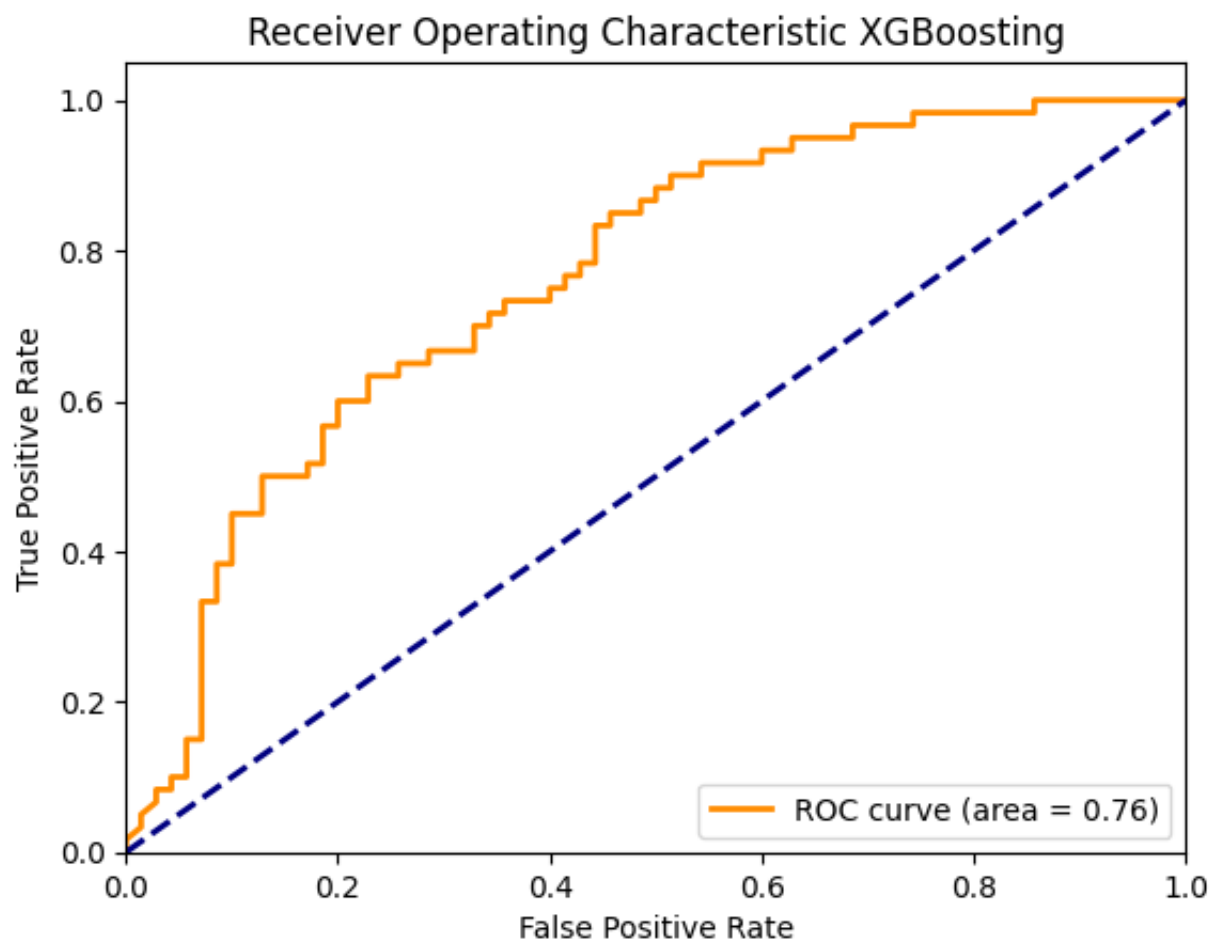
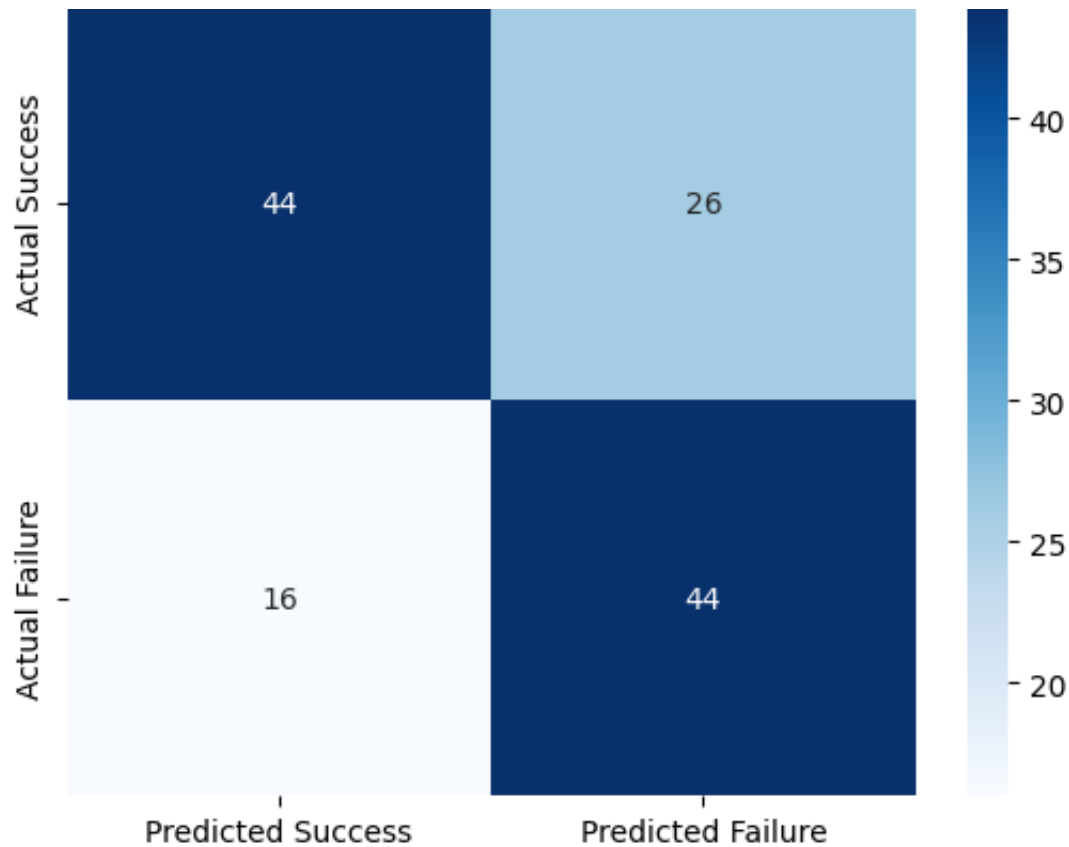
Training - Accuracy: 0.8619329388560157, Sensitivity: 0.8725099601593626, S  
 Metrics for manual threshold 0.5:

Accuracy: 0.676923076923077, Sensitivity: 0.7333333333333333, Specificity:  
 Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':  
 Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':  
 Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':  
 Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':  
 Threshold: 0.30, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':  
 Threshold: 0.35, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
 Threshold: 0.40, Metrics: {'Accuracy': 0.5923076923076923, 'Sensitivity': 0  
 Threshold: 0.45, Metrics: {'Accuracy': 0.676923076923077, 'Sensitivity': 0.  
 Threshold: 0.50, Metrics: {'Accuracy': 0.676923076923077, 'Sensitivity': 0.  
 Threshold: 0.55, Metrics: {'Accuracy': 0.7, 'Sensitivity': 0.6166666666666666  
 Threshold: 0.60, Metrics: {'Accuracy': 0.6923076923076923, 'Sensitivity': 0  
 Threshold: 0.65, Metrics: {'Accuracy': 0.5769230769230769, 'Sensitivity': 0  
 Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
 Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
 Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
 Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
 Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
 Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0  
 Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0

SHAP Summary for XGBoost



Confusion Matrix XGBoosting



```
Running evaluation with seed 44
Inside evaluate_xgboost function
Evaluating XGBoost...
```

```
Best parameters for XGBoost: {'colsample_bytree': 1, 'gamma': 0.1, 'learning_rate': 0.1, 'max_depth': 6, 'min_child_weight': 1, 'n_estimators': 100, 'objective': 'binary:logistic', 'random_state': 44, 'subsample': 1}
```

```
best parameters for xgboost: { colsample_bytree : 1, gamma : 0.1, learning
```

```
--- Dados ROC para copiar ---
```

```
FPR = [0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.028571428571
```

```
TPR = [0.0, 0.016666666666666666, 0.033333333333333333, 0.05, 0.066666666666
```

```
AUC = 0.7573809523809524
```

```
--- Fim dos Dados ROC ---
```

```
Training - Accuracy: 0.863905325443787, Sensitivity: 0.8725099601593626, Sp
Metrics for manual threshold 0.5:
```

```
Accuracy: 0.6692307692307692, Sensitivity: 0.75, Specificity: 0.6, F1: 0.67
```

```
Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':
```

```
Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':
```

```
Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':
```

```
Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':
```

```
Threshold: 0.30, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity':
```

```
Threshold: 0.35, Metrics: {'Accuracy': 0.5307692307692308, 'Sensitivity': 0
```

```
Threshold: 0.40, Metrics: {'Accuracy': 0.5846153846153846, 'Sensitivity': 0
```

```
Threshold: 0.45, Metrics: {'Accuracy': 0.6692307692307692, 'Sensitivity': 0
```

```
Threshold: 0.50, Metrics: {'Accuracy': 0.6692307692307692, 'Sensitivity': 0
```

```
Threshold: 0.55, Metrics: {'Accuracy': 0.676923076923077, 'Sensitivity': 0.
```

```
Threshold: 0.60, Metrics: {'Accuracy': 0.6846153846153846, 'Sensitivity': 0
```

```
Threshold: 0.65, Metrics: {'Accuracy': 0.5615384615384615, 'Sensitivity': 0
```

```
Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
```

```
Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
```

```
Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
```

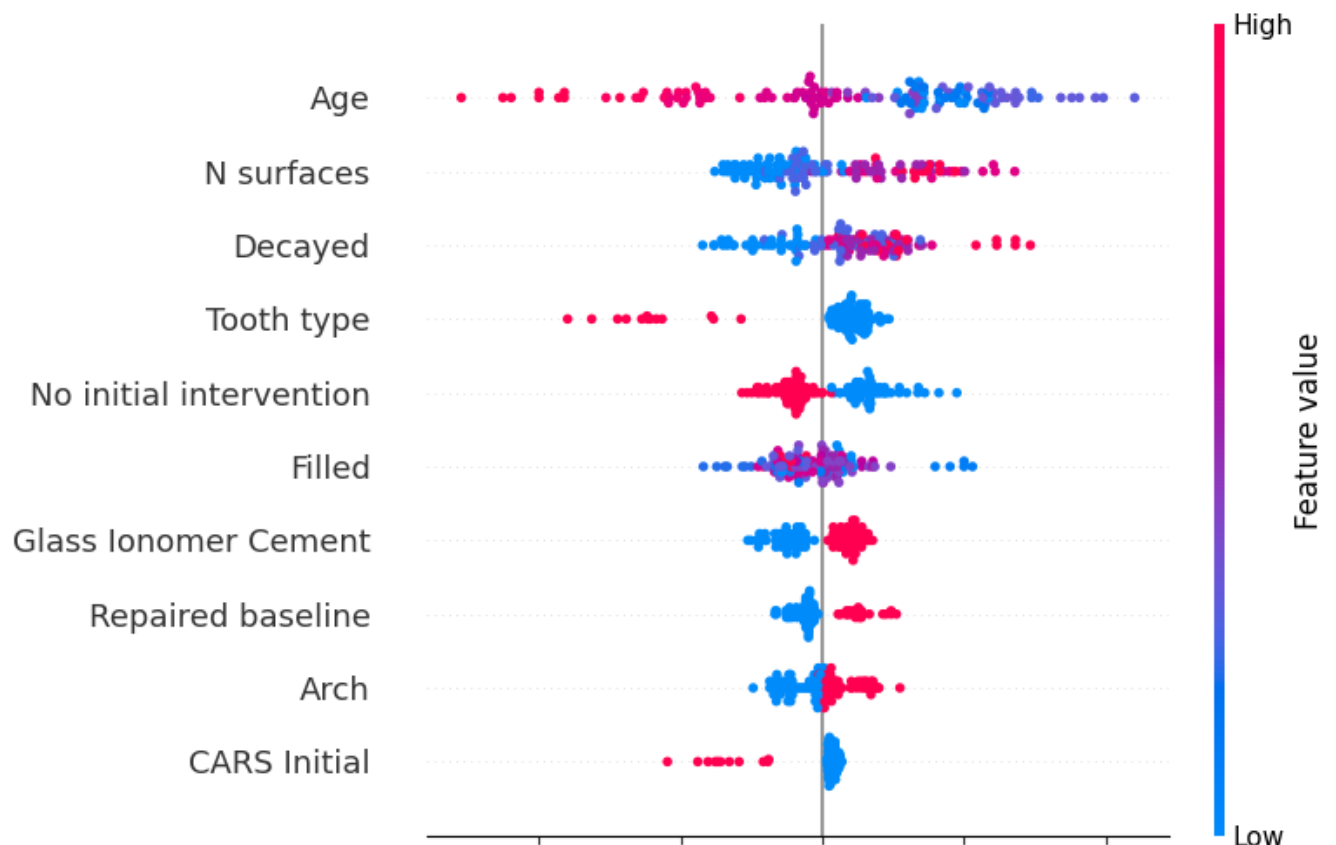
```
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
```

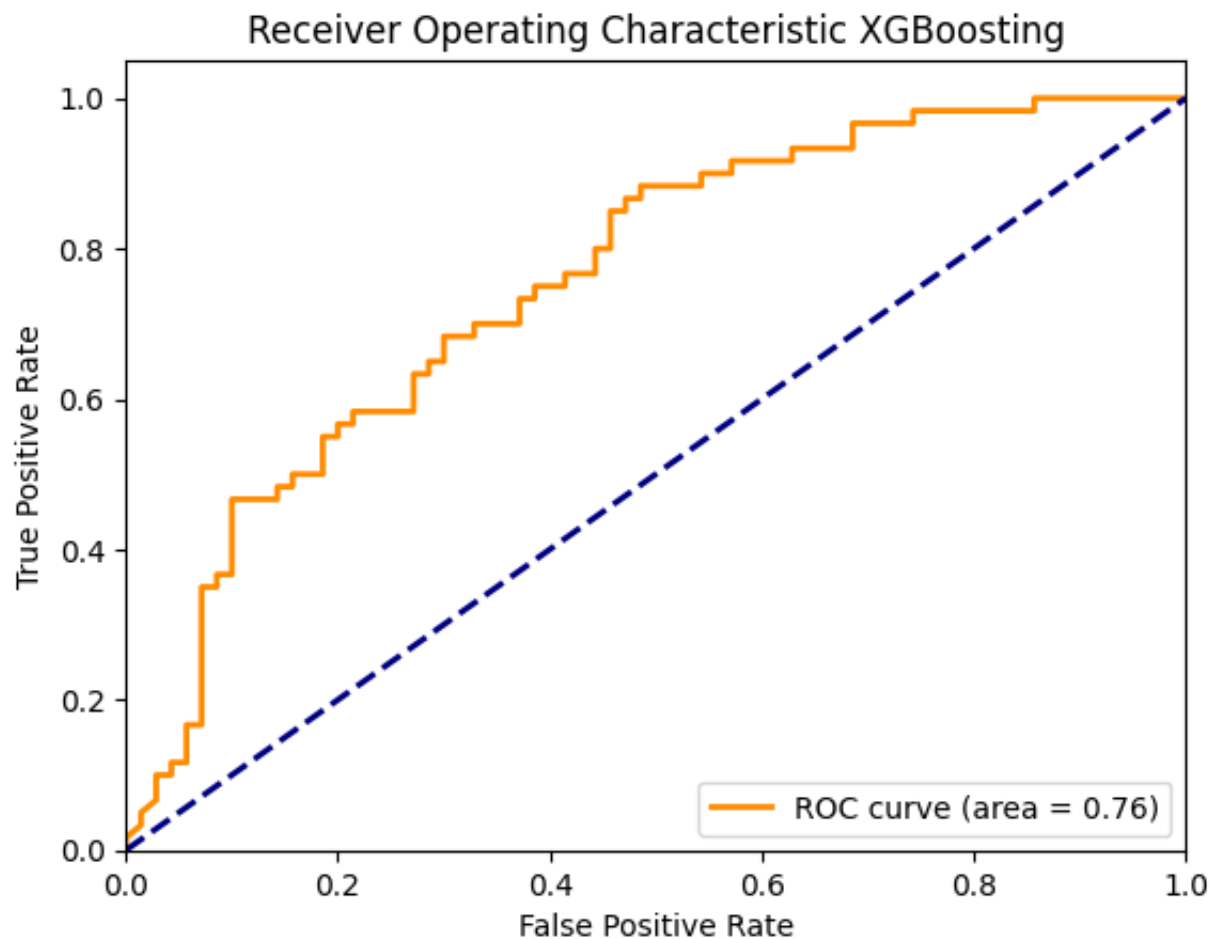
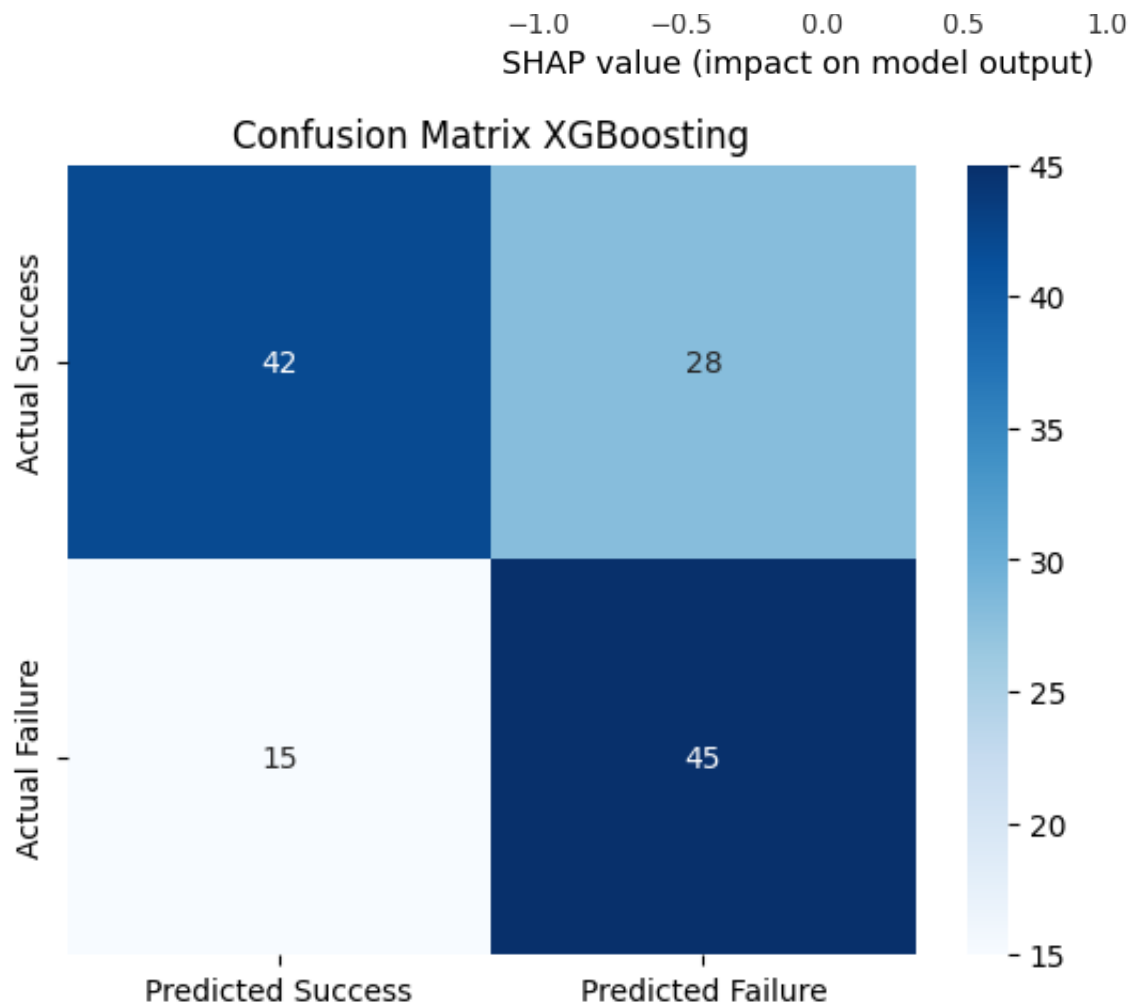
```
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
```

```
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
```

```
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0
```

```
SHAP Summary for XGBoost
```





```
Running evaluation with seed 45
Inside evaluate_xgboost function
Evaluating XGBoost...
Best parameters for XGBoost: {'colsample_bytree': 1, 'gamma': 0.1, 'learning_rate': 0.01, 'max_depth': 6, 'min_child_weight': 1, 'n_estimators': 100, 'objective': 'binary:logistic', 'random_state': 45, 'subsample': 0.8}
```

```
--- Dados ROC para copiar ---
```

```
FPR = [0.0, 0.014285714285714285, 0.014285714285714285, 0.02857142857142857,
```

```
TPR = [0.0, 0.016666666666666666, 0.06666666666666667, 0.08333333333333333,
```

```
AUC = 0.7607142857142857
```

```
--- Fim dos Dados ROC ---
```

```
Training - Accuracy: 0.8678500986193294, Sensitivity: 0.8844621513944223, Specificity: 0.8844621513944223, SHAP Metrics for manual threshold 0.5:
```

```
Accuracy: 0.6538461538461539, Sensitivity: 0.7333333333333333, Specificity: 0.6538461538461539,
```

```
Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156, 'Specificity': 0.46153846153846156,
```

```
Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156, 'Specificity': 0.46153846153846156,
```

```
Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156, 'Specificity': 0.46153846153846156,
```

```
Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156, 'Specificity': 0.46153846153846156,
```

```
Threshold: 0.30, Metrics: {'Accuracy': 0.46923076923076923, 'Sensitivity': 0.46923076923076923, 'Specificity': 0.46923076923076923,
```

```
Threshold: 0.35, Metrics: {'Accuracy': 0.5461538461538461, 'Sensitivity': 0.5461538461538461, 'Specificity': 0.5461538461538461,
```

```
Threshold: 0.40, Metrics: {'Accuracy': 0.5923076923076923, 'Sensitivity': 0.5923076923076923, 'Specificity': 0.5923076923076923,
```

```
Threshold: 0.45, Metrics: {'Accuracy': 0.6692307692307692, 'Sensitivity': 0.6692307692307692, 'Specificity': 0.6692307692307692,
```

```
Threshold: 0.50, Metrics: {'Accuracy': 0.6538461538461539, 'Sensitivity': 0.6538461538461539, 'Specificity': 0.6538461538461539,
```

```
Threshold: 0.55, Metrics: {'Accuracy': 0.7, 'Sensitivity': 0.6166666666666666, 'Specificity': 0.7,
```

```
Threshold: 0.60, Metrics: {'Accuracy': 0.6846153846153846, 'Sensitivity': 0.6846153846153846, 'Specificity': 0.6846153846153846,
```

```
Threshold: 0.65, Metrics: {'Accuracy': 0.5769230769230769, 'Sensitivity': 0.5769230769230769, 'Specificity': 0.5769230769230769,
```

```
Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384,
```

```
Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384,
```

```
Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384,
```

```
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384,
```

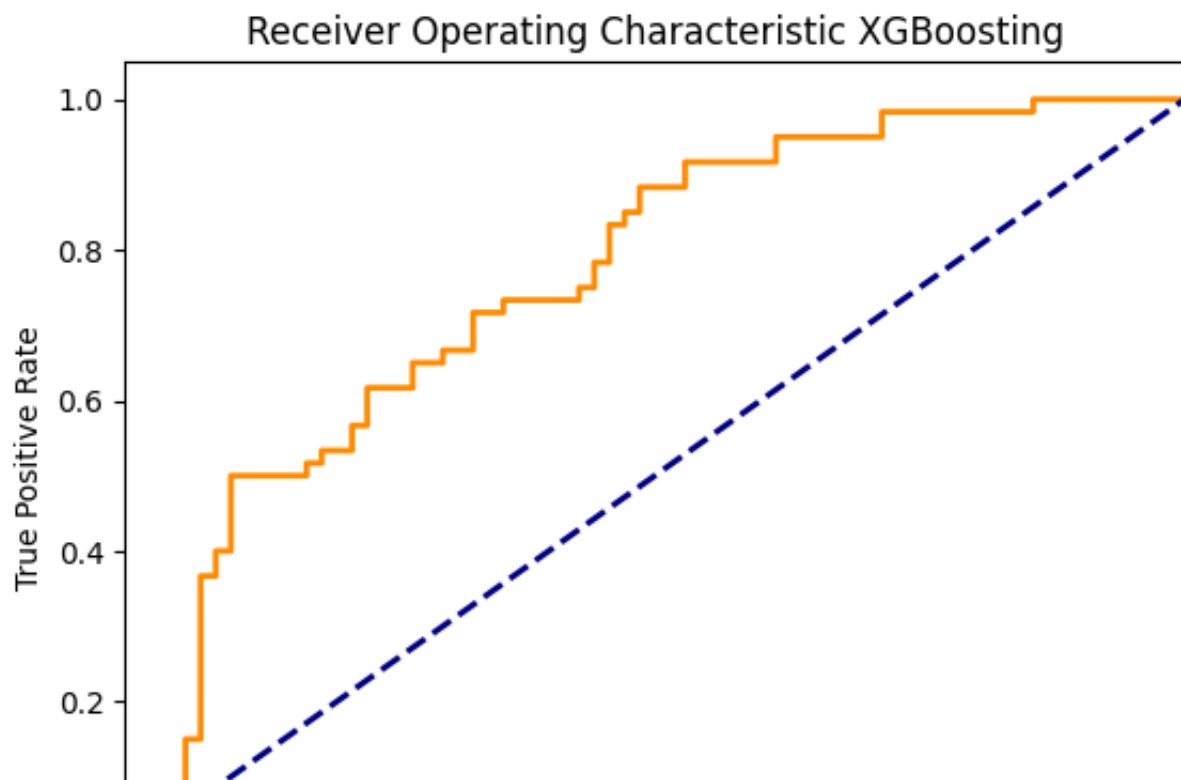
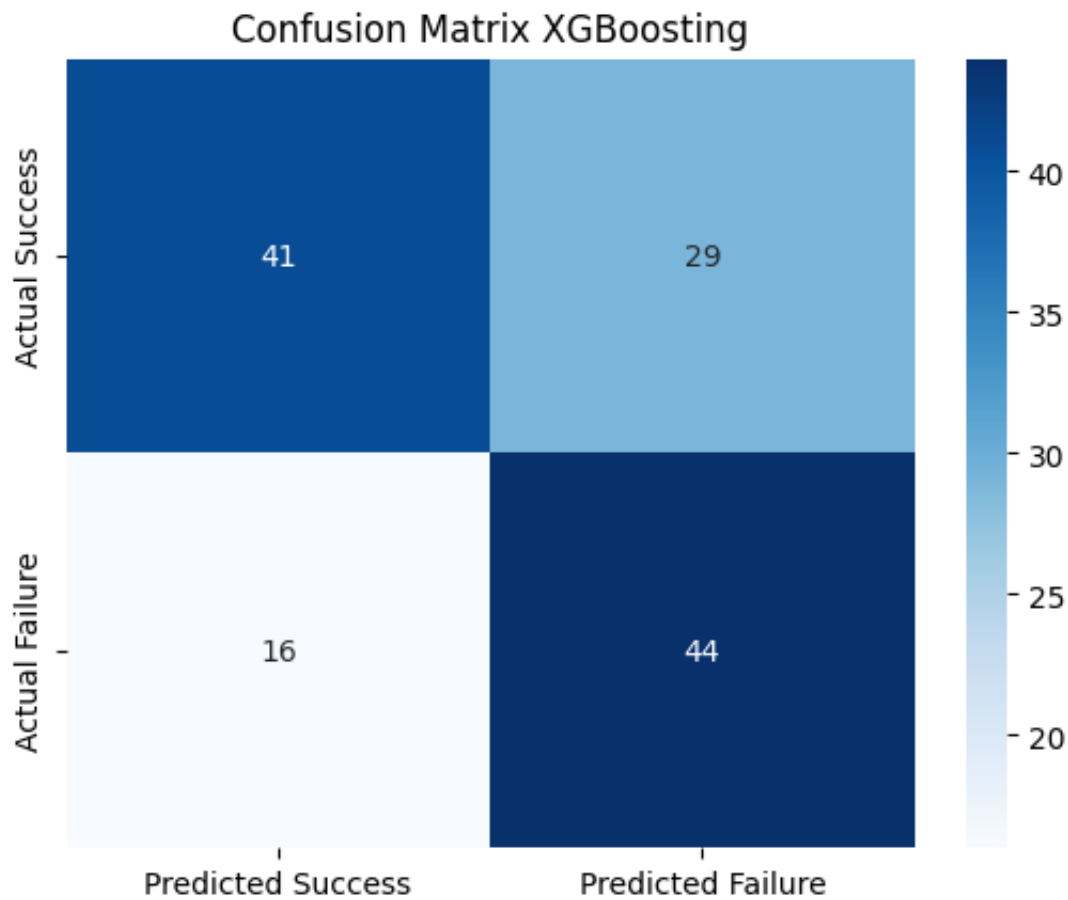
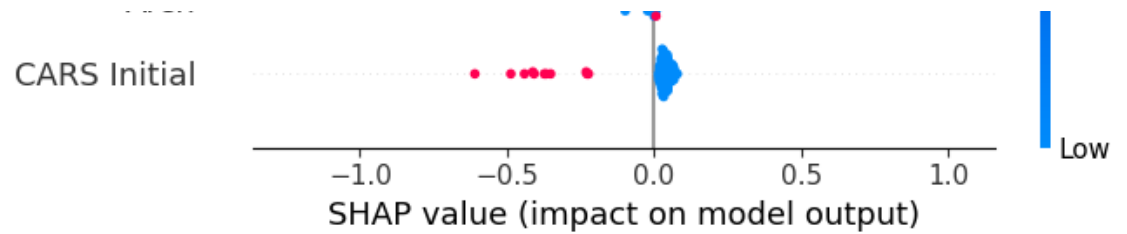
```
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384,
```

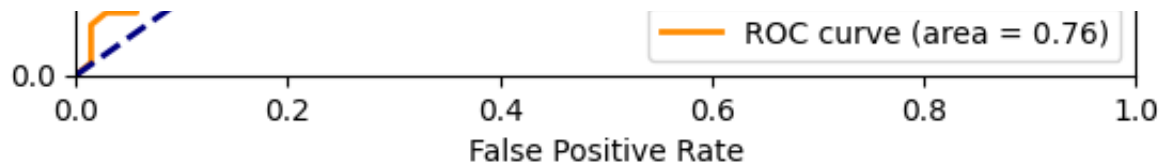
```
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384,
```

```
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384,
```

```
SHAP Summary for XGBoost
```







Running evaluation with seed 46

Inside evaluate\_xgboost function

Evaluating XGBoost...

