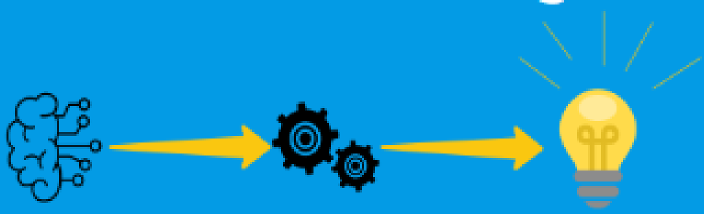
Machine Learning Basics

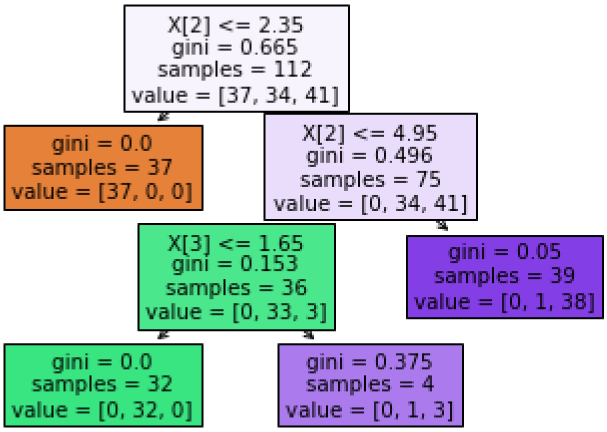


Decision Trees Classification, In-Depth Tree Structure Analysis

Learn How to Fit Decision Tree Classifier, Predict and Evaluate it. Learn How to visualize the structure and interpret it. Learn how to compute each element in the structure, using Python. Discover Decision_path and GridSearchCV.

Hanane D.

Contents



1 Introduction

I recommend you to read this article before [Everything You Need To Know About Decision Trees (1/2)](), in which you will learn:

- What are Decision Trees?
- How do we build a decision tree (Illustration part)?
- What is a recursive algorithm?
- Which algorithm is implemented in the Scikit-learn library?
- What is a stopping criterion?
- What are the Splitting tree criterions? also known as Attributes Selection Measures (ASM) (like Entropy, Information Gain, Gini Index metrics for Classification)

In the current tutorial, ***Decision Trees - In-Depth Tree Structure Analysis*** (2/2), we will practice Decision Trees for Classification using Python.
You will learn:

- How to fit the model, predict and evaluate it using the Scikit-learn library.
- How to visualize the tree structure and interpret it.
- How to compute the gini index, and the other values for each node using python.

You will also learn decision trees behind the scene: Understand deeply the tree structure using Python:

- The ***decision_path***: How is the prediction made precisely using python?.
- How to plot Decision Boundaries.
- How to tune Hyper-parameters using ***GridSearchCV***

For beginners, you can read up to "Decision Boundaries", and also have a look at the "Hyper-parameter tuning" at the end of the tutorial.

2 Load the dataset

Let’s use the Iris dataset to practice Decision Trees classifier.

First we load the packages we will use:

```
import pandas as pd
import numpy as np
from matplotlib import pyplot as plt

from sklearn.model_selection import train_test_split
from sklearn.datasets import load_iris
from sklearn.tree import DecisionTreeClassifier
from sklearn import tree

from sklearn.metrics import accuracy_score
```

```
from sklearn.datasets import load_iris

iris = load_iris()
X = iris.data
y = iris.target
print("# of observations:", X.shape[0])
print("# of features:", X.shape[1])
print("Features name:",iris.feature_names)
print("Classes to predict:",np.unique(y))
print("Target names:",iris.target_names)

# # of observations: 150
# # of features: 4
# Features name: ['sepal length (cm)', 'sepal width (cm)', 'petal length (cm)', 'petal width
(cm)']
# Classes to predict: [0 1 2]
# Target names: ['setosa' 'versicolor' 'virginica']
```

Here is an overview of the first 5 observations:

```
X[:5]
# array([[5.1, 3.5, 1.4, 0.2],
#        [4.9, 3. , 1.4, 0.2],
#        [4.7, 3.2, 1.3, 0.2],
#        [4.6, 3.1, 1.5, 0.2],
#        [5. , 3.6, 1.4, 0.2]])
```

For each class we have the same number of observations: 50 observations each.

```
np.unique(y, return_counts=True)
# (array([0, 1, 2]), array([50, 50, 50], dtype=int64))
```

Statistical description of the dataset:

```
pd.options.display.float_format = '{:,.2f}'.format
df.describe()
```

	sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)	target
count	150.00	150.00	150.00	150.00	150.00
mean	5.84	3.06	3.76	1.20	1.00
std	0.83	0.44	1.77	0.76	0.82
min	4.30	2.00	1.00	0.10	0.00
25%	5.10	2.80	1.60	0.30	0.00
50%	5.80	3.00	4.35	1.30	1.00
75%	6.40	3.30	5.10	1.80	2.00
max	7.90	4.40	6.90	2.50	2.00

The goal is to predict, given the measures (length and width), in which class the iris will fall.

