Welcome to the module 2b coding part: Decision Tree Classifier and Overfitting!

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OBJECTIVE OF THIS NOTEBOOK:

Now that we have learned how to make predictions using **Decision Trees**, we can take a look at what happens when we **overfit** or **underfit* *our data.

In this module we are going to continue using the 14 variables from the Cleveland dataset.

Below we have a brief description of what each of the features we are going to use mean. The numbers next to the features are the ones that were used in the original dataset.

- [1] #3 Age: age in years
- [2] #4 Sex: sex (1 = male; 0 = female)
- [3] #9 Chest_pain_type
  - Value 1: typical angina
  - Value 2: atypical angina
  - Value 3: non-anginal pain
  - Value 4: asymptomatic
- [4] #10 At_rest_bp: resting blood pressure (in mm Hg on admission to the hospital)
- [5] #12 Cholesterol: serum cholestoral in mg/dl
- [6] #16 Fast_blood_sug: (fasting blood sugar > 120 mg/dl) (1 = true; 0 = false)
- [7] #19 Rest_ecg: resting electrocardiographic results
  - Value 0: normal
  - Value 1: having ST-T wave abnormality (T wave inversions and/or ST elevation or depression of > 0.05 mV)
  - Value 2: showing probable or definite left ventricular hypertrophy by Estes' criteria
- [8] #32 Maxhr: thalach: maximum heart rate achieved
- [9] #38 Exer_angina: exang: exercise induced angina (1 = yes; 0 = no)
- [10] #40 Oldpeak: ST depression induced by exercise relative to rest
- [11] #41 Slope: the slope of the peak exercise ST segment
  - Value 1: upsloping
  - Value 2: flat
  - Value 3: downsloping
- [12] #44 Ca: number of major vessels (0-3) colored by flourosopy
- [13] #51 Thal: Thallium or stress test 3 = normal; 6 = fixed defect; 7 = reversable defect. See this website for more info on the thallium or stress test.
- [14] #58 Diag: num: diagnosis of heart disease (angiographic disease status)
  - Value 0: no vessel with 50% diameter narrowing
  - Value 1: one vessel with 50% diameter narrowing
  - Value 2,3,4: 2,3,4 vessels with 50% diameter narrowing

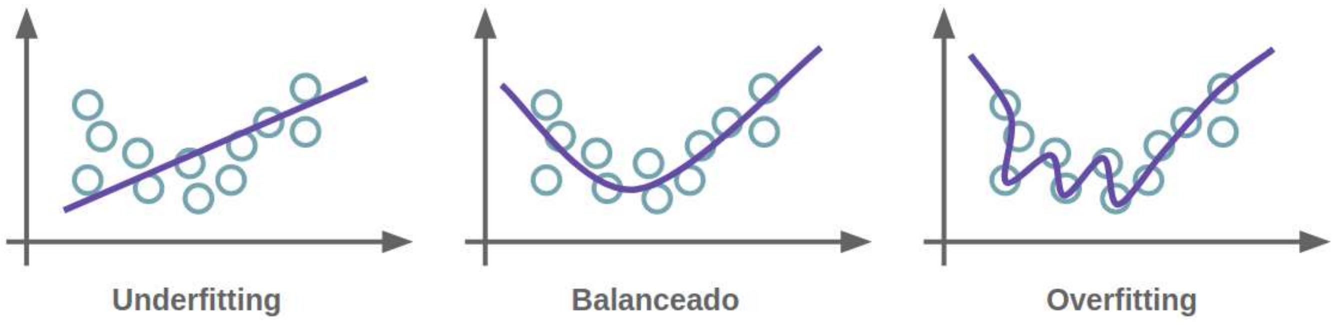
The **goal** of this notebook is to learn how overfitting works using the decision tree classifier model. I like decision trees because they are easier to understand than most other machine learning or statistical learning methods.

Your mission is to run each cell, see what happens, and answer some questions based on the code.

Let's look at the Cleveland dataset again with a focus on **overfitting**.

WHAT IS OVERFITTING?

