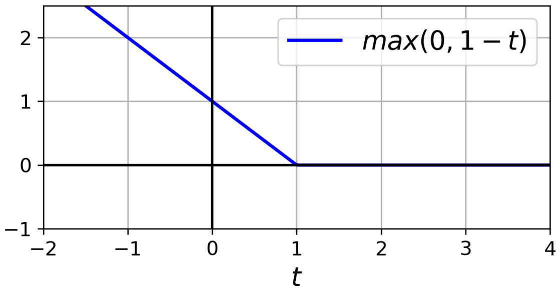

It is also possible to implement online kernelized SVMs—for example, using "Incremental and Decremental SVM Learning"[8] or "Fast Kernel Classifiers with Online and Active Learning."[9] However, these are implemented in Matlab and C++. For large-scale nonlinear problems, you may want to consider using neural networks instead (see Part II).

Exercises

1. What is the fundamental idea behind Support Vector Machines?
2. What is a support vector?
3. Why is it important to scale the inputs when using SVMs?
4. Can an SVM classifier output a confidence score when it classifies an instance? What about a probability?
5. Should you use the primal or the dual form of the SVM problem to train a model on a training set with millions of instances and hundreds of features?
6. Say you trained an SVM classifier with an RBF kernel. It seems to underfit the training set: should you increase or decrease γ (`gamma`)? What about `C`?
7. How should you set the QP parameters (**H**, **f**, **A**, and **b**) to solve the soft margin linear SVM classifier problem using an off-the-shelf QP solver?
8. Train a `LinearSVC` on a linearly separable dataset. Then train an `SVC` and a `SGDClassifier` on the same dataset. See if you can get them to produce roughly the same model.
9. Train an SVM classifier on the MNIST dataset. Since SVM classifiers are binary classifiers, you will need to use one-versus-all to classify all 10 digits. You may

[8] "Incremental and Decremental Support Vector Machine Learning," G. Cauwenberghs, T. Poggio (2001).

[9] "Fast Kernel Classifiers with Online and Active Learning," A. Bordes, S. Ertekin, J. Weston, L. Bottou (2005).

want to tune the hyperparameters using small validation sets to speed up the process. What accuracy can you reach?

10. Train an SVM regressor on the California housing dataset.

Solutions to these exercises are available in ???.

CHAPTER 6
Decision Trees

With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as he or she writes—so you can take advantage of these technologies long before the official release of these titles. The following will be Chapter 6 in the final release of the book.

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)
```

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