Best parameters for XGBoost: {'colsample\_bytree': 1, 'gamma': 0.1, 'learning\_rate': 0.1, 'max\_depth': 6, 'min\_child\_weight': 1, 'n\_estimators': 100, 'objective': 'binary:logistic', 'random\_state': 46, 'subsample': 0.8}

--- Dados ROC para copiar ---

FPR = [0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.02857142857142857, 0.04285714285714285, 0.05714285714285714, 0.07142857142857143, 0.08571428571428571, 0.1, 0.11428571428571428, 0.12857142857142858, 0.14285714285714285, 0.15714285714285714, 0.17142857142857143, 0.1857142857142857, 0.2, 0.21428571428571428, 0.22857142857142858, 0.24285714285714285, 0.25714285714285714, 0.27142857142857143, 0.2857142857142857, 0.3, 0.31428571428571428, 0.32857142857142858, 0.34285714285714285, 0.35714285714285714, 0.37142857142857143, 0.3857142857142857, 0.4, 0.41428571428571428, 0.42857142857142858, 0.44285714285714285, 0.45714285714285714, 0.47142857142857143, 0.4857142857142857, 0.5, 0.51428571428571428, 0.52857142857142858, 0.54285714285714285, 0.55714285714285714, 0.57142857142857143, 0.5857142857142857, 0.6, 0.61428571428571428, 0.62857142857142858, 0.64285714285714285, 0.65714285714285714, 0.67142857142857143, 0.6857142857142857, 0.7, 0.71428571428571428, 0.72857142857142858, 0.74285714285714285, 0.75714285714285714, 0.77142857142857143, 0.7857142857142857, 0.8, 0.81428571428571428, 0.82857142857142858, 0.84285714285714285, 0.85714285714285714, 0.87142857142857143, 0.8857142857142857, 0.9, 0.91428571428571428, 0.92857142857142858, 0.94285714285714285, 0.95714285714285714, 0.97142857142857143, 0.9857142857142857, 1.0]

TPR = [0.0, 0.016666666666666666, 0.03333333333333333, 0.05, 0.06666666666666666, 0.08333333333333333, 0.1, 0.11666666666666666, 0.13333333333333333, 0.15, 0.16666666666666666, 0.18333333333333333, 0.2, 0.21666666666666666, 0.23333333333333333, 0.25, 0.26666666666666666, 0.28333333333333333, 0.3, 0.31666666666666666, 0.33333333333333333, 0.35, 0.36666666666666666, 0.38333333333333333, 0.4, 0.41666666666666666, 0.43333333333333333, 0.45, 0.46666666666666666, 0.48333333333333333, 0.5, 0.51666666666666666, 0.53333333333333333, 0.55, 0.56666666666666666, 0.58333333333333333, 0.6, 0.61666666666666666, 0.63333333333333333, 0.65, 0.66666666666666666, 0.68333333333333333, 0.7, 0.71666666666666666, 0.73333333333333333, 0.75, 0.76666666666666666, 0.78333333333333333, 0.8, 0.81666666666666666, 0.83333333333333333, 0.85, 0.86666666666666666, 0.88333333333333333, 0.9, 0.91666666666666666, 0.93333333333333333, 0.95, 0.96666666666666666, 0.98333333333333333, 1.0]

AUC = 0.7666666666666667

--- Fim dos Dados ROC ---

Training - Accuracy: 0.8678500986193294, Sensitivity: 0.8844621513944223, Specificity: 0.67857142857142858, F1: 0.7692307692307692  
Metrics for manual threshold 0.5:

Accuracy: 0.6692307692307692, Sensitivity: 0.75, Specificity: 0.6, F1: 0.67

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.4, 'Specificity': 0.8, 'F1': 0.5384615384615384}

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.4, 'Specificity': 0.8, 'F1': 0.5384615384615384}

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.4, 'Specificity': 0.8, 'F1': 0.5384615384615384}

Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.4, 'Specificity': 0.8, 'F1': 0.5384615384615384}

Threshold: 0.30, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.4, 'Specificity': 0.8, 'F1': 0.5384615384615384}

Threshold: 0.35, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.6, 'Specificity': 0.4, 'F1': 0.5384615384615384}

Threshold: 0.40, Metrics: {'Accuracy': 0.5923076923076923, 'Sensitivity': 0.8, 'Specificity': 0.2, 'F1': 0.5923076923076923}

Threshold: 0.45, Metrics: {'Accuracy': 0.6923076923076923, 'Sensitivity': 1.0, 'Specificity': 0.0, 'F1': 0.6923076923076923}

Threshold: 0.50, Metrics: {'Accuracy': 0.6692307692307692, 'Sensitivity': 0.75, 'Specificity': 0.6, 'F1': 0.67}

Threshold: 0.55, Metrics: {'Accuracy': 0.6923076923076923, 'Sensitivity': 1.0, 'Specificity': 0.0, 'F1': 0.6923076923076923}

Threshold: 0.60, Metrics: {'Accuracy': 0.6769230769230769, 'Sensitivity': 0.8, 'Specificity': 0.4, 'F1': 0.6769230769230769}

Threshold: 0.65, Metrics: {'Accuracy': 0.5769230769230769, 'Sensitivity': 0.4, 'Specificity': 0.8, 'F1': 0.5769230769230769}

Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.2, 'Specificity': 1.0, 'F1': 0.5384615384615384}

Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.0, 'Specificity': 1.0, 'F1': 0.5384615384615384}

Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.0, 'Specificity': 1.0, 'F1': 0.5384615384615384}

Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.0, 'Specificity': 1.0, 'F1': 0.5384615384615384}

Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.0, 'Specificity': 1.0, 'F1': 0.5384615384615384}

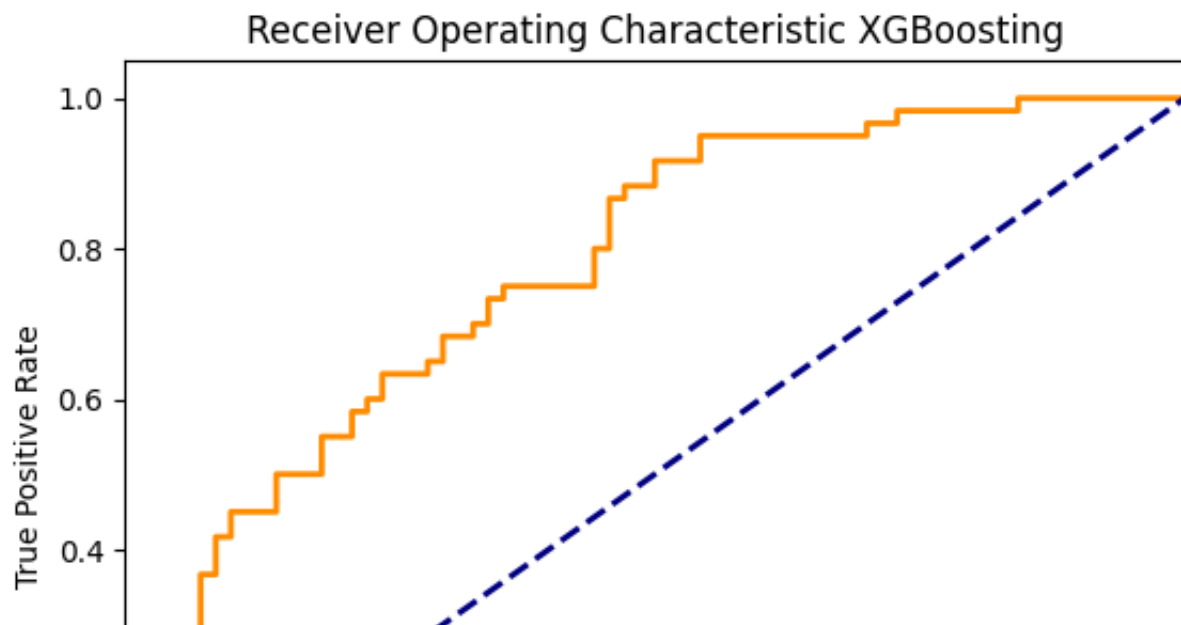
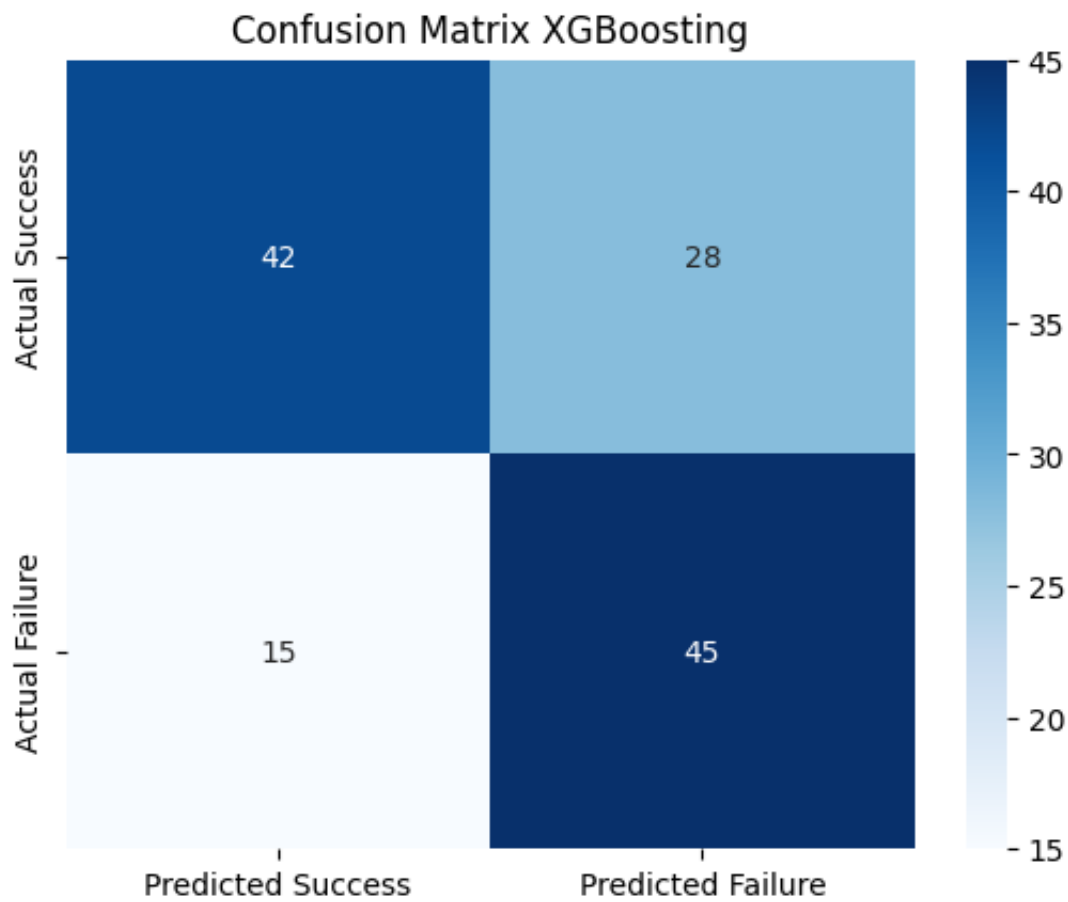
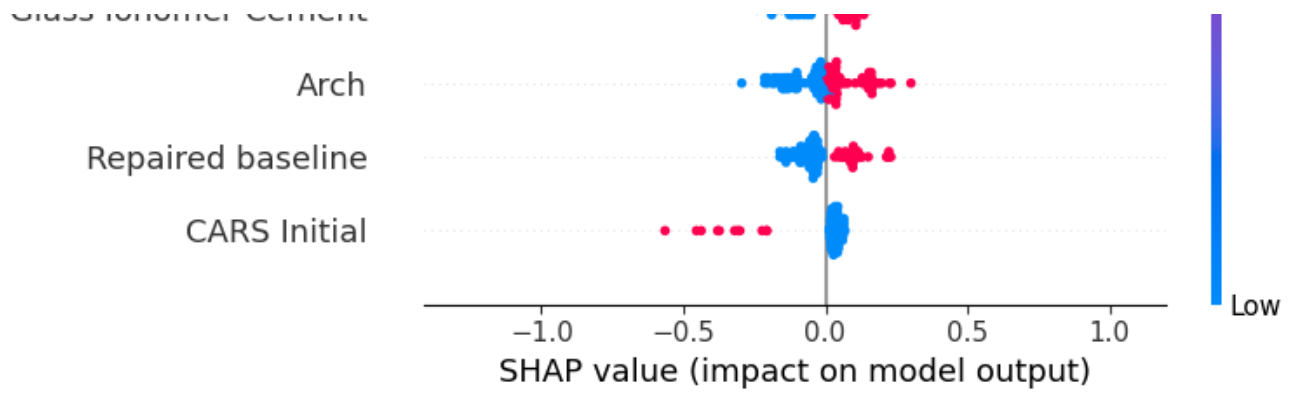
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.0, 'Specificity': 1.0, 'F1': 0.5384615384615384}

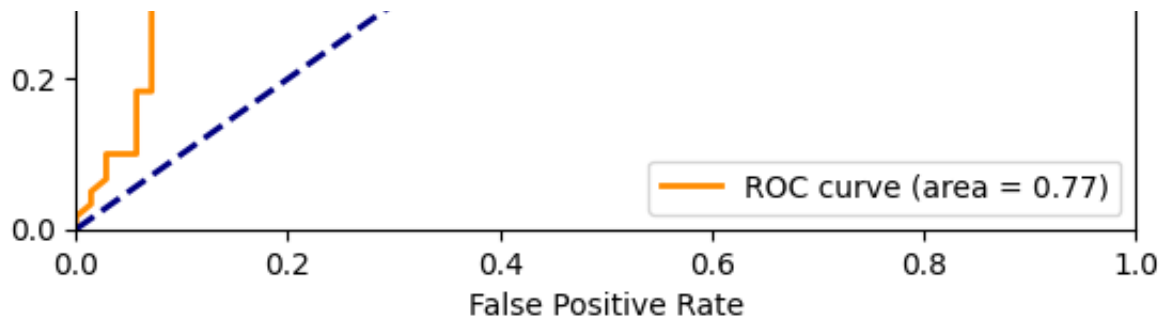
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.0, 'Specificity': 1.0, 'F1': 0.5384615384615384}

SHAP Summary for XGBoost









Running evaluation with seed 47

Inside evaluate\_xgboost function

Evaluating XGBoost...

Best parameters for XGBoost: {'colsample\_bytree': 1, 'gamma': 0.1, 'learning\_rate': 0.1, 'max\_depth': 6, 'min\_child\_weight': 1, 'n\_estimators': 100, 'objective': 'binary:logistic', 'random\_state': 47, 'subsample': 0.8}

--- Dados ROC para copiar ---

FPR = [0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.028571428571428571, 0.042857142857142856, 0.05714285714285714, 0.07142857142857143, 0.08571428571428571, 0.1, 0.11428571428571428, 0.12857142857142858, 0.14285714285714285, 0.15714285714285715, 0.17142857142857143, 0.18571428571428571, 0.2, 0.21428571428571428, 0.22857142857142858, 0.24285714285714285, 0.25714285714285715, 0.27142857142857143, 0.28571428571428571, 0.3, 0.31428571428571428, 0.32857142857142858, 0.34285714285714285, 0.35714285714285715, 0.37142857142857143, 0.38571428571428571, 0.4, 0.41428571428571428, 0.42857142857142858, 0.44285714285714285, 0.45714285714285715, 0.47142857142857143, 0.48571428571428571, 0.5, 0.51428571428571428, 0.52857142857142858, 0.54285714285714285, 0.55714285714285715, 0.57142857142857143, 0.58571428571428571, 0.6, 0.61428571428571428, 0.62857142857142858, 0.64285714285714285, 0.65714285714285715, 0.67142857142857143, 0.68571428571428571, 0.7, 0.71428571428571428, 0.72857142857142858, 0.74285714285714285, 0.75714285714285715, 0.77142857142857143, 0.78571428571428571, 0.8, 0.81428571428571428, 0.82857142857142858, 0.84285714285714285, 0.85714285714285715, 0.87142857142857143, 0.88571428571428571, 0.9, 0.91428571428571428, 0.92857142857142858, 0.94285714285714285, 0.95714285714285715, 0.97142857142857143, 0.98571428571428571, 1.0]

TPR = [0.0, 0.016666666666666666, 0.033333333333333333, 0.05, 0.066666666666666666, 0.08333333333333333, 0.1, 0.11666666666666666, 0.13333333333333333, 0.15, 0.16666666666666666, 0.18333333333333333, 0.2, 0.21666666666666666, 0.23333333333333333, 0.25, 0.26666666666666666, 0.28333333333333333, 0.3, 0.31666666666666666, 0.33333333333333333, 0.35, 0.36666666666666666, 0.38333333333333333, 0.4, 0.41666666666666666, 0.43333333333333333, 0.45, 0.46666666666666666, 0.48333333333333333, 0.5, 0.51666666666666666, 0.53333333333333333, 0.55, 0.56666666666666666, 0.58333333333333333, 0.6, 0.61666666666666666, 0.63333333333333333, 0.65, 0.66666666666666666, 0.68333333333333333, 0.7, 0.71666666666666666, 0.73333333333333333, 0.75, 0.76666666666666666, 0.78333333333333333, 0.8, 0.81666666666666666, 0.83333333333333333, 0.85, 0.86666666666666666, 0.88333333333333333, 0.9, 0.91666666666666666, 0.93333333333333333, 0.95, 0.96666666666666666, 0.98333333333333333, 1.0]

AUC = 0.7588095238095238

--- Fim dos Dados ROC ---

Training - Accuracy: 0.8678500986193294, Sensitivity: 0.8844621513944223, Specificity: 0.8714285714285714, Metrics for manual threshold 0.5:

Accuracy: 0.6615384615384615, Sensitivity: 0.7333333333333333, Specificity: 0.7333333333333333

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156, 'Specificity': 0.46153846153846156}

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156, 'Specificity': 0.46153846153846156}

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156, 'Specificity': 0.46153846153846156}

Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156, 'Specificity': 0.46153846153846156}

Threshold: 0.30, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156, 'Specificity': 0.46153846153846156}

Threshold: 0.35, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384}

Threshold: 0.40, Metrics: {'Accuracy': 0.5923076923076923, 'Sensitivity': 0.5923076923076923, 'Specificity': 0.5923076923076923}

Threshold: 0.45, Metrics: {'Accuracy': 0.6692307692307692, 'Sensitivity': 0.6692307692307692, 'Specificity': 0.6692307692307692}

Threshold: 0.50, Metrics: {'Accuracy': 0.6615384615384615, 'Sensitivity': 0.6615384615384615, 'Specificity': 0.6615384615384615}

Threshold: 0.55, Metrics: {'Accuracy': 0.6615384615384615, 'Sensitivity': 0.6615384615384615, 'Specificity': 0.6615384615384615}

Threshold: 0.60, Metrics: {'Accuracy': 0.6923076923076923, 'Sensitivity': 0.6923076923076923, 'Specificity': 0.6923076923076923}

Threshold: 0.65, Metrics: {'Accuracy': 0.5846153846153846, 'Sensitivity': 0.5846153846153846, 'Specificity': 0.5846153846153846}

Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384}

Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384}

Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384}

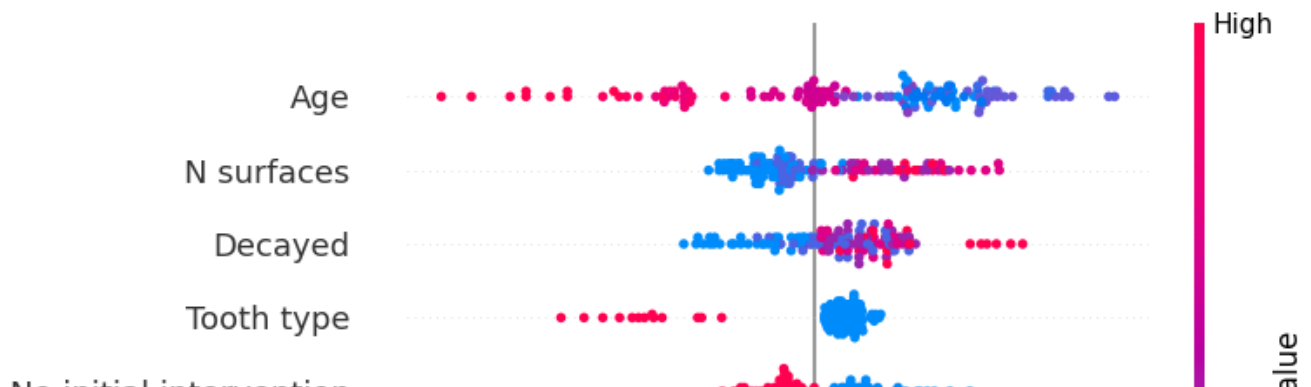
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384}

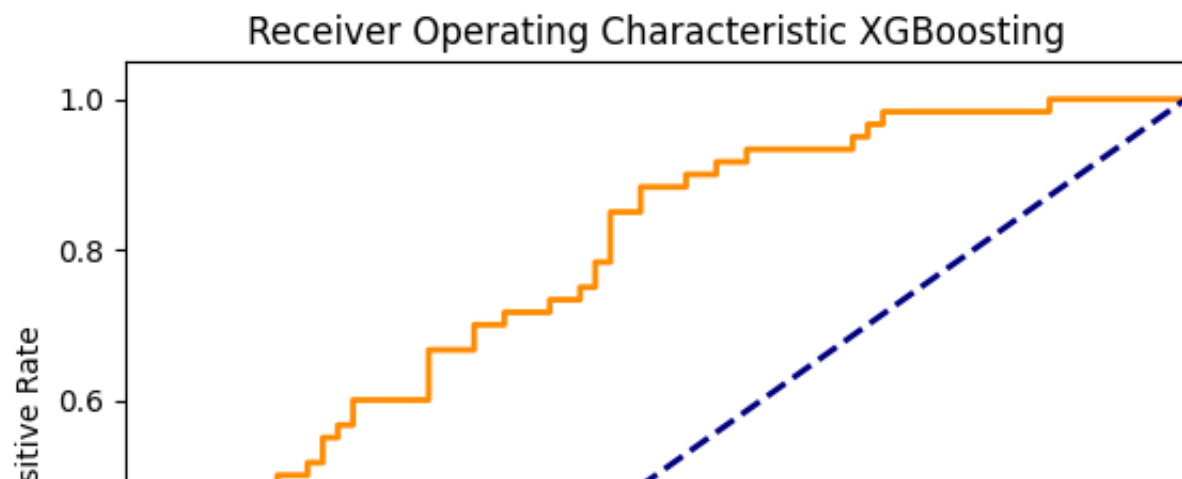
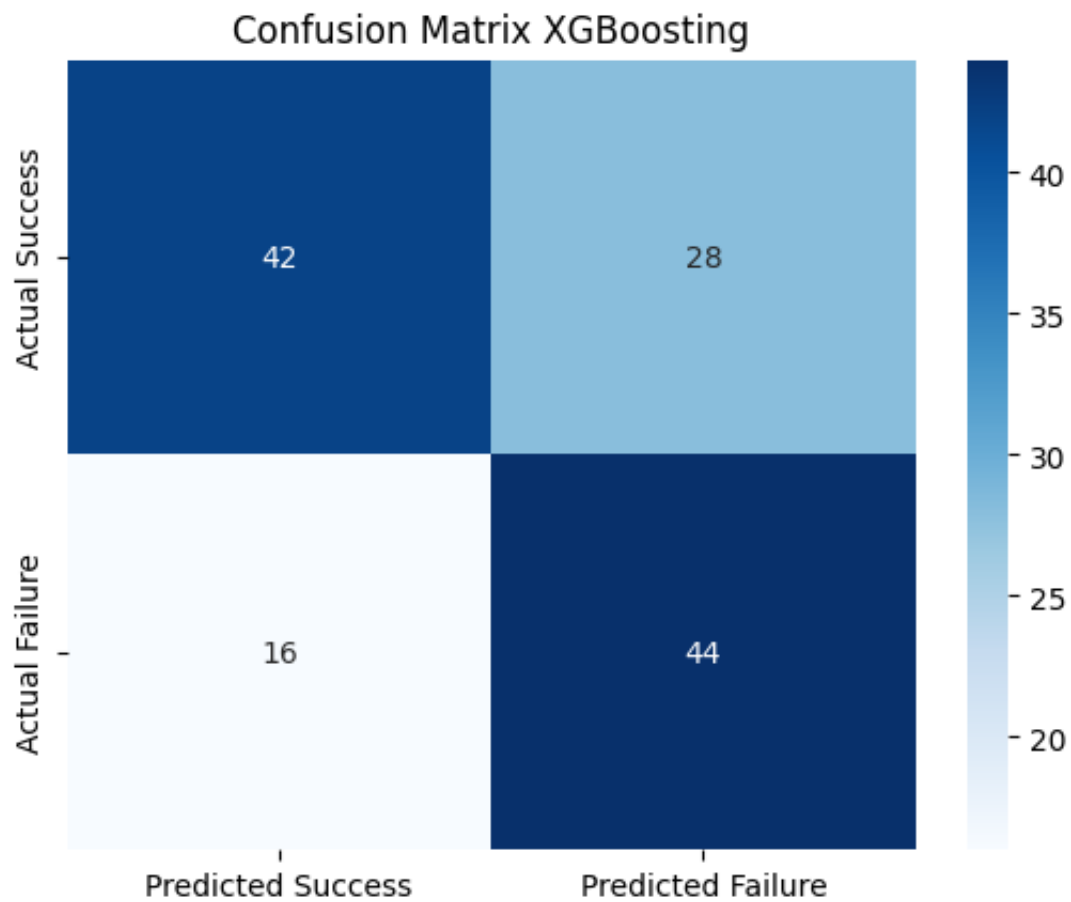
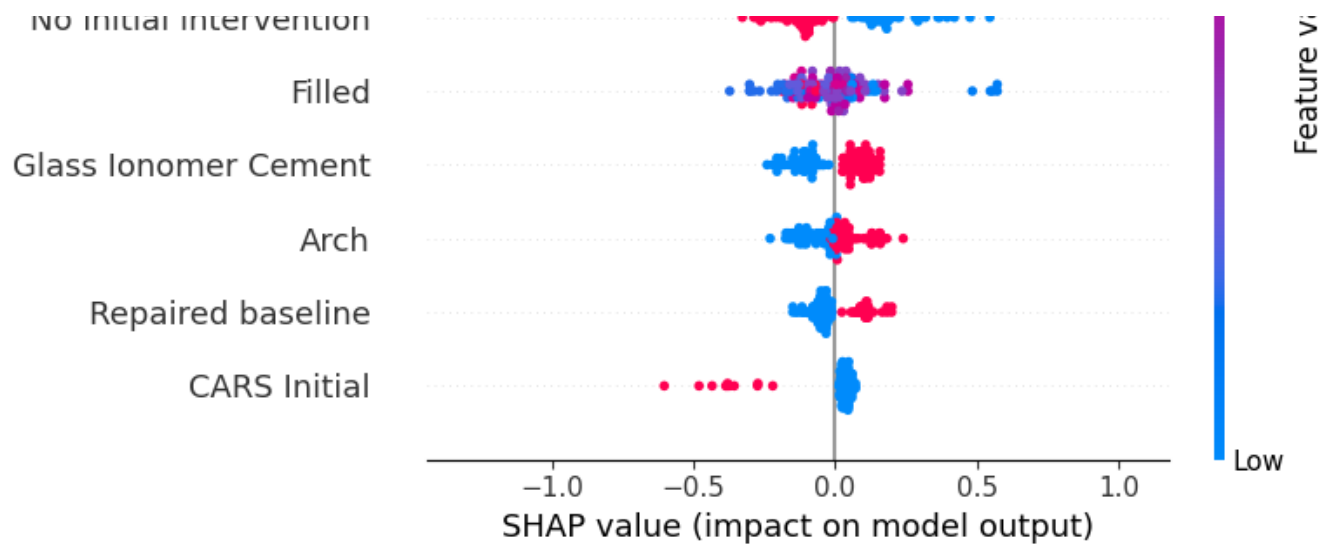
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384}

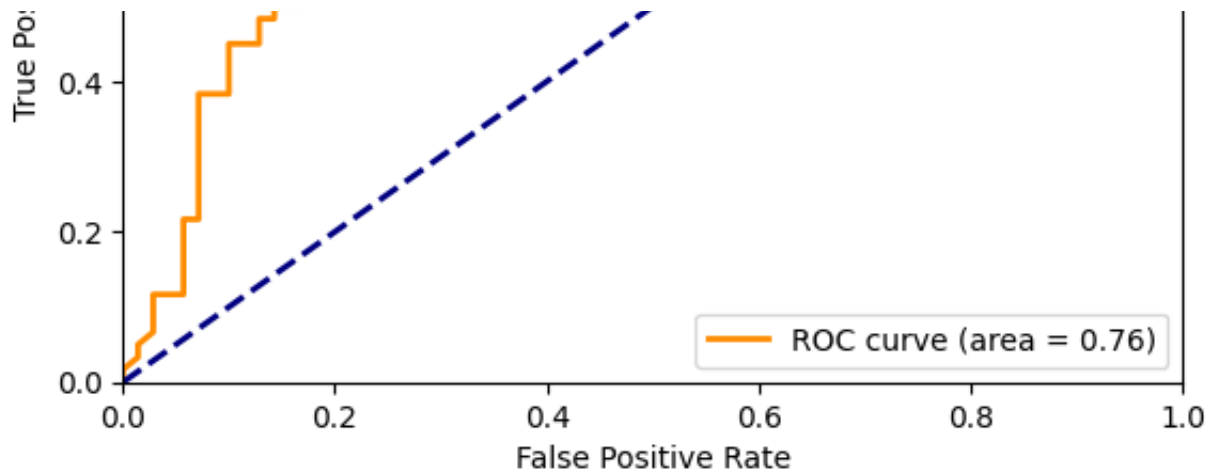
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384}

Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384}

SHAP Summary for XGBoost







Running evaluation with seed 48

Inside evaluate\_xgboost function

Evaluating XGBoost...