In machine learning it's important to train the models properly, not too much, not too little. For that reason, it's important to learn how to handle data that could be either overfitting or underfitting.



OVERFITTING: is a undesirable machine learning behavior, where our model follows too closely our training data, meaning it learns to predict our training data very well but it fails to make accurate predictions for new data.

UNDERFITTING: is a undesirable machine learning behavior, where our model does not get to learn enough from our training data, and therefore performs poorly when trying to make predictions for new data.

What we actually want is somewhere in the middle, we want it to fit just right like a nice shoe! We dont want our shoes to be so loose that we could loose them while walking (underfit) or so perfectly close to the shape of our foot that it feels too tight to walk comfortably (overfit).

You can find more information about overfitting and underfitting here: Scikit-learn: Underfitting vs. Overfitting

Step 1) Importing packages

Here we importing all the necessary packages– we'll explain what they do later when we use them.

```
# packages for data manipulation
import pandas as pd
import numpy as np

# packages for creating the machine learning model
from sklearn.tree import DecisionTreeClassifier
from sklearn.model_selection import train_test_split
from sklearn import metrics
from sklearn import tree

# packages for plotting
import matplotlib.pyplot as plt
import seaborn as sns
import graphviz

#hyperparameter tunning imports
from sklearn.model_selection import validation_curve
```

Step 2) Importing Cleveland dataset

First, we fetch the dataset from the 508 class github repository and state what columns we are interested in. The data are stored in a pandas data frame called "data".

```
# Loading our dataset again from github
columns = ["Age","Sex","Chest_pain_type","At_rest_bp","Cholesterol","Fast_blood_sug","Rest_ecg","Maxhr","Exer_angina","Oldpeak","Slope","Ca","Thal",'
data = pd.read_csv('https://raw.githubusercontent.com/pleunipennings/CSC508Data/main/processed.cleveland.data.txt',header=None,names=columns )
data.head()
```

	Age	Sex	Chest_pain_type	At_rest_bp	Cholesterol	Fast_blood_sug	Rest_ecg	Maxhr	Exer_angina	Oldpeak	Slope	Ca	Thal	Diag
0	63.0	1.0	1.0	145.0	233.0	1.0	2.0	150.0	0.0	2.3	3.0	0.0	6.0	0
1	67.0	1.0	4.0	160.0	286.0	0.0	2.0	108.0	1.0	1.5	2.0	3.0	3.0	2
2	67.0	1.0	4.0	120.0	229.0	0.0	2.0	129.0	1.0	2.6	2.0	2.0	7.0	1
3	37.0	1.0	3.0	130.0	250.0	0.0	0.0	187.0	0.0	3.5	3.0	0.0	3.0	0
4	41.0	0.0	2.0	130.0	204.0	0.0	2.0	172.0	0.0	1.4	1.0	0.0	3.0	0

後續步驟： 使用 data生成程式碼 查看建議的圖表 New interactive sheet

Step 3) Dealing with missing data

Next, we are going to do some work to deal with the missing data. Note that every dataset encodes **Missing values** differently, which is why it is a good idea sometimes to check exactly how missing values were encoded either from your data source, looking at the documentation about the data, etc.

In this case our dataset missing values, were encoded with a **"question mark (?)"**. Identify the columns having missing values

Task 1: Checking for missing data (Questions 1-3)

Question 1:

Is there missing data in the dataset, if so, how can you check that?

Which are the variables that have missing data?

```
#Code line to answer question 1
# Replace '?' with NaN
data.replace('?', np.nan, inplace=True)

# Convert the relevant columns to numeric types (for any further numerical analysis)
data = data.apply(pd.to_numeric, errors='ignore')

# Check for missing data
missing_data = data.isna().sum()

# Print the number of missing values in each column
print(missing_data)

# Identify which variables have missing data
columns_with_missing_data = missing_data[missing_data > 0].index.tolist()
print(f"Variables with missing data: {columns_with_missing_data}")
```

```
Age                0
Sex                0
Chest_pain_type    0
At_rest_bp         0
Cholesterol        0
Fast_blood_sug     0
Rest_ecg           0
Maxhr              0
Exer_angina        0
Oldpeak            0
Slope              0
Ca                 4
Thal               2
Diag               0
dtype: int64
Variables with missing data: ['Ca', 'Thal']
```