```
from sklearn.tree import export_graphviz

export_graphviz(
        tree_clf,
        out_file=image_path("iris_tree.dot"),
        feature_names=iris.feature_names[2:],
        class_names=iris.target_names,
        rounded=True,
        filled=True
    )
```

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.

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

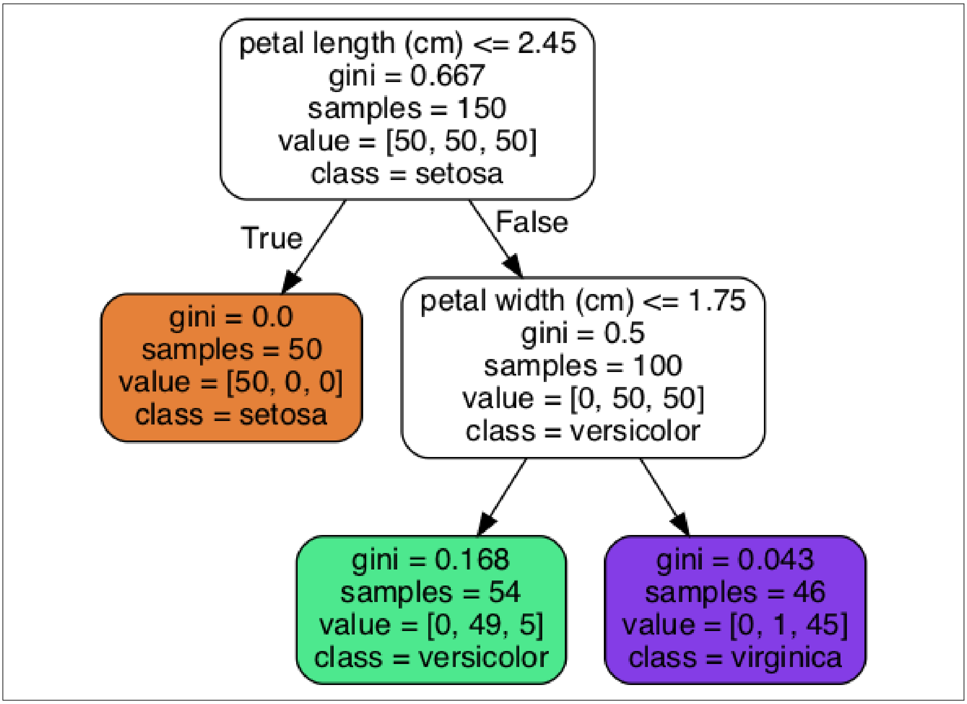

Figure 6-1. Iris Decision Tree

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.

Scikit-Learn uses the CART algorithm, which produces only *binary trees*: nonleaf nodes always have two children (i.e., questions only have yes/no answers). However, other algorithms such as ID3 can produce Decision Trees with nodes that have more than two children.

Figure 6-2 shows this Decision Tree's decision boundaries. The thick vertical line represents the decision boundary of the root node (depth 0): petal length = 2.45 cm. Since the left area is pure (only Iris-Setosa), it cannot be split any further. However, the right area is impure, so the depth-1 right node splits it at petal width = 1.75 cm (represented by the dashed line). Since `max_depth` was set to 2, the Decision Tree stops right there. However, if you set `max_depth` to 3, then the two depth-2 nodes would each add another decision boundary (represented by the dotted lines).

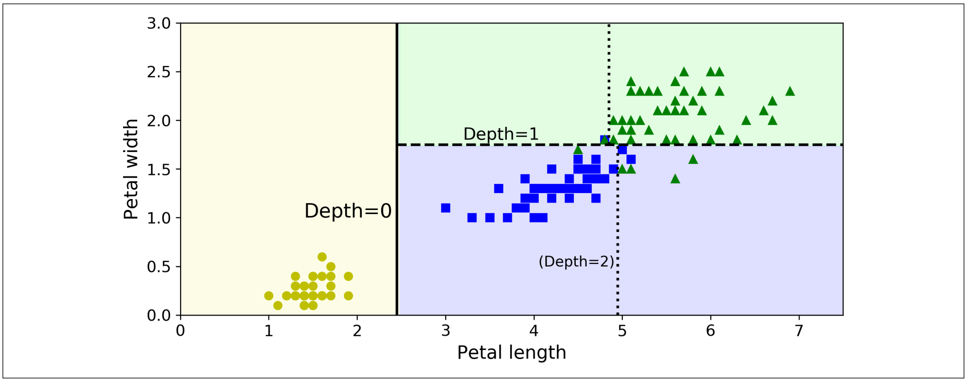

Figure 6-2. Decision Tree decision boundaries

Model Interpretation: White Box Versus Black Box

As you can see Decision Trees are fairly intuitive and their decisions are easy to interpret. Such models are often called *white box models*. In contrast, as we will see, Random Forests or neural networks are generally considered *black box models*. They make great predictions, and you can easily check the calculations that they performed to make these predictions; nevertheless, it is usually hard to explain in simple terms why the predictions were made. For example, if a neural network says that a particular person appears on a picture, it is hard to know what actually contributed to this prediction: did the model recognize that person's eyes? Her mouth? Her nose? Her shoes? Or even the couch that she was sitting on? Conversely, Decision Trees provide nice and simple classification rules that can even be applied manually if need be (e.g., for flower classification).

Estimating Class Probabilities

A Decision Tree can also estimate the probability that an instance belongs to a particular class *k*: first it traverses the tree to find the leaf node for this instance, and then it returns the ratio of training instances of class *k* in this node. For example, suppose you have found a flower whose petals are 5 cm long and 1.5 cm wide. The corresponding leaf node is the depth-2 left node, so the Decision Tree should output the following probabilities: 0% for Iris-Setosa (0/54), 90.7% for Iris-Versicolor (49/54), and 9.3% for Iris-Virginica (5/54). And of course if you ask it to predict the class, it should output Iris-Versicolor (class 1) since it has the highest probability. Let's check this:

```
>>> tree_clf.predict_proba([[5, 1.5]])
array([[0.        , 0.90740741, 0.09259259]])
```