3 Model

3.1 Split the dataset to train and test sets

```
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0) #test_size=25%
default
```

3.2 Fit the model

We fit the model with max_leaf_nodes=3 on the train set:

```
clf = DecisionTreeClassifier(max_leaf_nodes=3, random_state=0)
clf.fit(X_train, y_train)
```

3.3 Predict

```
y_predict=clf.predict(X_train)
```

3.4 Evaluate the model

Let's compute the accuracy score for our model.
There are many other measures to take into account: Recall, Precision, F1 score…We will keep it simple here, we use only the accuracy score to evaluate our model.
The accuracy score is the ratio of the correct classified samples among the total number of observations.

On the training set:

```
print(clf.score(X_train,y_train))
print(accuracy_score(y_train,y_predict))
# 0.9642857142857143
# 0.9642857142857143
```

Both methods give the same value.

The accuracy score 96.42% is very good. In real world datasets, it could be rare to get such a good score. Here, we are using a toy dataset, in which the data are cleaned and there is no missing.

On the testing set:

```
y_predict=clf.predict(X_test)
print(clf.score(X_test,y_test))
print(accuracy_score(y_test,y_predict))
# 0.8947368421052632
# 0.8947368421052632
```

The accuracy is about 89.5% which is still very high.

In reality, the model predicts a probability for each observation, and then applies the np.argmax to get the index of the maximum value. This index will be the predicted value.

For example, for the first observation:

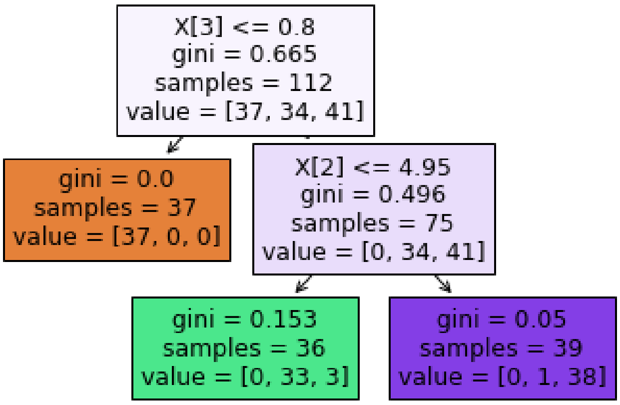
```
print("Probabilities: ",clf.predict_proba(X_test[0].reshape(1,-1)))
print("Index of the max value: ",np.argmax(clf.predict_proba(X_test[0].reshape(1,-1))))
```

In the meantime, the first value in y_predict is:

```
y_predict[0]
#2
```

3.5 Visualize the structure of the tree

```
tree.plot_tree(clf,filled=True)
plt.show()
```



This is the structure of the tree built by our classifier (clf with max_leaf_node=3).

There are 3 leaf nodes.

There are 2 nodes: the root node and one internal node.

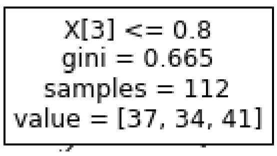
In each node and leaf, there is a useful information that helps understand the splitting logic:

- It gives the best feature and threshold chosen as separator (***X[3]<=0.8***)
- The gini index of the chosen feature/threshold (***gini***)
- Number of observations on the node (***samples***)
- The number of observations for each class (***value***)

3.6 Gini Index computation

By default, the metric chosen to split the tree is the ***Gini index*** *(You can modify it to use Entropy)*. To recall here, the lowest the value the best is the feature as a separator.

