Lab 3.7 - Student Notebook

Overview

This lab is a continuation of the guided labs in Module 3.

In this lab, you will create a hyperparameter tuning job to tune the model that you created previously. You will then compare the metrics of the two models.

Introduction to the business scenario

You work for a healthcare provider, and want to improve the detection of abnormalities in orthopedic patients.

You are tasked with solving this problem by using machine learning (ML). You have access to a dataset that contains six biomechanical features and a target of *normal* or *abnormal*. You can use this dataset to train an ML model to predict if a patient will have an abnormality.

About this dataset

This biomedical dataset was built by Dr. Henrique da Mota during a medical residence period in the Group of Applied Research in Orthopaedics (GARO) of the Centre Médico-Chirurgical de Réadaptation des Massues, Lyon, France. The data has been organized in two different, but related, classification tasks.

The first task consists in classifying patients as belonging to one of three categories:

- Normal (100 patients)
- Disk Hernia (60 patients)
- Spondylolisthesis (150 patients)

For the second task, the categories *Disk Hernia* and *Spondylolisthesis* were merged into a single category that is labeled as *abnormal*. Thus, the second task consists in classifying patients as belonging to one of two categories: *Normal* (100 patients) or *Abnormal* (210 patients).

Attribute information

Each patient is represented in the dataset by six biomechanical attributes that are derived from the shape and orientation of the pelvis and lumbar spine (in this order):

- Pelvic incidence
- Pelvic tilt
- Lumbar lordosis angle
- Sacral slope
- Pelvic radius
- Grade of spondylolisthesis

The following convention is used for the class labels:

- DH (Disk Hernia)
- Spondylolisthesis (SL)
- Normal (NO)
- Abnormal (AB)

For more information about this dataset, see the Vertebral Column dataset webpage.

Dataset attributions

This dataset was obtained from: Dua, D. and Graff, C. (2019). UCI Machine Learning Repository (http://archive.ics.uci.edu/ml). Irvine, CA: University of California, School of Information and Computer Science.

Lab setup

Because this solution is split across several labs in the module, you run the following cells so that you can load the data and train the model to be deployed.

Note: The setup can take up to 5 minutes to complete.

Importing the data, and training, testing and validating the model

By running the following cells, the data will be imported, and the model will be trained, tested and validated and ready for use.

Note: The following cells represent the key steps in the previous labs.

In order to tune the model it must be ready, then you can tweak the mdoel with hyperparameters later in step 2.

```
import warnings, requests, zipfile, io
warnings.simplefilter('ignore')
import pandas as pd
from scipy.io import arff

import os
import boto3
import sagemaker
from sagemaker.image_uris import retrieve
from sklearn.model_selection import train_test_split

from sklearn.metrics import roc_auc_score, roc_curve, auc, confusion_matrix
import seaborn as sns
import matplotlib.pyplot as plt

sagemaker.config INFO - Not applying SDK defaults from location: /etc/xdg/sagemake
```

r/config.yaml
sagemaker.config INFO - Not applying SDK defaults from location: /etc/xdg/sagemake
r/config.yaml
sagemaker.config INFO - Not applying SDK defaults from location: /home/ec2-user/.c
onfig/sagemaker/config.yaml

Matplotlib is building the font cache; this may take a moment.

Note: The following cell takes approximately **10** minutes to complete. Observe the code and how it processes, this will help you to better understand what is going on in the background. Keep in mind that this cell completes all the steps you did in previous labs in this module including:

