

Lab 3.6 - Student Notebook

Overview

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

In this lab, you will evaluate the model that you trained in previous modules. You will also calculate metrics based on the results of the test data.

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 the model

By running the following cells, the data will be imported and ready for use.

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

```
In [1]:
        bucket='c169682a4380823l11227747t1w845330842670-labbucket-fugeldmocqcm'
In [2]: import warnings, requests, zipfile, io
        warnings.simplefilter('ignore')
        import pandas as pd
        from scipy.io import arff
        import os
        import boto3
        import sagemaker
        import numpy as np
        from sklearn.metrics import roc_curve, auc
        import matplotlib.pyplot as plt
        from sagemaker.image uris import retrieve
        from sklearn.model selection import train test split
       sagemaker.config INFO - Not applying SDK defaults from location: /etc/xdg/sagem
       aker/config.yaml
       sagemaker.config INFO - Not applying SDK defaults from location: /home/ec2-use
       r/.config/sagemaker/config.yaml
In [3]: f zip = 'http://archive.ics.uci.edu/ml/machine-learning-databases/00212/verteb
        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
        test, validate = train test split(test and validate, test size=0.5, random sta
        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)).
```

```
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"}
s3 output location="s3://{}/{output/".format(bucket,prefix)
xgb model=sagemaker.estimator.Estimator(container,
                                       sagemaker.get execution role(),
                                       instance count=1,
                                       instance type='ml.m4.xlarge',
                                       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.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()
s3 = boto3.client('s3')
obj = s3.get object(Bucket=bucket, Key="{}/batch-out/{}".format(prefix,'batch-
```

Step 1: Exploring the results

The output from the model will be a probability. You must first convert that probability into one of the two classes, either 0 or 1. To do this, you can create a function to perform the conversion. Note the use of the threshold in the function.

```
In [4]: def binary convert(x):
            threshold = 0.3
            if x > threshold:
                return 1
            else:
                return 0
        target predicted binary = target predicted['class'].apply(binary convert)
        print(target predicted binary.head(5))
        test.head(5)
            1
            1
      1
       2
            1
      3
           1
      Name: class, dtype: int64
```

Out[4]:		class	pelvic_incidence	pelvic_tilt	lumbar_lordosis_angle	sacral_slope	pel
	136	1	88.024499	39.844669	81.774473	48.179830	1
	230	0	65.611802	23.137919	62.582179	42.473883	1
	134	1	52.204693	17.212673	78.094969	34.992020	1
	130	1	50.066786	9.120340	32.168463	40.946446	
	47	1	41.352504	16.577364	30.706191	24.775141	1

Based on these results, you can see that the initial model might not be that good. It's difficult to tell by comparing a few values.

Next, you will generate some metrics to see how well the model performs.

Step 2: Creating a confusion matrix

A *confusion matrix* is one of the key ways of measuring a classification model's performance. It's a table that maps out the correct and incorrect predictions. After you calculate a confusion matrix for your model, you can generate several other statistics. However, you will start by only creating the confusion matrix.

To create a confusion matrix, you need both the target values from your test data and the predicted value.

Get the targets from the test DataFrame.

```
In [5]: test_labels = test.iloc[:,0]
test_labels.head()

Out[5]: 136    1
    230    0
    134    1
    130    1
    47    1
    Name: class, dtype: int64
```

Now, you can use the *scikit-learn* library, which contains a function to create a confusion matrix.

```
In [6]: from sklearn.metrics import confusion_matrix

matrix = confusion_matrix(test_labels, target_predicted_binary)
df_confusion = pd.DataFrame(matrix, index=['Nnormal','Abnormal'],columns=['Nor
df_confusion
```

Out[6]:

	Normal	Abnormal	
Nnormal	7	3	
Abnormal	2	19	

You results will vary, but you should have results that are similiar to this example:

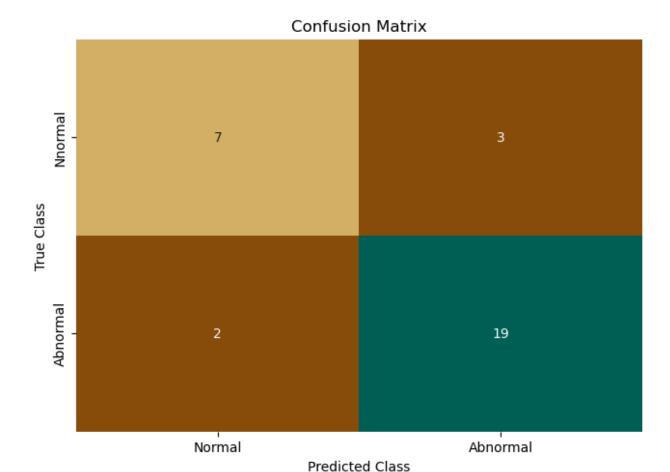
_	Normal	Abnormal	
Normal	7	3	
Abnormal	3	18	

The previous table shows that the model correctly predicted 7 Normal and 18 Abnormal values. However, it incorrectly predicted 3 Normal and 3 Abnormal values.

