CHAPTER 6

Decision Trees

Like SVMs, *Decision Trees* are versatile Machine Learning algorithms that can perform both classification and regression tasks, and even multioutput tasks. They are very powerful algorithms, capable of fitting complex datasets. For example, in Chapter 2 you trained a DecisionTreeRegressor model on the California housing dataset, fitting it perfectly (actually overfitting it).

Decision Trees are also the fundamental components of Random Forests (see Chapter 7), which are among the most powerful Machine Learning algorithms available today.

In this chapter we will start by discussing how to train, visualize, and make predictions with Decision Trees. Then we will go through the CART training algorithm used by Scikit-Learn, and we will discuss how to regularize trees and use them for regression tasks. Finally, we will discuss some of the limitations of Decision Trees.

Training and Visualizing a Decision Tree

To understand Decision Trees, let's just build one and take a look at how it makes predictions. The following code trains a DecisionTreeClassifier on the iris dataset (see Chapter 4):

```
from sklearn.datasets import load_iris
from sklearn.tree import DecisionTreeClassifier

iris = load_iris()
X = iris.data[:, 2:] # petal length and width
y = iris.target

tree_clf = DecisionTreeClassifier(max_depth=2)
tree_clf.fit(X, y)
```

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You can visualize the trained Decision Tree by first using the export_graphviz() method to output a graph definition file called *iris_tree.dot*:

Then you can convert this .dot file to a variety of formats such as PDF or PNG using the dot command-line tool from the *graphviz* package.¹ This command line converts the .dot file to a .png image file:

```
$ dot -Tpng iris_tree.dot -o iris_tree.png
```

Your first decision tree looks like Figure 6-1.

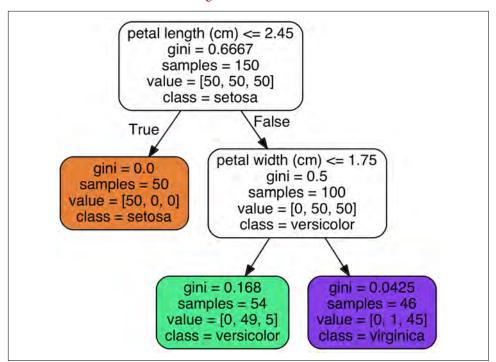


Figure 6-1. Iris Decision Tree

¹ Graphviz is an open source graph visualization software package, available at http://www.graphviz.org/.

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Making Predictions

Let's see how the tree represented in Figure 6-1 makes predictions. Suppose you find an iris flower and you want to classify it. You start at the *root node* (depth 0, at the top): this node asks whether the flower's petal length is smaller than 2.45 cm. If it is, then you move down to the root's left child node (depth 1, left). In this case, it is a *leaf node* (i.e., it does not have any children nodes), so it does not ask any questions: you can simply look at the predicted class for that node and the Decision Tree predicts that your flower is an Iris-Setosa (class=setosa).

Now suppose you find another flower, but this time the petal length is greater than 2.45 cm. You must move down to the root's right child node (depth 1, right), which is not a leaf node, so it asks another question: is the petal width smaller than 1.75 cm? If it is, then your flower is most likely an Iris-Versicolor (depth 2, left). If not, it is likely an Iris-Virginica (depth 2, right). It's really that simple.



One of the many qualities of Decision Trees is that they require very little data preparation. In particular, they don't require feature scaling or centering at all.

A node's samples attribute counts how many training instances it applies to. For example, 100 training instances have a petal length greater than 2.45 cm (depth 1, right), among which 54 have a petal width smaller than 1.75 cm (depth 2, left). A node's value attribute tells you how many training instances of each class this node applies to: for example, the bottom-right node applies to 0 Iris-Setosa, 1 Iris-Versicolor, and 45 Iris-Virginica. Finally, a node's gini attribute measures its *impurity*: a node is "pure" (gini=0) if all training instances it applies to belong to the same class. For example, since the depth-1 left node applies only to Iris-Setosa training instances, it is pure and its gini score is 0. Equation 6-1 shows how the training algorithm computes the gini score G_i of the ith node. For example, the depth-2 left node has a gini score equal to $1 - (0/54)^2 - (49/54)^2 - (5/54)^2 \approx 0.168$. Another *impurity measure* is discussed shortly.

Equation 6-1. Gini impurity

$$G_i = 1 - \sum_{k=1}^{n} p_{i,k}^2$$

• $p_{i,k}$ is the ratio of class k instances among the training instances in the i^{th} node.