Question 1 answer:

- `Ca`: 4 missing values
- `Thal`: 2 missing values

Question 2:

How can you display the missing values location?

```
#Code line to answer question 2
# Display the location of missing values
missing_locations = data.isna()

# Print the DataFrame showing missing values
print(missing_locations)
```

```
       Age    Sex  Chest_pain_type  At_rest_bp  Cholesterol  Fast_blood_sug  \
0    False  False            False       False        False           False
1    False  False            False       False        False           False
2    False  False            False       False        False           False
3    False  False            False       False        False           False
4    False  False            False       False        False           False
..     ...    ...              ...         ...          ...             ...
298  False  False            False       False        False           False
299  False  False            False       False        False           False
300  False  False            False       False        False           False
301  False  False            False       False        False           False
```

```
302  False  False           False       False        False          False

     Rest_ecg  Maxhr  Exer_angina  Oldpeak  Slope     Ca   Thal   Diag
0       False  False        False    False  False  False  False  False
1       False  False        False    False  False  False  False  False
2       False  False        False    False  False  False  False  False
3       False  False        False    False  False  False  False  False
4       False  False        False    False  False  False  False  False
..        ...    ...          ...      ...    ...    ...    ...    ...
298     False  False        False    False  False  False  False  False
299     False  False        False    False  False  False  False  False
300     False  False        False    False  False  False  False  False
301     False  False        False    False  False  False  False  False
302     False  False        False    False  False   True  False  False

[303 rows x 14 columns]
```

Question 2 answer:

Dealing with missing data, by replacing all missing values with the medians of the feature column.

```
# Replacing all the missing data with the median
data = data.replace('?', np.nan)
data['Thal'] = data['Thal'].fillna(data['Thal'].median())
data['Ca'] = data['Ca'].fillna(data['Ca'].median())
```

Question 3:

How can you verify that there is not missing values?

```
#Code line to answer question 3
# Check for missing values
missing_values_after_imputation = data.isna().sum()

# Print the number of missing values in each column
print(missing_values_after_imputation)

# Verify that there are no missing values
if missing_values_after_imputation.sum() == 0:
    print("There are no missing values in the dataset.")
else:
    print("There are still missing values in the dataset.")
```

```
Age                0
Sex                0
Chest_pain_type    0
At_rest_bp         0
Cholesterol        0
Fast_blood_sug     0
Rest_ecg           0
Maxhr              0
Exer_angina        0
Oldpeak            0
Slope              0
Ca                 0
Thal               0
Diag               0
dtype: int64
There are no missing values in the dataset.
```

Question 3 answer: There are no missing values in the dataset.

Task 2: Understanding how machine learning models work (Questions 4-8)

Question 4:

Write a list of the five basic steps there are before start training a machine learning model:

Question 4 answer:

1. Data Collection
2. Data Preprocessing
3. Feature Selection/Engineering

4. Exploratory Data Analysis (EDA)
5. Model Selection and Configuration

Step 4) Splitting target and features

Next we will separate our target variable from our features (variables used for predictions).

NOTE: We want to take the "Diag" column out of the features dataframe, because it is actually not a feature (in our analysis) but it is the "target" **Target** – what we want to predict.

```
# specifying target variable or label
labels = np.array(data["Diag"])

#Specifying feature variables
features = data.drop(columns='Diag')
features = features.astype('float64')
feats = np.array(features)

# For brevity we will rename them as X(features) and y(label)
X = features
y = labels
```

Next, we are converting the labels (stored in variable y) to binary values so that the model is trained just to predict the presence/absence of heart disease. All the values that are 1 or higher will just be 1 from here on. Recall that:

- **[0]** means no vessel with 50% diameter narrowing (No Heart Disease)
- **[1]** means one or more vessels with 50% diameter narrowing (Heart Disease)

```
# converting our target variable into 1 and 0
y = np.where(y >= 1,1,0)
```

Question 5:

Why did we need to change the label to [0] no heart disease and [1] heart disease for this Decision Tree Classifier model dataset?