- Importing the data
- Loading the data into a dataframe
- Splitting the data into training, test and validation datasets
- Uploading the split datasets to S3
- Training, testing and validating the model with the datasets

```
In [3]: %%time
        def plot roc(test labels, target predicted binary):
            TN, FP, FN, TP = confusion_matrix(test_labels, target_predicted_binary).ravel()
            # Sensitivity, hit rate, recall, or true positive rate
            Sensitivity = float(TP)/(TP+FN)*100
            # Specificity or true negative rate
            Specificity = float(TN)/(TN+FP)*100
            # Precision or positive predictive value
            Precision = float(TP)/(TP+FP)*100
            # Negative predictive value
            NPV = float(TN)/(TN+FN)*100
            # Fall out or false positive rate
            FPR = float(FP)/(FP+TN)*100
            # False negative rate
            FNR = float(FN)/(TP+FN)*100
            # False discovery rate
            FDR = float(FP)/(TP+FP)*100
            # Overall accuracy
            ACC = float(TP+TN)/(TP+FP+FN+TN)*100
```

```
print(f"Sensitivity or TPR: {Sensitivity}%")
   print(f"Specificity or TNR: {Specificity}%")
   print(f"Precision: {Precision}%")
   print(f"Negative Predictive Value: {NPV}%")
   print( f"False Positive Rate: {FPR}%")
   print(f"False Negative Rate: {FNR}%")
   print(f"False Discovery Rate: {FDR}%" )
   print(f"Accuracy: {ACC}%")
   test_labels = test.iloc[:,0];
   print("Validation AUC", roc_auc_score(test_labels, target_predicted_binary) )
   fpr, tpr, thresholds = roc_curve(test_labels, target_predicted_binary)
   roc_auc = auc(fpr, tpr)
   plt.figure()
   plt.plot(fpr, tpr, label='ROC curve (area = %0.2f)' % (roc_auc))
   plt.plot([0, 1], [0, 1], 'k--')
   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")
   # create the axis of thresholds (scores)
   ax2 = plt.gca().twinx()
   ax2.plot(fpr, thresholds, markeredgecolor='r',linestyle='dashed', color='r')
   ax2.set_ylabel('Threshold',color='r')
   ax2.set_ylim([thresholds[-1],thresholds[0]])
   ax2.set_xlim([fpr[0],fpr[-1]])
   print(plt.figure())
def plot_confusion_matrix(test_labels, target_predicted):
   matrix = confusion_matrix(test_labels, target_predicted)
   df confusion = pd.DataFrame(matrix)
   colormap = sns.color palette("BrBG", 10)
    sns.heatmap(df_confusion, annot=True, fmt='.2f', cbar=None, cmap=colormap)
   plt.title("Confusion Matrix")
   plt.tight_layout()
   plt.ylabel("True Class")
   plt.xlabel("Predicted Class")
   plt.show()
f_zip = 'http://archive.ics.uci.edu/ml/machine-learning-databases/00212/vertebral_c
r = requests.get(f_zip, stream=True)
Vertebral_zip = zipfile.ZipFile(io.BytesIO(r.content))
Vertebral zip.extractall()
data = arff.loadarff('column_2C_weka.arff')
df = pd.DataFrame(data[0])
class_mapper = {b'Abnormal':1,b'Normal':0}
df['class']=df['class'].replace(class_mapper)
```

```
cols = df.columns.tolist()
cols = cols[-1:] + cols[:-1]
df = df[cols]
train, test_and_validate = train_test_split(df, test_size=0.2, random_state=42, str
test, validate = train_test_split(test_and_validate, test_size=0.5, random_state=42
prefix='lab3'
train_file='vertebral_train.csv'
test file='vertebral test.csv'
validate_file='vertebral_validate.csv'
s3 resource = boto3.Session().resource('s3')
def upload_s3_csv(filename, folder, dataframe):
   csv_buffer = io.StringIO()
   dataframe.to_csv(csv_buffer, header=False, index=False )
   s3_resource.Bucket(bucket).Object(os.path.join(prefix, folder, filename)).put(B
upload_s3_csv(train_file, 'train', train)
upload_s3_csv(test_file, 'test', test)
upload_s3_csv(validate_file, 'validate', validate)
container = retrieve('xgboost',boto3.Session().region name,'1.0-1')
hyperparams={"num_round":"42",
             "eval metric": "auc",
             "objective": "binary:logistic",
             "silent" : 1}
s3_output_location="s3://{}/{}/output/".format(bucket,prefix)
xgb_model=sagemaker.estimator.Estimator(container,
                                       sagemaker.get_execution_role(),
                                       instance_count=1,
                                       instance_type='ml.m5.2xlarge',
                                       output path=s3 output location,
                                        hyperparameters=hyperparams,
                                        sagemaker_session=sagemaker.Session())
train_channel = sagemaker.inputs.TrainingInput(
    "s3://{}/{}/train/".format(bucket,prefix,train_file),
    content_type='text/csv')
validate_channel = sagemaker.inputs.TrainingInput(
    "s3://{}/validate/".format(bucket,prefix,validate_file),
   content_type='text/csv')
data_channels = {'train': train_channel, 'validation': validate_channel}
xgb_model.fit(inputs=data_channels, logs=False)
batch_X = test.iloc[:,1:];
batch X file='batch-in.csv'
upload_s3_csv(batch_X_file, 'batch-in', batch_X)
```

```
batch_output = "s3://{}/batch-out/".format(bucket,prefix)
batch input = "s3://{}/{}/batch-in/{}".format(bucket,prefix,batch X file)
xgb_transformer = xgb_model.transformer(instance_count=1,
                                      instance_type='ml.m5.2xlarge',
                                      strategy='MultiRecord',
                                      assemble_with='Line',
                                      output path=batch output)
xgb_transformer.transform(data=batch_input,
                        data_type='S3Prefix',
                        content_type='text/csv',
                        split_type='Line')
xgb transformer.wait(logs=False)
INFO:sagemaker:Creating training-job with name: sagemaker-xgboost-2025-08-17-13-12
-06-648
2025-08-17 13:12:07 Starting - Starting the training job..
2025-08-17 13:12:22 Starting - Preparing the instances for training..
2025-08-17 13:12:39 Downloading - Downloading input data..
2025-08-17 13:12:55 Downloading - Downloading the training image.....
2025-08-17 13:13:30 Training - Training image download completed. Training in prog
2025-08-17 13:13:56 Uploading - Uploading generated training model..
2025-08-17 13:14:09 Completed - Training job completed
INFO:sagemaker:Creating model with name: sagemaker-xgboost-2025-08-17-13-14-13-422
INFO:sagemaker:Creating transform job with name: sagemaker-xgboost-2025-08-17-13-1
4-14-041
CPU times: user 1.54 s, sys: 188 ms, total: 1.73 s
Wall time: 8min 6s
```