Best parameters for XGBoost: {'colsample\_bytree': 1, 'gamma': 0.1, 'learning\_rate': 0.1, 'max\_depth': 6, 'min\_child\_weight': 1, 'n\_estimators': 100, 'objective': 'binary:logistic', 'random\_state': 48, 'subsample': 0.8}

--- Dados ROC para copiar ---

FPR = [0.0, 0.014285714285714285, 0.014285714285714285, 0.02857142857142857, 0.02857142857142857, 0.04285714285714285, 0.04285714285714285, 0.05714285714285714, 0.05714285714285714, 0.07142857142857143, 0.07142857142857143, 0.08571428571428571, 0.08571428571428571, 0.1, 0.1, 0.11428571428571428, 0.11428571428571428, 0.12857142857142857, 0.12857142857142857, 0.14285714285714285, 0.14285714285714285, 0.15714285714285714, 0.15714285714285714, 0.17142857142857143, 0.17142857142857143, 0.18571428571428571, 0.18571428571428571, 0.2, 0.2, 0.21428571428571428, 0.21428571428571428, 0.22857142857142857, 0.22857142857142857, 0.24285714285714285, 0.24285714285714285, 0.25714285714285714, 0.25714285714285714, 0.27142857142857143, 0.27142857142857143, 0.28571428571428571, 0.28571428571428571, 0.3, 0.3, 0.31428571428571428, 0.31428571428571428, 0.32857142857142857, 0.32857142857142857, 0.34285714285714285, 0.34285714285714285, 0.35714285714285714, 0.35714285714285714, 0.37142857142857143, 0.37142857142857143, 0.38571428571428571, 0.38571428571428571, 0.4, 0.4, 0.41428571428571428, 0.41428571428571428, 0.42857142857142857, 0.42857142857142857, 0.44285714285714285, 0.44285714285714285, 0.45714285714285714, 0.45714285714285714, 0.47142857142857143, 0.47142857142857143, 0.48571428571428571, 0.48571428571428571, 0.5, 0.5, 0.51428571428571428, 0.51428571428571428, 0.52857142857142857, 0.52857142857142857, 0.54285714285714285, 0.54285714285714285, 0.55714285714285714, 0.55714285714285714, 0.57142857142857143, 0.57142857142857143, 0.58571428571428571, 0.58571428571428571, 0.6, 0.6, 0.61428571428571428, 0.61428571428571428, 0.62857142857142857, 0.62857142857142857, 0.64285714285714285, 0.64285714285714285, 0.65714285714285714, 0.65714285714285714, 0.67142857142857143, 0.67142857142857143, 0.68571428571428571, 0.68571428571428571, 0.7, 0.7, 0.71428571428571428, 0.71428571428571428, 0.72857142857142857, 0.72857142857142857, 0.74285714285714285, 0.74285714285714285, 0.75714285714285714, 0.75714285714285714, 0.77142857142857143, 0.77142857142857143, 0.78571428571428571, 0.78571428571428571, 0.8, 0.8, 0.81428571428571428, 0.81428571428571428, 0.82857142857142857, 0.82857142857142857, 0.84285714285714285, 0.84285714285714285, 0.85714285714285714, 0.85714285714285714, 0.87142857142857143, 0.87142857142857143, 0.88571428571428571, 0.88571428571428571, 0.9, 0.9, 0.91428571428571428, 0.91428571428571428, 0.92857142857142857, 0.92857142857142857, 0.94285714285714285, 0.94285714285714285, 0.95714285714285714, 0.95714285714285714, 0.97142857142857143, 0.97142857142857143, 0.98571428571428571, 0.98571428571428571, 1.0, 1.0]

AUC = 0.7614285714285713

--- Fim dos Dados ROC ---

Training - Accuracy: 0.8619329388560157, Sensitivity: 0.8605577689243028, Specificity: 0.8605577689243028, SHAP Summary for XGBoost

Metrics for manual threshold 0.5:

Accuracy: 0.6615384615384615, Sensitivity: 0.75, Specificity: 0.5857142857142857

Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156, 'Specificity': 0.46153846153846156}

Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156, 'Specificity': 0.46153846153846156}

Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156, 'Specificity': 0.46153846153846156}

Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156, 'Specificity': 0.46153846153846156}

Threshold: 0.30, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156, 'Specificity': 0.46153846153846156}

Threshold: 0.35, Metrics: {'Accuracy': 0.5307692307692308, 'Sensitivity': 0.5307692307692308, 'Specificity': 0.5307692307692308}

Threshold: 0.40, Metrics: {'Accuracy': 0.5923076923076923, 'Sensitivity': 0.5923076923076923, 'Specificity': 0.5923076923076923}

Threshold: 0.45, Metrics: {'Accuracy': 0.6461538461538462, 'Sensitivity': 0.6461538461538462, 'Specificity': 0.6461538461538462}

Threshold: 0.50, Metrics: {'Accuracy': 0.6615384615384615, 'Sensitivity': 0.6615384615384615, 'Specificity': 0.6615384615384615}

Threshold: 0.55, Metrics: {'Accuracy': 0.7, 'Sensitivity': 0.7, 'Specificity': 0.7}

Threshold: 0.60, Metrics: {'Accuracy': 0.7076923076923077, 'Sensitivity': 0.7076923076923077, 'Specificity': 0.7076923076923077}

Threshold: 0.65, Metrics: {'Accuracy': 0.5769230769230769, 'Sensitivity': 0.5769230769230769, 'Specificity': 0.5769230769230769}

Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384}

Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384}

Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384}

Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384}

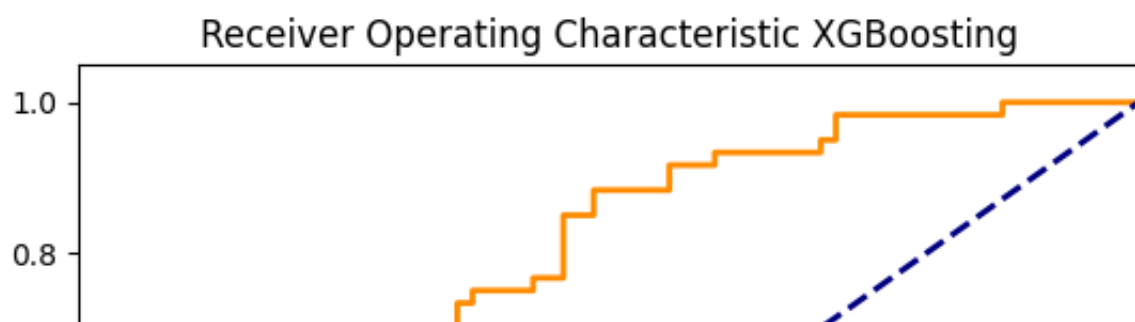
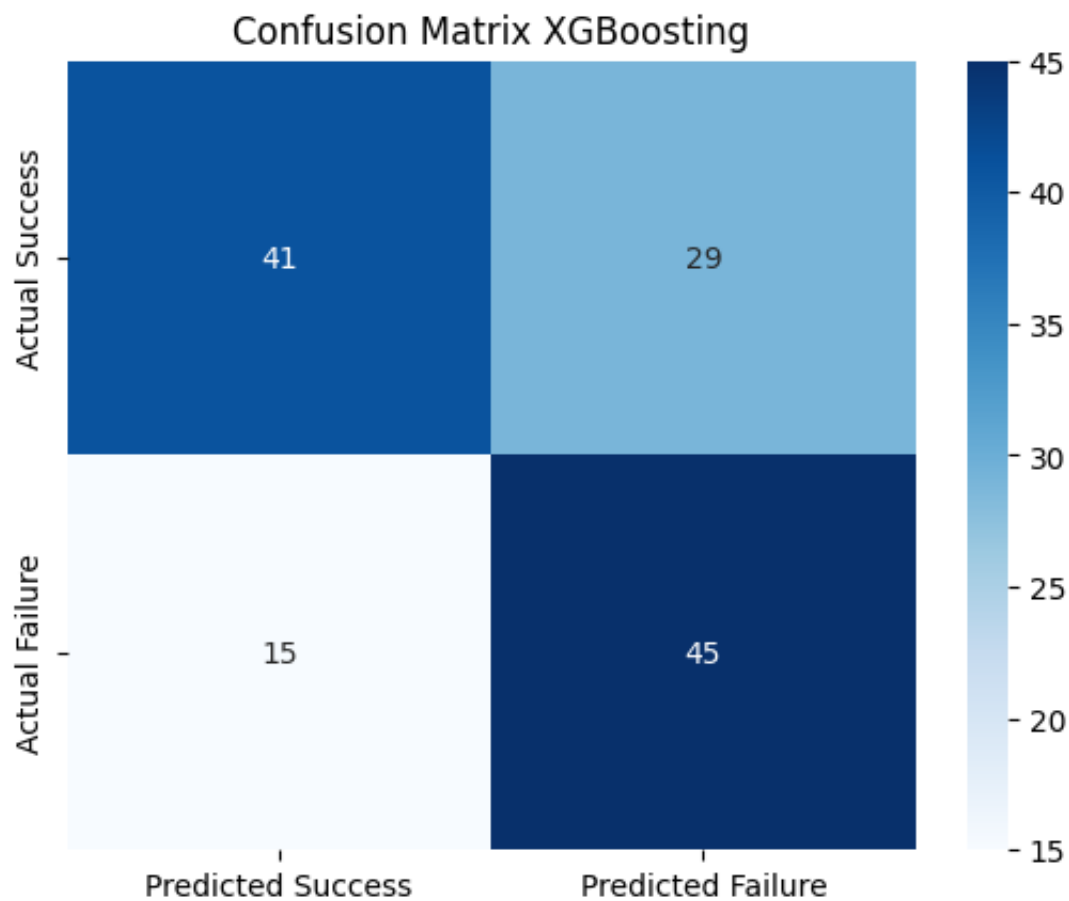
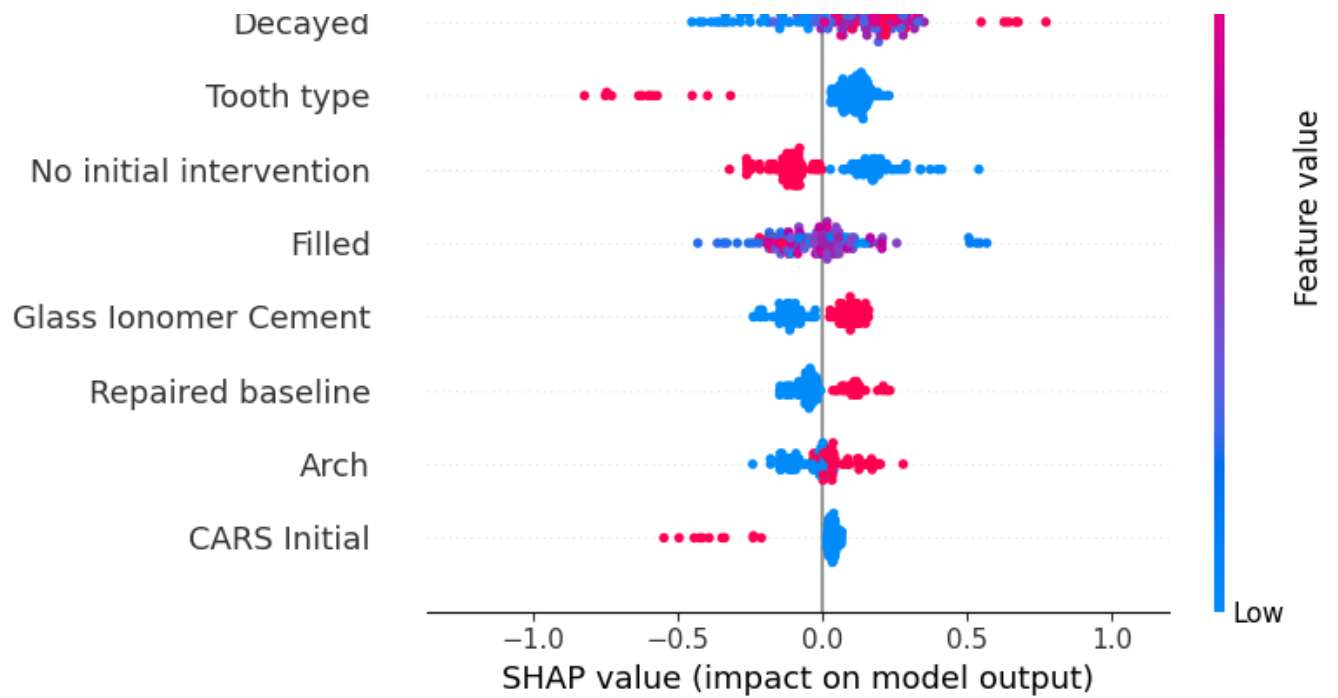
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384}

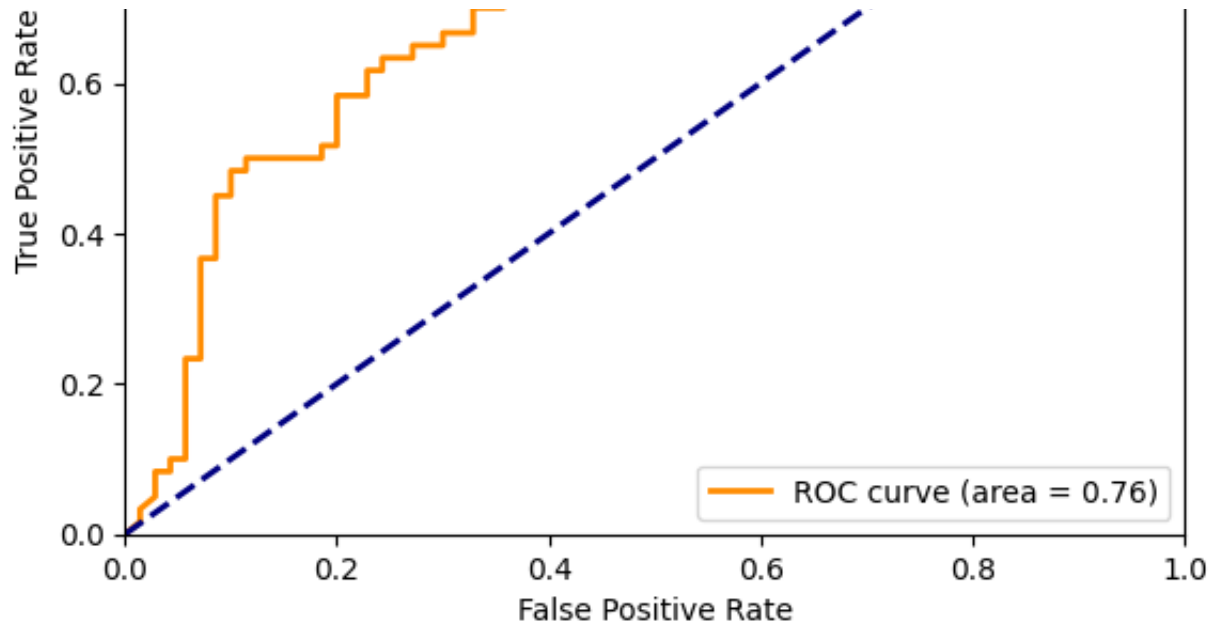
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384}

Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384}

SHAP Summary for XGBoost





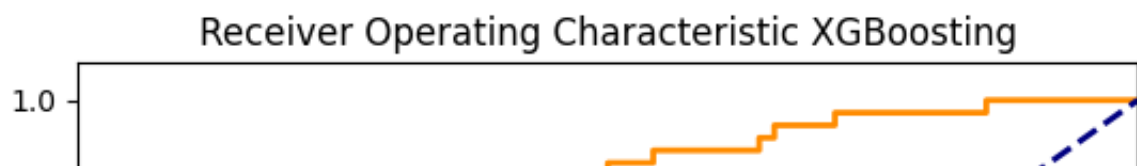
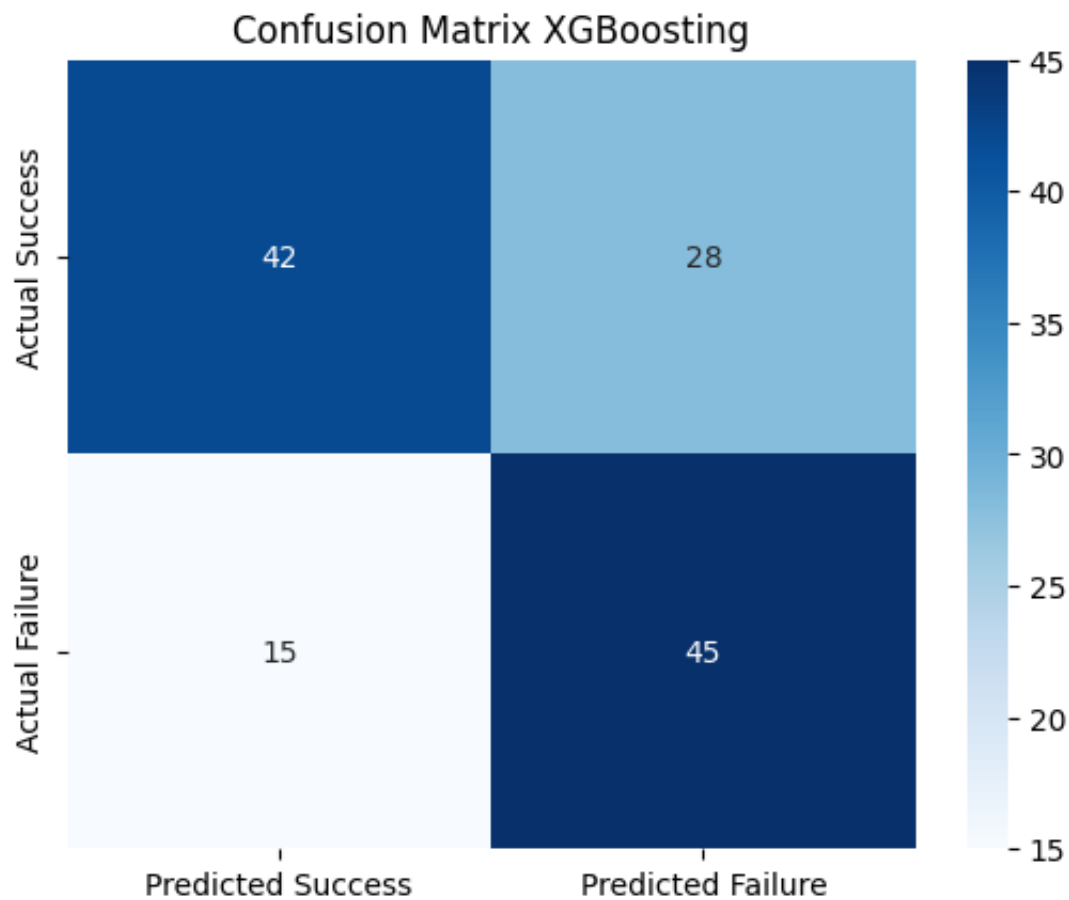
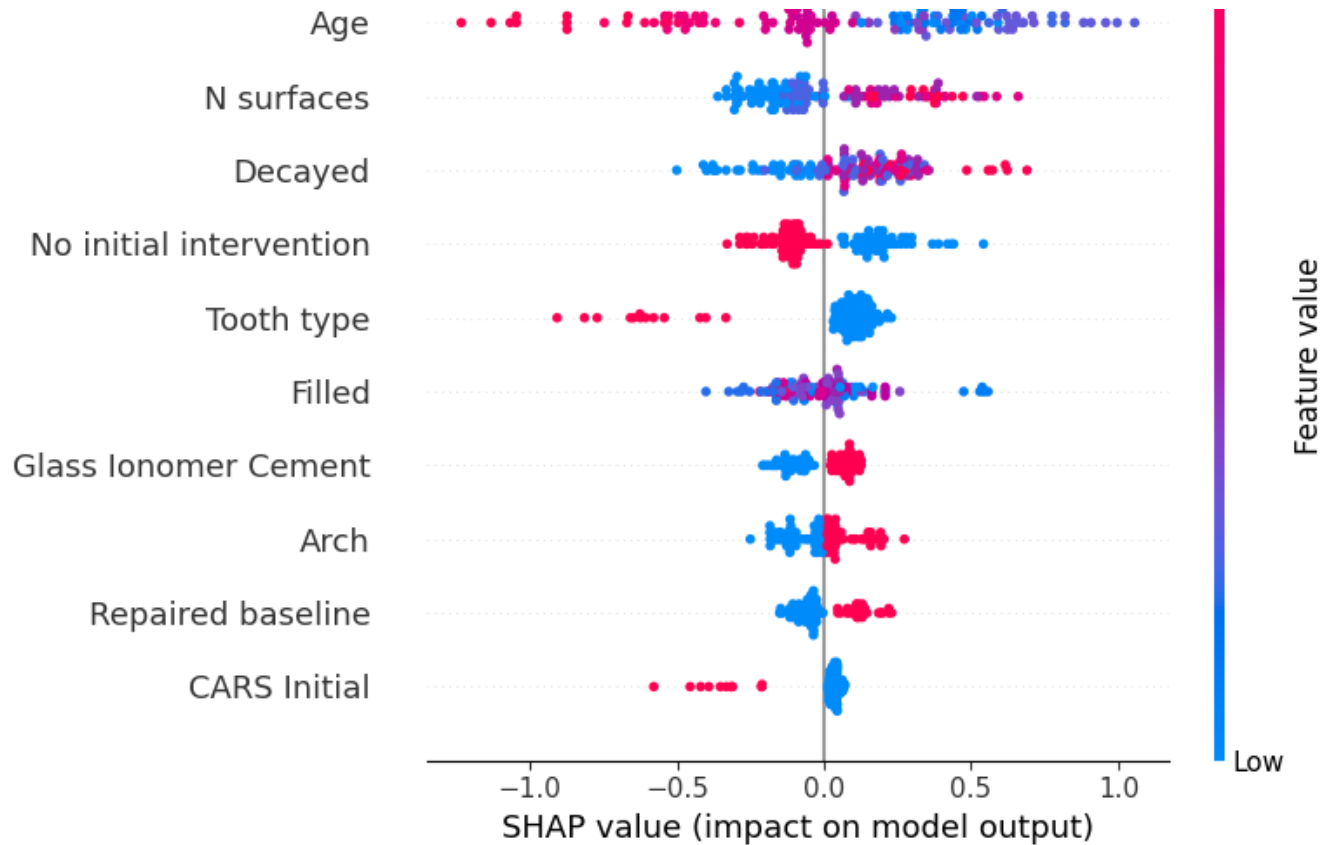