3.6.1 Root Node:



For the root node:

- The feature chosen is the 4th feature (*petal width*)
- The gini index of the training dataset before split: **0.665**
- We have **112** observations in this training set.
- There are **37** observations of class **0**, **34** of class **1** and **41** of class **2**

Using Python, we will compute each output for this node:

- Samples = 112

```
X_train.shape[0]
#112
```

- value=[37, 34, 41]

```
df_train=pd.DataFrame(data=X_train, columns=iris.feature_names)
df_train['target']=y_train
df_train.groupby(['target'])[['sepal length (cm)']].count()
```

target	sepal length (cm)
0	37
1	34
2	41

- gini=0.665

The following method computes the proportion of each class in the training sets. In other terms, it computes the probability of each class (also the p^2):

```
def compute_proprtion_class(df):
    df_proba=df.groupby(['target'])[['target']].count()/df.groupby(['target'])\
                                                        ['target'].count().sum()
    df_proba.columns=['proba']
    df_proba['proba^2']=df_proba['proba']**2
    return df_proba
```

For training set:

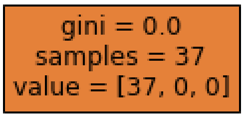
```
df_proba=compute_proprtion_class(df_train)
df_proba
```

target	proba	proba^2
0	0.330357	0.109136
1	0.303571	0.092156
2	0.366071	0.134008

Finally the Gini index for the root node is:

```
gini_index= 1-df_proba['proba^2'].sum()
gini_index
#0.6647002551020409
```

3.6.2 Left of the root node



- It's a leaf
- There are only observations (37) from class 0
- This subset is pure, so the Gini Index is 0

With Python:

- Samples = 37

```
df_train.loc[df_train.iloc[:,3]<=0.8,:].shape[0]
# 37
```

- value=[37, 0, 0]

There is only one class:

```
df_train.loc[df_train.iloc[:,3]<=0.8,:]['target'].unique()
# array([0])
```

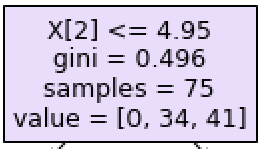
```
df_train.loc[df_train.iloc[:,3]<=0.8,:].groupby(['target'])[['target']].count().
rename(columns={'target':'count'})
```

	count
target	
0	37

- gini=0

As there is only one class (0), the probability to get this class is 1, so the gini index = 0.

3.6.3 Right of the root node



- It's an Internal node
- There are 75 observations, from class 1 and 2

With Python:

- Samples = 75

```
df_train.loc[df_train.iloc[:,3]>0.8,:].shape[0]
# 75
```

- value=[0, 37, 41]

```
df_train.loc[df_train.iloc[:,3]>0.8,:].groupby(['target'])[['target']].count()
```

	target
target	
1	34
2	41

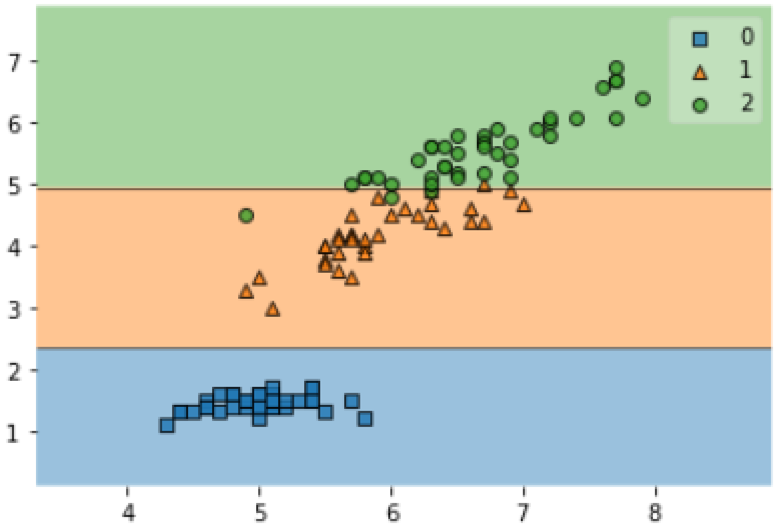
- gini=0.496

```
df_right=df_train.loc[df_train.iloc[:,3]>0.8,:]
df_proba=compute_proprtion_class(df_right)
gini_index= 1-df_proba['proba^2'].sum()
gini_index
#0.49564444444444455
```

3.7 Decision Boundaries

Here is a simple visualization of the decision trees boundaries by using only two variables of our dataset:

```
from mlxtend.plotting import plot_decision_regions

X_train_plot = X_train[:, [0, 2]]
clf_plot = DecisionTreeClassifier(max_leaf_nodes=3, random_state=0)
clf_plot.fit(X_train_plot, y_train)
plot_decision_regions(X_train_plot, y_train, clf_plot)
```