By using the *seaborn* and *matplotlib* Python libraries, you can plot these values in a chart to make them easier to read.

```
In [7]: import seaborn as sns
import matplotlib.pyplot as plt

colormap = sns.color_palette("BrBG", 10)
sns.heatmap(df_confusion, annot=True, cbar=None, cmap=colormap)
plt.title("Confusion Matrix")
plt.tight_layout()
plt.ylabel("True Class")
plt.xlabel("Predicted Class")
plt.show()
```



Tip: If the chart doesn't display the first time, try running the cell again.

If these results are good enough for your application, then the model might be good enough. However, because there are consequences from incorrectly predicting *Normal* values -- that is, no abnormality was found when there actually was one -- the focus should be on reducing this result.

Step 3: Calculating performance statistics

If you want to compare this model to the next model that you create, you need some metrics that you can record. For a binary classification problem, the confusion matrix data can be used to calculate various metrics.

To start, extract the values from the confusion matrix cells into variables.

```
In [8]: from sklearn.metrics import roc_auc_score, roc_curve, auc

TN, FP, FN, TP = confusion_matrix(test_labels, target_predicted_binary).ravel(
```

```
print(f"True Negative (TN) : {TN}")
print(f"False Positive (FP): {FP}")
print(f"False Negative (FN): {FN}")
print(f"True Positive (TP) : {TP}")
```

True Negative (TN): 7
False Positive (FP): 3
False Negative (FN): 2
True Positive (TP): 19

You can now calculate some statistics.

Sensitivity

Sensitivity is also known as hit rate, recall, or true positive rate (TPR). It measures the proportion of the actual positives that are correctly identified.

In this example, the sensitivity is the probablity of detecting an abnormality for patients with an abnormality.

```
In [9]: # Sensitivity, hit rate, recall, or true positive rate
    Sensitivity = float(TP)/(TP+FN)*100
    print(f"Sensitivity or TPR: {Sensitivity}%")
    print(f"There is a {Sensitivity}% chance of detecting patients with an abnorma
```

Sensitivity or TPR: 90.47619047619048%

There is a 90.47619047619048% chance of detecting patients with an abnormality have an abnormality

Question: Is the sensitivity good enough for this scenario?

Specificity

The next statistic is *specificity*, which is also known as the *true negative*. It measures the proportion of the actual negatives that are correctly identified.

In this example, the specificity is the probablity of detecting normal, for patients who are normal.

```
In [10]: # Specificity or true negative rate
    Specificity = float(TN)/(TN+FP)*100
    print(f"Specificity or TNR: {Specificity}%")
    print(f"There is a {Specificity}% chance of detecting normal patients are norm
```

Specificity or TNR: 70.0%

There is a 70.0% chance of detecting normal patients are normal.

Question: Is this specificity too low, exactly right, or too high? What value would you want to see here, given the scenario?

Positive and negative predictive values

The precision, or positive predictive value, is the proportion of positive results.

In this example, the positive predictive value is the probability that subjects with a positive screening test truly have an abnormality.

```
In [11]: # Precision or positive predictive value
         Precision = float(TP)/(TP+FP)*100
         print(f"Precision: {Precision}%")
         print(f"You have an abnormality, and the probablity that is correct is {Precis
```

Precision: 86.36363636363636%

You have an abnormality, and the probablity that is correct is 86.3636363636363 6%

The *negative predictive value* is the proportion of negative results.

In this example, the negative predictive value is the probability that subjects with a negative screening test truly have an abnormality.

```
In [12]: # Negative predictive value
         NPV = float(TN)/(TN+FN)*100
         print(f"Negative Predictive Value: {NPV}%")
         print(f"You don't have an abnormality, but there is a {NPV}% chance that is in
```

Negative Predictive Value: 77.7777777779%

You don't have an abnormality, but there is a 77.77777777779% chance that is incorrect

Think about the impact of these values. If you were a patient, how worried should you be if the test for an abnormality was positive? On the opposite side, how reassured should you be if you tested negative?

False positive rate

The false positive rate (FPR) is the probability that a false alarm will be raised, or that a positive result will be given when the true value is negative.

```
In [13]: # Fall out or false positive rate
         FPR = float(FP)/(FP+TN)*100
         print( f"False Positive Rate: {FPR}%")
         print( f"There is a {FPR}% chance that this positive result is incorrect.")
```

False Positive Rate: 30.0%

There is a 30.0% chance that this positive result is incorrect.