Question 5 answer: We changed the label to [0] for no heart disease and [1] for heart disease for the following reasons:

1. Binary Classification Requirement: The Decision Tree Classifier model works best when the target variable is binary.
2. Simplified Modeling: Having a binary label simplifies the modeling process.
3. Consistency with Model Output: Many classification algorithms expect binary labels for tasks such as calculating accuracy, precision, and recall.
4. Improved Interpretation: Converting the target variable into binary values makes the results easier to interpret.

Step 5) Separating train and test data

```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_state=2) # 70% training and 30% test
```

Up until now we have only reviewed what we have already done in the first part of the Notebook Module 2a

Now we are going observe differences in fitting our tree when we change the **max_deph** argument.

Question 6:

Why do we use more percentage for training?

Question 6 answer: When training a model, it's best to use a higher percentage for training, for example, 70%, because it helps the model learn better, improves performance, and enhances feature learning.

Question 7:

Why do we use less percentage for testing?

Question 7 answer: Using a smaller percentage for testing (e.g., 30%) is important because it ensures a substantial portion of the data is reserved for training, allows for efficient use of computational resources and time, and provides a fair estimate of how the model will perform on new, unseen data.

Question 8:

When we split the data into training and testing, does that mean that we start training from there, why or why not?

Question 8 answer:

1. Data Preparation
2. Model Selection and Configuration
3. Validation and Tuning
4. Initial Analysis

Step 6) Making the decision tree and making predictions with it

Task 3: Testing underfitted and overfitted decision trees (Questions 9-12)

Underfitted Decision Tree

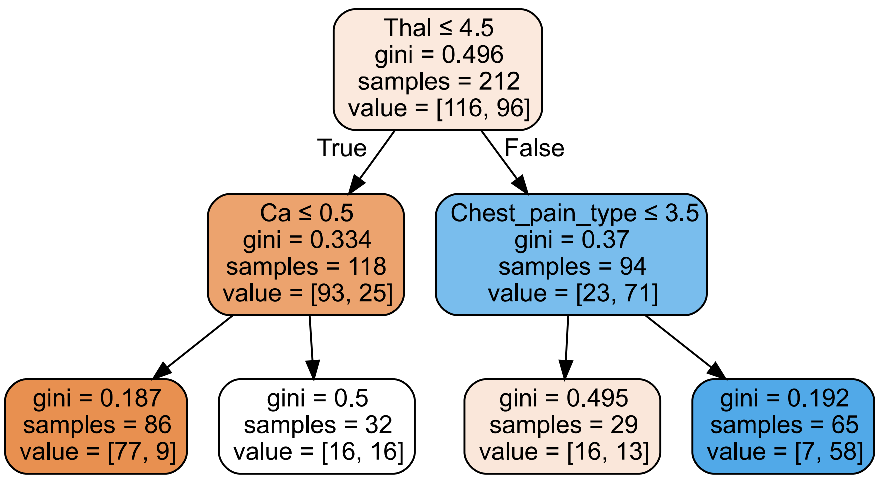
Here we will create a Decision Tree that is only 2 layers deep. Just as before we will create it, train it and graph it. Later we will compare how our tree performs by making predictions for the training data as well as for the testing data.

```
# Create Decision Tree classifer object
clf_under = DecisionTreeClassifier(max_depth=2, random_state=2)

# Train Decision Tree Classifer
clf_under = clf_under.fit(X_train,y_train)
```

Let's visualize our tree. Notice that because we specified that our tree should be at max 2 layers, the end gini values do not always reach to 0, unlike the first tree we made in the previous module, plus as expected we can see that there are only 2 layers 1 root node layer + 1 subsequent layer, before reaching the leaf nodes (prediction nodes). One layer, consists in all the nodes that are at the same height or level. For example: 2nd layer is composed of 2 nodes: ($Ca \leq 0.5$) and ($Chest\ pain\ type \leq 3.5$)

```
# Code to visualize our Decision Tree
dot_data_under = tree.export_graphviz(clf_under, out_file=None,
                                        feature_names=features.columns,
                                        filled=True, rounded=True,
                                        special_characters=True)
graph = graphviz.Source(dot_data_under)
graph.render("Classification tree")
display(graph)
```



a) Calculating Accuracy of Tree for training data

```
#Predict the response for training dataset
y_pred_train = clf_under.predict(X_train)

# Calculating Accuracy of our Tree
acc_under_train = round(100 * metrics.accuracy_score(y_train, y_pred_train),2)
print("Training Accuracy:",acc_under_train,"%")
```

```
Training Accuracy: 78.77 %
```