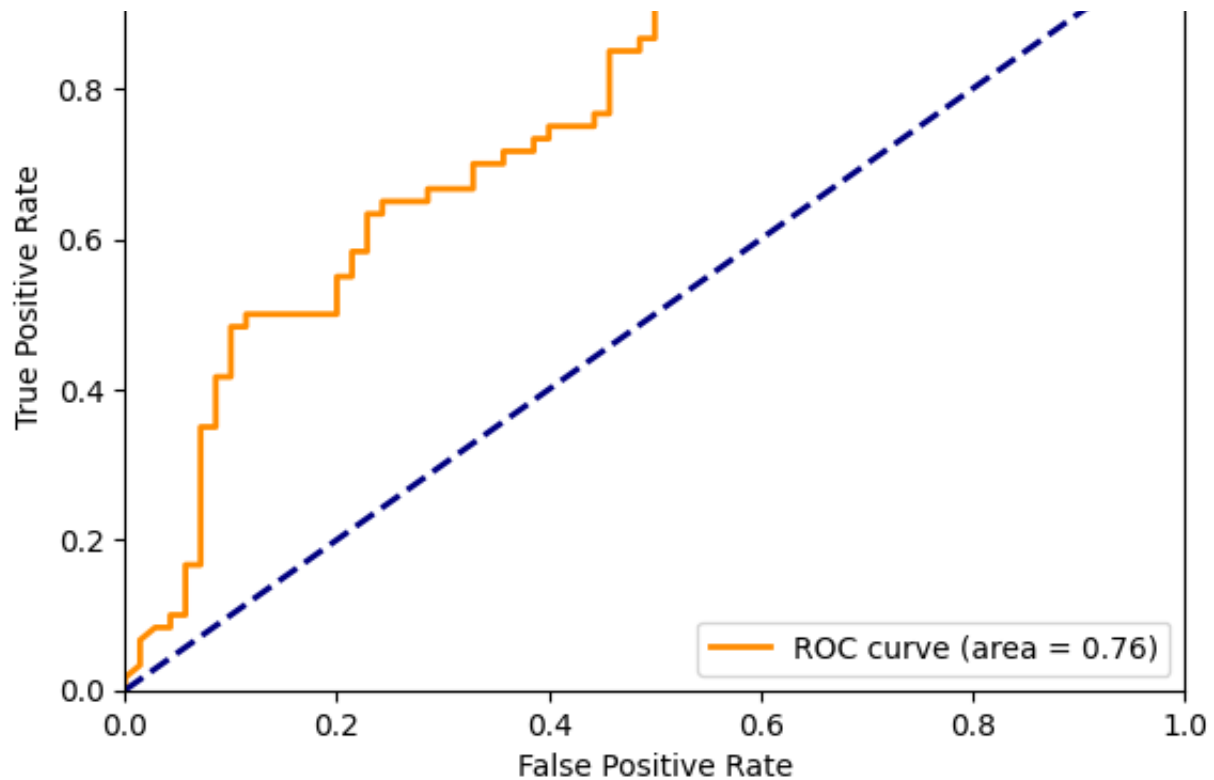
```
Running evaluation with seed 49
Inside evaluate_xgboost function
Evaluating XGBoost...
Best parameters for XGBoost: {'colsample_bytree': 1, 'gamma': 0.1, 'learning_rate': 0.1}

--- Dados ROC para copiar ---
FPR = [0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.028571428571428571, 0.042857142857142856, 0.05714285714285714, 0.07142857142857143, 0.08571428571428571, 0.1, 0.11428571428571428, 0.12857142857142858, 0.14285714285714287, 0.15714285714285715, 0.17142857142857143, 0.1857142857142857, 0.2, 0.21428571428571428, 0.22857142857142858, 0.24285714285714287, 0.25714285714285715, 0.27142857142857143, 0.2857142857142857, 0.3, 0.31428571428571428, 0.32857142857142858, 0.34285714285714287, 0.35714285714285715, 0.37142857142857143, 0.3857142857142857, 0.4, 0.41428571428571428, 0.42857142857142858, 0.44285714285714287, 0.45714285714285715, 0.47142857142857143, 0.4857142857142857, 0.5, 0.51428571428571428, 0.52857142857142858, 0.54285714285714287, 0.55714285714285715, 0.57142857142857143, 0.5857142857142857, 0.6, 0.61428571428571428, 0.62857142857142858, 0.64285714285714287, 0.65714285714285715, 0.67142857142857143, 0.6857142857142857, 0.7, 0.71428571428571428, 0.72857142857142858, 0.74285714285714287, 0.75714285714285715, 0.77142857142857143, 0.7857142857142857, 0.8, 0.81428571428571428, 0.82857142857142858, 0.84285714285714287, 0.85714285714285715, 0.87142857142857143, 0.8857142857142857, 0.9, 0.91428571428571428, 0.92857142857142858, 0.94285714285714287, 0.95714285714285715, 0.97142857142857143, 0.9857142857142857, 1.0]
TPR = [0.0, 0.016666666666666666, 0.03333333333333333, 0.06666666666666667, 0.1, 0.13333333333333333, 0.16666666666666666, 0.2, 0.23333333333333334, 0.26666666666666666, 0.3, 0.3333333333333333, 0.36666666666666664, 0.4, 0.4333333333333333, 0.46666666666666664, 0.5, 0.5333333333333333, 0.5666666666666666, 0.6, 0.6333333333333333, 0.6666666666666666, 0.7, 0.7333333333333333, 0.7666666666666666, 0.8, 0.8333333333333333, 0.8666666666666666, 0.9, 0.9333333333333333, 0.9666666666666666, 1.0]
AUC = 0.7642857142857143
--- Fim dos Dados ROC ---
```

```
Training - Accuracy: 0.8560157790927022, Sensitivity: 0.8645418326693227, Specificity: 0.8560157790927022, SHAP Summary for XGBoost
```

```
Accuracy: 0.6692307692307692, Sensitivity: 0.75, Specificity: 0.6, F1: 0.67
Threshold: 0.10, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156, 'Specificity': 0.46153846153846156, 'F1': 0.46153846153846156}
Threshold: 0.15, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156, 'Specificity': 0.46153846153846156, 'F1': 0.46153846153846156}
Threshold: 0.20, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156, 'Specificity': 0.46153846153846156, 'F1': 0.46153846153846156}
Threshold: 0.25, Metrics: {'Accuracy': 0.46153846153846156, 'Sensitivity': 0.46153846153846156, 'Specificity': 0.46153846153846156, 'F1': 0.46153846153846156}
Threshold: 0.30, Metrics: {'Accuracy': 0.46923076923076923, 'Sensitivity': 0.46923076923076923, 'Specificity': 0.46923076923076923, 'F1': 0.46923076923076923}
Threshold: 0.35, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384, 'F1': 0.5384615384615384}
Threshold: 0.40, Metrics: {'Accuracy': 0.5923076923076923, 'Sensitivity': 0.5923076923076923, 'Specificity': 0.5923076923076923, 'F1': 0.5923076923076923}
Threshold: 0.45, Metrics: {'Accuracy': 0.6769230769230769, 'Sensitivity': 0.6769230769230769, 'Specificity': 0.6769230769230769, 'F1': 0.6769230769230769}
Threshold: 0.50, Metrics: {'Accuracy': 0.6692307692307692, 'Sensitivity': 0.6692307692307692, 'Specificity': 0.6692307692307692, 'F1': 0.6692307692307692}
Threshold: 0.55, Metrics: {'Accuracy': 0.7076923076923077, 'Sensitivity': 0.7076923076923077, 'Specificity': 0.7076923076923077, 'F1': 0.7076923076923077}
Threshold: 0.60, Metrics: {'Accuracy': 0.6923076923076923, 'Sensitivity': 0.6923076923076923, 'Specificity': 0.6923076923076923, 'F1': 0.6923076923076923}
Threshold: 0.65, Metrics: {'Accuracy': 0.5769230769230769, 'Sensitivity': 0.5769230769230769, 'Specificity': 0.5769230769230769, 'F1': 0.5769230769230769}
Threshold: 0.70, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384, 'F1': 0.5384615384615384}
Threshold: 0.75, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384, 'F1': 0.5384615384615384}
Threshold: 0.80, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384, 'F1': 0.5384615384615384}
Threshold: 0.85, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384, 'F1': 0.5384615384615384}
Threshold: 0.90, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384, 'F1': 0.5384615384615384}
Threshold: 0.95, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384, 'F1': 0.5384615384615384}
Threshold: 1.00, Metrics: {'Accuracy': 0.5384615384615384, 'Sensitivity': 0.5384615384615384, 'Specificity': 0.5384615384615384, 'F1': 0.5384615384615384}
SHAP Summary for XGBoost
```





Aggregated Test Set Metrics Across Seeds:

	accuracy	sensitivity	specificity	f1	roc_auc
0	0.661538	0.750000	0.585714	0.671642	0.754048
1	0.661538	0.750000	0.585714	0.671642	0.752619
2	0.661538	0.733333	0.600000	0.666667	0.760952
3	0.676923	0.733333	0.628571	0.676923	0.763571
4	0.669231	0.750000	0.600000	0.676692	0.757381
5	0.653846	0.733333	0.585714	0.661654	0.760714
6	0.669231	0.750000	0.600000	0.676692	0.766667
7	0.661538	0.733333	0.600000	0.666667	0.758810
8	0.661538	0.750000	0.585714	0.671642	0.761429
9	0.669231	0.750000	0.600000	0.676692	0.764286

Summary of Test Set Metrics (Mean, Standard Error, 95% Confidence Interval)

Accuracy: Mean = 0.665, SE = 0.002, 95% CI = [0.660, 0.669]

Sensitivity: Mean = 0.743, SE = 0.003, 95% CI = [0.737, 0.749]

Specificity: Mean = 0.597, SE = 0.004, 95% CI = [0.588, 0.607]

F1: Mean = 0.672, SE = 0.002, 95% CI = [0.668, 0.675]

Roc\_auc: Mean = 0.760, SE = 0.001, 95% CI = [0.757, 0.763]



```
# Set seeds for reproducibility
seed_value = 42
np.random.seed(seed_value)
random.seed(seed_value)
```

```

tf.random.set_seed(seed_value)

# Define a function to build, train, and evaluate a neural network model.
def evaluate_neural_network(X_train, y_train, X_test, y_test, threshold_list):
    # Initialize the neural network model with specified layers.
    model = Sequential([
        Dense(128, activation='relu', kernel_regularizer=l2(0.01), input_shape=(
        BatchNormalization(),
        Dropout(0.3),
        Dense(64, activation='relu', kernel_regularizer=l2(0.01)),
        BatchNormalization(),
        Dropout(0.3),
        Dense(1, activation='sigmoid')
    ])

    # Compile the model specifying the optimizer, loss function, and metrics.
    model.compile(optimizer='adam', loss='binary_crossentropy', metrics=['accura

    # Define callbacks for early stopping and learning rate reduction.
    early_stopping = EarlyStopping(monitor='val_loss', patience=10, restore_best
    reduce_lr = ReduceLROnPlateau(monitor='val_loss', factor=0.2, patience=5, mi

    # Train the model with a validation split, epochs, batch size, and callbacks
    model.fit(X_train, y_train, validation_split=0.2, epochs=30, batch_size=32,

    # Training set evaluation
    y_train_probs = model.predict(X_train).ravel()
    y_train_pred = (y_train_probs >= threshold_list[-1]).astype(int) # Use the
    train_acc = accuracy_score(y_train, y_train_pred)
    train_sens = sensitivity(y_train, y_train_pred)
    train_spec = specificity(y_train, y_train_pred)
    train_f1 = f1_score(y_train, y_train_pred)
    train_roc_auc = roc_auc_score(y_train, y_train_probs)

    # Test set evaluation for multiple thresholds
    y_probs = model.predict(X_test).ravel()
    thresholds_metrics = []

    # Calcular FPR, TPR e AUC
    fpr, tpr, thresholds = roc_curve(y_test, y_probs)
    roc_auc = auc(fpr, tpr)

    # Imprimir os valores de FPR, TPR e AUC de forma fácil de copiar
    print("\n--- Dados ROC para copiar ---")
    print("FPR =", fpr.tolist())
    print("TPR =", tpr.tolist())
    print("AUC =", roc_auc)
    print("--- Fim dos Dados ROC ---\n")

```

```

for threshold in threshold_list:
    y_pred = (y_probs >= threshold).astype(int)
    acc = accuracy_score(y_test, y_pred)
    sens = sensitivity(y_test, y_pred)
    spec = specificity(y_test, y_pred)
    f1 = f1_score(y_test, y_pred)
    thresholds_metrics.append({
        'threshold': threshold,
        'accuracy': acc,
        'sensitivity': sens,
        'specificity': spec,
        'f1_score': f1
    })

# Print training set metrics
print(f"Training - Accuracy: {train_acc:.4f}, Sensitivity: {train_sens:.4f},

# Test set ROC AUC
test_roc_auc = roc_auc_score(y_test, y_probs)

# Print test set metrics for each threshold
for metrics in thresholds_metrics:
    print(f"Threshold: {metrics['threshold']:.2f}, Accuracy: {metrics['accur

return model, train_acc, train_sens, train_spec, train_f1, train_roc_auc, te

# Plotting functions for confusion matrix and ROC curve visualization.
def plot_confusion_matrix(y_true, y_pred):
    matrix = confusion_matrix(y_true, y_pred)
    sns.heatmap(matrix, annot=True, fmt='d', cmap='Blues',
                 xticklabels=['Predicted Success', 'Predicted Failure'],
                 yticklabels=['Actual Success', 'Actual Failure'])
    plt.title('Confusion Matrix Neural Network')
    plt.show()

def plot_roc_curve(y_true, y_probs):
    fpr, tpr, thresholds = roc_curve(y_true, y_probs)
    roc_auc = auc(fpr, tpr)

    plt.figure()
    plt.plot(fpr, tpr, color='darkorange', lw=2, label=f'ROC curve (area = {roc_
    plt.plot([0, 1], [0, 1], color='navy', lw=2, linestyle='--')
    plt.xlim([0.0, 1.0])
    plt.ylim([0.0, 1.05])
    plt.xlabel('False Positive Rate')
    plt.ylabel('True Positive Rate')
    plt.title('Receiver Operating Characteristic Neural Network')
    plt.legend(loc='lower right')

```

```
plt.legend(loc='lower right',
plt.show()
```

```
# Main function where the evaluation process is initiated.
```

```
def main(X_train, y_train, X_test, y_test):
```

```
    # Define a list of thresholds to evaluate
```

```
    threshold_list = np.arange(0.1, 1.05, 0.05)
```

```
    aggregated_metrics = []
```

```
    for seed_value in range(40, 50):
```

```
        np.random.seed(seed_value)
```

```
        random.seed(seed_value)
```

```
        tf.random.set_seed(seed_value)
```

```
    # Evaluate the neural network model and store its performance metrics.
```

```
    model, train_acc, train_sens, train_spec, train_f1, train_roc_auc, test_
```

```
    # Choose a threshold for detailed evaluation
```

```
    chosen_threshold = 0.45
```

```
    y_test_probs = model.predict(X_test).ravel()
```

```
    y_test_pred = (y_test_probs >= chosen_threshold).astype(int)
```

```
    # Calculate and print the metrics for the chosen threshold
```

```
    chosen_acc = accuracy_score(y_test, y_test_pred)
```

```
    chosen_sens = sensitivity(y_test, y_test_pred)
```

```
    chosen_spec = specificity(y_test, y_test_pred)
```

```
    chosen_f1 = f1_score(y_test, y_test_pred)
```

```
    print(f"\nMetrics for chosen threshold {chosen_threshold}:")
```

```
    print(f"Accuracy: {chosen_acc:.4f}, Sensitivity: {chosen_sens:.4f}, Spec
```

```
    # Append the chosen test metrics for aggregation
```

```
    test_metrics = {
```

```
        "accuracy": chosen_acc,
```

```
        "sensitivity": chosen_sens,
```

```
        "specificity": chosen_spec,
```

```
        "f1": chosen_f1,
```

```
        "roc_auc": test_roc_auc
```

```
    }
```

```
    aggregated_metrics.append(test_metrics)
```

```
    # Plotting functions assuming they are defined elsewhere
```

```
    plot_confusion_matrix(y_test, y_test_pred)
```

```
    plot_roc_curve(y_test, y_test_probs)
```

```
# Aggregate results across seeds
```

```
results_df = pd.DataFrame(aggregated_metrics)
```

```
n = len(results_df)
```

```
print("\nAggregated Test Set Metrics Across Seeds:")
```

```

print(results_df)

# Compute mean, standard error, and 95% confidence interval for each metric
def summarize_metric(metric_values):
    mean_val = metric_values.mean()
    std_val = metric_values.std(ddof=1)
    se = std_val / np.sqrt(n)
    t_crit = stats.t.ppf(0.975, df=n - 1)
    ci_lower = mean_val - t_crit * se
    ci_upper = mean_val + t_crit * se
    return mean_val, se, (ci_lower, ci_upper)

metrics_summary = {}
for metric in results_df.columns:
    mean_val, se, ci = summarize_metric(results_df[metric])
    metrics_summary[metric] = {
        "Mean": mean_val,
        "Standard Error": se,
        "95% CI": ci
    }

print("\nSummary of Test Set Metrics (Mean, Standard Error, 95% Confidence I
for metric, summary in metrics_summary.items():
    print(f"{metric.capitalize()}: Mean = {summary['Mean']:.4f}, SE = {summa

# Entry point of the script to run the main function.
if __name__ == '__main__':
    main(X_train, y_train, X_test, y_test)























```

```

➡ /usr/local/lib/python3.11/dist-packages/keras/src/layers/core/dense.py:87:
    super().__init__(activity_regularizer=activity_regularizer, **kwargs)
Epoch 1/30
13/13 ————— 4s 48ms/step - accuracy: 0.5086 - loss: 2.0989 -
Epoch 2/30
13/13 ————— 0s 16ms/step - accuracy: 0.6734 - loss: 1.8383 -
Epoch 3/30
13/13 ————— 0s 15ms/step - accuracy: 0.7051 - loss: 1.7589 -
Epoch 4/30
13/13 ————— 0s 14ms/step - accuracy: 0.6936 - loss: 1.7038 -
Epoch 5/30
13/13 ————— 0s 15ms/step - accuracy: 0.7085 - loss: 1.6292 -
Epoch 6/30
13/13 ————— 0s 17ms/step - accuracy: 0.7388 - loss: 1.5911 -
Epoch 7/30
13/13 ————— 0s 15ms/step - accuracy: 0.7382 - loss: 1.4999 -
Epoch 8/30
13/13 ————— 0s 16ms/step - accuracy: 0.7651 - loss: 1.4798 -
Epoch 9/30
13/13 ————— 0s 12ms/step - accuracy: 0.7644 - loss: 1.4070 -

```

```

Epoch 10/30
13/13  0s 9ms/step - accuracy: 0.7694 - loss: 1.3464 -
Epoch 11/30
13/13  0s 9ms/step - accuracy: 0.7153 - loss: 1.3720 -
Epoch 12/30
13/13  0s 9ms/step - accuracy: 0.7501 - loss: 1.2866 -
Epoch 13/30
13/13  0s 9ms/step - accuracy: 0.7415 - loss: 1.2845 -
Epoch 14/30
13/13  0s 10ms/step - accuracy: 0.7749 - loss: 1.2227 -
Epoch 15/30
13/13  0s 10ms/step - accuracy: 0.7625 - loss: 1.2023 -
Epoch 16/30
13/13  0s 12ms/step - accuracy: 0.7657 - loss: 1.2051 -
Epoch 17/30
13/13  0s 9ms/step - accuracy: 0.7925 - loss: 1.0891 -
Epoch 18/30
13/13  0s 9ms/step - accuracy: 0.7870 - loss: 1.0877 -
Epoch 19/30
13/13  0s 11ms/step - accuracy: 0.7871 - loss: 1.1080 -
Epoch 20/30
13/13  0s 13ms/step - accuracy: 0.7894 - loss: 1.0091 -
Epoch 21/30
13/13  0s 10ms/step - accuracy: 0.7959 - loss: 1.0219 -
Epoch 22/30
13/13  0s 10ms/step - accuracy: 0.7777 - loss: 1.0230 -
Epoch 23/30
13/13  0s 12ms/step - accuracy: 0.8096 - loss: 0.9915 -
Epoch 24/30
13/13  0s 10ms/step - accuracy: 0.8145 - loss: 0.9585 -
Epoch 25/30
13/13  0s 10ms/step - accuracy: 0.8315 - loss: 0.9332 -
Epoch 26/30
13/13  0s 9ms/step - accuracy: 0.8061 - loss: 0.9258 -
Epoch 27/30
13/13  0s 9ms/step - accuracy: 0.8106 - loss: 0.9196 -
Epoch 28/30
13/13  0s 9ms/step - accuracy: 0.7950 - loss: 0.8941 -
Epoch 29/30
13/13  0s 13ms/step - accuracy: 0.8474 - loss: 0.8310 -
Epoch 30/30
13/13  0s 9ms/step - accuracy: 0.8493 - loss: 0.8405 -
16/16  0s 7ms/step
5/5  0s 6ms/step

```

--- Dados ROC para copiar ---

FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.0285714


TPR = [0.0, 0.016666666666666666, 0.03333333333333333, 0.05, 0.183333333333

AUC = 0.7254761904761905

--- Fim dos Dados ROC ---

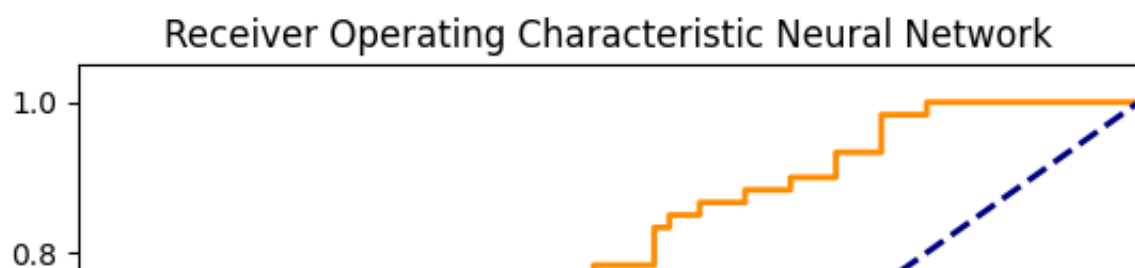
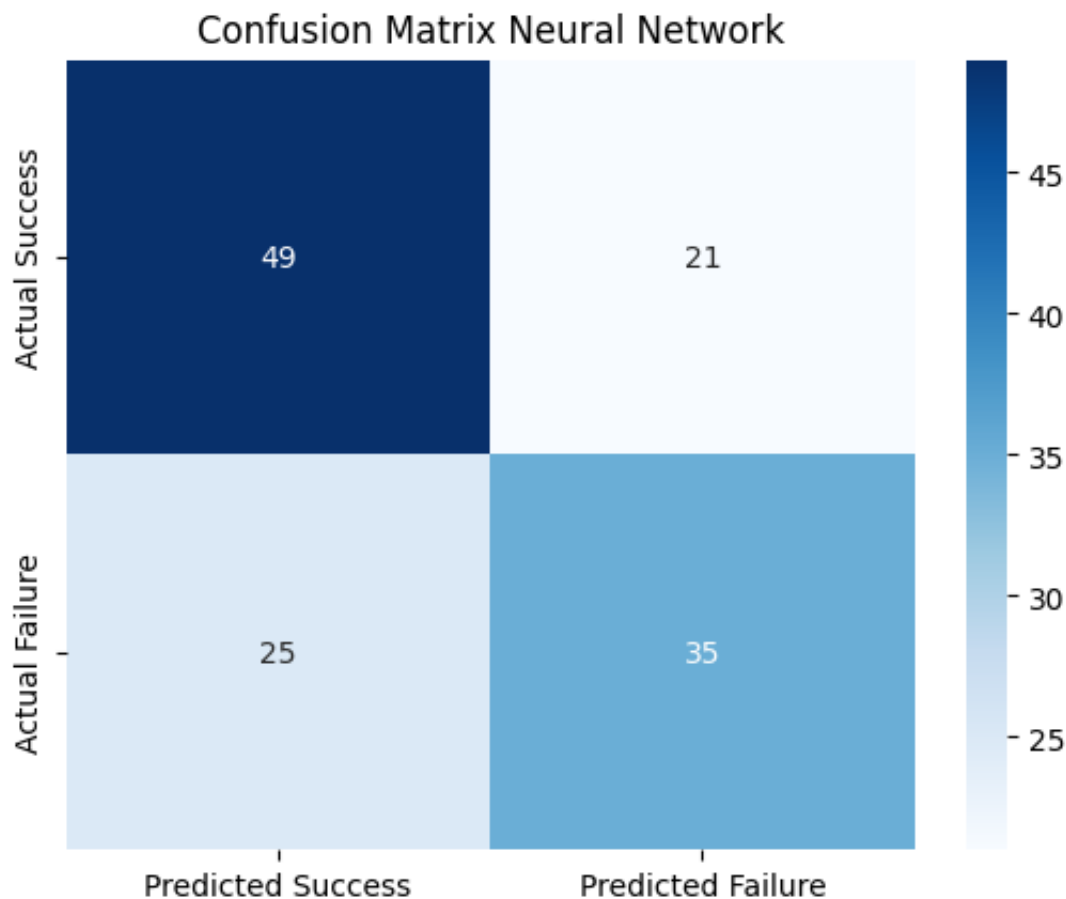
Training - Accuracy: 0.5049, Sensitivity: 0.0000, Specificity: 1.0000, F1:  
Threshold: 0.10, Accuracy: 0.5154, Sensitivity: 1.0000, Specificity: 0.1000  
Threshold: 0.15, Accuracy: 0.5462, Sensitivity: 1.0000, Specificity: 0.1571

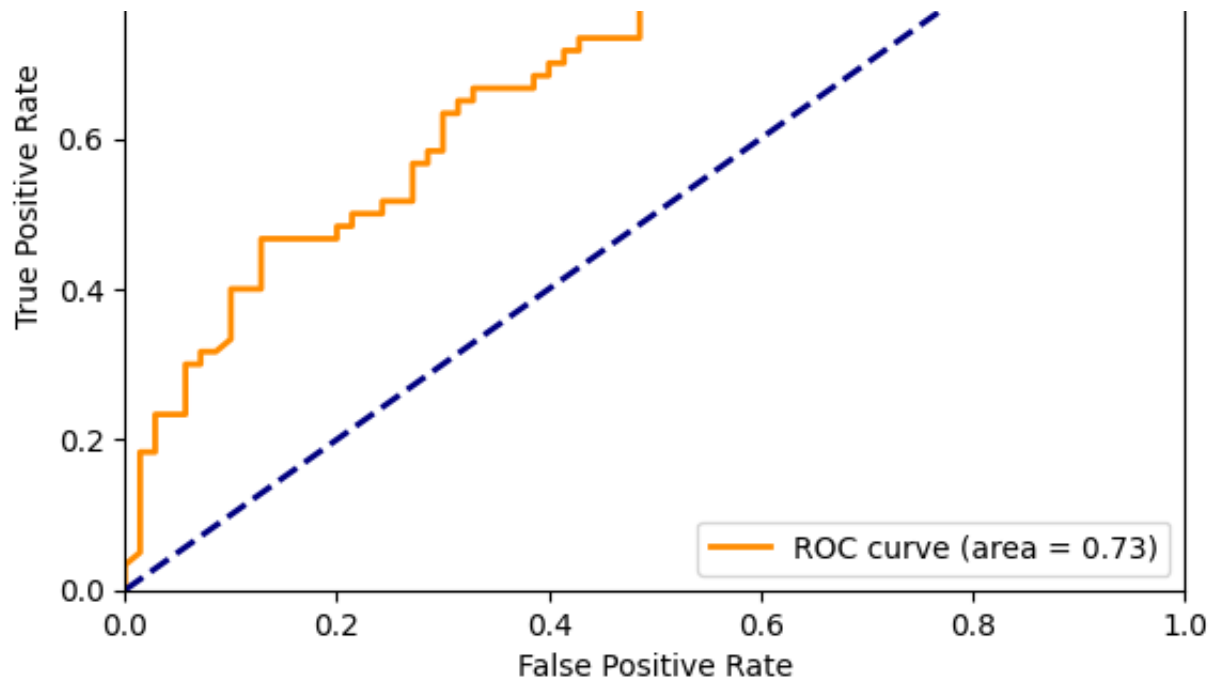
Threshold: 0.20, Accuracy: 0.5846, Sensitivity: 0.9833, Specificity: 0.2429  
Threshold: 0.25, Accuracy: 0.5923, Sensitivity: 0.9000, Specificity: 0.3286  
Threshold: 0.30, Accuracy: 0.6231, Sensitivity: 0.8500, Specificity: 0.4286  
Threshold: 0.35, Accuracy: 0.6154, Sensitivity: 0.7833, Specificity: 0.4714  
Threshold: 0.40, Accuracy: 0.6385, Sensitivity: 0.7167, Specificity: 0.5714  
Threshold: 0.45, Accuracy: 0.6462, Sensitivity: 0.5833, Specificity: 0.7000  
Threshold: 0.50, Accuracy: 0.6538, Sensitivity: 0.4667, Specificity: 0.8143  
Threshold: 0.55, Accuracy: 0.6846, Sensitivity: 0.4667, Specificity: 0.8714  
Threshold: 0.60, Accuracy: 0.6692, Sensitivity: 0.4000, Specificity: 0.9000  
Threshold: 0.65, Accuracy: 0.6385, Sensitivity: 0.3167, Specificity: 0.9143  
Threshold: 0.70, Accuracy: 0.6385, Sensitivity: 0.2833, Specificity: 0.9429  
Threshold: 0.75, Accuracy: 0.6154, Sensitivity: 0.2000, Specificity: 0.9714  
Threshold: 0.80, Accuracy: 0.5769, Sensitivity: 0.1000, Specificity: 0.9857  
Threshold: 0.85, Accuracy: 0.5538, Sensitivity: 0.0500, Specificity: 0.9857  
Threshold: 0.90, Accuracy: 0.5385, Sensitivity: 0.0000, Specificity: 1.0000  
Threshold: 0.95, Accuracy: 0.5385, Sensitivity: 0.0000, Specificity: 1.0000  
Threshold: 1.00, Accuracy: 0.5385, Sensitivity: 0.0000, Specificity: 1.0000

5/5  0s 7ms/step

Metrics for chosen threshold 0.45:

Accuracy: 0.6462, Sensitivity: 0.5833, Specificity: 0.7000, F1: 0.6034, ROC





Epoch 1/30

```
/usr/local/lib/python3.11/dist-packages/keras/src/layers/core/dense.py:87:
super().__init__(activity_regularizer=activity_regularizer, **kwargs)
```

13/13 ————— 3s 37ms/step - accuracy: 0.5119 - loss: 2.1441 -

Epoch 2/30

13/13 ————— 0s 9ms/step - accuracy: 0.6365 - loss: 1.8846 -

Epoch 3/30

13/13 ————— 0s 9ms/step - accuracy: 0.6955 - loss: 1.7827 -

Epoch 4/30

13/13 ————— 0s 12ms/step - accuracy: 0.6312 - loss: 1.7600 -

Epoch 5/30

13/13 ————— 0s 10ms/step - accuracy: 0.7123 - loss: 1.6380 -

Epoch 6/30

13/13 ————— 0s 10ms/step - accuracy: 0.6744 - loss: 1.6064 -

Epoch 7/30

13/13 ————— 0s 10ms/step - accuracy: 0.7121 - loss: 1.5266 -

Epoch 8/30

13/13 ————— 0s 9ms/step - accuracy: 0.6523 - loss: 1.5357 -

Epoch 9/30

13/13 ————— 0s 14ms/step - accuracy: 0.7204 - loss: 1.4699 -

Epoch 10/30

13/13 ————— 0s 16ms/step - accuracy: 0.7516 - loss: 1.3927 -

Epoch 11/30

13/13 ————— 0s 17ms/step - accuracy: 0.7398 - loss: 1.3899 -

Epoch 12/30

13/13 ————— 0s 14ms/step - accuracy: 0.7524 - loss: 1.3142 -

Epoch 13/30

13/13 ————— 0s 16ms/step - accuracy: 0.7408 - loss: 1.3336 -

Epoch 14/30

13/13 ————— 0s 16ms/step - accuracy: 0.7366 - loss: 1.2775 -

Epoch 15/30

13/13 ————— 0s 16ms/step - accuracy: 0.7621 - loss: 1.2403 -

Epoch 16/30

13/13 ————— 0s 16ms/step - accuracy: 0.7639 - loss: 1.2047 -

Epoch 17/30



```

13/13 _____ 0s 19ms/step - accuracy: 0.7362 - loss: 1.1868 -
Epoch 18/30
13/13 _____ 0s 16ms/step - accuracy: 0.6972 - loss: 1.1922 -
Epoch 19/30
13/13 _____ 0s 9ms/step - accuracy: 0.7522 - loss: 1.1494 -
Epoch 20/30
13/13 _____ 0s 9ms/step - accuracy: 0.7733 - loss: 1.0939 -
Epoch 21/30
13/13 _____ 0s 10ms/step - accuracy: 0.7748 - loss: 1.0970 -
Epoch 22/30
13/13 _____ 0s 9ms/step - accuracy: 0.7701 - loss: 1.0659 -
Epoch 23/30
13/13 _____ 0s 9ms/step - accuracy: 0.8240 - loss: 0.9895 -
Epoch 24/30
13/13 _____ 0s 10ms/step - accuracy: 0.7854 - loss: 1.0312 -
Epoch 25/30
13/13 _____ 0s 9ms/step - accuracy: 0.8032 - loss: 1.0126 -
Epoch 26/30
13/13 _____ 0s 12ms/step - accuracy: 0.8176 - loss: 0.9315 -
Epoch 27/30
13/13 _____ 0s 9ms/step - accuracy: 0.8100 - loss: 0.9266 -
Epoch 28/30
13/13 _____ 0s 13ms/step - accuracy: 0.7840 - loss: 0.9528 -
Epoch 29/30
13/13 _____ 0s 11ms/step - accuracy: 0.7987 - loss: 0.9416 -
Epoch 30/30
13/13 _____ 0s 11ms/step - accuracy: 0.7958 - loss: 0.8942 -
16/16 _____ 0s 8ms/step
5/5 _____ 0s 8ms/step