```
>>> tree_clf.predict([[5, 1.5]])
array([1])
```

Perfect! Notice that the estimated probabilities would be identical anywhere else in the bottom-right rectangle of Figure 6-2—for example, if the petals were 6 cm long and 1.5 cm wide (even though it seems obvious that it would most likely be an Iris-Virginica in this case).

The CART Training Algorithm

Scikit-Learn uses the *Classification And Regression Tree* (CART) algorithm to train Decision Trees (also called "growing" trees). The idea is really quite simple: the algorithm first splits the training set in two subsets using a single feature k and a threshold t_k (e.g., "petal length ≤ 2.45 cm"). How does it choose k and t_k? It searches for the pair (k, t_k) that produces the purest subsets (weighted by their size). The cost function that the algorithm tries to minimize is given by Equation 6-2.

Equation 6-2. CART cost function for classification

$$J(k, t_k) = \frac{m_{\text{left}}}{m} G_{\text{left}} + \frac{m_{\text{right}}}{m} G_{\text{right}}$$

$$\text{where } \begin{cases} G_{\text{left/right}} \text{ measures the impurity of the left/right subset,} \\ m_{\text{left/right}} \text{ is the number of instances in the left/right subset.} \end{cases}$$

Once it has successfully split the training set in two, it splits the subsets using the same logic, then the sub-subsets and so on, recursively. It stops recursing once it reaches the maximum depth (defined by the `max_depth` hyperparameter), or if it cannot find a split that will reduce impurity. A few other hyperparameters (described in a moment) control additional stopping conditions (`min_samples_split`, `min_samples_leaf`, `min_weight_fraction_leaf`, and `max_leaf_nodes`).

As you can see, the CART algorithm is a *greedy algorithm*: it greedily searches for an optimum split at the top level, then repeats the process at each level. It does not check whether or not the split will lead to the lowest possible impurity several levels down. A greedy algorithm often produces a reasonably good solution, but it is not guaranteed to be the optimal solution.

Unfortunately, finding the optimal tree is known to be an *NP-Complete* problem:[2] it requires $O(\exp(m))$ time, making the problem intractable even for fairly small training sets. This is why we must settle for a "reasonably good" solution.

Computational Complexity

Making predictions requires traversing the Decision Tree from the root to a leaf. Decision Trees are generally approximately balanced, so traversing the Decision Tree requires going through roughly $O(log_2(m))$ nodes.[3] Since each node only requires checking the value of one feature, the overall prediction complexity is just $O(log_2(m))$, independent of the number of features. So predictions are very fast, even when dealing with large training sets.

However, the training algorithm compares all features (or less if `max_features` is set) on all samples at each node. This results in a training complexity of $O(n \times m\ log(m))$. For small training sets (less than a few thousand instances), Scikit-Learn can speed up training by presorting the data (set `presort=True`), but this slows down training considerably for larger training sets.

Gini Impurity or Entropy?

By default, the Gini impurity measure is used, but you can select the *entropy* impurity measure instead by setting the `criterion` hyperparameter to `"entropy"`. The concept of entropy originated in thermodynamics as a measure of molecular disorder: entropy approaches zero when molecules are still and well ordered. It later spread to a wide variety of domains, including Shannon's *information theory*, where it measures the average information content of a message:[4] entropy is zero when all messages are identical. In Machine Learning, it is frequently used as an impurity measure: a set's

[2] P is the set of problems that can be solved in polynomial time. NP is the set of problems whose solutions can be verified in polynomial time. An NP-Hard problem is a problem to which any NP problem can be reduced in polynomial time. An NP-Complete problem is both NP and NP-Hard. A major open mathematical question is whether or not P = NP. If P ≠ NP (which seems likely), then no polynomial algorithm will ever be found for any NP-Complete problem (except perhaps on a quantum computer).

[3] log_2 is the binary logarithm. It is equal to $log_2(m) = log(m) / log(2)$.

[4] A reduction of entropy is often called an *information gain*.

entropy is zero when it contains instances of only one class. Equation 6-3 shows the definition of the entropy of the i$^{\text{th}}$ node. For example, the depth-2 left node in Figure 6-1 has an entropy equal to $-\frac{49}{54}\log_2\left(\frac{49}{54}\right)-\frac{5}{54}\log_2\left(\frac{5}{54}\right)\approx 0.445$.

Equation 6-3. Entropy

$$H_i = -\sum_{\substack{k=1 \\ p_{i,k}\neq 0}}^{n} p_{i,k}\log_2\left(p_{i,k}\right)$$

So should you use Gini impurity or entropy? The truth is, most of the time it does not make a big difference: they lead to similar trees. Gini impurity is slightly faster to compute, so it is a good default. However, when they differ, Gini impurity tends to isolate the most frequent class in its own branch of the tree, while entropy tends to produce slightly more balanced trees.[5]

Regularization Hyperparameters

Decision Trees make very few assumptions about the training data (as opposed to linear models, which obviously assume that the data is linear, for example). If left unconstrained, the tree structure will adapt itself to the training data, fitting it very closely, and most likely overfitting it. Such a model is often called a *nonparametric model*, not because it does not have any parameters (it often has a lot) but because the number of parameters is not determined prior to training, so the model structure is free to stick closely to the data. In contrast, a *parametric model* such as a linear model has a predetermined number of parameters, so its degree of freedom is limited, reducing the risk of overfitting (but increasing the risk of underfitting).

To avoid overfitting the training data, you need to restrict the Decision Tree's freedom during training. As you know by now, this is called regularization. The regularization hyperparameters depend on the algorithm used, but generally you can at least restrict the maximum depth of the Decision Tree. In Scikit-Learn, this is controlled by the `max_depth` hyperparameter (the default value is `None`, which means unlimited). Reducing `max_depth` will regularize the model and thus reduce the risk of overfitting.

The `DecisionTreeClassifier` class has a few other parameters that similarly restrict the shape of the Decision Tree: `min_samples_split` (the minimum number of samples a node must have before it can be split), `min_samples_leaf` (the minimum number of samples a leaf node must have), `min_weight_fraction_leaf` (same as `min_samples_leaf` but expressed as a fraction of the total number of weighted

[5] See Sebastian Raschka's interesting analysis for more details.