False negative rate

The false negative rate -- or miss rate -- is the probability that a true positive will be missed by the test.

```
In [14]: # False negative rate
FNR = float(FN)/(TP+FN)*100
print(f"False Negative Rate: {FNR}%")
print(f"There is a {FNR}% chance that this negative result is incorrect.")
```

False Negative Rate: 9.523809523809524% There is a 9.523809523809524% chance that this negative result is incorrect.

False discovery rate

In this example, the false discovery rate is the probability of predicting an abnormality when the patient doesn't have one.

```
In [15]: # False discovery rate
FDR = float(FP)/(TP+FP)*100
print(f"False Discovery Rate: {FDR}%" )
print(f"You have an abnormality, but there is a {FDR}% chance this is incorrect
```

False Discovery Rate: 13.6363636363635%

You have an abnormality, but there is a 13.6363636363635% chance this is incorrect.

Overall accuracy

How accuracte is your model?

```
In [16]: # Overall accuracy
ACC = float(TP+TN)/(TP+FP+FN+TN)*100
print(f"Accuracy: {ACC}%")
```

Accuracy: 83.87096774193549%

In summary, you calculated the following metrics from your model:

```
In [17]: 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}%")
```

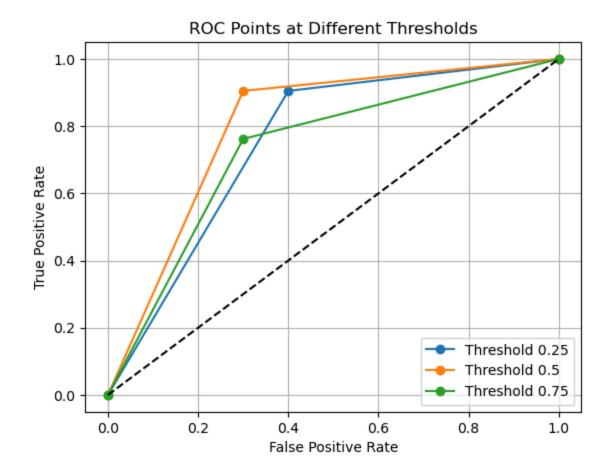
Sensitivity or TPR: 90.47619047619048% Specificity or TNR: 70.0% Precision: 86.36363636363636% Negative Predictive Value: 77.77777777777779% False Positive Rate: 30.0% False Negative Rate: 9.523809523809524% False Discovery Rate: 13.636363636363635% Accuracy: 83.87096774193549%

Challenge task: Record the previous values, then go back to step 1 and change the value used for the threshold. Values you should try are .25 and .75.

Did those threshold values make a difference?

```
In [20]: from sklearn.metrics import classification report, confusion matrix, roc curve
         import numpy as np
         import matplotlib.pyplot as plt
         def evaluate threshold(threshold):
             preds binary = (target predicted >= threshold).astype(int)
             print(f"\n--- Threshold: {threshold} ---")
             print("Classification Report:")
             print(classification report(test labels, preds binary))
             print("Confusion Matrix:")
             print(confusion matrix(test labels, preds binary))
             fpr, tpr, _ = roc_curve(test_labels, preds binary)
             plt.plot(fpr, tpr, marker='o', label=f'Threshold {threshold}')
         thresholds to try = [0.25, 0.5, 0.75]
         plt.figure()
         for thresh in thresholds to try:
             evaluate threshold(thresh)
         plt.plot([0, 1], [0, 1], 'k--')
         plt.xlabel('False Positive Rate')
         plt.ylabel('True Positive Rate')
         plt.title('ROC Points at Different Thresholds')
         plt.legend(loc='lower right')
         plt.grid(True)
         plt.show()
```

Threshold: 0 Classification Re	eport:	recall	f1-score	support
0 1	0.75 0.83	0.60 0.90	0.67 0.86	10 21
accuracy macro avg weighted avg	0.79 0.80	0.75 0.81	0.81 0.77 0.80	31 31 31
Confusion Matrix [[6 4] [2 19]]	:			
Threshold: 0 Classification Re	eport:	recall	f1-score	support
0 1	0.78 0.86	0.70 0.90	0.74 0.88	10 21
accuracy macro avg weighted avg	0.82 0.84	0.80 0.84	0.84 0.81 0.84	31 31 31
Confusion Matrix [[7 3] [2 19]]	:			
Threshold: 0 Classification Ro		recall	f1-score	support
0 1	0.58 0.84	0.70 0.76	0.64 0.80	10 21
accuracy macro avg weighted avg	0.71 0.76	0.73 0.74	0.74 0.72 0.75	31 31 31
Confusion Matrix [[7 3] [5 16]]	:			



Step 4: Calculating the AUC-ROC Curve

The scikit-learn library has functions that can help you compute the *area under the* receiver operating characteristic curve (AUC-ROC).