```

--- Dados ROC para copiar ---

FPR = [0.0, 0.0, 0.02857142857142857, 0.02857142857142857, 0.04285714285714

TPR = [0.0, 0.016666666666666666, 0.016666666666666666, 0.033333333333333333

AUC = 0.7926190476190477

--- Fim dos Dados ROC ---

```

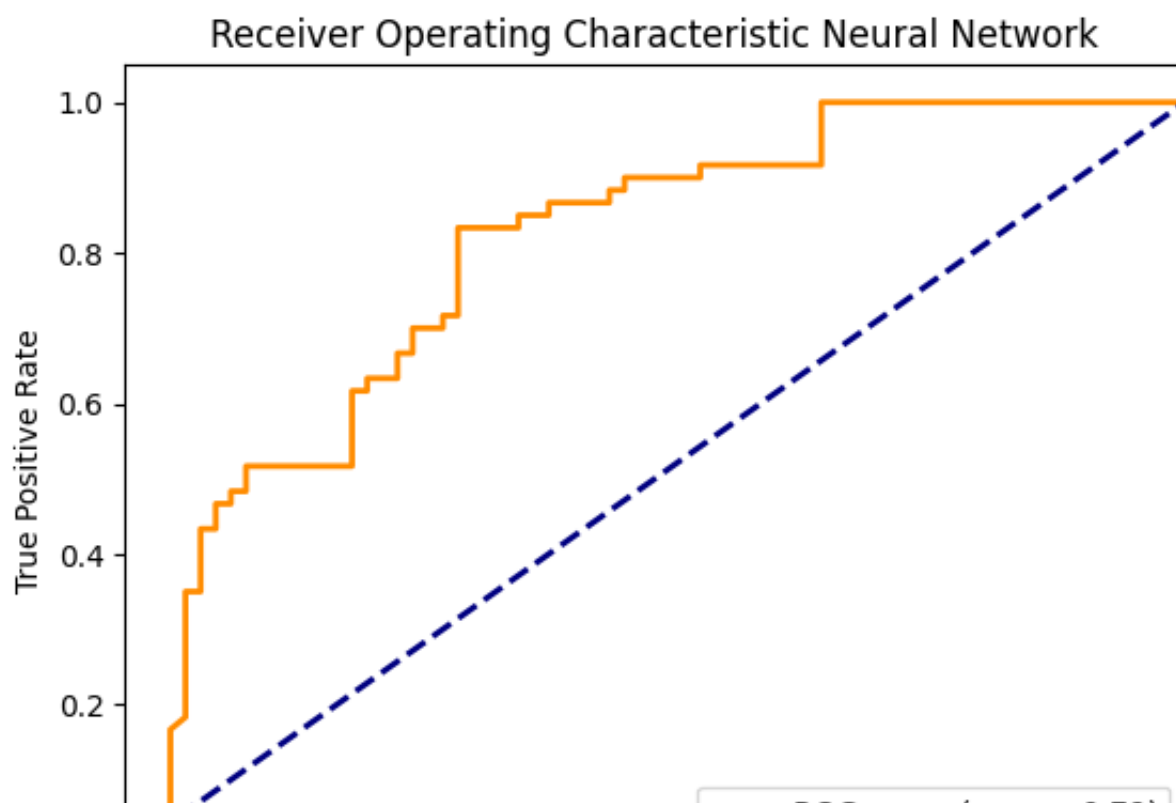
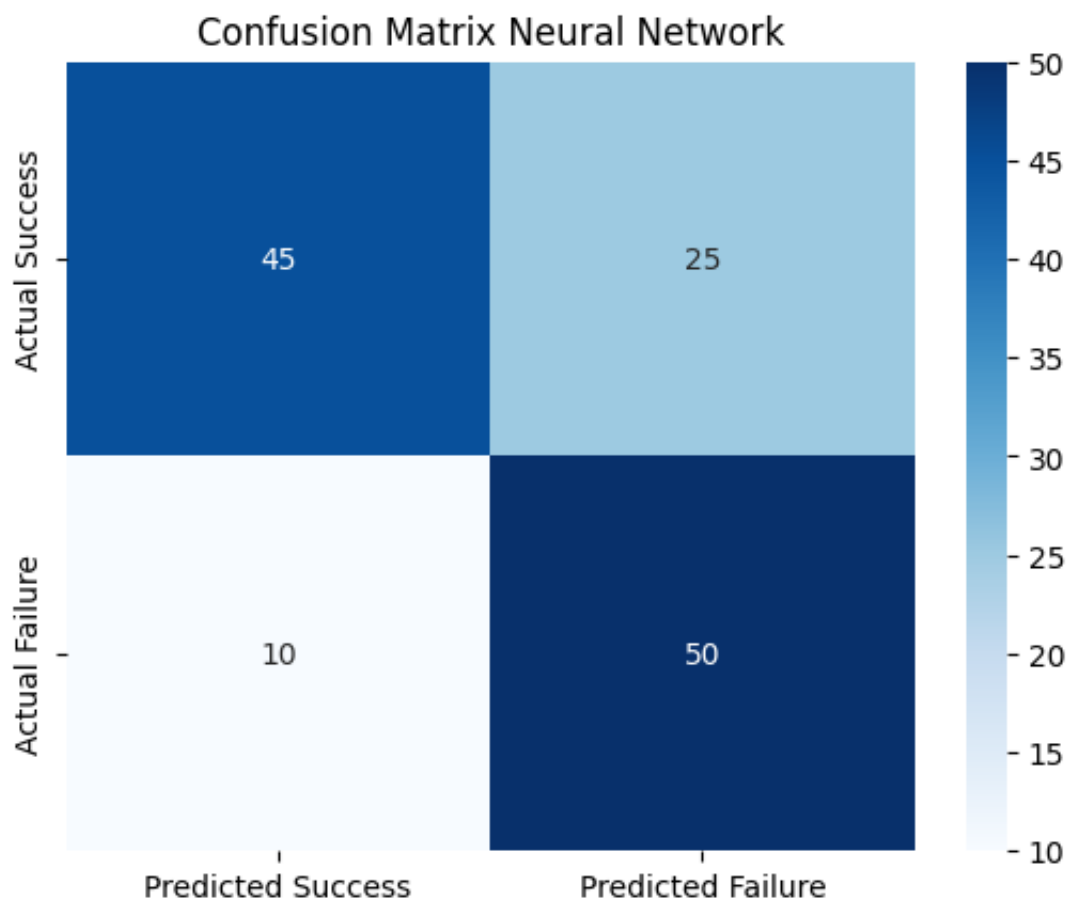
Training - Accuracy: 0.5049, Sensitivity: 0.0000, Specificity: 1.0000, F1:
Threshold: 0.10, Accuracy: 0.4923, Sensitivity: 1.0000, Specificity: 0.0571
Threshold: 0.15, Accuracy: 0.5462, Sensitivity: 1.0000, Specificity: 0.1571
Threshold: 0.20, Accuracy: 0.5615, Sensitivity: 1.0000, Specificity: 0.1857
Threshold: 0.25, Accuracy: 0.6231, Sensitivity: 1.0000, Specificity: 0.3000
Threshold: 0.30, Accuracy: 0.6154, Sensitivity: 0.9167, Specificity: 0.3571
Threshold: 0.35, Accuracy: 0.6692, Sensitivity: 0.9000, Specificity: 0.4714
Threshold: 0.40, Accuracy: 0.6923, Sensitivity: 0.8667, Specificity: 0.5429
Threshold: 0.45, Accuracy: 0.7308, Sensitivity: 0.8333, Specificity: 0.6429
Threshold: 0.50, Accuracy: 0.7231, Sensitivity: 0.7667, Specificity: 0.6857
Threshold: 0.55, Accuracy: 0.7154, Sensitivity: 0.7000, Specificity: 0.7286
Threshold: 0.60, Accuracy: 0.7000, Sensitivity: 0.6167, Specificity: 0.7714
Threshold: 0.65, Accuracy: 0.6615, Sensitivity: 0.5167, Specificity: 0.7857
Threshold: 0.70, Accuracy: 0.7000, Sensitivity: 0.4833, Specificity: 0.8857
Threshold: 0.75, Accuracy: 0.6846, Sensitivity: 0.4000, Specificity: 0.9286
Threshold: 0.80, Accuracy: 0.6308, Sensitivity: 0.2667, Specificity: 0.9429
Threshold: 0.85, Accuracy: 0.5462, Sensitivity: 0.0667, Specificity: 0.9571
Threshold: 0.90, Accuracy: 0.5385, Sensitivity: 0.0167, Specificity: 0.9857

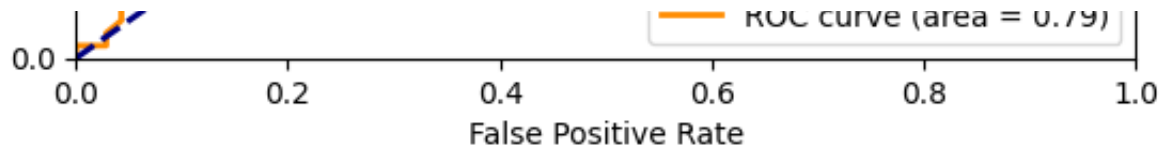
```

Threshold: 0.95, Accuracy: 0.5385, Sensitivity: 0.0000, Specificity: 1.0000  
Threshold: 1.00, Accuracy: 0.5385, Sensitivity: 0.0000, Specificity: 1.0000  
5/5 ————— 0s 7ms/step

Metrics for chosen threshold 0.45:

Accuracy: 0.7308, Sensitivity: 0.8333, Specificity: 0.6429, F1: 0.7407, ROC





Epoch 1/30

```
/usr/local/lib/python3.11/dist-packages/keras/src/layers/core/dense.py:87:
    super().__init__(activity_regularizer=activity_regularizer, **kwargs)
```

13/13 ██████████ 3s 32ms/step - accuracy: 0.5682 - loss: 2.1212 -

Epoch 2/30

13/13 ██████████ 0s 13ms/step - accuracy: 0.6392 - loss: 1.8197 -

Epoch 3/30

13/13 ██████████ 0s 12ms/step - accuracy: 0.6403 - loss: 1.7688 -

Epoch 4/30

13/13 ██████████ 0s 10ms/step - accuracy: 0.6855 - loss: 1.6640 -

Epoch 5/30

13/13 ██████████ 0s 10ms/step - accuracy: 0.6925 - loss: 1.6139 -

Epoch 6/30

13/13 ██████████ 0s 11ms/step - accuracy: 0.7221 - loss: 1.5381 -

Epoch 7/30

13/13 ██████████ 0s 10ms/step - accuracy: 0.7384 - loss: 1.5077 -

Epoch 8/30

13/13 ██████████ 0s 10ms/step - accuracy: 0.7065 - loss: 1.5191 -

Epoch 9/30

13/13 ██████████ 0s 10ms/step - accuracy: 0.7399 - loss: 1.4094 -

Epoch 10/30

13/13 ██████████ 0s 10ms/step - accuracy: 0.7210 - loss: 1.3922 -

Epoch 11/30

13/13 ██████████ 0s 9ms/step - accuracy: 0.7357 - loss: 1.3954 -

Epoch 12/30

13/13 ██████████ 0s 9ms/step - accuracy: 0.7794 - loss: 1.2919 -

Epoch 13/30

13/13 ██████████ 0s 12ms/step - accuracy: 0.7450 - loss: 1.2893 -

Epoch 14/30

13/13 ██████████ 0s 11ms/step - accuracy: 0.7822 - loss: 1.2232 -

Epoch 15/30

13/13 ██████████ 0s 10ms/step - accuracy: 0.8046 - loss: 1.1764 -

Epoch 16/30

13/13 ██████████ 0s 10ms/step - accuracy: 0.7271 - loss: 1.2373 -

Epoch 17/30

13/13 ██████████ 0s 14ms/step - accuracy: 0.8297 - loss: 1.1086 -

Epoch 18/30

13/13 ██████████ 0s 16ms/step - accuracy: 0.7667 - loss: 1.1388 -

Epoch 19/30

13/13 ██████████ 0s 18ms/step - accuracy: 0.7962 - loss: 1.0652 -

Epoch 20/30

13/13 ██████████ 0s 15ms/step - accuracy: 0.7900 - loss: 1.0504 -

Epoch 21/30

13/13 ██████████ 0s 18ms/step - accuracy: 0.7993 - loss: 1.0368 -

Epoch 22/30

13/13 ██████████ 0s 17ms/step - accuracy: 0.7766 - loss: 1.0408 -

Epoch 23/30

13/13 ██████████ 0s 19ms/step - accuracy: 0.8018 - loss: 0.9764 -

Epoch 24/30

13/13 ██████████ 0s 17ms/step - accuracy: 0.8243 - loss: 0.9573 -

```

13/13 ----- 0s 17ms/step - accuracy: 0.8167 - loss: 0.9637 -
Epoch 25/30
13/13 ----- 0s 17ms/step - accuracy: 0.8167 - loss: 0.9637 -
Epoch 26/30
13/13 ----- 0s 18ms/step - accuracy: 0.8128 - loss: 0.9058 -
Epoch 27/30
13/13 ----- 0s 11ms/step - accuracy: 0.8197 - loss: 0.9272 -
Epoch 28/30
13/13 ----- 0s 11ms/step - accuracy: 0.8244 - loss: 0.8984 -
Epoch 29/30
13/13 ----- 0s 13ms/step - accuracy: 0.8519 - loss: 0.8512 -
Epoch 30/30
13/13 ----- 0s 10ms/step - accuracy: 0.8293 - loss: 0.8398 -
16/16 ----- 0s 7ms/step
5/5 ----- 0s 7ms/step

```

--- Dados ROC para copiar ---

```

FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.0285714
TPR = [0.0, 0.016666666666666666, 0.05, 0.06666666666666667, 0.13333333333333
AUC = 0.7392857142857143

```

--- Fim dos Dados ROC ---

```

Training - Accuracy: 0.5049, Sensitivity: 0.0000, Specificity: 1.0000, F1:
Threshold: 0.10, Accuracy: 0.5000, Sensitivity: 1.0000, Specificity: 0.0714
Threshold: 0.15, Accuracy: 0.5385, Sensitivity: 1.0000, Specificity: 0.1429
Threshold: 0.20, Accuracy: 0.5615, Sensitivity: 1.0000, Specificity: 0.1857
Threshold: 0.25, Accuracy: 0.5846, Sensitivity: 0.9500, Specificity: 0.2714
Threshold: 0.30, Accuracy: 0.5923, Sensitivity: 0.9333, Specificity: 0.3000
Threshold: 0.35, Accuracy: 0.6077, Sensitivity: 0.9167, Specificity: 0.3429
Threshold: 0.40, Accuracy: 0.6154, Sensitivity: 0.8167, Specificity: 0.4429
Threshold: 0.45, Accuracy: 0.6385, Sensitivity: 0.8167, Specificity: 0.4857
Threshold: 0.50, Accuracy: 0.6769, Sensitivity: 0.7833, Specificity: 0.5857
Threshold: 0.55, Accuracy: 0.6615, Sensitivity: 0.6667, Specificity: 0.6571
Threshold: 0.60, Accuracy: 0.6385, Sensitivity: 0.5833, Specificity: 0.6857
Threshold: 0.65, Accuracy: 0.6615, Sensitivity: 0.5333, Specificity: 0.7714
Threshold: 0.70, Accuracy: 0.6615, Sensitivity: 0.4500, Specificity: 0.8429
Threshold: 0.75, Accuracy: 0.6538, Sensitivity: 0.3667, Specificity: 0.9000
Threshold: 0.80, Accuracy: 0.6154, Sensitivity: 0.2333, Specificity: 0.9429
Threshold: 0.85, Accuracy: 0.5846, Sensitivity: 0.1333, Specificity: 0.9714
Threshold: 0.90, Accuracy: 0.5692, Sensitivity: 0.0833, Specificity: 0.9857
Threshold: 0.95, Accuracy: 0.5462, Sensitivity: 0.0167, Specificity: 1.0000
Threshold: 1.00, Accuracy: 0.5385, Sensitivity: 0.0000, Specificity: 1.0000
5/5 ----- 0s 7ms/step

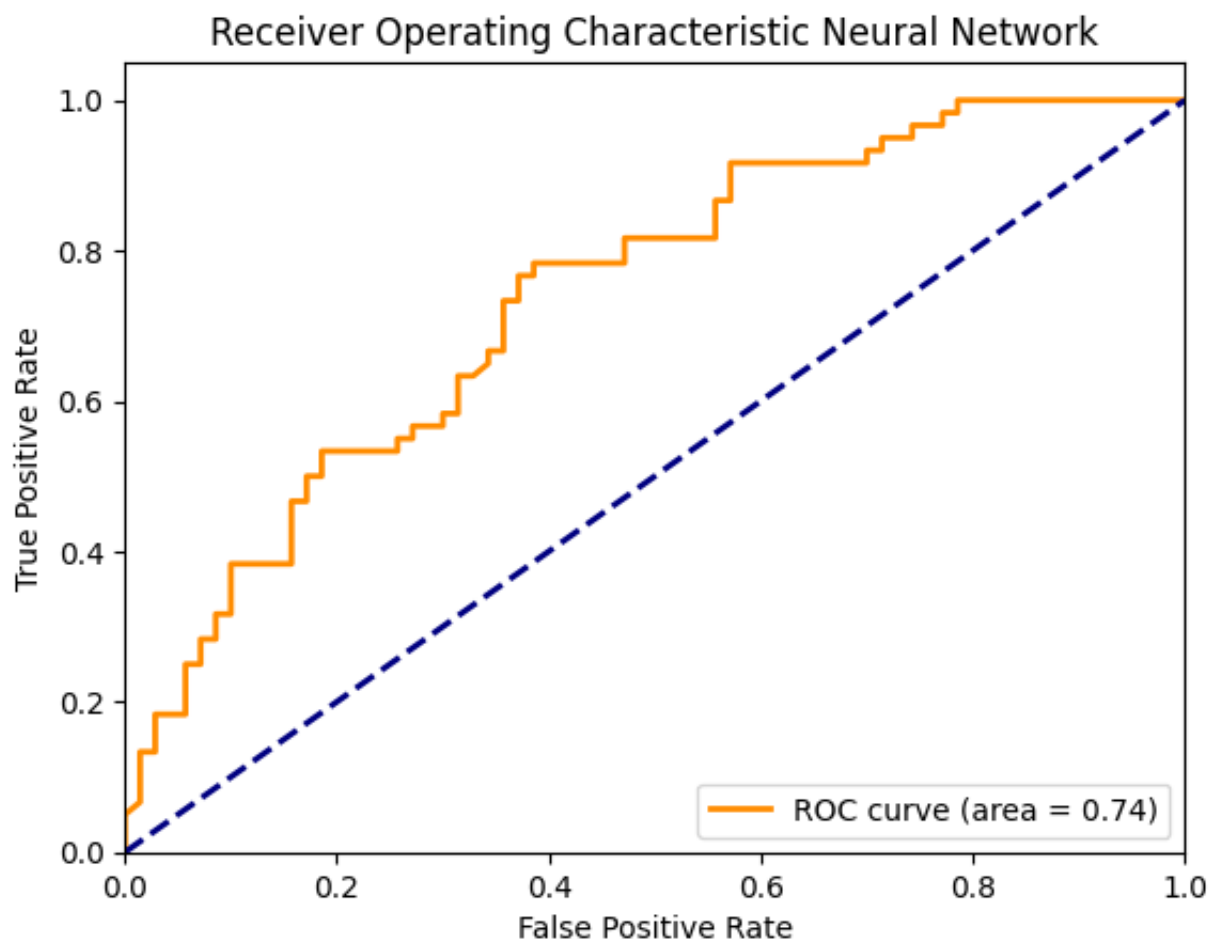
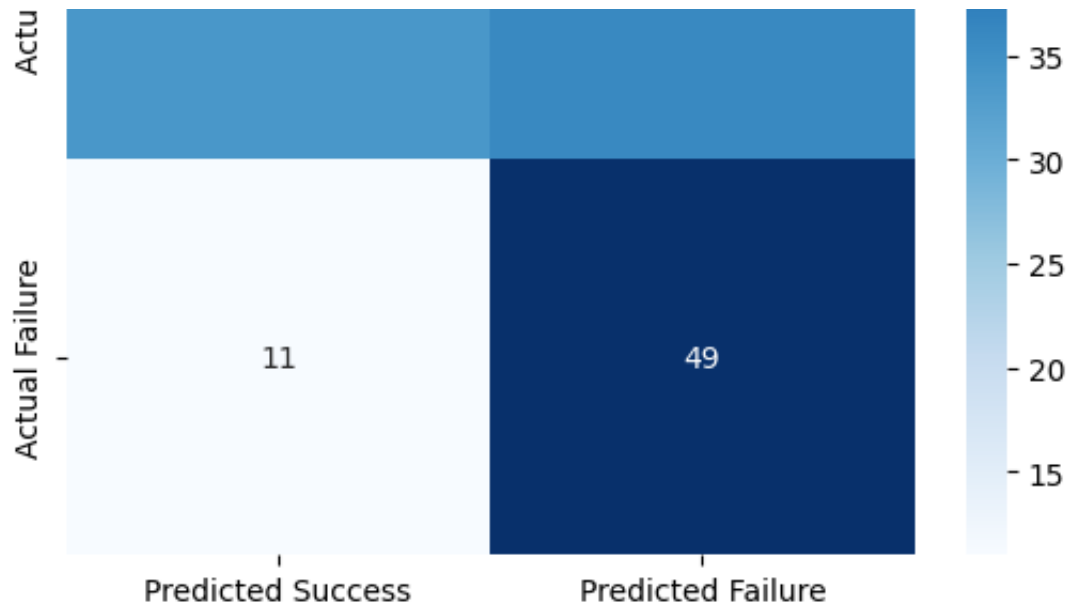
```

Metrics for chosen threshold 0.45:

Accuracy: 0.6385, Sensitivity: 0.8167, Specificity: 0.4857, F1: 0.6759, ROC

Confusion Matrix Neural Network





Epoch 1/30

```
/usr/local/lib/python3.11/dist-packages/keras/src/layers/core/dense.py:87:
    super().__init__(activity_regularizer=activity_regularizer, **kwargs)
```

```
13/13 ───────────────── 3s 33ms/step - accuracy: 0.5418 - loss: 2.0681 -
```

Epoch 2/30

```
13/13 ───────────────── 0s 9ms/step - accuracy: 0.5981 - loss: 1.9176 -
```





















Epoch 3/30

```
13/13 ───────────────── 0s 10ms/step - accuracy: 0.6430 - loss: 1.7329 -
```

Epoch 4/30

```
13/13 ───────────────── 0s 9ms/step - accuracy: 0.6618 - loss: 1.6970 -
```

```

Epoch 5/30
13/13  0s 9ms/step - accuracy: 0.6712 - loss: 1.6605 -
Epoch 6/30
13/13  0s 10ms/step - accuracy: 0.7124 - loss: 1.5369 -
Epoch 7/30
13/13  0s 10ms/step - accuracy: 0.6727 - loss: 1.5878 -
Epoch 8/30
13/13  0s 10ms/step - accuracy: 0.7574 - loss: 1.4031 -
Epoch 9/30
13/13  0s 12ms/step - accuracy: 0.7446 - loss: 1.3933 -
Epoch 10/30
13/13  0s 10ms/step - accuracy: 0.6992 - loss: 1.3609 -
Epoch 11/30
13/13  0s 13ms/step - accuracy: 0.7376 - loss: 1.3128 -
Epoch 12/30
13/13  0s 14ms/step - accuracy: 0.7924 - loss: 1.2587 -
Epoch 13/30
13/13  0s 10ms/step - accuracy: 0.7457 - loss: 1.2373 -
Epoch 14/30
13/13  0s 11ms/step - accuracy: 0.7540 - loss: 1.1990 -
Epoch 15/30
13/13  0s 11ms/step - accuracy: 0.7798 - loss: 1.1675 -
Epoch 16/30
13/13  0s 11ms/step - accuracy: 0.7645 - loss: 1.1218 -
Epoch 17/30
13/13  0s 10ms/step - accuracy: 0.7941 - loss: 1.0942 -
Epoch 18/30
13/13  0s 10ms/step - accuracy: 0.8207 - loss: 1.0490 -
Epoch 19/30
13/13  0s 10ms/step - accuracy: 0.8351 - loss: 1.0368 -
Epoch 20/30
13/13  0s 10ms/step - accuracy: 0.8225 - loss: 0.9981 -
Epoch 21/30
13/13  0s 15ms/step - accuracy: 0.7919 - loss: 1.0126 -
Epoch 22/30
13/13  0s 17ms/step - accuracy: 0.8204 - loss: 0.9708 -
Epoch 23/30
13/13  0s 17ms/step - accuracy: 0.8341 - loss: 0.9103 -
Epoch 24/30
13/13  0s 15ms/step - accuracy: 0.8468 - loss: 0.8920 -
Epoch 25/30
13/13  0s 15ms/step - accuracy: 0.8594 - loss: 0.8561 -
Epoch 26/30
13/13  0s 14ms/step - accuracy: 0.8617 - loss: 0.8770 -
Epoch 27/30
13/13  0s 14ms/step - accuracy: 0.8505 - loss: 0.8414 -
Epoch 28/30
13/13  0s 17ms/step - accuracy: 0.8377 - loss: 0.8215 -
Epoch 29/30
13/13  0s 17ms/step - accuracy: 0.8561 - loss: 0.8078 -
Epoch 30/30
13/13  0s 16ms/step - accuracy: 0.8695 - loss: 0.7752 -
16/16  0s 8ms/step
5/5  0s 7ms/step