Step 1: Getting model statistics

Before you tune the model, re-familiarize yourself with the current model's metrics.

The setup performed a batch prediction, so you must read in the results from Amazon Simple Storage Service (Amazon S3).

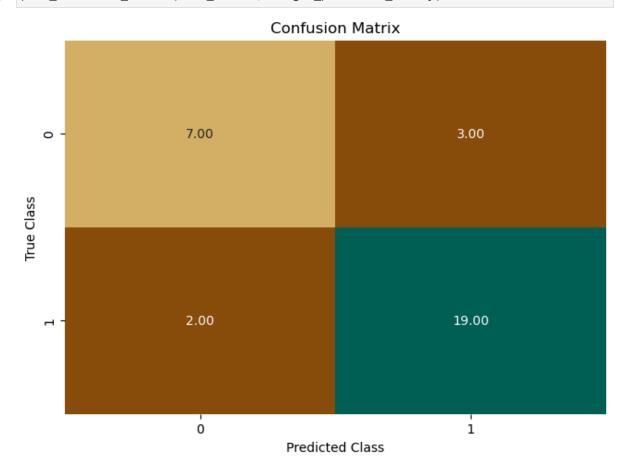
```
In [4]:
    s3 = boto3.client('s3')
    obj = s3.get_object(Bucket=bucket, Key="{}/batch-out/{}".format(prefix,'batch-in.cs
    target_predicted = pd.read_csv(io.BytesIO(obj['Body'].read()),names=['class'])

def binary_convert(x):
    threshold = 0.5
    if x > threshold:
        return 1
    else:
        return 0
```

```
target_predicted_binary = target_predicted['class'].apply(binary_convert)
test_labels = test.iloc[:,0]
```

Plot the confusion matrix and the receiver operating characteristic (ROC) curve for the original model.