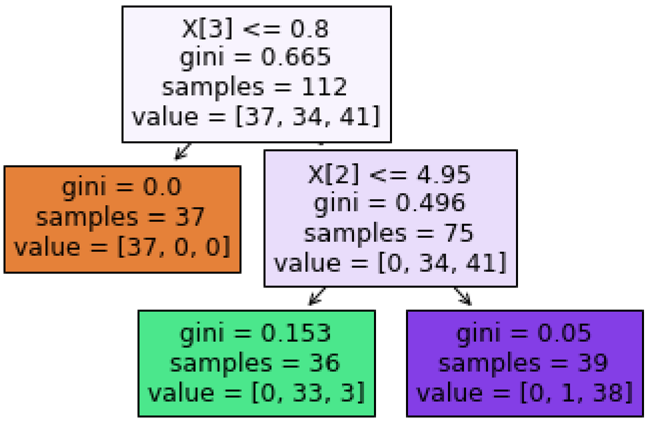
4 Decision Tree behind the scene

Let’s discover how to find the details of the tree structure using Python. We want to know:

- If the current node, is a node or a leaf,
- If it's in the left or the right of the parent node,
- Which feature is the one chosen to separate the node
- The threshold values…

A lot of indicators that we can find by deeply analyzing this object: ***clf.tree_.***

In our dataset and our fitted classifier, we had this structure:



- The number of node : 5

```
clf.tree_.node_count
#5
```

It starts with the root node, with index=0. The second node is the orange one, with index=1. It ends with the purple node, index=4.

- The number of final leaves: 3

```
clf.tree_.n_leaves
#3
```

- For each node: is there a ***left*** leaf?

```
clf.tree_.children_left
# array([ 1, -1,  3, -1, -1], dtype=int64)
```

Here is the explanation of the array:
➢ If it's -1, meaning, no left leaf.
➢ If it's different from -1, it indicates the index of the left leaf.

For example:
➢ The first value in the array concerns the root node. As you can see in the tree, It did have a 1 left descendante leaf. Thus, the first value of the array indicates the index of the left leaf: 1. Which is the orange leaf.

➢ The second value concerns the second node in the tree, which is the orange leaf. So the leaf has no left leaf, thus the value is -1.

➢ The third value concerns the third node (the one with X[2]<=4.95). This node has a left leaf, which has index 3. Thus this is the value you have on the array.

➢ etc, etc

- For each node: is there a ***right*** leaf?

```
clf.tree_.children_right
# array([ 2, -1,  4, -1, -1], dtype=int64)
```

➢ For the root node, it did have a right leaf, with the index =2. This is the first value in the array
➢ For the second leaf (orange), there is not right leaf, so the value is -1
➢ For the third node (first purple), there is a right leaf, which is the purple value with index=4.

From these two arrays, we know that the 2nd, 4th and 5th nodes are **terminal leaves**.

- What are the features chosen for each node?

```
clf.tree_.feature
# array([ 3, -2,  2, -2, -2], dtype=int64)
```

- ➢ For the first node, the feature with index equal to 3 (4th feature) is the one chosen as a separator
- ➢ For the second node, the value is -2, meaning there is no feature. It's a terminal leaf.
- ➢ For the third node, the feature is the 3th one (idx=2)

.

- What are the thresholds chosen for each node (and for the chosen feature)?

```
clf.tree_.threshold
# array([ 0.80000001, -2. ,  4.95000005, -2. , -2.])
```

- ➢ The first value 0.8 is the threshold applied to the feature in the index 3.
- ➢ When it's -2, meaning the node is actually a final leaf.

- The number of observations in each node:

```
clf.tree_.n_node_samples
# array([112,  37,  75,  36,  39], dtype=int64)
```

- The gini impurity for each node/leaf:

```
clf.tree_.impurity
# array([0.66470026, 0.        , 0.49564444, 0.15277778, 0.04996713])
```

5 Decision path

5.1 How is the prediction made precisely?

Each observation in the test samples will go through the tree structure.
Given the sample features values, each node will decide if the sample goes left or right until it meets a final leaf. The majority class in the terminal leaf to which the sample belongs will be the predicted value.

```
sample_id=0
print("First sample features in the test set", X_test[sample_id].reshape(1,-1))
```

```
predict_class=clf.predict(X_test[sample_id].reshape(1,-1))[0]
print("The predict class for the sample=",sample_id," :",predict_class)

leaf_id=clf.apply(X_test[sample_id].reshape(1,-1))
print("The final leaf on which the observation falls", leaf_id)

# First sample features in the test set [[5.8 2.8 5.1 2.4]]
# The predict class for the sample= 0  : 2
# The final leaf on which the observation falls [4]
```