```

--- Dados ROC para copiar ---

FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.0285714

TPR = [0.0, 0.016666666666666666, 0.066666666666666667, 0.06666666666666667,

AUC = 0.7647619047619048

--- Fim dos Dados ROC ---

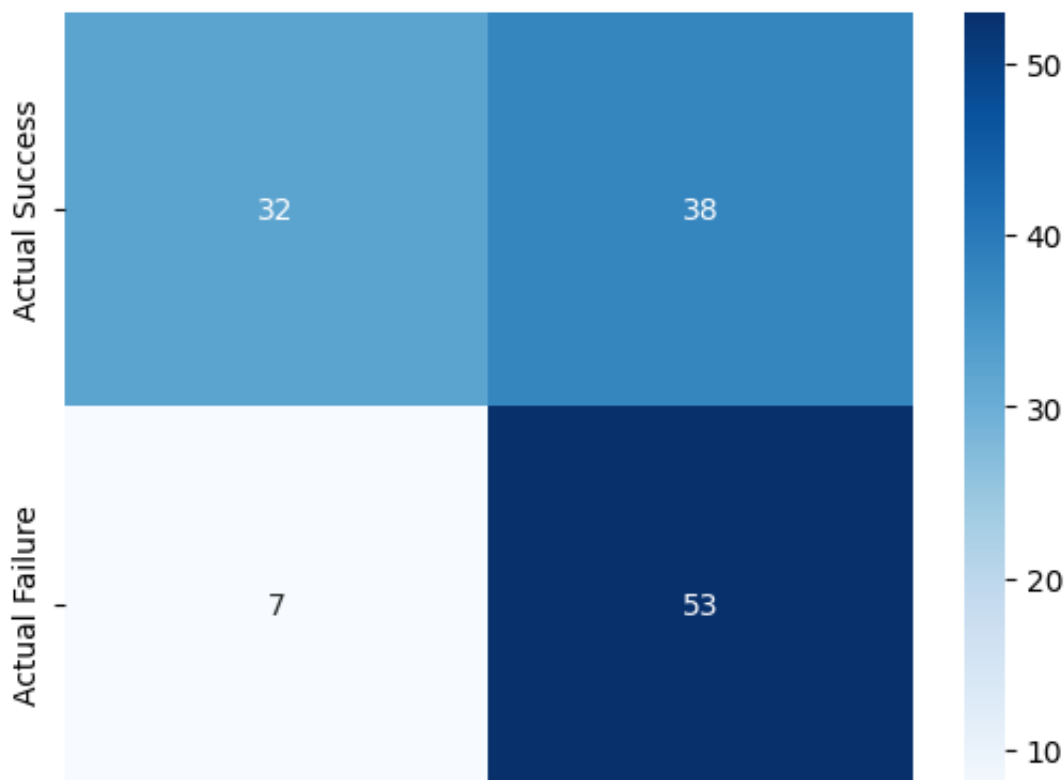
Training - Accuracy: 0.5049, Sensitivity: 0.0000, Specificity: 1.0000, F1:  
 Threshold: 0.10, Accuracy: 0.4846, Sensitivity: 1.0000, Specificity: 0.0429  
 Threshold: 0.15, Accuracy: 0.5231, Sensitivity: 1.0000, Specificity: 0.1143  
 Threshold: 0.20, Accuracy: 0.5231, Sensitivity: 1.0000, Specificity: 0.1143  
 Threshold: 0.25, Accuracy: 0.5385, Sensitivity: 0.9667, Specificity: 0.1714  
 Threshold: 0.30, Accuracy: 0.5769, Sensitivity: 0.9667, Specificity: 0.2429  
 Threshold: 0.35, Accuracy: 0.5769, Sensitivity: 0.9167, Specificity: 0.2857  
 Threshold: 0.40, Accuracy: 0.5923, Sensitivity: 0.9000, Specificity: 0.3286  
 Threshold: 0.45, Accuracy: 0.6538, Sensitivity: 0.8833, Specificity: 0.4571  
 Threshold: 0.50, Accuracy: 0.6615, Sensitivity: 0.8500, Specificity: 0.5000  
 Threshold: 0.55, Accuracy: 0.6923, Sensitivity: 0.8333, Specificity: 0.5714  
 Threshold: 0.60, Accuracy: 0.7000, Sensitivity: 0.7500, Specificity: 0.6571  
 Threshold: 0.65, Accuracy: 0.7308, Sensitivity: 0.7167, Specificity: 0.7429  
 Threshold: 0.70, Accuracy: 0.7154, Sensitivity: 0.6667, Specificity: 0.7571  
 Threshold: 0.75, Accuracy: 0.7077, Sensitivity: 0.5167, Specificity: 0.8714  
 Threshold: 0.80, Accuracy: 0.6385, Sensitivity: 0.3333, Specificity: 0.9000  
 Threshold: 0.85, Accuracy: 0.5846, Sensitivity: 0.1333, Specificity: 0.9714  
 Threshold: 0.90, Accuracy: 0.5692, Sensitivity: 0.0667, Specificity: 1.0000  
 Threshold: 0.95, Accuracy: 0.5385, Sensitivity: 0.0000, Specificity: 1.0000  
 Threshold: 1.00, Accuracy: 0.5385, Sensitivity: 0.0000, Specificity: 1.0000

5/5  0s 7ms/step

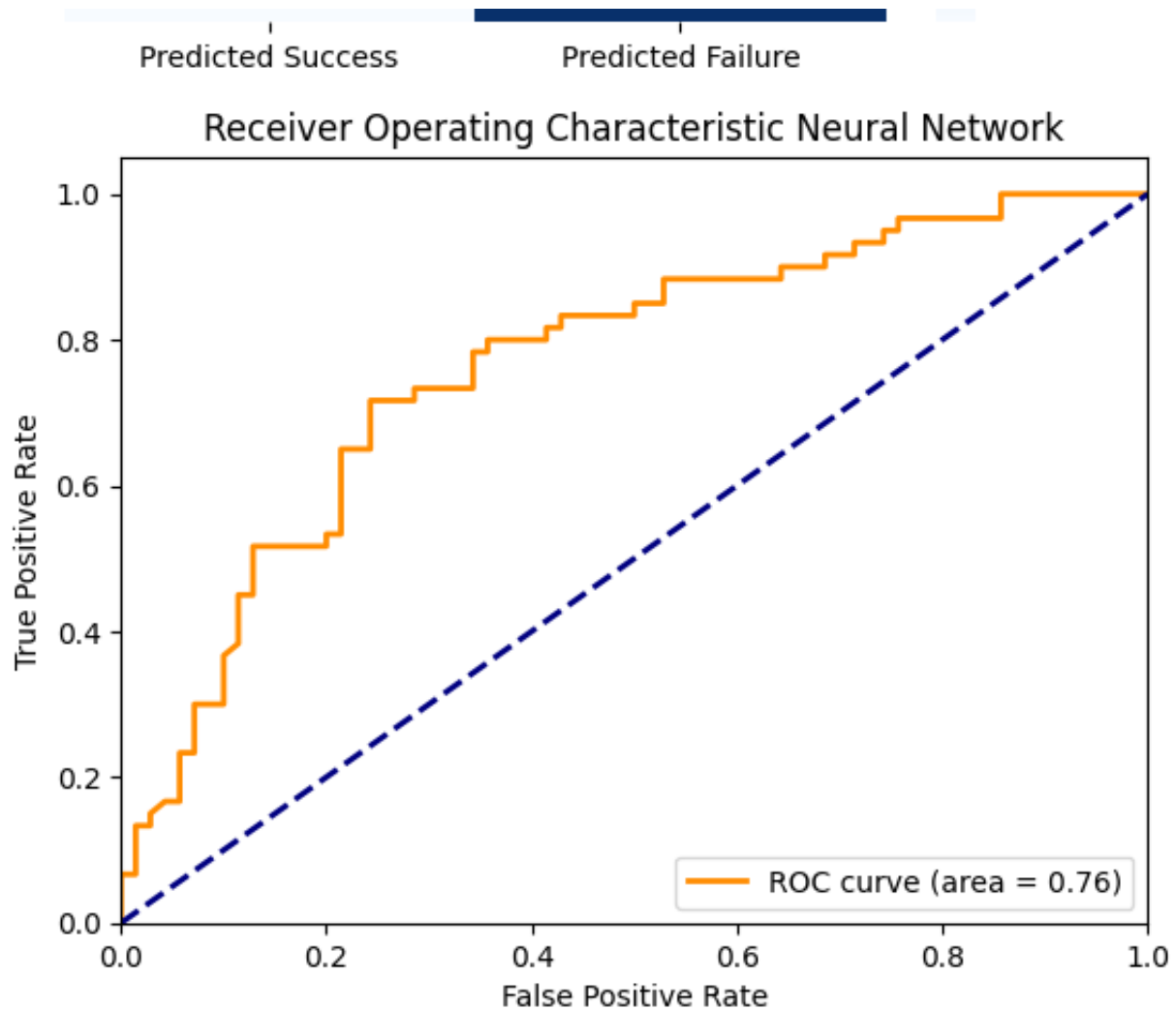
Metrics for chosen threshold 0.45:

Accuracy: 0.6538, Sensitivity: 0.8833, Specificity: 0.4571, F1: 0.7020, ROC

Confusion Matrix Neural Network







Epoch 1/30

```
/usr/local/lib/python3.11/dist-packages/keras/src/layers/core/dense.py:87:
super().__init__(activity_regularizer=activity_regularizer, **kwargs)
```

13/13 ————— 3s 33ms/step - accuracy: 0.4700 - loss: 2.2802 -

Epoch 2/30

13/13 ————— 0s 10ms/step - accuracy: 0.6087 - loss: 1.9446 -

Epoch 3/30

13/13 ————— 0s 10ms/step - accuracy: 0.6965 - loss: 1.7472 -

Epoch 4/30

13/13 ————— 0s 12ms/step - accuracy: 0.6885 - loss: 1.7105 -

Epoch 5/30

13/13 ————— 0s 10ms/step - accuracy: 0.7276 - loss: 1.6210 -

Epoch 6/30

13/13 ————— 0s 13ms/step - accuracy: 0.7140 - loss: 1.5967 -

Epoch 7/30

13/13 ————— 0s 10ms/step - accuracy: 0.7274 - loss: 1.5602 -

Epoch 8/30

13/13 ————— 0s 10ms/step - accuracy: 0.7250 - loss: 1.5112 -

Epoch 9/30

13/13 ————— 0s 10ms/step - accuracy: 0.7869 - loss: 1.4561 -

Epoch 10/30

13/13 ————— 0s 12ms/step - accuracy: 0.7144 - loss: 1.4304 -

Epoch 11/30

13/13 ————— 0s 10ms/step - accuracy: 0.7321 - loss: 1.3675 -

Epoch 12/30



```

-
13/13 _____ 0s 10ms/step - accuracy: 0.7881 - loss: 1.2989 -
Epoch 13/30
13/13 _____ 0s 12ms/step - accuracy: 0.7621 - loss: 1.2982 -
Epoch 14/30
13/13 _____ 0s 10ms/step - accuracy: 0.7592 - loss: 1.3112 -
Epoch 15/30
13/13 _____ 0s 10ms/step - accuracy: 0.8041 - loss: 1.2182 -
Epoch 16/30
13/13 _____ 0s 10ms/step - accuracy: 0.7889 - loss: 1.1982 -
Epoch 17/30
13/13 _____ 0s 10ms/step - accuracy: 0.8172 - loss: 1.1173 -
Epoch 18/30
13/13 _____ 0s 10ms/step - accuracy: 0.7839 - loss: 1.1571 -
Epoch 19/30
13/13 _____ 0s 10ms/step - accuracy: 0.8135 - loss: 1.1138 -
Epoch 20/30
13/13 _____ 0s 10ms/step - accuracy: 0.8049 - loss: 1.1112 -
Epoch 21/30
13/13 _____ 0s 10ms/step - accuracy: 0.8167 - loss: 1.0430 -
Epoch 22/30
13/13 _____ 0s 10ms/step - accuracy: 0.8196 - loss: 1.0689 -
Epoch 23/30
13/13 _____ 0s 11ms/step - accuracy: 0.8408 - loss: 1.0037 -
Epoch 24/30
13/13 _____ 0s 10ms/step - accuracy: 0.7800 - loss: 1.0104 -
Epoch 25/30
13/13 _____ 0s 11ms/step - accuracy: 0.8473 - loss: 0.9659 -
Epoch 26/30
13/13 _____ 0s 10ms/step - accuracy: 0.8330 - loss: 0.9497 -
Epoch 27/30
13/13 _____ 0s 9ms/step - accuracy: 0.7989 - loss: 0.9561 -
Epoch 28/30
13/13 _____ 0s 10ms/step - accuracy: 0.8580 - loss: 0.8809 -
Epoch 29/30
13/13 _____ 0s 15ms/step - accuracy: 0.8166 - loss: 0.9267 -
Epoch 30/30
13/13 _____ 0s 16ms/step - accuracy: 0.8533 - loss: 0.8662 -
16/16 _____ 0s 12ms/step
5/5 _____ 0s 10ms/step

```

--- Dados ROC para copiar ---

FPR = [0.0, 0.014285714285714285, 0.014285714285714285, 0.04285714285714286

TPR = [0.0, 0.016666666666666666, 0.15, 0.15, 0.16666666666666666, 0.166666

AUC = 0.7666666666666667

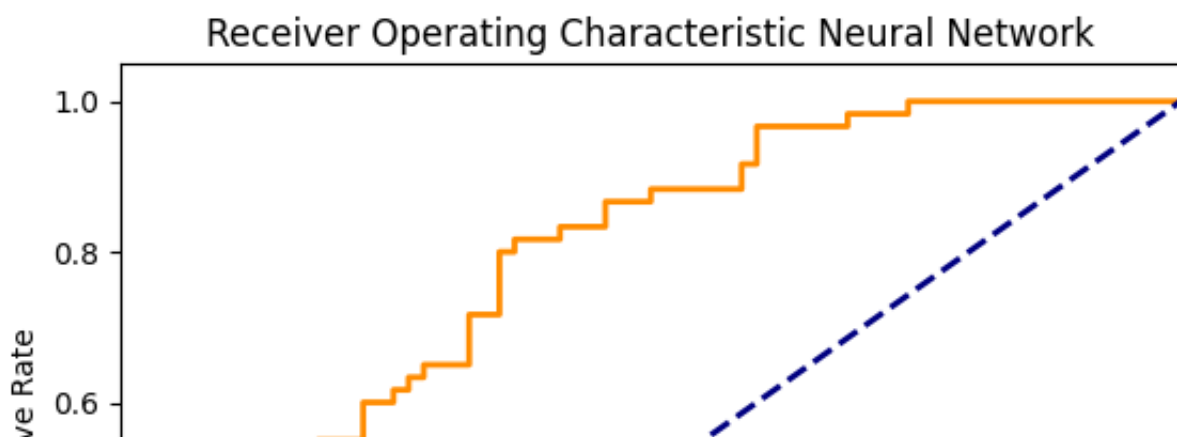
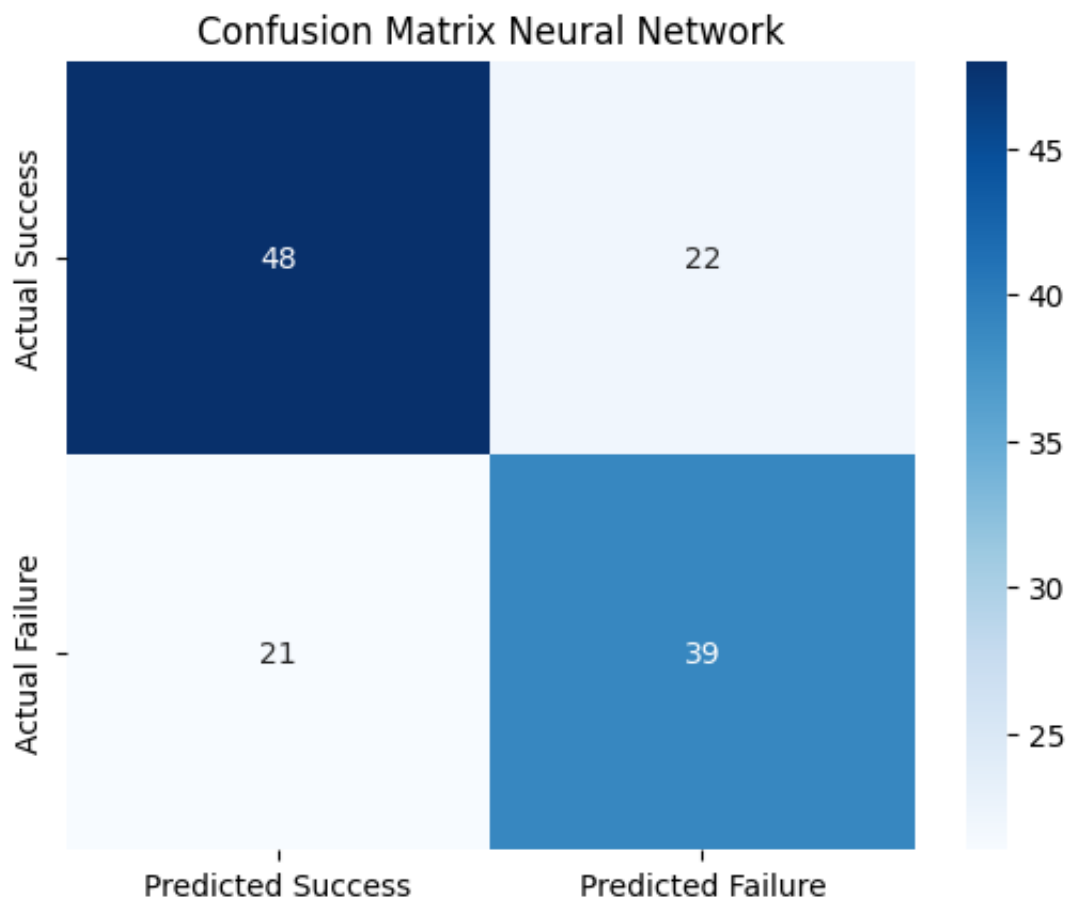
--- Fim dos Dados ROC ---

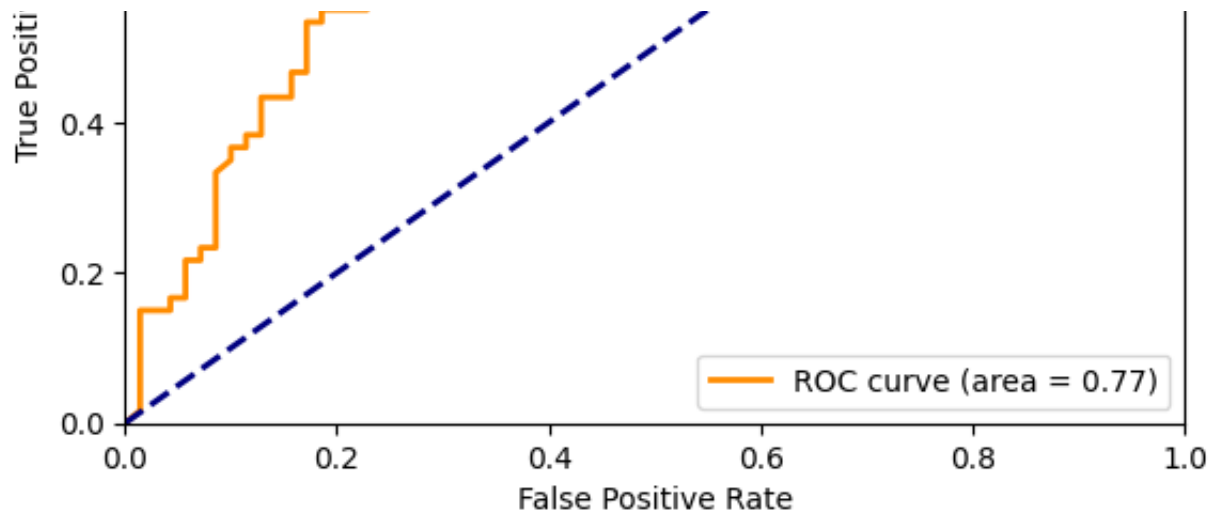
Training - Accuracy: 0.5049, Sensitivity: 0.0000, Specificity: 1.0000, F1:  
 Threshold: 0.10, Accuracy: 0.5615, Sensitivity: 1.0000, Specificity: 0.1857  
 Threshold: 0.15, Accuracy: 0.5846, Sensitivity: 1.0000, Specificity: 0.2286  
 Threshold: 0.20, Accuracy: 0.6077, Sensitivity: 0.9833, Specificity: 0.2857  
 Threshold: 0.25, Accuracy: 0.6538, Sensitivity: 0.9667, Specificity: 0.3857  
 Threshold: 0.30, Accuracy: 0.6308, Sensitivity: 0.8833, Specificity: 0.4143  
 Threshold: 0.35, Accuracy: 0.6846, Sensitivity: 0.8500, Specificity: 0.5429  
 Threshold: 0.40, Accuracy: 0.7154, Sensitivity: 0.8000, Specificity: 0.6429

```
Threshold: 0.45, Accuracy: 0.6692, Sensitivity: 0.6500, Specificity: 0.6857
Threshold: 0.50, Accuracy: 0.6769, Sensitivity: 0.6000, Specificity: 0.7429
Threshold: 0.55, Accuracy: 0.6923, Sensitivity: 0.5500, Specificity: 0.8143
Threshold: 0.60, Accuracy: 0.6615, Sensitivity: 0.4500, Specificity: 0.8429
Threshold: 0.65, Accuracy: 0.6462, Sensitivity: 0.3833, Specificity: 0.8714
Threshold: 0.70, Accuracy: 0.6231, Sensitivity: 0.2833, Specificity: 0.9143
Threshold: 0.75, Accuracy: 0.6000, Sensitivity: 0.2333, Specificity: 0.9143
Threshold: 0.80, Accuracy: 0.5846, Sensitivity: 0.1500, Specificity: 0.9571
Threshold: 0.85, Accuracy: 0.5692, Sensitivity: 0.0833, Specificity: 0.9857
Threshold: 0.90, Accuracy: 0.5385, Sensitivity: 0.0167, Specificity: 0.9857
Threshold: 0.95, Accuracy: 0.5385, Sensitivity: 0.0167, Specificity: 0.9857
Threshold: 1.00, Accuracy: 0.5385, Sensitivity: 0.0000, Specificity: 1.0000
5/5 ————— 0s 10ms/step
```

Metrics for chosen threshold 0.45:

Accuracy: 0.6692, Sensitivity: 0.6500, Specificity: 0.6857, F1: 0.6446, ROC





```

/usr/local/lib/python3.11/dist-packages/keras/src/layers/core/dense.py:87:
    super().__init__(activity_regularizer=activity_regularizer, **kwargs)
Epoch 1/30
13/13 ————— 3s 35ms/step - accuracy: 0.5495 - loss: 2.1584 -
Epoch 2/30
13/13 ————— 0s 13ms/step - accuracy: 0.6460 - loss: 1.8967 -
Epoch 3/30
13/13 ————— 0s 10ms/step - accuracy: 0.7103 - loss: 1.7326 -
Epoch 4/30
13/13 ————— 0s 10ms/step - accuracy: 0.6574 - loss: 1.7173 -
Epoch 5/30
13/13 ————— 0s 13ms/step - accuracy: 0.6823 - loss: 1.6882 -
Epoch 6/30
13/13 ————— 0s 11ms/step - accuracy: 0.7146 - loss: 1.5614 -
Epoch 7/30
13/13 ————— 0s 11ms/step - accuracy: 0.6954 - loss: 1.5630 -
Epoch 8/30
13/13 ————— 0s 12ms/step - accuracy: 0.7045 - loss: 1.5072 -
Epoch 9/30
13/13 ————— 0s 11ms/step - accuracy: 0.7262 - loss: 1.4283 -
Epoch 10/30
13/13 ————— 0s 12ms/step - accuracy: 0.7474 - loss: 1.4104 -
Epoch 11/30
13/13 ————— 0s 10ms/step - accuracy: 0.7616 - loss: 1.3134 -
Epoch 12/30
13/13 ————— 0s 14ms/step - accuracy: 0.7464 - loss: 1.3337 -
Epoch 13/30
13/13 ————— 0s 11ms/step - accuracy: 0.7469 - loss: 1.3068 -
Epoch 14/30
13/13 ————— 0s 10ms/step - accuracy: 0.7676 - loss: 1.2278 -
Epoch 15/30
13/13 ————— 0s 11ms/step - accuracy: 0.7591 - loss: 1.2235 -
Epoch 16/30
13/13 ————— 0s 10ms/step - accuracy: 0.7655 - loss: 1.1926 -
Epoch 17/30
13/13 ————— 0s 10ms/step - accuracy: 0.7902 - loss: 1.1295 -
Epoch 18/30
13/13 ————— 0s 12ms/step - accuracy: 0.7880 - loss: 1.1369 -
Epoch 19/30
13/13 ————— 0s 11ms/step - accuracy: 0.7867 - loss: 1.0824 -

```

```

13/13 ----- vs 11ms/step - accuracy: 0.7797 - loss: 1.0654 -
Epoch 20/30
13/13 ----- 0s 10ms/step - accuracy: 0.7792 - loss: 1.0771 -
Epoch 21/30
13/13 ----- 0s 10ms/step - accuracy: 0.7903 - loss: 1.0465 -
Epoch 22/30
13/13 ----- 0s 10ms/step - accuracy: 0.7902 - loss: 1.0368 -
Epoch 23/30
13/13 ----- 0s 13ms/step - accuracy: 0.7882 - loss: 1.0198 -
Epoch 24/30
13/13 ----- 0s 11ms/step - accuracy: 0.7746 - loss: 0.9969 -
Epoch 25/30
13/13 ----- 0s 10ms/step - accuracy: 0.8124 - loss: 0.9506 -
Epoch 26/30
13/13 ----- 0s 10ms/step - accuracy: 0.8005 - loss: 0.9381 -
Epoch 27/30
13/13 ----- 0s 11ms/step - accuracy: 0.8151 - loss: 0.9073 -
Epoch 28/30
13/13 ----- 0s 13ms/step - accuracy: 0.8180 - loss: 0.8958 -
Epoch 29/30
13/13 ----- 0s 12ms/step - accuracy: 0.8465 - loss: 0.8803 -
Epoch 30/30
13/13 ----- 0s 11ms/step - accuracy: 0.8501 - loss: 0.8481 -
16/16 ----- 0s 9ms/step
5/5 ----- 0s 12ms/step

```

--- Dados ROC para copiar ---

```

FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.0285714
TPR = [0.0, 0.016666666666666666, 0.066666666666666667, 0.08333333333333333,
AUC = 0.7861904761904762

```

--- Fim dos Dados ROC ---

```

Training - Accuracy: 0.5049, Sensitivity: 0.0000, Specificity: 1.0000, F1:
Threshold: 0.10, Accuracy: 0.4846, Sensitivity: 1.0000, Specificity: 0.0429
Threshold: 0.15, Accuracy: 0.5385, Sensitivity: 1.0000, Specificity: 0.1429
Threshold: 0.20, Accuracy: 0.5538, Sensitivity: 1.0000, Specificity: 0.1714
Threshold: 0.25, Accuracy: 0.6308, Sensitivity: 1.0000, Specificity: 0.3143
Threshold: 0.30, Accuracy: 0.6231, Sensitivity: 0.9667, Specificity: 0.3286
Threshold: 0.35, Accuracy: 0.6462, Sensitivity: 0.9167, Specificity: 0.4143
Threshold: 0.40, Accuracy: 0.6769, Sensitivity: 0.9167, Specificity: 0.4714
Threshold: 0.45, Accuracy: 0.6923, Sensitivity: 0.9000, Specificity: 0.5143
Threshold: 0.50, Accuracy: 0.6923, Sensitivity: 0.7833, Specificity: 0.6143
Threshold: 0.55, Accuracy: 0.6769, Sensitivity: 0.7000, Specificity: 0.6571
Threshold: 0.60, Accuracy: 0.7000, Sensitivity: 0.6500, Specificity: 0.7429
Threshold: 0.65, Accuracy: 0.7077, Sensitivity: 0.6000, Specificity: 0.8000
Threshold: 0.70, Accuracy: 0.7000, Sensitivity: 0.5333, Specificity: 0.8429
Threshold: 0.75, Accuracy: 0.6923, Sensitivity: 0.4667, Specificity: 0.8857
Threshold: 0.80, Accuracy: 0.6538, Sensitivity: 0.3833, Specificity: 0.8857
Threshold: 0.85, Accuracy: 0.6231, Sensitivity: 0.2667, Specificity: 0.9286
Threshold: 0.90, Accuracy: 0.6000, Sensitivity: 0.1500, Specificity: 0.9857
Threshold: 0.95, Accuracy: 0.5462, Sensitivity: 0.0167, Specificity: 1.0000
Threshold: 1.00, Accuracy: 0.5385, Sensitivity: 0.0000, Specificity: 1.0000
5/5 ----- 0s 13ms/step

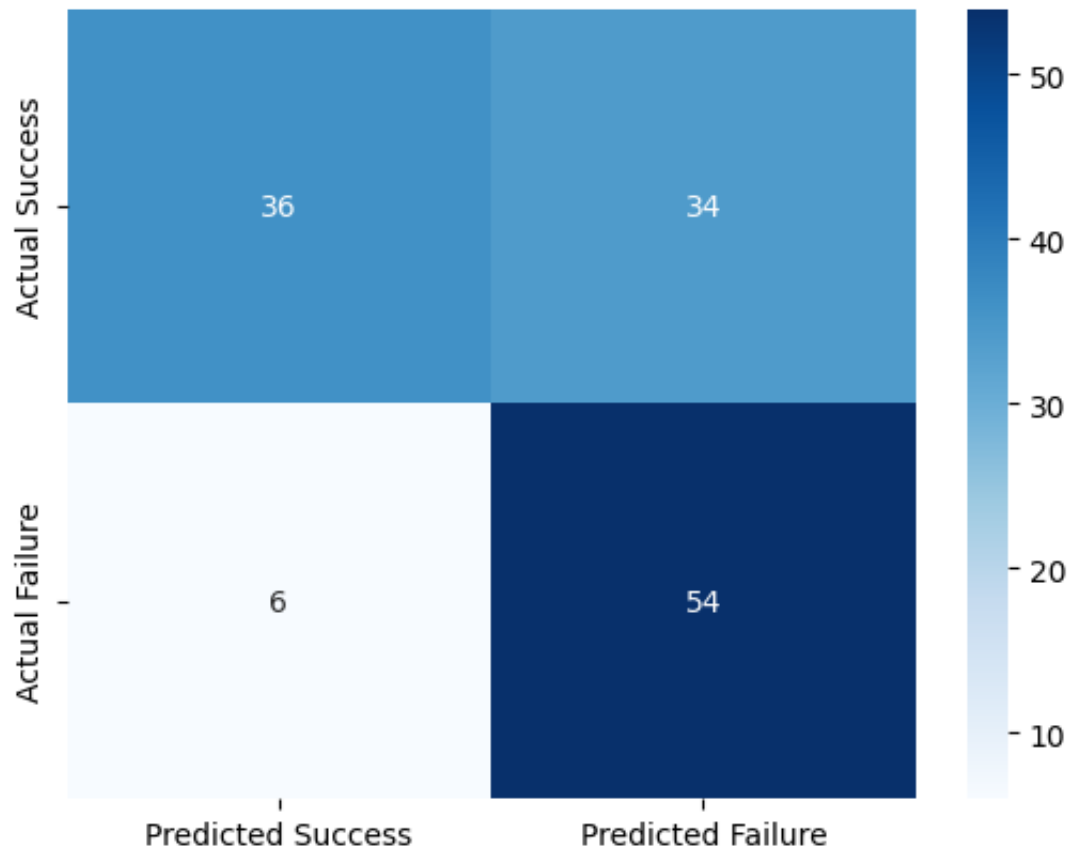
```