In [5]: plot_confusion_matrix(test_labels, target_predicted_binary)



In [6]: plot_roc(test_labels, target_predicted_binary)

Sensitivity or TPR: 90.47619047619048%

Specificity or TNR: 70.0% Precision: 86.36363636363636

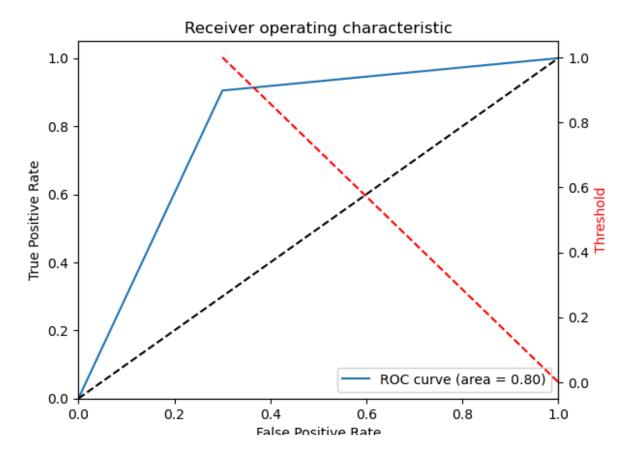
Negative Predictive Value: 77.77777777779%

False Positive Rate: 30.0%

Accuracy: 83.87096774193549% Validation AUC 0.8023809523809523

```
Traceback (most recent call last) -
in <module>:1
) 1 plot_roc(test_labels, target_predicted_binary)
in plot roc:49
/home/ec2-user/anaconda3/envs/python3/lib/python3.10/site-packages/matplotli
in set_ylim
  4049
                   if top is not None:
                       raise TypeError("Cannot pass both 'top' and 'ymax'")
  4050
  4051
                   top = ymax
) 4052
               return self.yaxis. set lim(bottom, top, emit=emit, auto=auto)
  4053
  4054
           get_yscale = _axis_method_wrapper("yaxis", "get_scale")
           set yscale = axis method wrapper("yaxis", " set axes scale")
  4055
/home/ec2-user/anaconda3/envs/python3/lib/python3.10/site-packages/matplotli
set lim
  1214
               self.axes. process unit info([(name, (v0, v1))], convert=Fals
  1215
               v0 = self.axes._validate_converted_limits(v0, self.convert_un
  1216
1217
               v1 = self.axes. validate converted limits(v1, self.convert un
  1218
  1219
               if v0 is None or v1 is None:
  1220
                   # Axes init calls set_xlim(0, 1) before get_xlim() can be
/home/ec2-user/anaconda3/envs/python3/lib/python3.10/site-packages/matplotli
in _validate_converted_limits
                       converted_limit = converted_limit.squeeze()
  3736
  3737
                   if (isinstance(converted_limit, Real)
                           and not np.isfinite(converted limit)):
  3738
3739
                       raise ValueError("Axis limits cannot be NaN or Inf")
  3740
                   return converted limit
  3741
  3742
           def set xlim(self, left=None, right=None, *, emit=True, auto=Fals
```

ValueError: Axis limits cannot be NaN or Inf



This plot gives you a starting point. Make a note of the *Validation area under the curve (AUC)*. You will use it later to check your tuned model to see if it's better.

Step 2: Creating a hyperparameter tuning job

A hyperparameter tuning job can take several hours to complete, depending on the value ranges that you provide. To simplify this task, the parameters used in this step are a subset of the recommended ranges. They were tuned to give good results in this lab, without taking multiple hours to complete.

For more information about the parameters to tune for XGBoost, see Tune an XGBoost Model in the AWS Documentation.

Because this next cell can take approximately **45** minutes to complete, go ahead and run the cell. You will examine what's happening, and why these hyperparameter ranges were chosen.

```
instance_type='ml.m4.xlarge',
                                    output_path='s3://{}/output'.format(bucket,
                                    sagemaker session=sagemaker.Session())
xgb.set_hyperparameters(eval_metric='error@.40',
                        objective='binary:logistic',
                        num round=42)
hyperparameter_ranges = { 'alpha': ContinuousParameter(0, 100),
                         'min_child_weight': ContinuousParameter(1, 5),
                         'subsample': ContinuousParameter(0.5, 1),
                         'eta': ContinuousParameter(0.1, 0.3),
                         'num_round': IntegerParameter(1,50)
objective_metric_name = 'validation:error'
objective_type = 'Minimize'
tuner = HyperparameterTuner(xgb,
                            objective_metric_name,
                            hyperparameter_ranges,
                            max_jobs=10, # Set this to 10 or above depending upon b
                            max_parallel_jobs=1,
                            objective_type=objective_type,
                            early stopping type='Auto')
tuner.fit(inputs=data_channels, include_cls_metadata=False)
tuner.wait()
```

First, you will create the model that you want to tune.