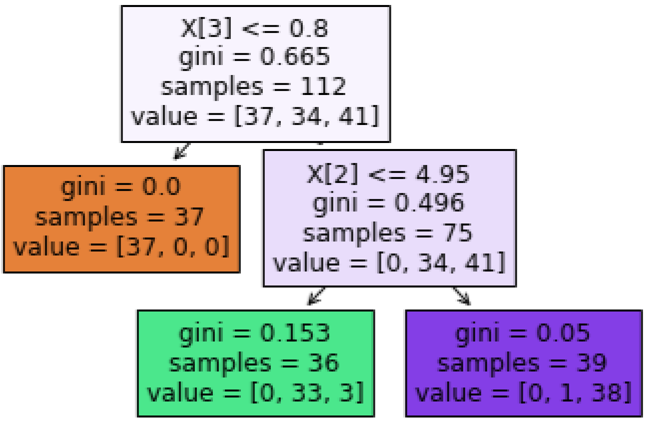
Let’s use deicion_path methods to determine the nodes through which the sample passed :

```
for idx, node_id in enumerate(node_index):
    is_leaf="It's not a leaf"
    idx_feature=clf.tree_.feature[node_id]
    majority_class=None

    if clf.tree_.feature[node_id]==-2:
        is_leaf="It's a leaf"
        majority_class=np.argmax(clf.tree_.value[node_id])

    if node_id in clf.tree_.children_left:
        sens_leave='Left Node'
    elif node_id in clf.tree_.children_right:
        sens_leave='Right Node'
    else:
        sens_leave='Root Node'

    to_print= majority_class

    if majority_class==None:
        print(
            "Step=",idx,"\n",
            "     We are in the",sens_leave,\
            ",node_id=",node_id,",",is_leaf,\
            ", Best feature idx=",idx_feature,\
            ", # of samples per class",clf.tree_.value[node_id],\
              )
    else:
         print(
            "Step=",idx,"\n",
            "     We are in the",sens_leave,\
            ",node_id=",node_id,",",is_leaf,\
            ", # of samples per class",clf.tree_.value[node_id],\
            ", majority class= predicted value", np.argmax(clf.tree_.value[node_id])\
              )

# Step= 0
#       We are in the Root Node ,node_id= 0 , It's not a leaf , Best feature idx= 3 , # of
samples per class [[37. 34. 41.]]
# Step= 1
#       We are in the Right Node ,node_id= 2 , It's not a leaf , Best feature idx= 2 , # of
samples per class [[ 0. 34. 41.]]
```

```
# Step= 2
#       We are in the Right Node ,node_id= 4 , It's a leaf , # of samples per class [[ 0.  1.
38.]] , majority class= predicted value 2
```

Let’s recall here the values of this observation:
First sample features in the test set [[5.8 2.8 5.1 2.4]]

- At the beginning, the sample goes naturally through the root node, node_id=0.
- As the value of the fourth feature is 2.4, more than 0.8, the sample falls in the node at the right side, node_id=2.
- Then the value of the third feature is 5.1 which is more than the threshold at this node 4.95, so the feature goes to the right side again. It falls on the purple final leaf, node_id=4, on which class=2 has the majority vote. Thus the predicted value of the this observation is 2



6 Hyper-parameters Tuning

Hyper-parameters are not learnt by the model, they are input to the model (like 'max_depth', 'max_leaf_nodes' for Decision Trees).

We don’t know which value will give the best estimator. Thus, we need to test several values as inputs to the model and keep the one giving the best performance.

6.1 GridSearchCV

GridSearchCV helps perform this search, while cross-validating the data (using 5-fold by default).

We input a grid of parameters to GridSearchCV. It fits the model, with all the possible combinations of parameter values, to our dataset. It evaluates each combination and keeps the best one in memory.

Let's practice:

```
from sklearn.model_selection import GridSearchCV
```

We will test several values of max_depth, min_samples_leaf and max_leaf_nodes.

```
X = iris.data
y = iris.target

X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0) #(25% default)

parameters = {'max_depth':[2,3,4,5,6],
'min_samples_leaf':[10,5,1],'max_leaf_nodes':[3,4,5,7,10]}
dt = DecisionTreeClassifier()
clf = GridSearchCV(dt, parameters)
clf.fit(X_train,y_train)
```

We can then retrieve the best parameters and the best score:

```
best_params=clf.best_params_
best_params
# {'max_depth': 3, 'max_leaf_nodes': 4, 'min_samples_leaf': 1}
```

We have the best estimator when max_depth=3, max_leaf_nodes=4 ,min_samples_leaf=1.