Metrics for chosen threshold 0.45:

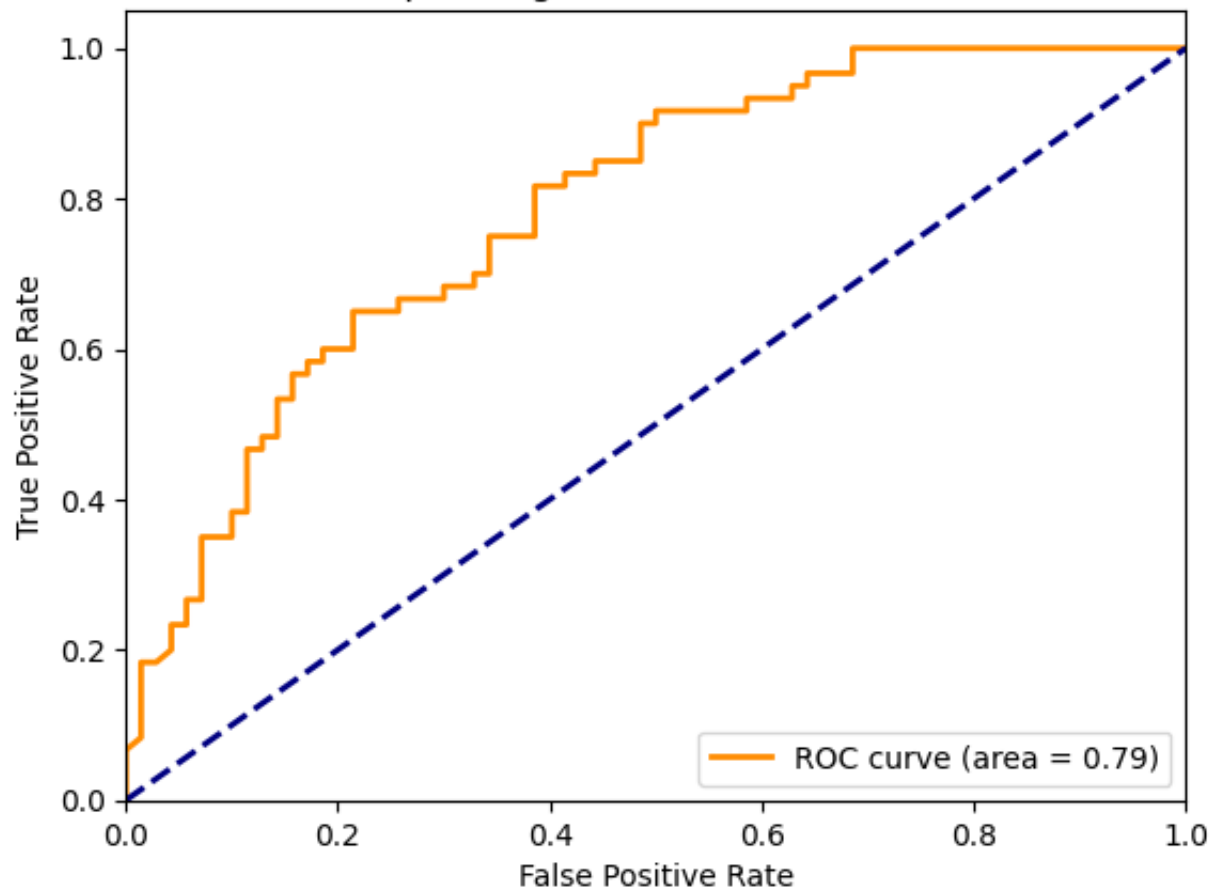
metrics for chosen threshold 0.45:

Accuracy: 0.6923, Sensitivity: 0.9000, Specificity: 0.5143, F1: 0.7297, ROC



























Confusion Matrix Neural Network



Receiver Operating Characteristic Neural Network



```

Epoch 1/30
/usr/local/lib/python3.11/dist-packages/keras/src/layers/core/dense.py:87:
    super().__init__(activity_regularizer=activity_regularizer, **kwargs)
13/13  3s 32ms/step - accuracy: 0.4735 - loss: 2.1764 -
Epoch 2/30
13/13  0s 9ms/step - accuracy: 0.5942 - loss: 1.9289 -
Epoch 3/30
13/13  0s 13ms/step - accuracy: 0.6256 - loss: 1.7993 -
Epoch 4/30
13/13  0s 10ms/step - accuracy: 0.6417 - loss: 1.7814 -
Epoch 5/30
13/13  0s 10ms/step - accuracy: 0.6731 - loss: 1.6785 -
Epoch 6/30
13/13  0s 10ms/step - accuracy: 0.6792 - loss: 1.6658 -
Epoch 7/30
13/13  0s 10ms/step - accuracy: 0.6836 - loss: 1.5624 -
Epoch 8/30
13/13  0s 11ms/step - accuracy: 0.7113 - loss: 1.5461 -
Epoch 9/30
13/13  0s 11ms/step - accuracy: 0.7099 - loss: 1.4486 -
Epoch 10/30
13/13  0s 11ms/step - accuracy: 0.7511 - loss: 1.3663 -
Epoch 11/30
13/13  0s 11ms/step - accuracy: 0.7295 - loss: 1.3722 -
Epoch 12/30
13/13  0s 11ms/step - accuracy: 0.6892 - loss: 1.4068 -
Epoch 13/30
13/13  0s 12ms/step - accuracy: 0.7310 - loss: 1.3329 -
Epoch 14/30
13/13  0s 11ms/step - accuracy: 0.7116 - loss: 1.3756 -
Epoch 15/30
13/13  0s 10ms/step - accuracy: 0.7302 - loss: 1.2664 -
Epoch 16/30
13/13  0s 10ms/step - accuracy: 0.7321 - loss: 1.2188 -
Epoch 17/30
13/13  0s 13ms/step - accuracy: 0.7518 - loss: 1.1935 -
Epoch 18/30
13/13  0s 10ms/step - accuracy: 0.7754 - loss: 1.1605 -
Epoch 19/30
13/13  0s 10ms/step - accuracy: 0.8205 - loss: 1.1282 -
Epoch 20/30
13/13  0s 10ms/step - accuracy: 0.7537 - loss: 1.1307 -
Epoch 21/30
13/13  0s 12ms/step - accuracy: 0.8031 - loss: 1.0750 -
Epoch 22/30
13/13  0s 11ms/step - accuracy: 0.7660 - loss: 1.0997 -
Epoch 23/30
13/13  0s 10ms/step - accuracy: 0.8121 - loss: 1.0427 -
Epoch 24/30
13/13  0s 9ms/step - accuracy: 0.7953 - loss: 1.0313 -
Epoch 25/30
13/13  0s 10ms/step - accuracy: 0.7761 - loss: 1.0037 -
Epoch 26/30
13/13  0s 10ms/step - accuracy: 0.7718 - loss: 1.0332 -

```

```

Epoch 27/30
13/13 ————— 0s 12ms/step - accuracy: 0.8267 - loss: 0.9694 -
Epoch 28/30
13/13 ————— 0s 10ms/step - accuracy: 0.8014 - loss: 0.9387 -
Epoch 29/30
13/13 ————— 0s 9ms/step - accuracy: 0.7903 - loss: 0.9660 -
Epoch 30/30
13/13 ————— 0s 10ms/step - accuracy: 0.8299 - loss: 0.9280 -
16/16 ————— 0s 8ms/step
5/5 ————— 0s 7ms/step

```

--- Dados ROC para copiar ---

```

FPR = [0.0, 0.0, 0.0, 0.02857142857142857, 0.02857142857142857, 0.042857142
TPR = [0.0, 0.016666666666666666, 0.03333333333333333, 0.03333333333333333,
AUC = 0.7622619047619047

```

--- Fim dos Dados ROC ---

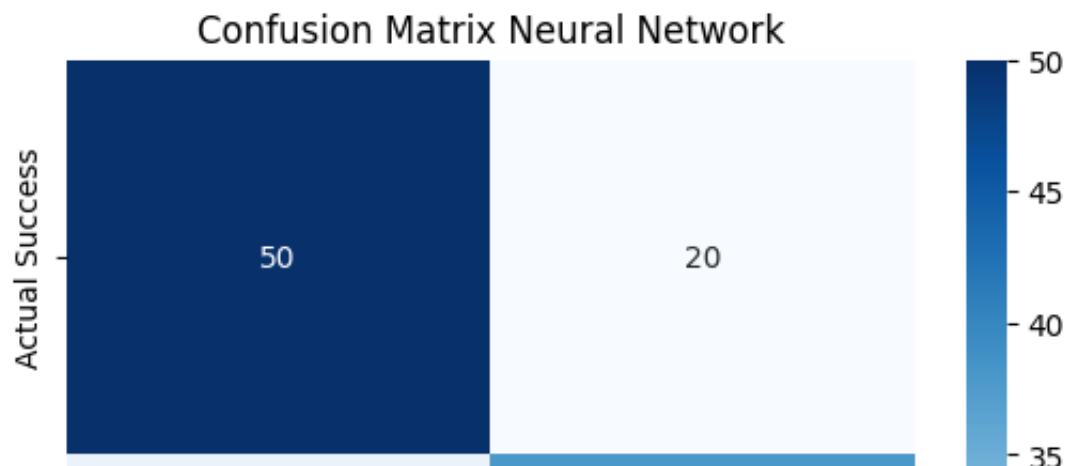
```

Training - Accuracy: 0.5049, Sensitivity: 0.0000, Specificity: 1.0000, F1:
Threshold: 0.10, Accuracy: 0.5308, Sensitivity: 1.0000, Specificity: 0.1286
Threshold: 0.15, Accuracy: 0.5692, Sensitivity: 0.9667, Specificity: 0.2286
Threshold: 0.20, Accuracy: 0.5769, Sensitivity: 0.9500, Specificity: 0.2571
Threshold: 0.25, Accuracy: 0.6308, Sensitivity: 0.9500, Specificity: 0.3571
Threshold: 0.30, Accuracy: 0.6462, Sensitivity: 0.8500, Specificity: 0.4714
Threshold: 0.35, Accuracy: 0.6692, Sensitivity: 0.7667, Specificity: 0.5857
Threshold: 0.40, Accuracy: 0.6923, Sensitivity: 0.7333, Specificity: 0.6571
Threshold: 0.45, Accuracy: 0.6769, Sensitivity: 0.6333, Specificity: 0.7143
Threshold: 0.50, Accuracy: 0.6769, Sensitivity: 0.6167, Specificity: 0.7286
Threshold: 0.55, Accuracy: 0.7000, Sensitivity: 0.5833, Specificity: 0.8000
Threshold: 0.60, Accuracy: 0.7000, Sensitivity: 0.5333, Specificity: 0.8429
Threshold: 0.65, Accuracy: 0.6923, Sensitivity: 0.4833, Specificity: 0.8714
Threshold: 0.70, Accuracy: 0.6846, Sensitivity: 0.4500, Specificity: 0.8857
Threshold: 0.75, Accuracy: 0.6769, Sensitivity: 0.3667, Specificity: 0.9429
Threshold: 0.80, Accuracy: 0.6231, Sensitivity: 0.2333, Specificity: 0.9571
Threshold: 0.85, Accuracy: 0.6077, Sensitivity: 0.2000, Specificity: 0.9571
Threshold: 0.90, Accuracy: 0.5692, Sensitivity: 0.1000, Specificity: 0.9714
Threshold: 0.95, Accuracy: 0.5462, Sensitivity: 0.0167, Specificity: 1.0000
Threshold: 1.00, Accuracy: 0.5385, Sensitivity: 0.0000, Specificity: 1.0000
5/5 ————— 0s 8ms/step

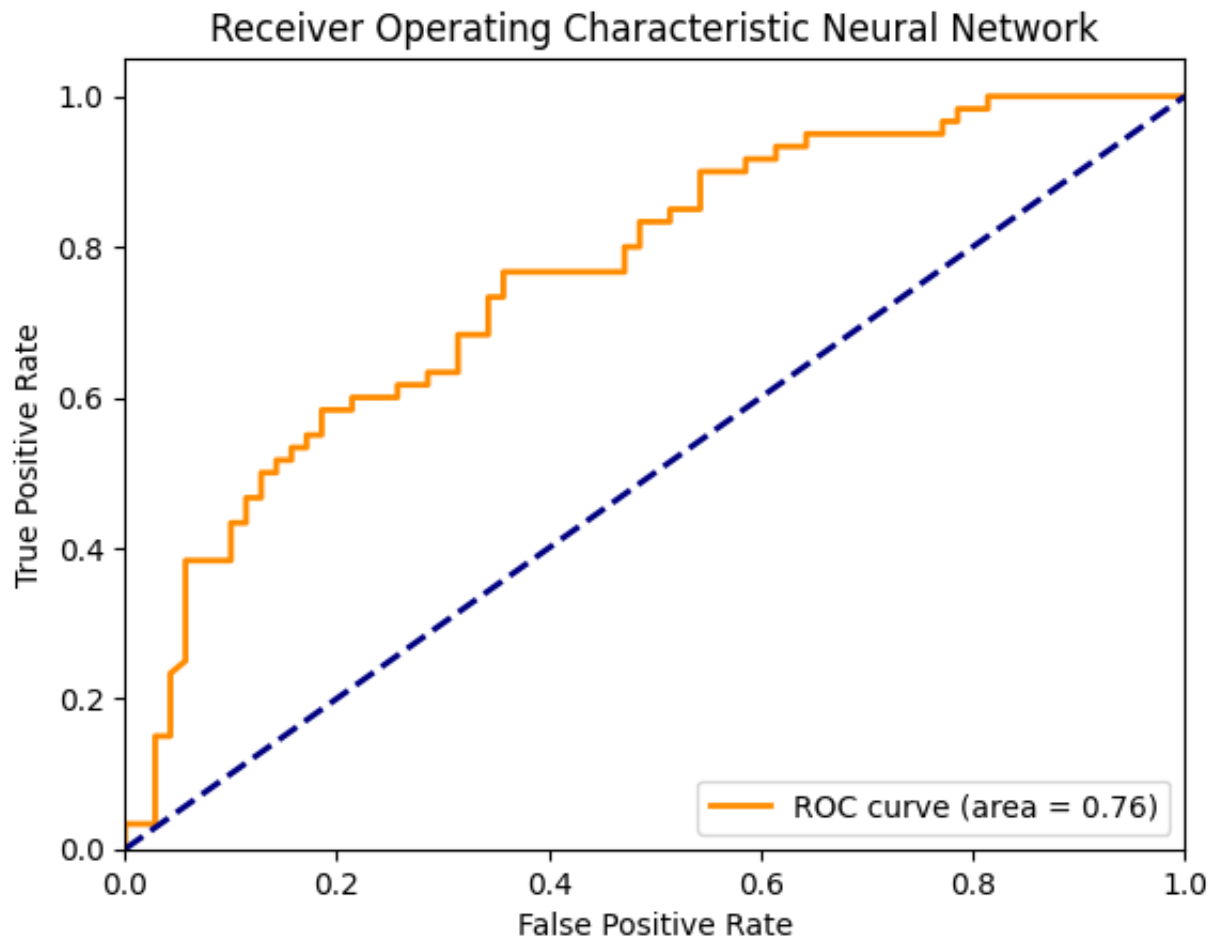
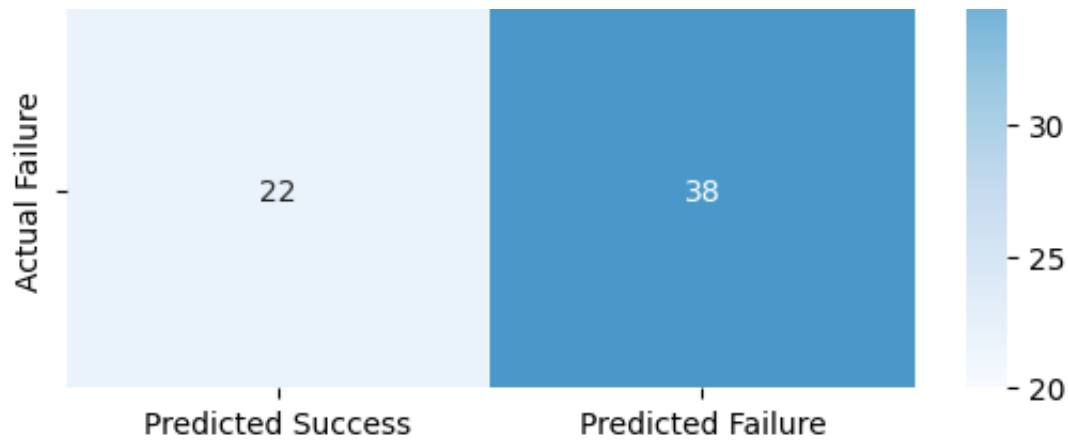
```

Metrics for chosen threshold 0.45:

Accuracy: 0.6769, Sensitivity: 0.6333, Specificity: 0.7143, F1: 0.6441, ROC







Epoch 1/30

```
/usr/local/lib/python3.11/dist-packages/keras/src/layers/core/dense.py:87:
super().__init__(activity_regularizer=activity_regularizer, **kwargs)
```

13/13 ————— 4s 31ms/step - accuracy: 0.5876 - loss: 2.0551 -

Epoch 2/30

13/13 ————— 0s 10ms/step - accuracy: 0.6123 - loss: 1.9082 -

Epoch 3/30

13/13 ————— 0s 10ms/step - accuracy: 0.6976 - loss: 1.7679 -

Epoch 4/30

13/13 ————— 0s 10ms/step - accuracy: 0.6721 - loss: 1.7501 -

Epoch 5/30

13/13 ————— 0s 10ms/step - accuracy: 0.7193 - loss: 1.6352 -

Epoch 6/30

13/13 ————— 0s 10ms/step - accuracy: 0.6539 - loss: 1.6049 -

Epoch 7/30



```

13/13 _____ 0s 10ms/step - accuracy: 0.7276 - loss: 1.5181 -
Epoch 8/30
13/13 _____ 0s 10ms/step - accuracy: 0.7282 - loss: 1.4801 -
Epoch 9/30
13/13 _____ 0s 11ms/step - accuracy: 0.7468 - loss: 1.3992 -
Epoch 10/30
13/13 _____ 0s 10ms/step - accuracy: 0.7202 - loss: 1.4187 -
Epoch 11/30
13/13 _____ 0s 10ms/step - accuracy: 0.6842 - loss: 1.3812 -
Epoch 12/30
13/13 _____ 0s 10ms/step - accuracy: 0.7446 - loss: 1.2832 -
Epoch 13/30
13/13 _____ 0s 10ms/step - accuracy: 0.7596 - loss: 1.2542 -
Epoch 14/30
13/13 _____ 0s 10ms/step - accuracy: 0.7635 - loss: 1.2453 -
Epoch 15/30
13/13 _____ 0s 13ms/step - accuracy: 0.7437 - loss: 1.2473 -
Epoch 16/30
13/13 _____ 0s 10ms/step - accuracy: 0.7580 - loss: 1.1825 -
Epoch 17/30
13/13 _____ 0s 10ms/step - accuracy: 0.8022 - loss: 1.1206 -
Epoch 18/30
13/13 _____ 0s 10ms/step - accuracy: 0.7844 - loss: 1.0930 -
Epoch 19/30
13/13 _____ 0s 11ms/step - accuracy: 0.7941 - loss: 1.0979 -
Epoch 20/30
13/13 _____ 0s 10ms/step - accuracy: 0.8047 - loss: 1.0161 -
Epoch 21/30
13/13 _____ 0s 14ms/step - accuracy: 0.8118 - loss: 1.0157 -
Epoch 22/30
13/13 _____ 0s 10ms/step - accuracy: 0.8148 - loss: 0.9764 -
Epoch 23/30
13/13 _____ 0s 12ms/step - accuracy: 0.8306 - loss: 0.9503 -
Epoch 24/30
13/13 _____ 0s 10ms/step - accuracy: 0.8521 - loss: 0.9170 -
Epoch 25/30
13/13 _____ 0s 13ms/step - accuracy: 0.8003 - loss: 0.9647 -
Epoch 26/30
13/13 _____ 0s 11ms/step - accuracy: 0.8008 - loss: 0.9003 -
Epoch 27/30
13/13 _____ 0s 13ms/step - accuracy: 0.8337 - loss: 0.9029 -
Epoch 28/30
13/13 _____ 0s 13ms/step - accuracy: 0.8373 - loss: 0.8710 -
Epoch 29/30
13/13 _____ 0s 13ms/step - accuracy: 0.8039 - loss: 0.8811 -
Epoch 30/30
13/13 _____ 0s 11ms/step - accuracy: 0.8626 - loss: 0.7907 -
16/16 _____ 0s 9ms/step
5/5 _____ 0s 8ms/step

```


--- Dados ROC para copiar ---

```

FPR = [0.0, 0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.0285714
TPR = [0.0, 0.016666666666666666, 0.06666666666666667, 0.08333333333333333,
AUC = 0.7569047619047619

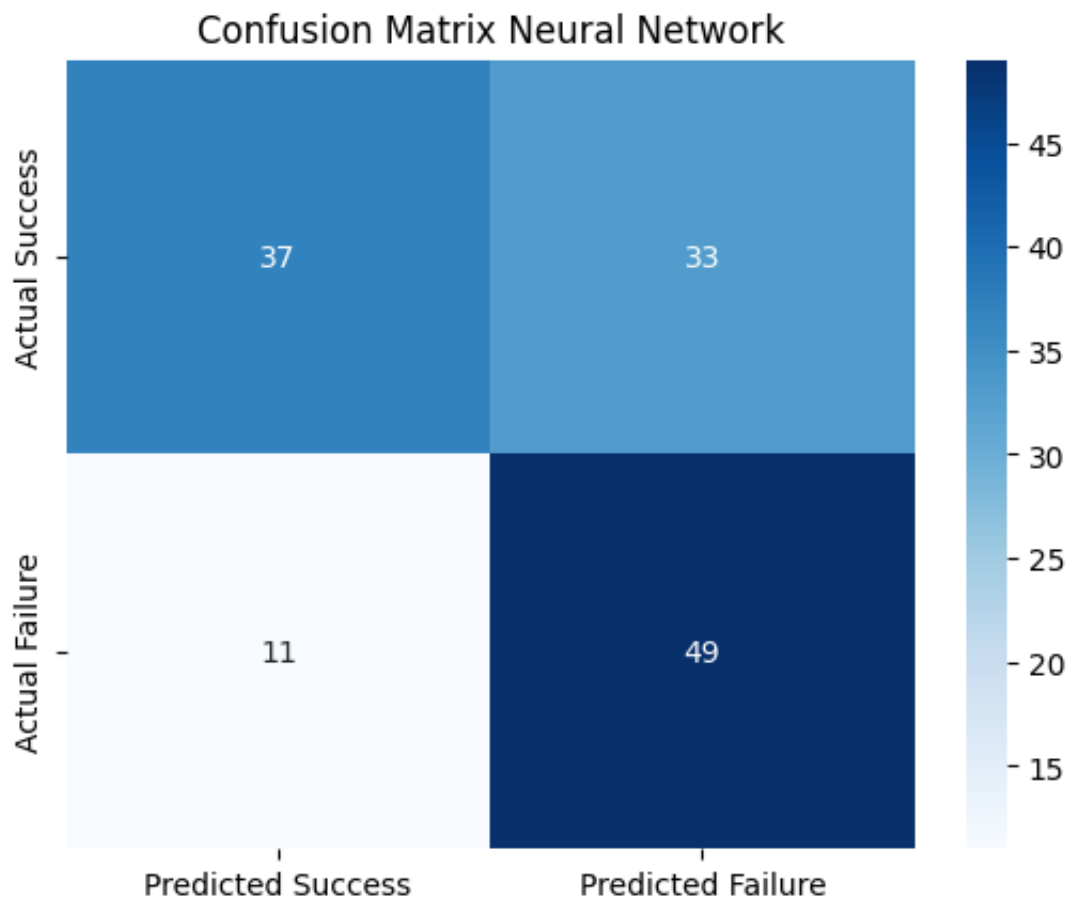
```

--- Fim dos Dados ROC ---

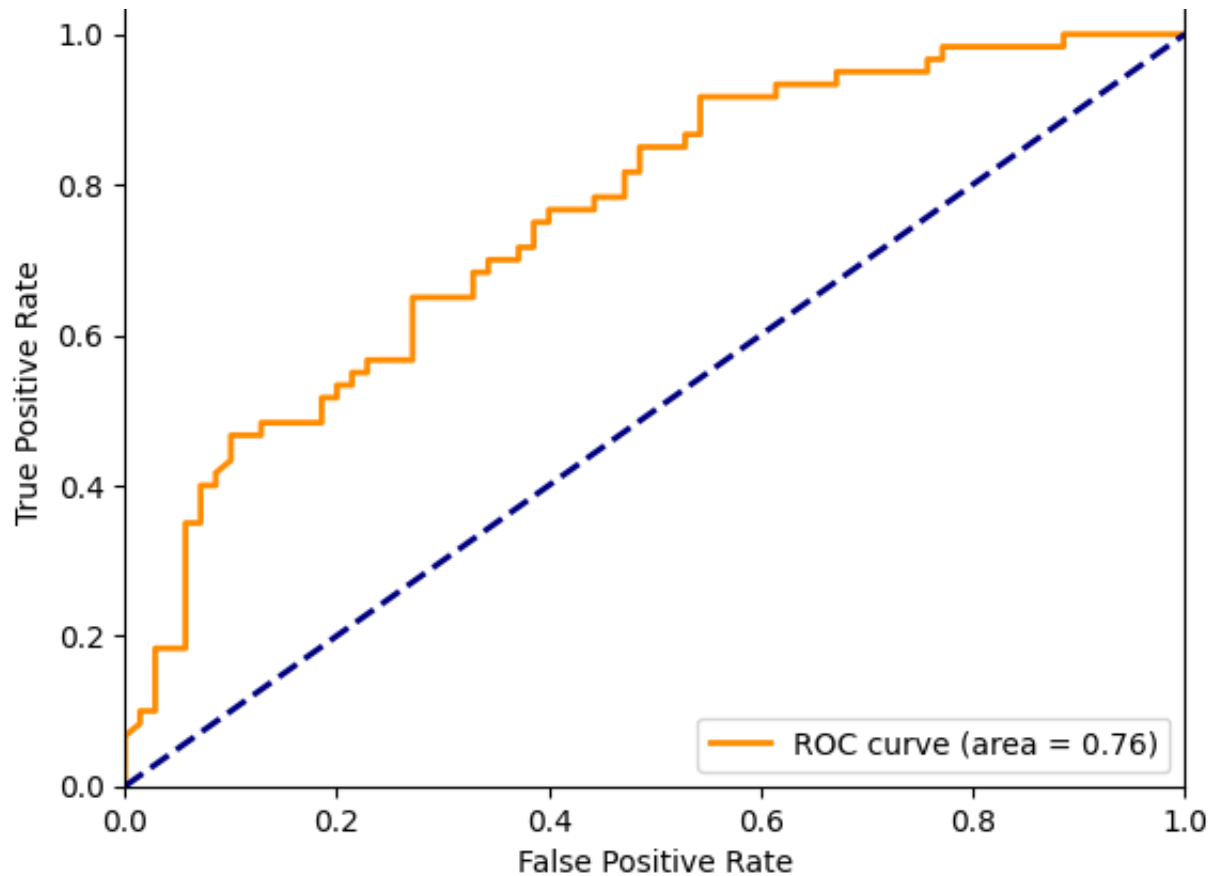
Training - Accuracy: 0.5049, Sensitivity: 0.0000, Specificity: 1.0000, F1:  
Threshold: 0.10, Accuracy: 0.5077, Sensitivity: 1.0000, Specificity: 0.0857  
Threshold: 0.15, Accuracy: 0.5231, Sensitivity: 1.0000, Specificity: 0.1143  
Threshold: 0.20, Accuracy: 0.5154, Sensitivity: 0.9833, Specificity: 0.1143  
Threshold: 0.25, Accuracy: 0.5692, Sensitivity: 0.9833, Specificity: 0.2143  
Threshold: 0.30, Accuracy: 0.6077, Sensitivity: 0.9500, Specificity: 0.3143  
Threshold: 0.35, Accuracy: 0.6385, Sensitivity: 0.9167, Specificity: 0.4000  
Threshold: 0.40, Accuracy: 0.6538, Sensitivity: 0.8667, Specificity: 0.4714  
Threshold: 0.45, Accuracy: 0.6615, Sensitivity: 0.8167, Specificity: 0.5286  
Threshold: 0.50, Accuracy: 0.6692, Sensitivity: 0.7333, Specificity: 0.6143  
Threshold: 0.55, Accuracy: 0.6692, Sensitivity: 0.7000, Specificity: 0.6429  
Threshold: 0.60, Accuracy: 0.6615, Sensitivity: 0.5833, Specificity: 0.7286  
Threshold: 0.65, Accuracy: 0.6692, Sensitivity: 0.5000, Specificity: 0.8143  
Threshold: 0.70, Accuracy: 0.7000, Sensitivity: 0.4667, Specificity: 0.9000  
Threshold: 0.75, Accuracy: 0.6462, Sensitivity: 0.3000, Specificity: 0.9429  
Threshold: 0.80, Accuracy: 0.5923, Sensitivity: 0.1833, Specificity: 0.9429  
Threshold: 0.85, Accuracy: 0.5769, Sensitivity: 0.1167, Specificity: 0.9714  
Threshold: 0.90, Accuracy: 0.5462, Sensitivity: 0.0167, Specificity: 1.0000  
Threshold: 0.95, Accuracy: 0.5385, Sensitivity: 0.0000, Specificity: 1.0000  
Threshold: 1.00, Accuracy: 0.5385, Sensitivity: 0.0000, Specificity: 1.0000  
5/5  0s 8ms/step