- The ROC is a probability curve.
- The AUC tells you how well the model can distinguish between classes.

The AUC can be calculated. As you will see in the next lab, it can be used to measure the performance of the model.

In this example, the higher the AUC, the better the model is at distinguishing between abnormal and normal patients.

Depending on the value you set for the threshold, the AUC can change. You can plot the AUC by using the probability instead of your converted class.

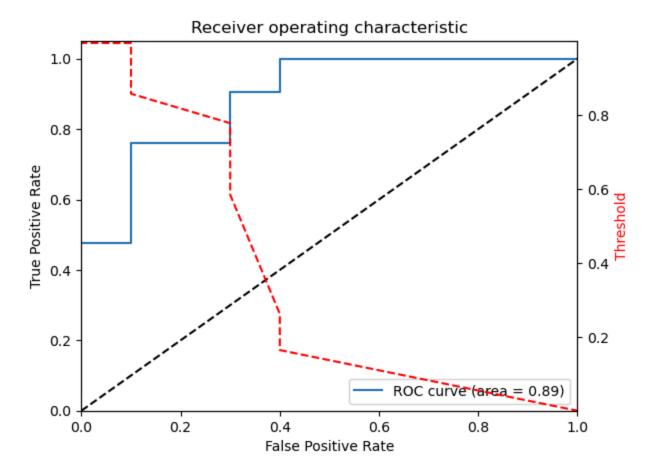
```
In [18]: test_labels = test.iloc[:,0];
print("Validation AUC", roc_auc_score(test_labels, target_predicted) )
```

Validation AUC 0.8904761904761904

Typically, the ROC curve is plotted with the TPR against the FPR, where the TPR is on the y-axis and the FPR is on the x-axis.

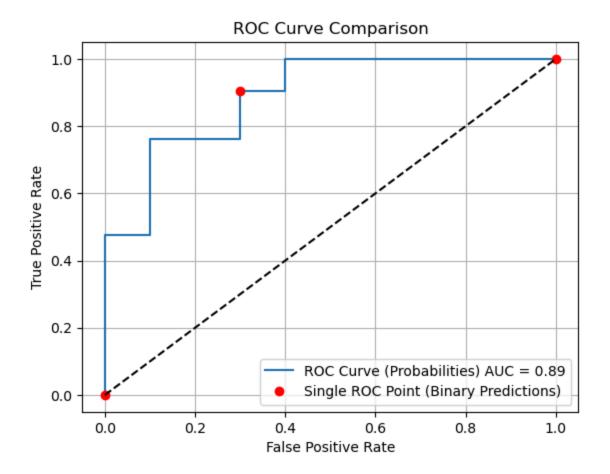
scikit-learn has the **roc curve** function to help generate those values to plot.

```
In [19]: fpr, tpr, thresholds = roc curve(test labels, target predicted)
         finite indices = np.isfinite(thresholds)
         fpr finite = fpr[finite indices]
         tpr finite = tpr[finite indices]
         thresholds finite = thresholds[finite indices]
         plt.figure()
         plt.plot(fpr finite, tpr finite, label='ROC curve (area = %0.2f)' % auc(fpr fi
         plt.plot([0, 1], [0, 1], 'k--') # Dashed diagonal
         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")
         roc auc = auc(fpr, tpr)
         if thresholds finite.size > 0:
             ax2 = plt.gca().twinx()
             ax2.plot(fpr finite, thresholds finite, markeredgecolor='r', linestyle='de
             ax2.set ylabel('Threshold', color='r')
             ax2.set ylim([thresholds finite[-1], thresholds finite[0]])
             ax2.set xlim([fpr finite[0], fpr finite[-1]])
         plt.show()
```



Challenge task: Update the previous code to use *target_predicted_binary* instead of *target_predicted*. How does that change the graph? Which is the most useful?

```
In [21]:
        from sklearn.metrics import roc curve, auc
         fpr prob, tpr prob, thresholds prob = roc curve(test labels, target predicted)
         roc auc prob = auc(fpr prob, tpr prob)
         target_predicted_binary = (target_predicted >= 0.5).astype(int)
         fpr bin, tpr bin, thresholds bin = roc curve(test labels, target predicted bir
         roc auc bin = auc(fpr bin, tpr bin)
         plt.figure()
         plt.plot(fpr prob, tpr prob, label=f'ROC Curve (Probabilities) AUC = {roc auc
         plt.plot(fpr bin, tpr bin, 'ro', label='Single ROC Point (Binary Predictions)'
         plt.plot([0, 1], [0, 1], 'k--')
         plt.xlabel('False Positive Rate')
         plt.ylabel('True Positive Rate')
         plt.title('ROC Curve Comparison')
         plt.legend(loc='lower right')
         plt.grid(True)
         plt.show()
```



Congratulations!

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