Question 9:

What is the training accuracy %?

Question 9 answer: 78.77 %

b) Calculating Accuracy of Tree for testing data

```
#Predict the response for test dataset
y_pred = clf_under.predict(X_test)

# Calculating Accuracy of our Tree
acc_under_test = round(100 * metrics.accuracy_score(y_test, y_pred),2)
print("Test Accuracy:",acc_under_test,"%")
```

```
Test Accuracy: 73.63 %
```

Question 10:

What is the testing accuracy %?

Question 10 answer: 73.63 %

As we can see, our model is not great at predicting the training data nor the testing data. This is a case of **underfitting**.

Overfitted Decision Tree

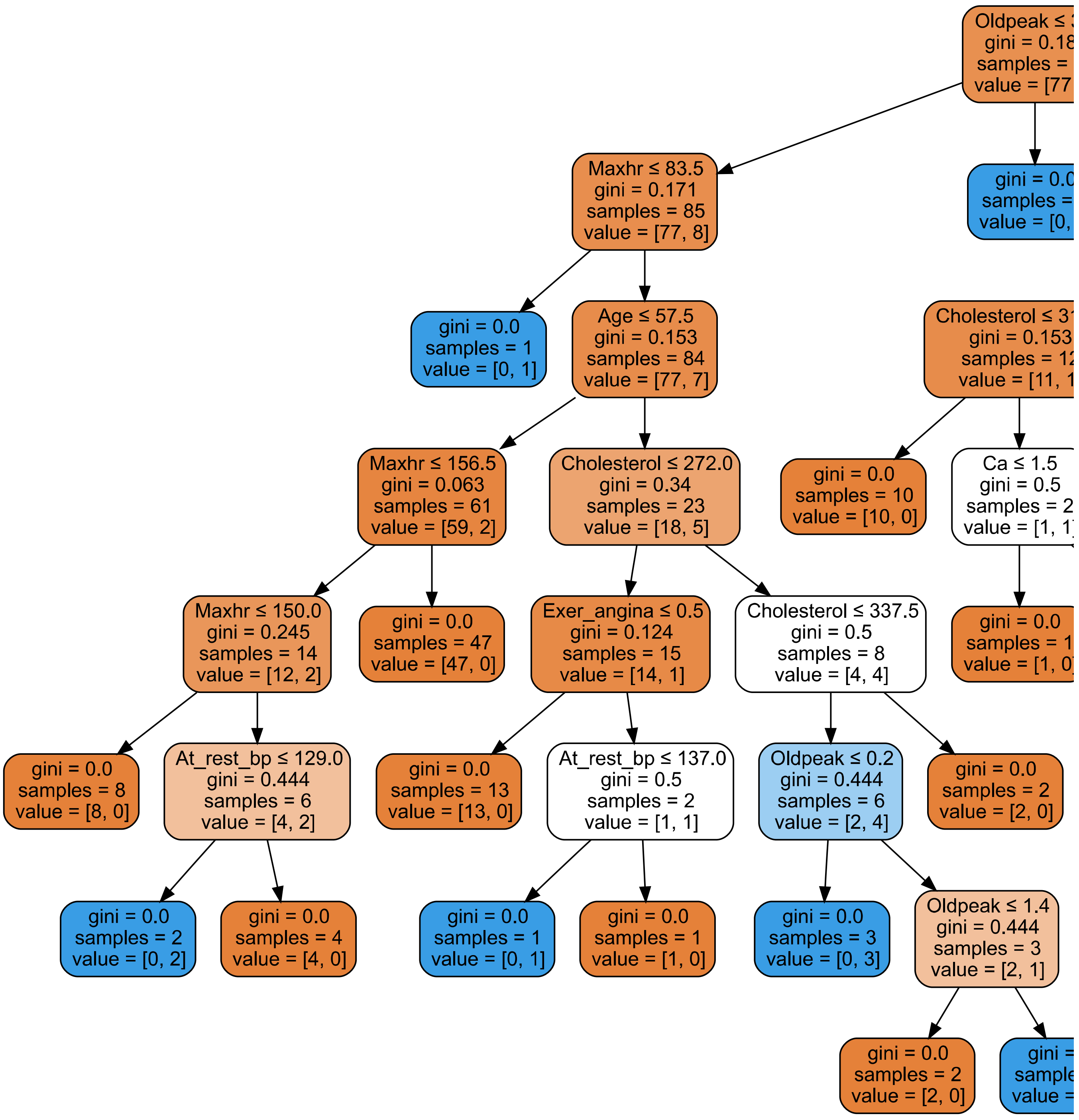
Here we will create a Decision Tree that is only 10 layers deep. Just as before we will train it, and then use our test data to make predictions to check our accuracy of our model.

```
# Create Decision Tree classifer object
clf_over = DecisionTreeClassifier(max_depth=10, random_state=2)

# Train Decision Tree Classifer
clf_over = clf_over.fit(X_train,y_train)
```