Metrics for chosen threshold 0.45:

Accuracy: 0.6615, Sensitivity: 0.8167, Specificity: 0.5286, F1: 0.6901, ROC



Receiver Operating Characteristic Neural Network



Epoch 1/30

```
/usr/local/lib/python3.11/dist-packages/keras/src/layers/core/dense.py:87:
super().__init__(activity_regularizer=activity_regularizer, **kwargs)
```

13/13 ————— 4s 34ms/step - accuracy: 0.5820 - loss: 2.0933 -

Epoch 2/30

13/13 ————— 0s 11ms/step - accuracy: 0.6300 - loss: 1.9992 -

Epoch 3/30

13/13 ————— 0s 10ms/step - accuracy: 0.6705 - loss: 1.8165 -

Epoch 4/30

13/13 ————— 0s 11ms/step - accuracy: 0.7124 - loss: 1.7261 -

Epoch 5/30

13/13 ————— 0s 9ms/step - accuracy: 0.6767 - loss: 1.7591 -

Epoch 6/30

13/13 ————— 0s 10ms/step - accuracy: 0.6989 - loss: 1.6073 -

Epoch 7/30

13/13 ————— 0s 10ms/step - accuracy: 0.6664 - loss: 1.6151 -

Epoch 8/30

13/13 ————— 0s 11ms/step - accuracy: 0.7359 - loss: 1.4982 -

Epoch 9/30

13/13 ————— 0s 12ms/step - accuracy: 0.7117 - loss: 1.4637 -

Epoch 10/30

13/13 ————— 0s 15ms/step - accuracy: 0.6850 - loss: 1.5023 -

Epoch 11/30

13/13 ————— 0s 13ms/step - accuracy: 0.7269 - loss: 1.4122 -

Epoch 12/30

13/13 ————— 0s 11ms/step - accuracy: 0.6957 - loss: 1.3863 -

Epoch 13/30

13/13 ————— 0s 10ms/step - accuracy: 0.7583 - loss: 1.2970 -

Epoch 14/30

13/13 ————— 0s 10ms/step - accuracy: 0.7000 - loss: 1.3346 -

```

13/13 ----- 0s 10ms/step - accuracy: 0.7089 - loss: 1.3240 -
Epoch 15/30
13/13 ----- 0s 10ms/step - accuracy: 0.7855 - loss: 1.2575 -
Epoch 16/30
13/13 ----- 0s 14ms/step - accuracy: 0.7254 - loss: 1.2374 -
Epoch 17/30
13/13 ----- 0s 10ms/step - accuracy: 0.7775 - loss: 1.1986 -
Epoch 18/30
13/13 ----- 0s 10ms/step - accuracy: 0.7922 - loss: 1.1831 -
Epoch 19/30
13/13 ----- 0s 10ms/step - accuracy: 0.8048 - loss: 1.0975 -
Epoch 20/30
13/13 ----- 0s 10ms/step - accuracy: 0.7434 - loss: 1.1419 -
Epoch 21/30
13/13 ----- 0s 11ms/step - accuracy: 0.7560 - loss: 1.1205 -
Epoch 22/30
13/13 ----- 0s 10ms/step - accuracy: 0.7902 - loss: 1.0650 -
Epoch 23/30
13/13 ----- 0s 10ms/step - accuracy: 0.7794 - loss: 1.0587 -
Epoch 24/30
13/13 ----- 0s 10ms/step - accuracy: 0.7965 - loss: 1.0136 -
Epoch 25/30
13/13 ----- 0s 13ms/step - accuracy: 0.7883 - loss: 1.0029 -
Epoch 26/30
13/13 ----- 0s 11ms/step - accuracy: 0.7947 - loss: 0.9764 -
Epoch 27/30
13/13 ----- 0s 10ms/step - accuracy: 0.8069 - loss: 0.9434 -
Epoch 28/30
13/13 ----- 0s 10ms/step - accuracy: 0.8072 - loss: 0.9467 -
Epoch 29/30
13/13 ----- 0s 13ms/step - accuracy: 0.7772 - loss: 0.9336 -
Epoch 30/30
13/13 ----- 0s 10ms/step - accuracy: 0.8073 - loss: 0.9251 -
16/16 ----- 0s 8ms/step
5/5 ----- 0s 7ms/step

```

--- Dados ROC para copiar ---

FPR = [0.0, 0.014285714285714285, 0.02857142857142857, 0.02857142857142857,

TPR = [0.0, 0.016666666666666666, 0.016666666666666666, 0.21666666666666667

AUC = 0.7495238095238095

--- Fim dos Dados ROC ---

```

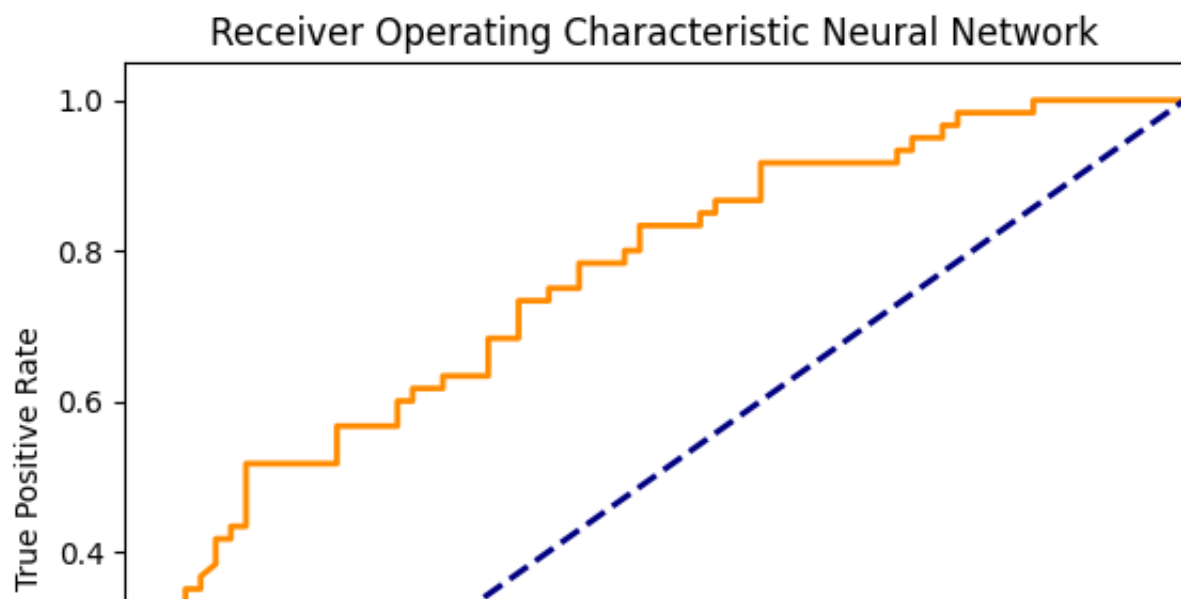
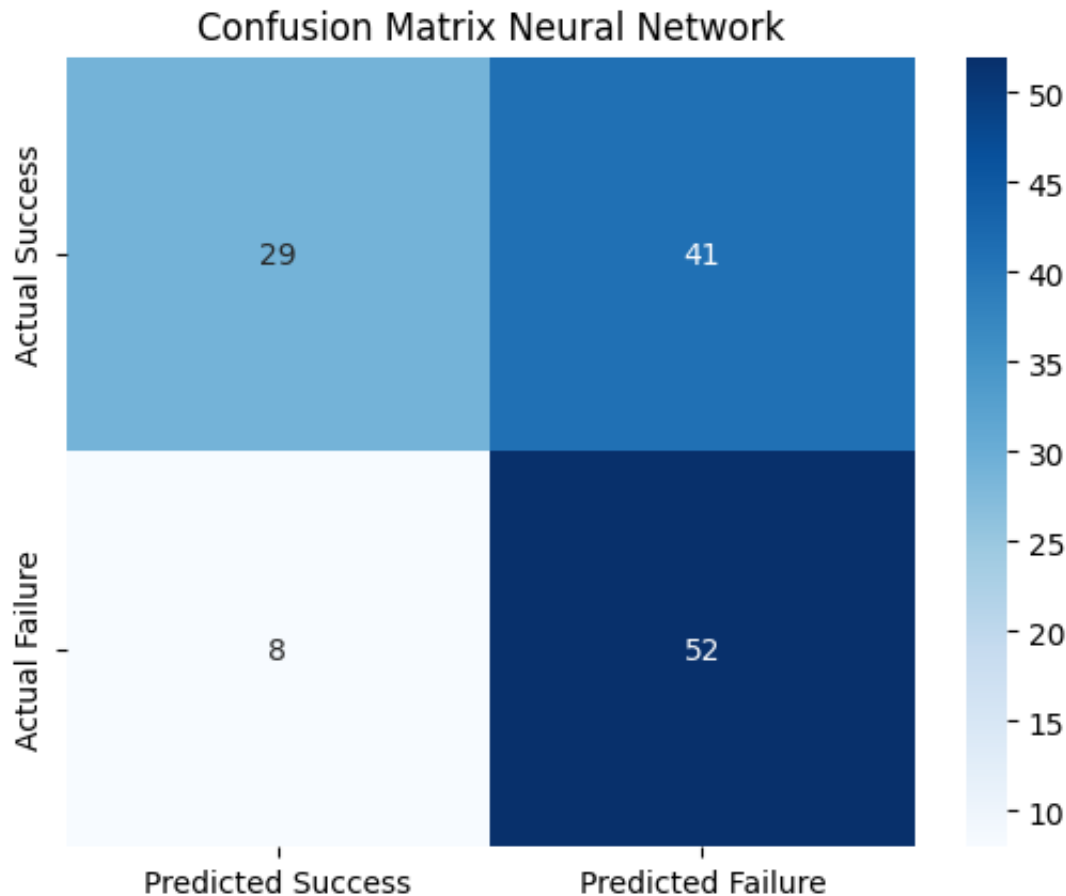
Training - Accuracy: 0.5049, Sensitivity: 0.0000, Specificity: 1.0000, F1:
Threshold: 0.10, Accuracy: 0.4923, Sensitivity: 1.0000, Specificity: 0.0571
Threshold: 0.15, Accuracy: 0.5385, Sensitivity: 1.0000, Specificity: 0.1429
Threshold: 0.20, Accuracy: 0.5462, Sensitivity: 0.9833, Specificity: 0.1714
Threshold: 0.25, Accuracy: 0.5615, Sensitivity: 0.9833, Specificity: 0.2000
Threshold: 0.30, Accuracy: 0.5615, Sensitivity: 0.9500, Specificity: 0.2286
Threshold: 0.35, Accuracy: 0.5692, Sensitivity: 0.9167, Specificity: 0.2714
Threshold: 0.40, Accuracy: 0.6077, Sensitivity: 0.9167, Specificity: 0.3429
Threshold: 0.45, Accuracy: 0.6231, Sensitivity: 0.8667, Specificity: 0.4143
Threshold: 0.50, Accuracy: 0.6538, Sensitivity: 0.8167, Specificity: 0.5143
Threshold: 0.55, Accuracy: 0.6692, Sensitivity: 0.7333, Specificity: 0.6143
Threshold: 0.60, Accuracy: 0.6462, Sensitivity: 0.6333, Specificity: 0.6571
Threshold: 0.65, Accuracy: 0.6600, Sensitivity: 0.5667, Specificity: 0.7571

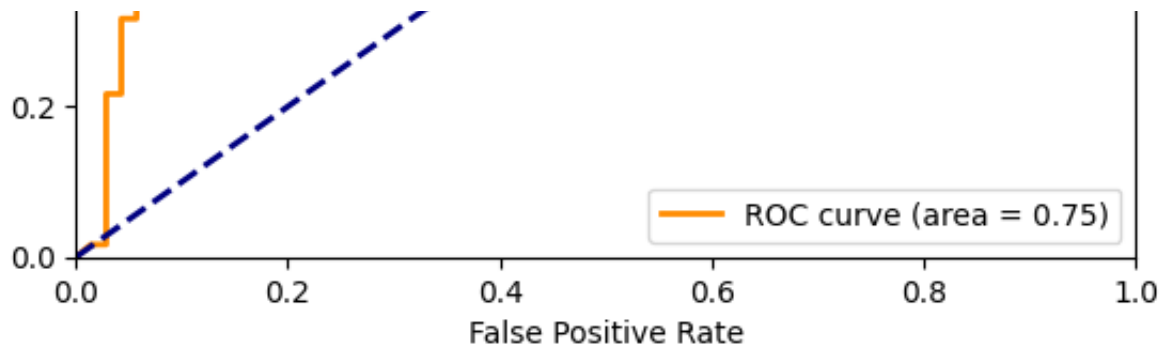
```

```
Threshold: 0.65, Accuracy: 0.6692, Sensitivity: 0.5667, Specificity: 0.7571
Threshold: 0.70, Accuracy: 0.6923, Sensitivity: 0.5167, Specificity: 0.8429
Threshold: 0.75, Accuracy: 0.7077, Sensitivity: 0.5000, Specificity: 0.8857
Threshold: 0.80, Accuracy: 0.6615, Sensitivity: 0.3333, Specificity: 0.9429
Threshold: 0.85, Accuracy: 0.5923, Sensitivity: 0.1500, Specificity: 0.9714
Threshold: 0.90, Accuracy: 0.5538, Sensitivity: 0.0667, Specificity: 0.9714
Threshold: 0.95, Accuracy: 0.5385, Sensitivity: 0.0000, Specificity: 1.0000
Threshold: 1.00, Accuracy: 0.5385, Sensitivity: 0.0000, Specificity: 1.0000
5/5 ————— 0s 9ms/step
```

Metrics for chosen threshold 0.45:

Accuracy: 0.6231, Sensitivity: 0.8667, Specificity: 0.4143, F1: 0.6797, ROC





Epoch 1/30

```
/usr/local/lib/python3.11/dist-packages/keras/src/layers/core/dense.py:87:
super().__init__(activity_regularizer=activity_regularizer, **kwargs)
```

```
13/13 ————— 5s 45ms/step - accuracy: 0.4572 - loss: 2.3356 -
```

Epoch 2/30

```
13/13 ————— 0s 10ms/step - accuracy: 0.6653 - loss: 1.8524 -
```

Epoch 3/30

```
13/13 ————— 0s 10ms/step - accuracy: 0.6542 - loss: 1.8147 -
```

Epoch 4/30

```
13/13 ————— 0s 13ms/step - accuracy: 0.6482 - loss: 1.6993 -
```

Epoch 5/30

```
13/13 ————— 0s 13ms/step - accuracy: 0.7080 - loss: 1.6293 -
```

Epoch 6/30

```
13/13 ————— 0s 13ms/step - accuracy: 0.6663 - loss: 1.6126 -
```

Epoch 7/30

```
13/13 ————— 0s 12ms/step - accuracy: 0.7615 - loss: 1.5127 -
```

Epoch 8/30

```
13/13 ————— 0s 10ms/step - accuracy: 0.7101 - loss: 1.4593 -
```

Epoch 9/30

```
13/13 ————— 0s 13ms/step - accuracy: 0.7223 - loss: 1.4421 -
```

Epoch 10/30

```
13/13 ————— 0s 10ms/step - accuracy: 0.7347 - loss: 1.4103 -
```

Epoch 11/30

```
13/13 ————— 0s 11ms/step - accuracy: 0.7979 - loss: 1.2864 -
```

Epoch 12/30

```
13/13 ————— 0s 13ms/step - accuracy: 0.7689 - loss: 1.2795 -
```

Epoch 13/30

```
13/13 ————— 0s 10ms/step - accuracy: 0.7712 - loss: 1.2544 -
```

Epoch 14/30

```
13/13 ————— 0s 10ms/step - accuracy: 0.7692 - loss: 1.2603 -
```

Epoch 15/30

```
13/13 ————— 0s 10ms/step - accuracy: 0.7675 - loss: 1.1830 -
```

Epoch 16/30

```
13/13 ————— 0s 10ms/step - accuracy: 0.7699 - loss: 1.2111 -
```

Epoch 17/30

```
13/13 ————— 0s 10ms/step - accuracy: 0.7804 - loss: 1.1415 -
```

Epoch 18/30

```
13/13 ————— 0s 13ms/step - accuracy: 0.8022 - loss: 1.1195 -
```

Epoch 19/30

```
13/13 ————— 0s 10ms/step - accuracy: 0.8259 - loss: 1.0513 -
```












Epoch 20/30

```
13/13 ————— 0s 11ms/step - accuracy: 0.8286 - loss: 1.0658 -
```

Epoch 21/30

```
13/13 ————— 0s 10ms/step - accuracy: 0.8131 - loss: 1.0186 -
```

```

Epoch 22/30
13/13  0s 10ms/step - accuracy: 0.8056 - loss: 1.0375 -
Epoch 23/30
13/13  0s 10ms/step - accuracy: 0.7966 - loss: 0.9970 -
Epoch 24/30
13/13  0s 10ms/step - accuracy: 0.8312 - loss: 0.9458 -
Epoch 25/30
13/13  0s 11ms/step - accuracy: 0.8496 - loss: 0.9309 -
Epoch 26/30
13/13  0s 10ms/step - accuracy: 0.8151 - loss: 0.9297 -
Epoch 27/30
13/13  0s 10ms/step - accuracy: 0.8328 - loss: 0.9132 -
Epoch 28/30
13/13  0s 14ms/step - accuracy: 0.8374 - loss: 0.8998 -
Epoch 29/30
13/13  0s 10ms/step - accuracy: 0.8369 - loss: 0.8788 -
Epoch 30/30
13/13  0s 14ms/step - accuracy: 0.8361 - loss: 0.8533 -
16/16  0s 8ms/step
5/5  0s 8ms/step

```

--- Dados ROC para copiar ---


```

FPR = [0.0, 0.0, 0.014285714285714285, 0.014285714285714285, 0.028571428571
TPR = [0.0, 0.016666666666666666, 0.033333333333333333, 0.16666666666666666,
AUC = 0.7892857142857144

```

--- Fim dos Dados ROC ---

```

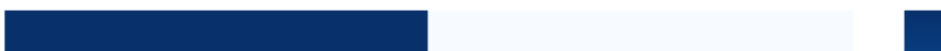
Training - Accuracy: 0.5049, Sensitivity: 0.0000, Specificity: 1.0000, F1:
Threshold: 0.10, Accuracy: 0.5462, Sensitivity: 1.0000, Specificity: 0.1571
Threshold: 0.15, Accuracy: 0.5769, Sensitivity: 0.9833, Specificity: 0.2286
Threshold: 0.20, Accuracy: 0.5846, Sensitivity: 0.9667, Specificity: 0.2571
Threshold: 0.25, Accuracy: 0.6308, Sensitivity: 0.9500, Specificity: 0.3571
Threshold: 0.30, Accuracy: 0.6538, Sensitivity: 0.8833, Specificity: 0.4571
Threshold: 0.35, Accuracy: 0.6923, Sensitivity: 0.8500, Specificity: 0.5571
Threshold: 0.40, Accuracy: 0.7231, Sensitivity: 0.7667, Specificity: 0.6857
Threshold: 0.45, Accuracy: 0.7231, Sensitivity: 0.6833, Specificity: 0.7571
Threshold: 0.50, Accuracy: 0.7231, Sensitivity: 0.6333, Specificity: 0.8000
Threshold: 0.55, Accuracy: 0.6923, Sensitivity: 0.5333, Specificity: 0.8286
Threshold: 0.60, Accuracy: 0.7000, Sensitivity: 0.4833, Specificity: 0.8857
Threshold: 0.65, Accuracy: 0.6769, Sensitivity: 0.4000, Specificity: 0.9143
Threshold: 0.70, Accuracy: 0.6385, Sensitivity: 0.3167, Specificity: 0.9143
Threshold: 0.75, Accuracy: 0.6308, Sensitivity: 0.2667, Specificity: 0.9429
Threshold: 0.80, Accuracy: 0.6000, Sensitivity: 0.1833, Specificity: 0.9571
Threshold: 0.85, Accuracy: 0.6077, Sensitivity: 0.1833, Specificity: 0.9714
Threshold: 0.90, Accuracy: 0.5692, Sensitivity: 0.0833, Specificity: 0.9857
Threshold: 0.95, Accuracy: 0.5385, Sensitivity: 0.0000, Specificity: 1.0000
Threshold: 1.00, Accuracy: 0.5385, Sensitivity: 0.0000, Specificity: 1.0000
5/5  0s 8ms/step

```

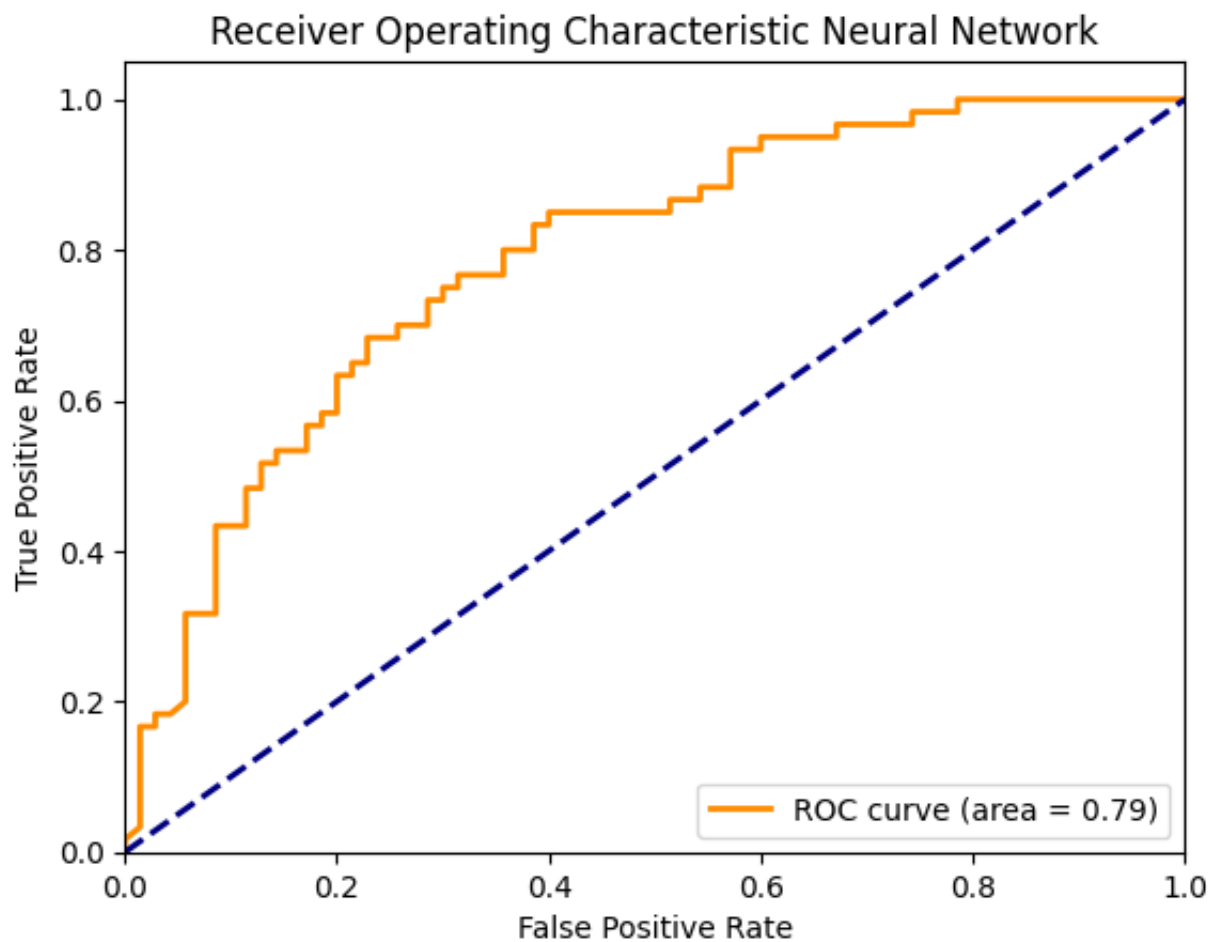
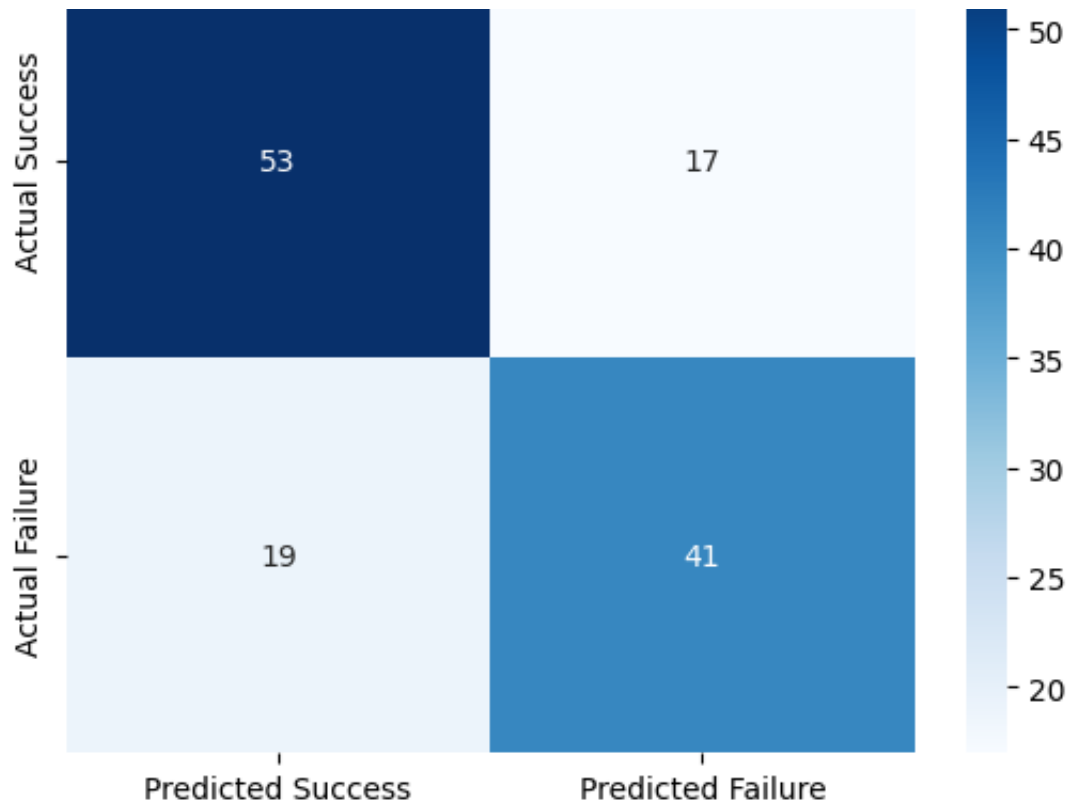
Metrics for chosen threshold 0.45:

Accuracy: 0.7231, Sensitivity: 0.6833, Specificity: 0.7571, F1: 0.6949, ROC

## Confusion Matrix Neural Network







Aggregated Test Set Metrics Across Seeds:

	accuracy	sensitivity	specificity	f1	roc_auc
0	0.646154	0.583333	0.700000	0.603448	0.725476
1	0.730769	0.833333	0.642857	0.740741	0.792619



2	0.638462	0.816667	0.485714	0.675862	0.739286
3	0.653846	0.883333	0.457143	0.701987	0.764762
4	0.669231	0.650000	0.685714	0.644628	0.766667
5	0.692308	0.900000	0.514286	0.729730	0.786190
6	0.676923	0.633333	0.714286	0.644068	0.762262
7	0.661538	0.816667	0.528571	0.690141	0.756905
8	0.623077	0.866667	0.414286	0.679739	0.749524
9	0.723077	0.683333	0.757143	0.694915	0.789286

Summary of Test Set Metrics (Mean, Standard Error, 95% Confidence Interval)

Accuracy: Mean = 0.6715, SE = 0.0111, 95% CI = [0.6464, 0.6967]

Sensitivity: Mean = 0.7667, SE = 0.0369, 95% CI = [0.6831, 0.8502]

Specificity: Mean = 0.5900, SE = 0.0389, 95% CI = [0.5020, 0.6780]

F1: Mean = 0.6805, SE = 0.0131, 95% CI = [0.6509, 0.7101]

Roc\_auc: Mean = 0.7633, SE = 0.0069, 95% CI = [0.7476, 0.7790]