Notice that the *eval_metric* of the model was changed to *error@.40*, with a goal of minimizing that value.

error is the binary classification error rate. It's calculated as #(wrong cases)/#(all cases). For predictions, the evaluation will consider the instances that have a prediction value larger

than 0.4 to be positive instances, and the others as negative instances.

Next, you must specify the hyperparameters that you want to tune, in addition to the ranges that you must select for each parameter.

The hyperparameters that have the largest effect on XGBoost objective metrics are:

- alpha
- min_child_weight
- subsample
- eta
- num round

The recommended tuning ranges can be found in the AWS Documentation at Tune an XGBoost Model.

For this lab, you will use a *subset* of values. These values were obtained by running the tuning job with the full range, then minimizing the range so that you can use fewer iterations to get better performance. Though this practice isn't strictly realistic, it prevents you from waiting several hours in this lab for the tuning job to complete.

You must specify how you are rating the model. You could use several different objective metrics, a subset of which applies to a binary classification problem. Because the evaluation metric is **error**, you set the objective to *error*.

```
objective_metric_name = 'validation:error'
objective_type = 'Minimize'
```

Finally, you run the tuning job.

```
tuner.fit(inputs=data_channels, include_cls_metadata=False)
tuner.wait()
```

Wait until the training job is finished. It might take up to **45** minutes. While you are waiting, observe the job status in the console, as described in the following instructions.

To monitor hyperparameter optimization jobs:

- 1. In the AWS Management Console, on the **Services** menu, choose **Amazon SageMaker**.
- 2. Choose **Training > Hyperparameter tuning jobs**.
- 3. You can check the status of each hyperparameter tuning job, its objective metric value, and its logs.

After the training job is finished, check the job and make sure that it completed successfully.

Step 3: Investigating the tuning job results

Now that the job is complete, there should be 10 completed jobs. One of the jobs should be marked as the best.

You can examine the metrics by getting *HyperparameterTuningJobAnalytics* and loading that data into a pandas DataFrame.

```
In [9]: from pprint import pprint
from sagemaker.analytics import HyperparameterTuningJobAnalytics

tuner_analytics = HyperparameterTuningJobAnalytics(tuner.latest_tuning_job.name, sa

df_tuning_job_analytics = tuner_analytics.dataframe()

# Sort the tuning job analytics by the final metrics value

df_tuning_job_analytics.sort_values(
    by=['FinalObjectiveValue'],
    inplace=True,
    ascending=False if tuner.objective_type == "Maximize" else True)

# Show detailed analytics for the top 20 models

df_tuning_job_analytics.head(20)
```

Out[9]:		alpha	eta	min_child_weight	num_round	subsample	TrainingJobName	TrainingJobSt
	0	10.950396	0.117005	3.952173	48.0	0.923327	sagemaker- xgboost-250817- 1322-010- 90670033	Compl
	1	8.530900	0.250943	2.691228	30.0	0.931734	sagemaker- xgboost-250817- 1322-009- 124d00f1	Compl
	3	13.310649	0.123024	3.239096	45.0	0.758787	sagemaker- xgboost-250817- 1322-007- c1af2c62	Compl
	2	0.000000	0.288789	1.372494	43.0	0.734033	sagemaker- xgboost-250817- 1322-008- ed81853e	Compl
	4	25.319327	0.105476	4.631399	37.0	0.816182	sagemaker- xgboost-250817- 1322-006- 2b8a201a	Compl
	5	85.829524	0.112860	1.967791	11.0	0.891646	sagemaker- xgboost-250817- 1322-005- 4e2c3fac	Stoţ
	6	83.236067	0.115312	2.967319	15.0	0.612255	sagemaker- xgboost-250817- 1322-004- efb687a8	Compl
	7	53.905240	0.279767	3.699243	6.0	0.631864	sagemaker- xgboost-250817- 1322-003- 081756b6	Stoŗ
	8	84.594289	0.162824	1.793102	44.0	0.707728	sagemaker- xgboost-250817- 1322-002- a06c9350	Stoŗ
	9	62.823638	0.197017	3.350466	27.0	0.585030	sagemaker- xgboost-250817- 1322-001- 3eecc02f	Compl