The score corresponding to these best parameters :

```
clf.best_score_
# 0.9644268774703558
```

Here is the best classifier:

```
clf.best_estimator_
# DecisionTreeClassifier(max_depth=3, max_leaf_nodes=4)
```

6.2 Fit the best estimator, Predict and Evaluate

We will fit our training by this best estimator, test and evaluate the model :

```
clf_best = clf.best_estimator_
clf_best.fit(X_train,y_train)
clf_best.score(X_train,y_train)
# 0.9821428571428571
```

The training accuracy is **98.2%**. It is much higher than the first model 96.4% with max_leaf_nodes=3, and without any tuning.

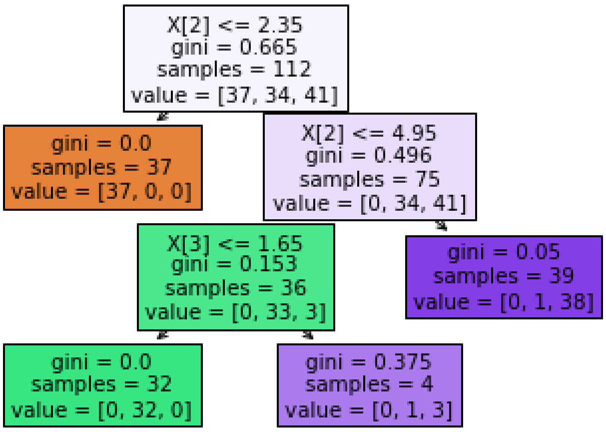
The predicted values of the test set:

```
y_predict=clf_best.predict(X_test)
print(clf_best.score(X_test,y_test))
print(accuracy_score(y_test,y_predict))
# 0.9736842105263158
# 0.9736842105263158
```

Also, the test accuracy is way better than the first model: **97.37%** vs 89.5%

6.3 Visualize the structure

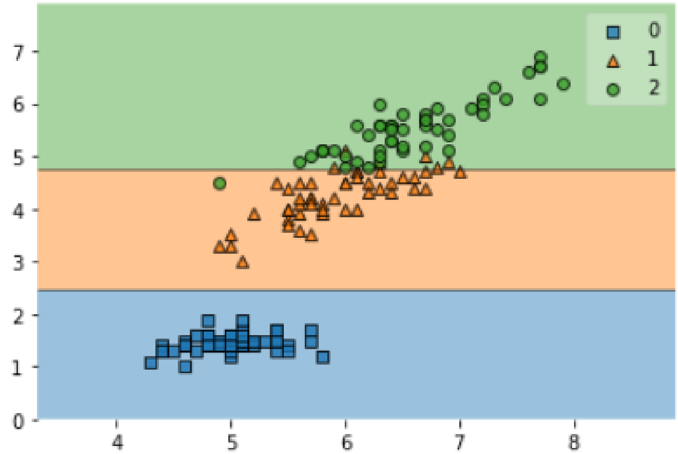
Here is the structure of this best classifier:



7 Decision Boundaries

```
from mlxtend.plotting import plot_decision_regions

# X = iris.data[:, [0, 2]]
# y = iris.target

X_train_plot = X_train[:, [0, 2]]
clf_plot=DecisionTreeClassifier(max_depth=3, max_leaf_nodes=4)
clf_plot.fit(X, y)
```

```
plot_decision_regions(X, y, clf_plot)
```



8 Summary

In this tutorial, you leaned, within Python, how to use a decision tree classifier:

- How to fit, predict evaluate the model;
- How to visualize the tree structure and compute each element using python, including the gini impurity metric
- How to plot a decision boundaries
- How to hack more deeply the tree structure
- How to use decision_path to understand the way in the tree the observations are following to get the prediction
- How to tune the hyper-parameters using Grid Search and find the best model

If you want to understand the concepts behind the decision trees and the metrics used to split the trees, you can have a look at the following articles:

- Gini Index
- Entropy
- Information Gain
- Everything You Need To Know About Decision Trees (1/2)

I hope you enjoyed reading this tutorial. I would appreciate it if you could leave a comment, in one of my articles, telling me if it meets your expectations.