Below we will graph our tree as before. This time note that the gini values for our tree do reach to 0, unlike the underfitted Decision tree. When we do not specify the depth of our created tree, the default is to run our tree until it reaches a gini value of 0. But we will see that this doesn't always mean that we have the most optimal model. What we actually care about is having a high accuracy when predicting TESTING Data.

```
# Code to visualize our Decision Tree
dot_data_over = tree.export_graphviz(clf_over, out_file=None,
                                      feature_names=features.columns,
                                      filled=True, rounded=True,
                                      special_characters=True)
graph2 = graphviz.Source(dot_data_over)
graph2.render("Classification tree")
display(graph2)
```



a) Calculating Accuracy of Tree for training data

```
#Predict the response for training dataset
y_pred_train2 = clf_over.predict(X_train)

# Calculating Accuracy of our Tree
acc_over_train = round(100 * metrics.accuracy_score(y_train, y_pred_train2),2)
print("Training Accuracy:",acc_over_train,"%")
```

```
Training Accuracy: 100.0 %
```

Question 11:

What is the training accuracy %?

Question 11 answer: 100.0 %

b) Calculating Accuracy of Tree for testing data

```
#Predict the response for test dataset
y_pred2 = clf_over.predict(X_test)

# Calculating Accuracy of our Tree
acc_over_test = round(100 * metrics.accuracy_score(y_test, y_pred2),2)
print("Test Accuracy:",acc_over_test,"%")
```

```
Test Accuracy: 70.33 %
```

Question 12:

What is the training accuracy %?

Question 12 answer: 70.33 %

As we can see, our model is amazing at predicting the training data, however the accuracy for the testing data is not great. This is a case of **overfitting**.

Task 4: Final thoughts (Questions 13-15)

Finding the Best Fitting Tree

There are different methods to find the best fitting Decision Tree, the task of finding the best fitting Machine Learning Model in general is called **Hyper parameter tunning**. Each kind of machine learning model has different kinds of hyperparameters to tune. We will comeback to this concept in later modules. But for our example, we are trying to tune the **max_depth** of our Decision Tree Classifier. So how do we know what number to pick for max_depth?