You should be able to see the hyperparameters that were used for each job, along with the score. You could use those parameters and create a model, or you can get the best model from the hyperparameter tuning job.

In [10]: attached_tuner = HyperparameterTuner.attach(tuner.latest_tuning_job.name, sagemaker

```
best_training_job = attached_tuner.best_training_job()
```

Now, you must attach to the best training job and create the model.

```
In [11]: from sagemaker.estimator import Estimator
algo_estimator = Estimator.attach(best_training_job)

best_algo_model = algo_estimator.create_model(env={'SAGEMAKER_DEFAULT_INVOCATIONS_A

2025-08-17 13:32:55 Starting - Found matching resource for reuse
2025-08-17 13:32:55 Downloading - Downloading the training image
2025-08-17 13:32:55 Training - Training image download completed. Training in prog
ress.
2025-08-17 13:32:55 Uploading - Uploading generated training model
2025-08-17 13:32:55 Completed - Resource reused by training job: sagemaker-xgboost
-250817-1322-009-124d00f1
```

Then, you can use the transform method to perform a batch prediction by using your testing data. Remember that the testing data is data that the model has never seen before.

```
In [12]: %%time
         batch_output = "s3://{}/{}/batch-out/".format(bucket,prefix)
         batch_input = "s3://{}/{}/batch-in/{}".format(bucket,prefix,batch_X_file)
         xgb transformer = best algo model.transformer(instance count=1,
                                               instance type='ml.m4.xlarge',
                                               strategy='MultiRecord',
                                               assemble with='Line',
                                               output_path=batch_output)
         xgb transformer.transform(data=batch input,
                                 data_type='S3Prefix',
                                 content_type='text/csv',
                                 split_type='Line')
         xgb_transformer.wait(logs=False)
         INFO:sagemaker:Creating model with name: sagemaker-xgboost-2025-08-17-13-34-45-343
         INFO:sagemaker:Creating transform job with name: sagemaker-xgboost-2025-08-17-13-3
         4-45-826
         ......
         . . !
         CPU times: user 723 ms, sys: 21.5 ms, total: 745 ms
         Wall time: 6min 28s
```

Get the predicted target and the test labels of the model.

```
In [13]:
    s3 = boto3.client('s3')
    obj = s3.get_object(Bucket=bucket, Key="{}/batch-out/{}".format(prefix,'batch-in.cs
    best_target_predicted = pd.read_csv(io.BytesIO(obj['Body'].read()),names=['class'])

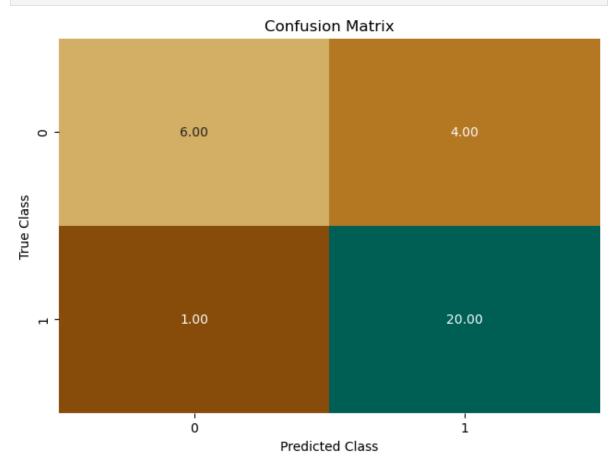
def binary_convert(x):
    threshold = 0.5
    if x > threshold:
        return 1
```

```
else:
    return 0

best_target_predicted_binary = best_target_predicted['class'].apply(binary_convert)
test_labels = test.iloc[:,0]
```

Plot a confusion matrix for your best_target_predicted and test_labels.