Validation Curve

One possibility would be to use a **validation curve**. In this method we essentially fit our tree using a range of depths. We saw in the previous part that choosing 2 produced underfitting and choosing 10 was overfitting, thus the optimal depth must be in between. So why don't we test a range from 1 to 10?

```
# Setting figure size
sns.set(rc={'figure.figsize':(11.7,8.27)})

# Choosing a range from 1 to 10 to test
tree_depths = range(1,11)
```

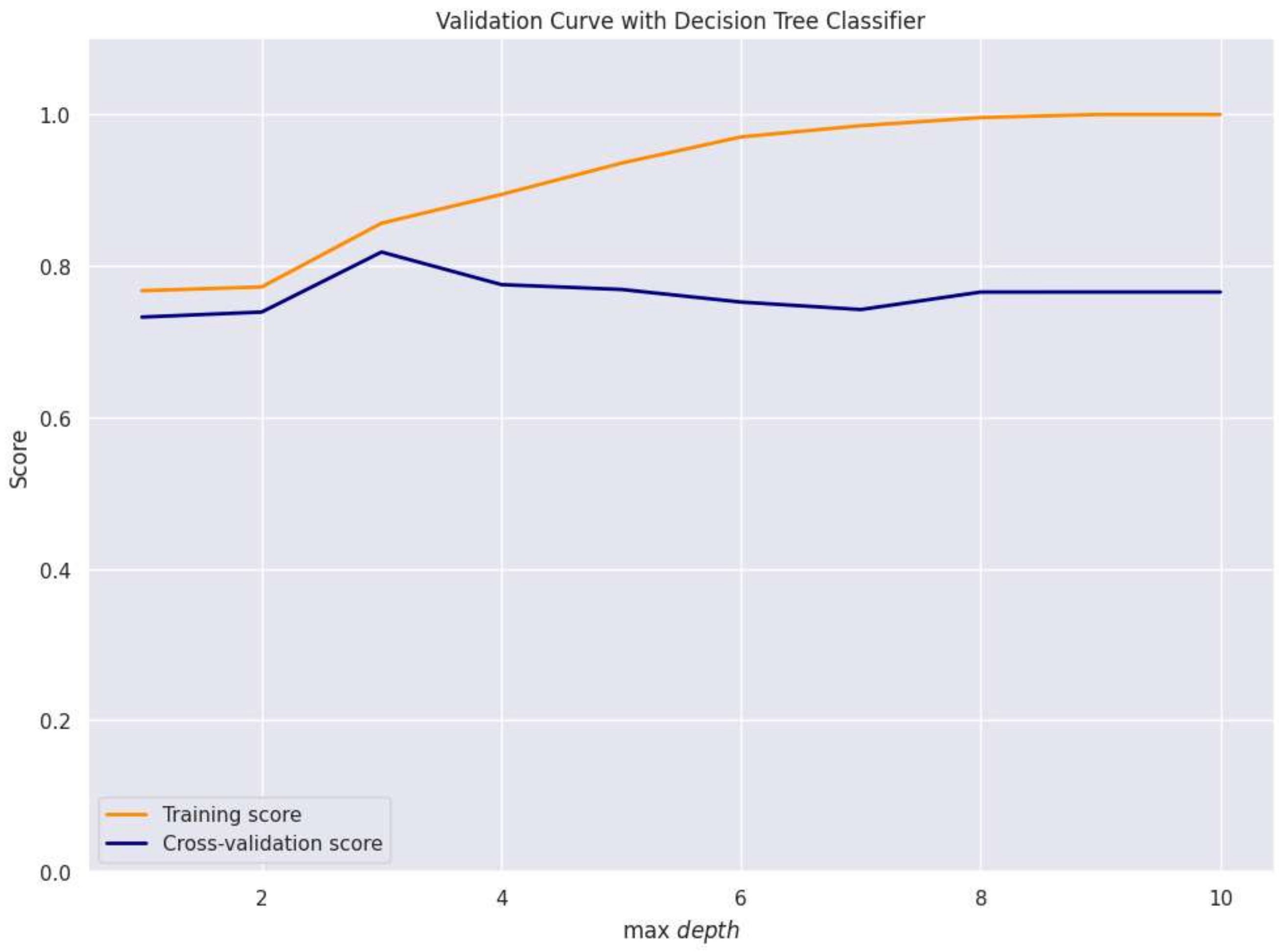
Once we have the range we want to test we can start plotting our validation curve. This plot is created by using our complete data and splits it randomly a certain amount of times (the default is 5), into 2 portions: **Training** data and **Validation** data chunks. The Validation data is essentially similar to testing data. Doing the different splits lets us essentially create simulated "testing data chunks" from data that we already have, so it's inherently biased but in this way we can have at least an idea of how the depth of a tree influences the accuracy of our predictions.

```
# create validation curve
train_scores, test_scores = validation_curve(
        DecisionTreeClassifier(random_state=2),
        X,
        y,
    ),
        param_name="max_depth",
        param_range=tree_depths,
        scoring="accuracy")

# storing scores mean scores(from default 5 random splits)
train_scores_mean = np.mean(train_scores, axis=1)
validation_scores_mean = np.mean(test_scores, axis=1)

# plot titles and labels
plt.title("Validation Curve with Decision Tree Classifier")
plt.xlabel(r"$\max \ depth$")
plt.ylabel("Score")
plt.ylim(0.0, 1.1)
plt.plot(tree_depths, train_scores_mean, label="Training score", color="darkorange", lw=2)
plt.plot(tree_depths, validation_scores_mean, label="Cross-validation score", color="navy", lw=2)

# plot legend
plt.legend(loc="lower left")
plt.show()
```



Question 13:

Can you tell with max depth is underfitting and overfitting just by looking at this graph, explain how?

Question 13 answer: Underfitting (high bias) occurs when the model is too simple with low max depth values (1 and 2). Overfitting (high variance) happens as the max depth increases beyond 5. The optimal point is usually found around max depth = 3-4, where the cross-validation score is highest.

- Based on the graph above we can see that indeed choosing a max depth of 2 was underfitting , because both the **training score and the crossvalidation score** were in the around the **70'ish percent**.
- Choosing 10 was overtfitting because we see the **lines diverge** dramatically, the training is as expected perfect 100% but the testing was not going in the same direction.
- the optimal spot accordding to our validation curve would be around 3, because we can see that both **lines are not diverging** and they are the **highest accuracy score before diversion**.

Therefore lets try using max_depth = 3 and see what results we get in our Decision Tree Classifier. Remember that what our ideal is to have high training and testing accuracy.

```
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3, random_state=2)

# Create Decision Tree classifer object
clf_best = DecisionTreeClassifier(max_depth=3, random_state=2)

# Train Decision Tree Classifer
clf_best = clf_best.fit(X_train,y_train)
```

a) Calculating Accuracy of Tree for training data

```
#Predict the response for training dataset
y_pred_train3 = clf_best.predict(X_train)

# Calculating Accuracy of our Tree
acc_best_train = round(100 * metrics.accuracy_score(y_train, y_pred_train3),2)
print("Training Accuracy:",acc_best_train,"%")
```

```
Training Accuracy: 85.85 %
```

b) Calculating Accuracy of Tree for testing data

```
#Predict the response for test dataset
y_pred_best = clf_best.predict(X_test)

# Calculating Accuracy of our Tree
acc_best_test = round(100 * metrics.accuracy_score(y_test, y_pred_best),2)
print("Test Accuracy:",acc_best_test,"%")
```

```
Test Accuracy: 80.22 %
```

As we can see we have bumped our testing accuracy from low 70's% in both cases of (underfitting and overfitting) to 80.22% with the help of our cross validation curve!

Question 14:

Did you find this module understandable or do you believe it requires more details and explanation?

Question 14 answer: Yes, it's really easy to understand.

Question 15:

Write down one thing you learned today and one thing that confuses you. (I know, I ask this all the time, but it is important to think about it for a few seconds!)

Question 15 answer:

Learned

1. I learned that adjusting parameters like `max_depth` in decision tree models can make the splits more complex and improve accuracy on the training data, but it may not necessarily improve performance on the test data. This helps me understand overfitting and its impact on model generalization.

Confused

2. I'm still unsure about fine-tuning decision tree hyperparameters for optimal accuracy and generalization without overfitting, especially when balancing training and test accuracy. It feels like a delicate balance that needs more clarity.

🙂 Congratulations! You just finished working on the first machine learning model Decision Trees. You should be proud of how much you have learned (even if you feel like some of this is still confusing, it's going to get easier with practice)