In [14]: plot_confusion_matrix(test_labels, best_target_predicted_binary)



Plot the ROC chart.

```
In [15]: plot_roc(test_labels, best_target_predicted_binary)
```

Sensitivity or TPR: 95.23809523809523%

Specificity or TNR: 60.0% Precision: 83.3333333333334%

Negative Predictive Value: 85.71428571428571%

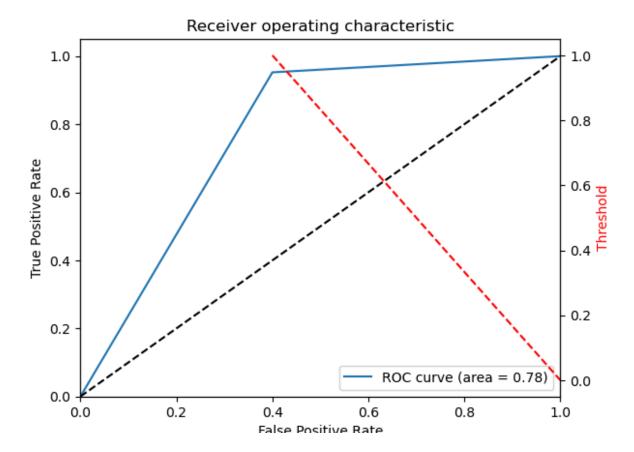
False Positive Rate: 40.0%

False Negative Rate: 4.761904761904762% False Discovery Rate: 16.66666666666664%

Accuracy: 83.87096774193549% Validation AUC 0.7761904761904761

```
Traceback (most recent call last) -
in <module>:1
) 1 plot_roc(test_labels, best_target_predicted_binary)
in plot roc:49
/home/ec2-user/anaconda3/envs/python3/lib/python3.10/site-packages/matplotli
in set_ylim
  4049
                   if top is not None:
                       raise TypeError("Cannot pass both 'top' and 'ymax'")
  4050
  4051
                   top = ymax
) 4052
               return self.yaxis. set lim(bottom, top, emit=emit, auto=auto)
  4053
  4054
           get_yscale = _axis_method_wrapper("yaxis", "get_scale")
           set yscale = axis method wrapper("yaxis", " set axes scale")
  4055
/home/ec2-user/anaconda3/envs/python3/lib/python3.10/site-packages/matplotli
set lim
  1214
               self.axes. process unit info([(name, (v0, v1))], convert=Fals
  1215
               v0 = self.axes._validate_converted_limits(v0, self.convert_un
  1216
1217
               v1 = self.axes. validate converted limits(v1, self.convert un
  1218
  1219
               if v0 is None or v1 is None:
  1220
                   # Axes init calls set_xlim(0, 1) before get_xlim() can be
/home/ec2-user/anaconda3/envs/python3/lib/python3.10/site-packages/matplotli
in _validate_converted_limits
                       converted_limit = converted_limit.squeeze()
  3736
  3737
                   if (isinstance(converted_limit, Real)
                           and not np.isfinite(converted limit)):
  3738
                       raise ValueError("Axis limits cannot be NaN or Inf")
3739
  3740
                   return converted limit
  3741
  3742
           def set xlim(self, left=None, right=None, *, emit=True, auto=Fals
```

ValueError: Axis limits cannot be NaN or Inf



Question: How do these results differ from the original? Are these results better or worse?

You might not always see an improvement. There are a few reasons for this result:

- The model might already be good from the initial pass (what counts as *good* is subjective).
- You don't have a large amount of data to train with.
- You are using a subset of the hyperparameter tuning ranges to save time in this lab.

Increasing the hyperparameter ranges (as recommended by the documentation) and running more than 30 jobs will typically improve the model. However, this process will take 2-3 hours to complete.

Congratulations!

You have completed this lab, and you can now end the lab by following the lab guide instructions.

In []: