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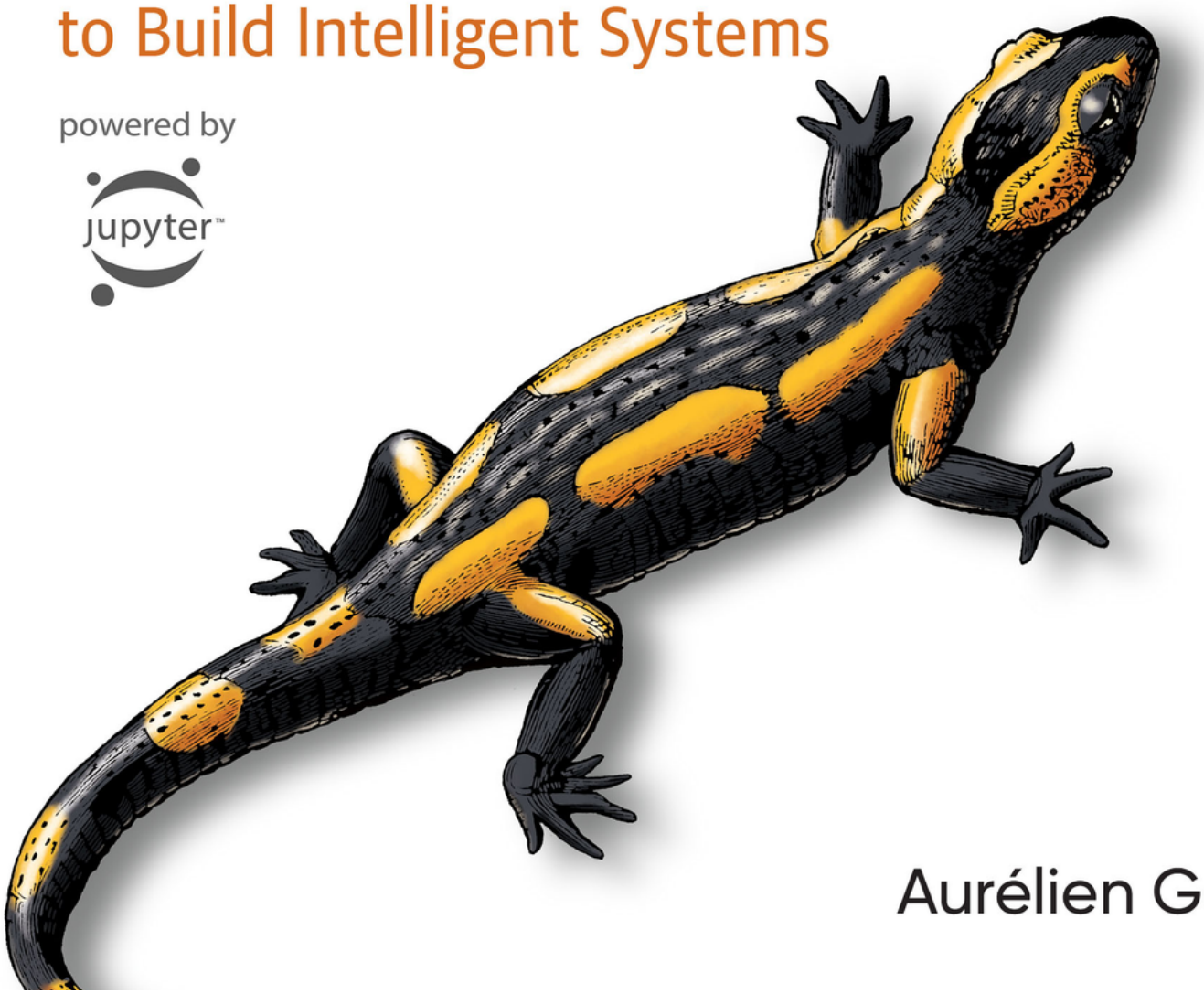

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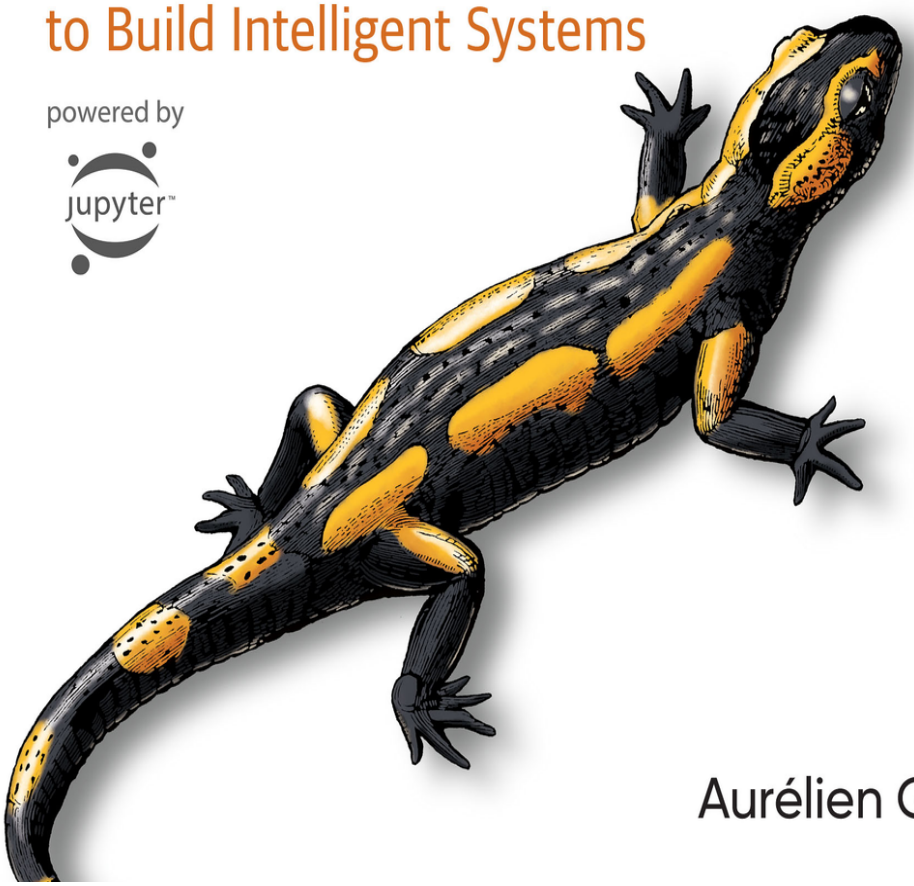

Aurélien Géron

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Concepts, Tools, and Techniques to Build Intelligent Systems

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Beijing • Boston • Farnham • Sebastopol • Tokyo

Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow

by Aurélien Géron

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Chapter 6. Decision Trees

Decision trees are versatile machine learning algorithms that can perform both classification and regression tasks, and even multioutput tasks. They are 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 explore 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 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(as_frame=True)
X_iris = iris.data[["petal length (cm)", "petal width (cm)"]].values
y_iris = iris.target

tree_clf = DecisionTreeClassifier(max_depth=2, random_state=42)
tree_clf.fit(X_iris, y_iris)
```

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

```
from sklearn.tree import export_graphviz

export_graphviz(
        tree_clf,
        out_file="iris_tree.dot",
        feature_names=["petal length (cm)", "petal width (cm)"],
        class_names=iris.target_names,
        rounded=True,
```

```
        filled=True
    )
```

Then you can use `graphviz.Source.from_file()` to load and display the file in a Jupyter notebook:

```
from graphviz import Source

Source.from_file("iris_tree.dot")
```

Graphviz is an open source graph visualization software package. It also includes a `dot` command-line tool to convert *.dot* files to a variety of formats, such as PDF or PNG.

Your first decision tree looks like Figure 6-1.

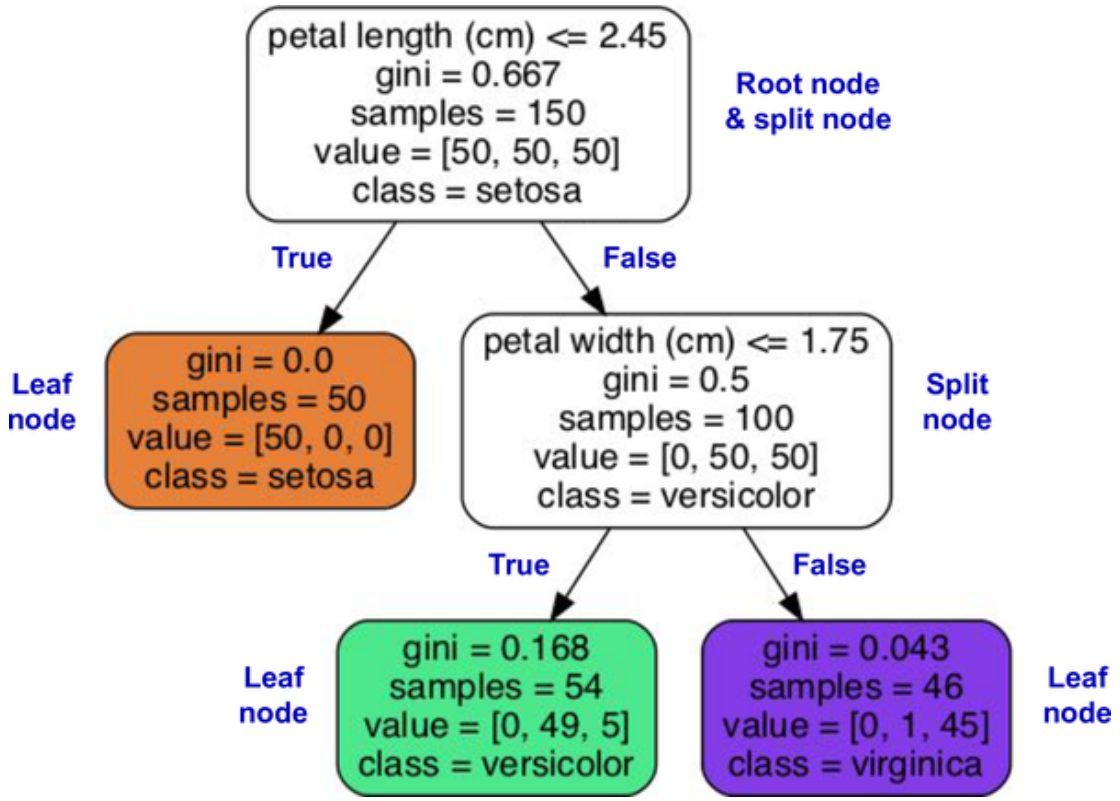

Figure 6-1. Iris decision tree

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 based on its petals. 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 child nodes), so it does not ask any questions: 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, and this time the petal length is greater than 2.45 cm. You again start at the root but now move down to its right child node (depth 1, right). This is not a leaf node, it's a *split 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.

> **NOTE**
>
> One of the many qualities of decision trees is that they require very little data preparation. In fact, 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), and of those 100, 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 *Gini 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 impurity is 0. Equation 6-1 shows how the training algorithm computes the Gini impurity G_i of the i^{th} node. The depth-2 left node has a Gini impurity equal to $1 - (0/54)^2 - (49/54)^2 - (5/54)^2 \approx 0.168$.

Equation 6-1. Gini impurity

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

In this equation:

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

> **NOTE**
>
> Scikit-Learn uses the CART algorithm, which produces only *binary trees*, meaning trees where split nodes always have exactly 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 lefthand area is pure (only *Iris setosa*), it cannot be split any further. However, the righthand 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. If you set `max_depth` to 3, then the two depth-2 nodes would each add another decision boundary (represented by the two vertical dotted lines).

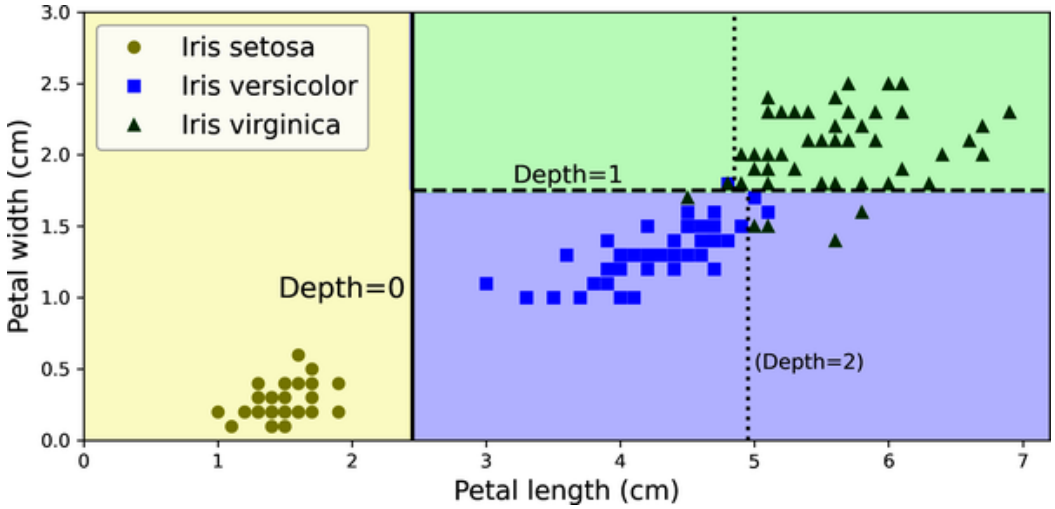

Figure 6-2. Decision tree decision boundaries

> **TIP**
>
> The tree structure, including all the information shown in Figure 6-1, is available via the classifier's `tree_` attribute. Type **`help(tree_clf.tree_)`** for details, and see the this chapter's notebook for an example.

MODEL INTERPRETATION: WHITE BOX VERSUS BLACK BOX

Decision trees are intuitive, and their decisions are easy to interpret. Such models are often called *white box models*. In contrast, as you will see, random forests and 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 in a picture, it is hard to know what contributed to this prediction: Did the model recognize that person's eyes? Their mouth? Their nose? Their shoes? Or even the couch that they were sitting on? Conversely, decision trees provide nice, simple classification rules that can even be applied manually if need be (e.g., for flower classification). The field of *interpretable ML* aims at creating ML systems that can explain their decisions in a way humans can understand. This is important in many domains—for example, to ensure the system does not make unfair decisions.

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 outputs 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 if you ask it to predict the class, it outputs *Iris versicolor* (class 1) because it has the highest probability. Let's check this:

```
>>> tree_clf.predict_proba([[5, 1.5]]).round(3)
array([[0.   , 0.907, 0.093]])
>>> 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 algorithm works by first splitting the training set into 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. Equation 6-2 gives the cost function that the algorithm tries to minimize.

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 the CART algorithm 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`.

> **WARNING**
>
> 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 subsequent 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 solution that's reasonably good but not guaranteed to be optimal.
>
> Unfortunately, finding the optimal tree is known to be an *NP-complete* problem.[1] It requires $O(\exp(m))$ time, making the problem intractable even for small training sets. This is why we must settle for a "reasonably good" solution when training decision trees.

Computational Complexity

Making predictions requires traversing the decision tree from the root to a leaf. Decision trees generally are approximately balanced, so traversing the decision tree requires going through roughly $O(\log_2(m))$ nodes, where $\log_2(m)$ is the *binary logarithm* of m, equal to $\log(m) / \log(2)$. Since each node only requires checking the value of one feature, the overall prediction complexity is $O(\log_2(m))$, independent of

the number of features. So predictions are very fast, even when dealing with large training sets.

The training algorithm compares all features (or less if `max_features` is set) on all samples at each node. Comparing all features on all samples at each node results in a training complexity of $O(n \times m \log_2(m))$.

Gini Impurity or Entropy?

By default, the `DecisionTreeClassifier` class uses the Gini impurity measure, 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. Entropy later spread to a wide variety of domains, including in Shannon's information theory, where it measures the average information content of a message, as we saw in Chapter 4. Entropy is zero when all messages are identical. In machine learning, entropy is frequently used as an impurity measure: a set's entropy is zero when it contains instances of only one class. Equation 6-3 shows the definition of the entropy of the i^{th} node. For example, the depth-2 left node in Figure 6-1 has an entropy equal to $-(49/54) \log_2 (49/54) - (5/54) \log_2 (5/54) \approx 0.445$.

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.[2]

Regularization Hyperparameters

Decision trees make very few assumptions about the training data (as opposed to linear models, which 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—indeed, 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:

`max_features`

: Maximum number of features that are evaluated for splitting at each node

`max_leaf_nodes`

: Maximum number of leaf nodes

`min_samples_split`

: Minimum number of samples a node must have before it can be split

`min_samples_leaf`

: Minimum number of samples a leaf node must have to be created

`min_weight_fraction_leaf`

: Same as `min_samples_leaf` but expressed as a fraction of the total number of weighted instances

Increasing `min_*` hyperparameters or reducing `max_*` hyperparameters will regularize the model.

> **NOTE**
>
> Other algorithms work by first training the decision tree without restrictions, then *pruning* (deleting) unnecessary nodes. A node whose children are all leaf nodes is considered unnecessary if the purity improvement it provides is not statistically significant. Standard statistical tests, such as the χ^2 *test* (chi-squared test), are used to estimate the probability that the improvement is purely the result of chance (which is called the *null hypothesis*). If this probability, called the *p-value*, is higher than a given threshold (typically 5%, controlled by a hyperparameter), then the node is considered unnecessary and its children are deleted. The pruning continues until all unnecessary nodes have been pruned.

Let's test regularization on the moons dataset, introduced in Chapter 5. We'll train one decision tree without regularization, and another with `min_samples_leaf=5`. Here's the code; Figure 6-3 shows the decision boundaries of each tree:

```
from sklearn.datasets import make_moons

X_moons, y_moons = make_moons(n_samples=150, noise=0.2, random_state=42)

tree_clf1 = DecisionTreeClassifier(random_state=42)
tree_clf2 = DecisionTreeClassifier(min_samples_leaf=5, random_state=42)
tree_clf1.fit(X_moons, y_moons)
tree_clf2.fit(X_moons, y_moons)
```

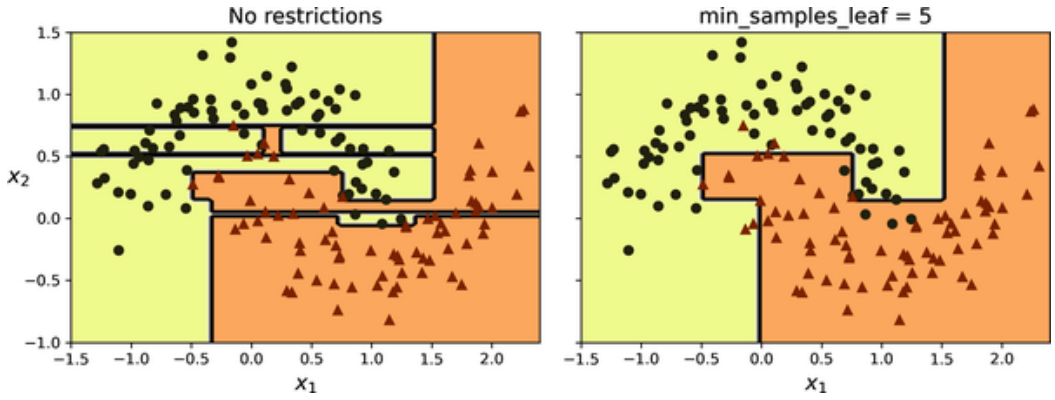

Figure 6-3. Decision boundaries of an unregularized tree (left) and a regularized tree (right)

The unregularized model on the left is clearly overfitting, and the regularized model on the right will probably generalize better. We can verify this by evaluating both trees on a test set generated using a different random seed:

```
>>> X_moons_test, y_moons_test = make_moons(n_samples=1000, noise=0.2,
...                                         random_state=43)
...
>>> tree_clf1.score(X_moons_test, y_moons_test)
0.898
>>> tree_clf2.score(X_moons_test, y_moons_test)
0.92
```

Indeed, the second tree has a better accuracy on the test set.

Regression

Decision trees are also capable of performing regression tasks. Let's build a regression tree using Scikit-Learn's `DecisionTreeRegressor` class, training it on a noisy quadratic dataset with `max_depth=2`:

```
import numpy as np
from sklearn.tree import DecisionTreeRegressor

np.random.seed(42)
X_quad = np.random.rand(200, 1) - 0.5  # a single random input feature
y_quad = X_quad ** 2 + 0.025 * np.random.randn(200, 1)

tree_reg = DecisionTreeRegressor(max_depth=2, random_state=42)
tree_reg.fit(X_quad, y_quad)
```

The resulting tree is represented in Figure 6-4.

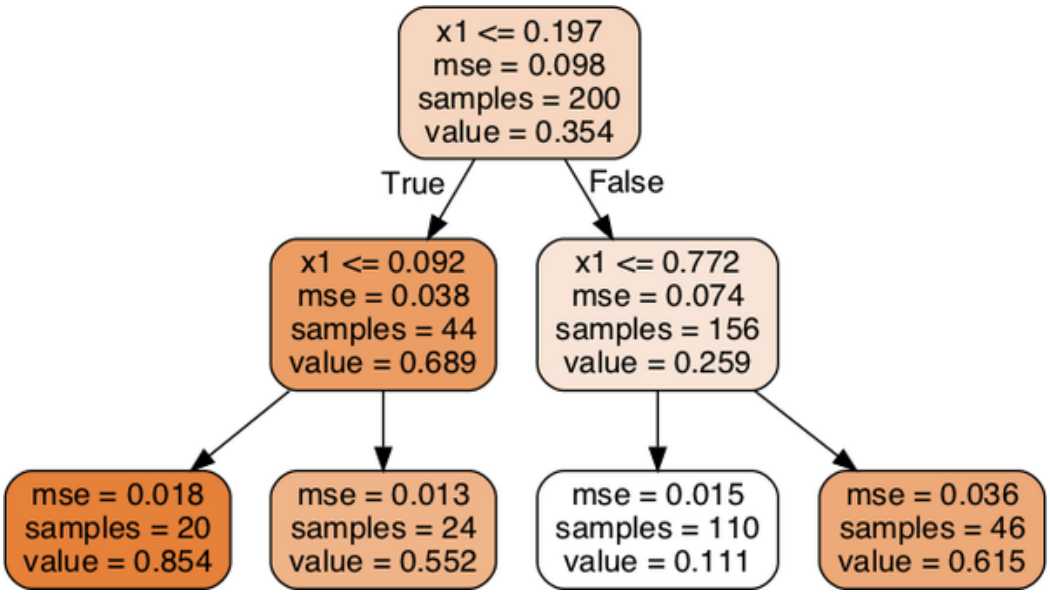

Figure 6-4. A decision tree for regression

This tree looks very similar to the classification tree you built earlier. The main difference is that instead of predicting a class in each node, it predicts a value. For example, suppose you want to make a prediction for a new instance with $x_1 = 0.2$. The root node asks whether $x_1 \leq 0.197$. Since it is not, the algorithm goes to the right child node, which asks whether $x_1 \leq 0.772$. Since it is, the algorithm goes to the left child node. This is a leaf node, and it predicts `value=0.111`. This prediction is the average

target value of the 110 training instances associated with this leaf node, and it results in a mean squared error equal to 0.015 over these 110 instances.

This model's predictions are represented on the left in Figure 6-5. If you set `max_depth=3`, you get the predictions represented on the right. Notice how the predicted value for each region is always the average target value of the instances in that region. The algorithm splits each region in a way that makes most training instances as close as possible to that predicted value.

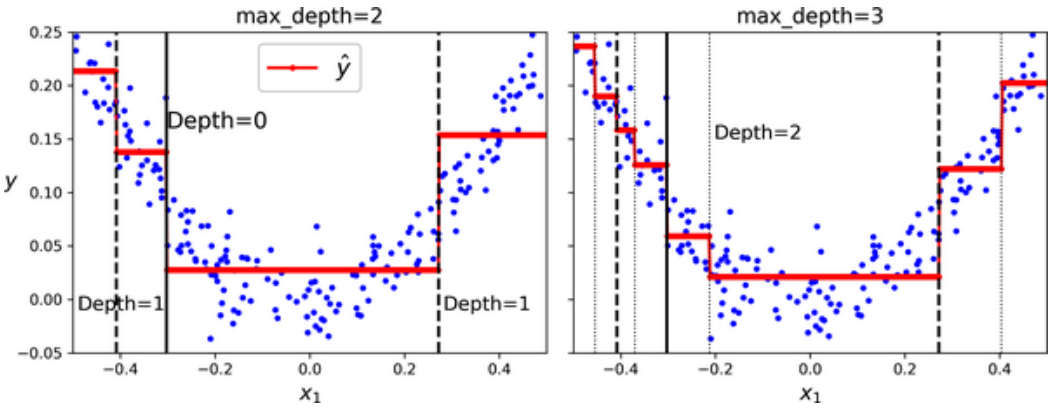

Figure 6-5. Predictions of two decision tree regression models

The CART algorithm works as described earlier, except that instead of trying to split the training set in a way that minimizes impurity, it now tries to split the training set in a way that minimizes the MSE. Equation 6-4 shows the cost function that the algorithm tries to minimize.

Equation 6-4. CART cost function for regression

$$J\left(k, t_k\right) = \frac{m_{\text{left}}}{m}\text{MSE}_{\text{left}} + \frac{m_{\text{right}}}{m}\text{MSE}_{\text{right}} \quad \text{where} \quad \text{MSE}_{\text{node}} = \frac{\sum_{i \in \text{node}}\left(\hat{y}_{\text{node}} - y^{(i)}\right)^2}{m_{\text{node}}}$$
$$\hat{y}_{\text{node}} = \frac{\sum_{i \in \text{node}} y^{(i)}}{m_{\text{node}}}$$

Just like for classification tasks, decision trees are prone to overfitting when dealing with regression tasks. Without any regularization (i.e., using the default hyperparameters), you get the predictions on the left in Figure 6-6. These predictions are obviously overfitting the training set very badly. Just setting `min_samples_leaf=10` results in a much more reasonable model, represented on the right in Figure 6-6.

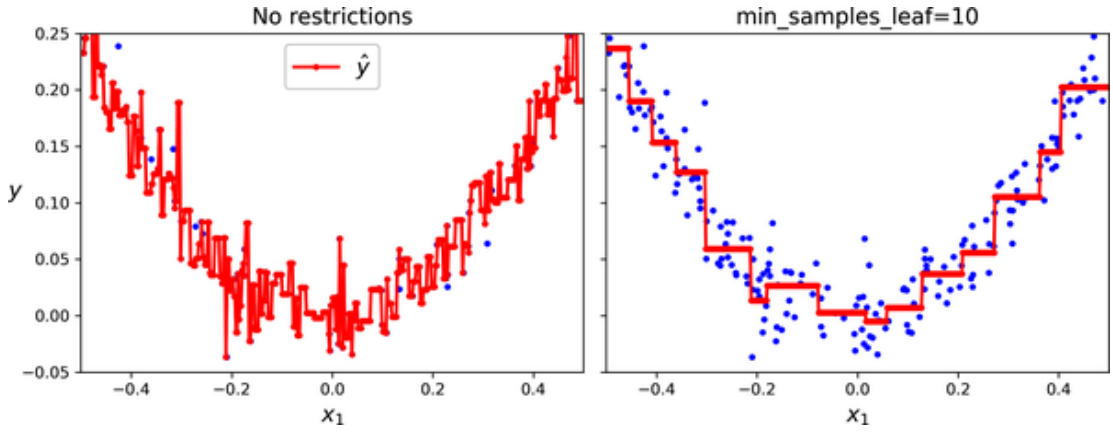

Figure 6-6. Predictions of an unregularized regression tree (left) and a regularized tree (right)

Sensitivity to Axis Orientation

Hopefully by now you are convinced that decision trees have a lot going for them: they are relatively easy to understand and interpret, simple to use, versatile, and powerful. However, they do have a few limitations. First, as you may have noticed, decision trees love orthogonal decision boundaries (all splits are perpendicular to an axis), which makes them sensitive to the data's orientation. For example, Figure 6-7 shows a simple linearly separable dataset: on the left, a decision tree can split it easily, while on the right, after the dataset is rotated by 45°, the decision boundary looks unnecessarily convoluted. Although both decision trees fit the training set perfectly, it is very likely that the model on the right will not generalize well.

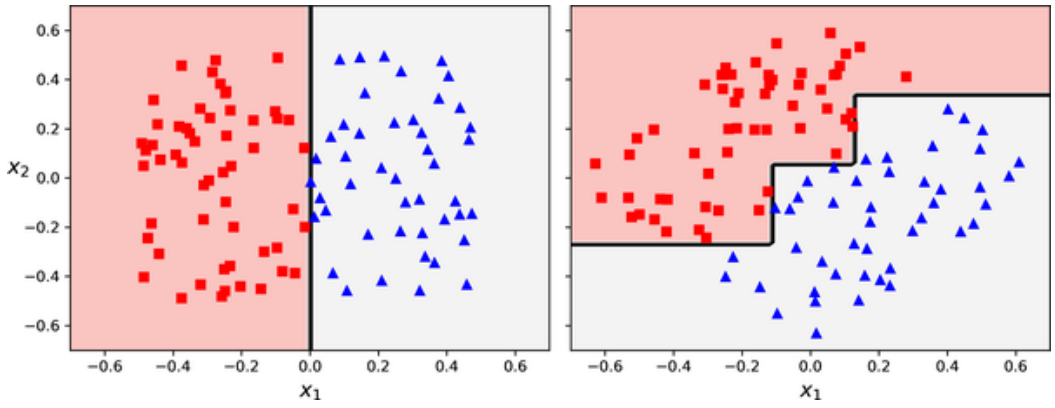

Figure 6-7. Sensitivity to training set rotation

One way to limit this problem is to scale the data, then apply a principal component analysis transformation. We will look at PCA in detail in Chapter 8, but for now you only need to know that it rotates the data in a way that reduces the correlation between the features, which often (not always) makes things easier for trees.

Let's create a small pipeline that scales the data and rotates it using PCA, then train a `DecisionTreeClassifier` on that data. Figure 6-8 shows the decision boundaries of that tree: as you can see, the rotation makes it possible to fit the dataset pretty well using only one feature, z_1, which is a linear function of the original petal length and width. Here's the code:

```
from sklearn.decomposition import PCA
from sklearn.pipeline import make_pipeline
from sklearn.preprocessing import StandardScaler

pca_pipeline = make_pipeline(StandardScaler(), PCA())
X_iris_rotated = pca_pipeline.fit_transform(X_iris)
tree_clf_pca = DecisionTreeClassifier(max_depth=2, random_state=42)
tree_clf_pca.fit(X_iris_rotated, y_iris)
```

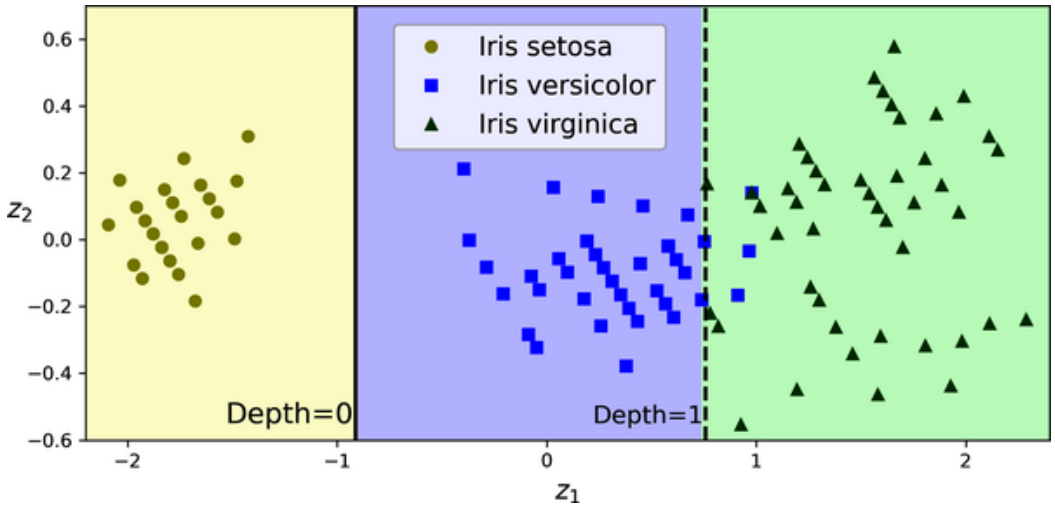

Figure 6-8. A tree's decision boundaries on the scaled and PCA-rotated iris dataset

Decision Trees Have a High Variance

More generally, the main issue with decision trees is that they have quite a high variance: small changes to the hyperparameters or to the data may produce very different models. In fact, since the training algorithm used by Scikit-Learn is stochastic—it randomly selects the set of features to evaluate at each node—even retraining the same decision tree on the exact same data may produce a very different model, such as the one represented in Figure 6-9 (unless you set the `random_state` hyperparameter). As you can see, it looks very different from the previous decision tree (Figure 6-2).

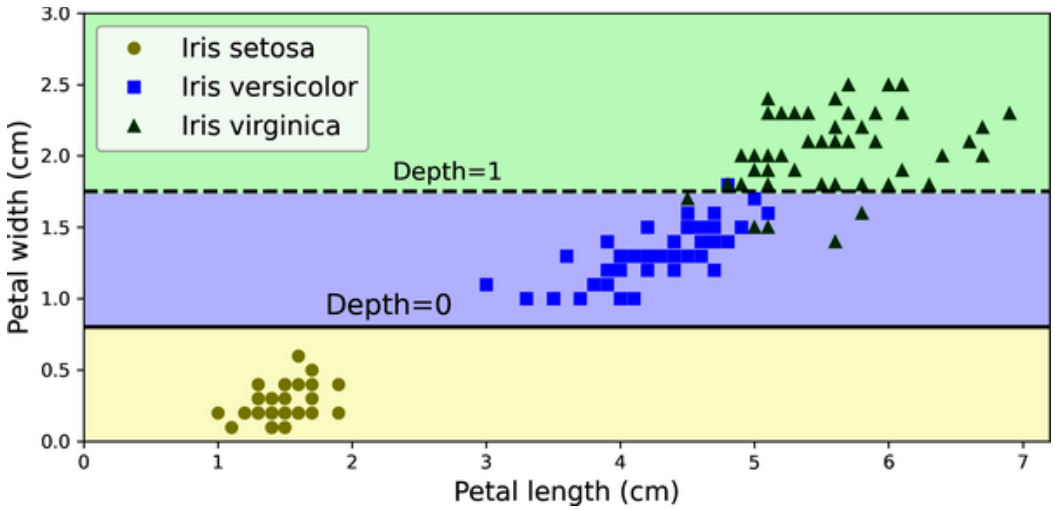

Figure 6-9. Retraining the same model on the same data may produce a very different model

Luckily, by averaging predictions over many trees, it's possible to reduce variance significantly. Such an *ensemble* of trees is called a *random forest*, and it's one of the most powerful types of models available today, as you will see in the next chapter.

Exercises

1. What is the approximate depth of a decision tree trained (without restrictions) on a training set with one million instances?
2. Is a node's Gini impurity generally lower or higher than its parent's? Is it *generally* lower/higher, or *always* lower/higher?
3. If a decision tree is overfitting the training set, is it a good idea to try decreasing `max_depth`?
4. If a decision tree is underfitting the training set, is it a good idea to try scaling the input features?
5. If it takes one hour to train a decision tree on a training set containing one million instances, roughly how much time will it take to train another decision tree on a training set containing ten million instances? Hint: consider the CART algorithm's computational complexity.
6. If it takes one hour to train a decision tree on a given training set, roughly how much time will it take if you double the number of features?
7. Train and fine-tune a decision tree for the moons dataset by following these steps:

a. Use `make_moons(n_samples=10000, noise=0.4)` to generate a moons dataset.

b. Use `train_test_split()` to split the dataset into a training set and a test set.

c. Use grid search with cross-validation (with the help of the `GridSearchCV` class) to find good hyperparameter values for a `DecisionTreeClassifier`. Hint: try various values for `max_leaf_nodes`.

d. Train it on the full training set using these hyperparameters, and measure your model's performance on the test set. You should get roughly 85% to 87% accuracy.

8. Grow a forest by following these steps:

a. Continuing the previous exercise, generate 1,000 subsets of the training set, each containing 100 instances selected randomly. Hint: you can use Scikit-Learn's `ShuffleSplit` class for this.

b. Train one decision tree on each subset, using the best hyperparameter values found in the previous exercise. Evaluate these 1,000 decision trees on the test set. Since they were trained on smaller sets, these decision trees will likely perform worse than the first decision tree, achieving only about 80% accuracy.

c. Now comes the magic. For each test set instance, generate the predictions of the 1,000 decision trees, and keep only the most frequent prediction (you can use SciPy's `mode()` function for this). This approach gives you *majority-vote predictions* over the test set.

d. Evaluate these predictions on the test set: you should obtain a slightly higher accuracy than your first model (about 0.5 to 1.5% higher). Congratulations, you have trained a random forest classifier!

Solutions to these exercises are available at the end of this chapter's notebook, at *https://homl.info/colab3*.

---

1 P is the set of problems that can be solved in *polynomial time* (i.e., a polynomial of the dataset size). NP is the set of problems whose solutions can be verified in polynomial time. An NP-hard problem is a problem that can be reduced to a known NP-hard problem 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 one day on a quantum computer).

2 See Sebastian Raschka's interesting analysis for more details.

Chapter 7. Ensemble Learning and Random Forests

Suppose you pose a complex question to thousands of random people, then aggregate their answers. In many cases you will find that this aggregated answer is better than an expert's answer. This is called the *wisdom of the crowd*. Similarly, if you aggregate the predictions of a group of predictors (such as classifiers or regressors), you will often get better predictions than with the best individual predictor. A group of predictors is called an *ensemble*; thus, this technique is called *ensemble learning*, and an ensemble learning algorithm is called an *ensemble method*.

As an example of an ensemble method, you can train a group of decision tree classifiers, each on a different random subset of the training set. You can then obtain the predictions of all the individual trees, and the class that gets the most votes is the ensemble's prediction (see the last exercise in Chapter 6). Such an ensemble of decision trees is called a *random forest*, and despite its simplicity, this is one of the most powerful machine learning algorithms available today.

As discussed in Chapter 2, you will often use ensemble methods near the end of a project, once you have already built a few good predictors, to combine them into an even better predictor. In fact, the winning solutions in machine learning competitions often involve several ensemble methods—most famously in the Netflix Prize competition.

In this chapter we will examine the most popular ensemble methods, including voting classifiers, bagging and pasting ensembles, random forests, and boosting, and stacking ensembles.

Voting Classifiers

Suppose you have trained a few classifiers, each one achieving about 80% accuracy. You may have a logistic regression classifier, an SVM classifier, a random forest classifier, a *k*-nearest neighbors classifier, and perhaps a few more (see Figure 7-1).

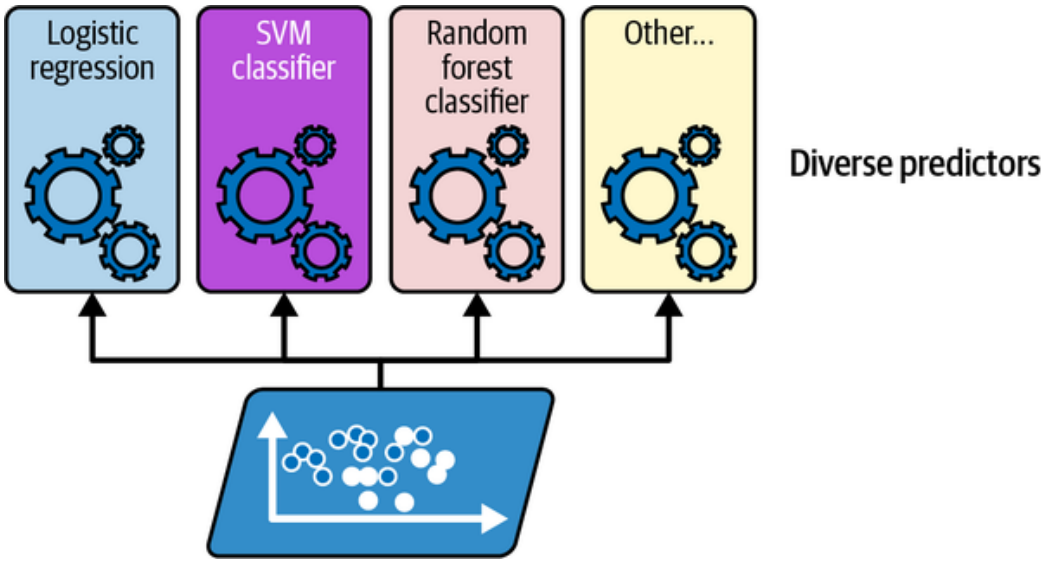

Figure 7-1. Training diverse classifiers

A very simple way to create an even better classifier is to aggregate the predictions of each classifier: the class that gets the most votes is the ensemble's prediction. This majority-vote classifier is called a *hard voting* classifier (see Figure 7-2).

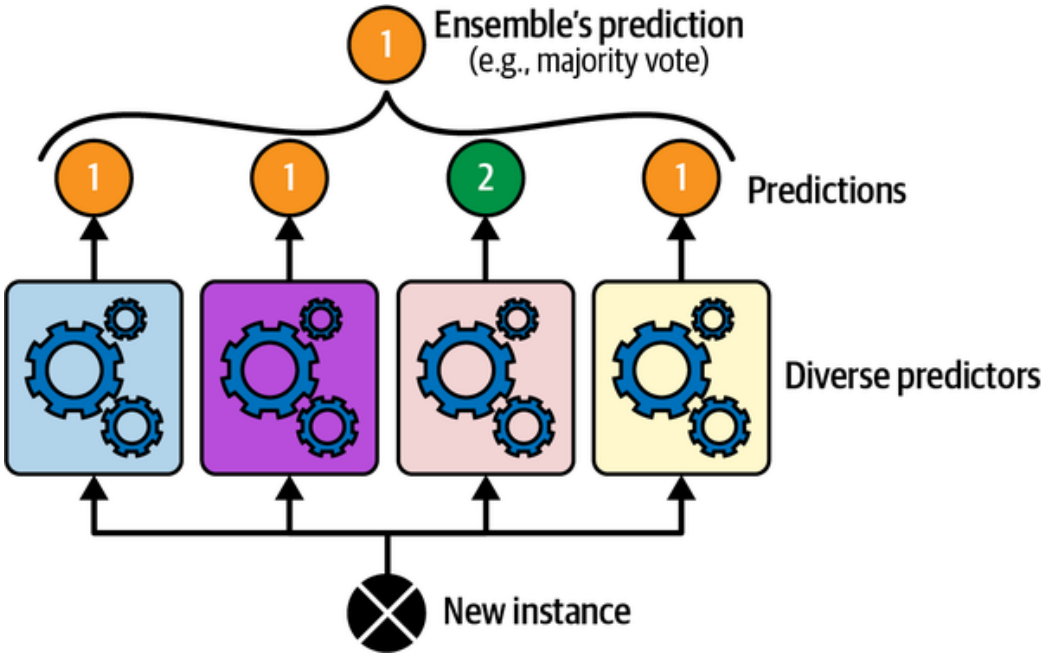

Figure 7-2. Hard voting classifier predictions

Somewhat surprisingly, this voting classifier often achieves a higher accuracy than the best classifier in the ensemble. In fact, even if each classifier is a *weak learner* (meaning it does only slightly better than random guessing), the ensemble can still be a *strong learner* (achieving high accuracy), provided there are a sufficient number of weak learners in the ensemble and they are sufficiently diverse.

How is this possible? The following analogy can help shed some light on this mystery. Suppose you have a slightly biased coin that has a 51% chance of coming up heads and 49% chance of coming up tails. If you toss it 1,000 times, you will generally get more or less 510 heads and 490 tails, and hence a majority of heads. If you do the math, you will find that the probability of obtaining a majority of heads after 1,000 tosses is close to 75%. The more you toss the coin, the higher the probability (e.g., with 10,000 tosses, the probability climbs over 97%). This is due to the *law of large numbers*: as you keep tossing the coin, the ratio of heads gets closer and closer to the probability of heads (51%). Figure 7-3 shows 10 series of biased coin tosses. You can see that as the number of tosses increases, the ratio of heads approaches 51%. Eventually all 10 series end up so close to 51% that they are consistently above 50%.

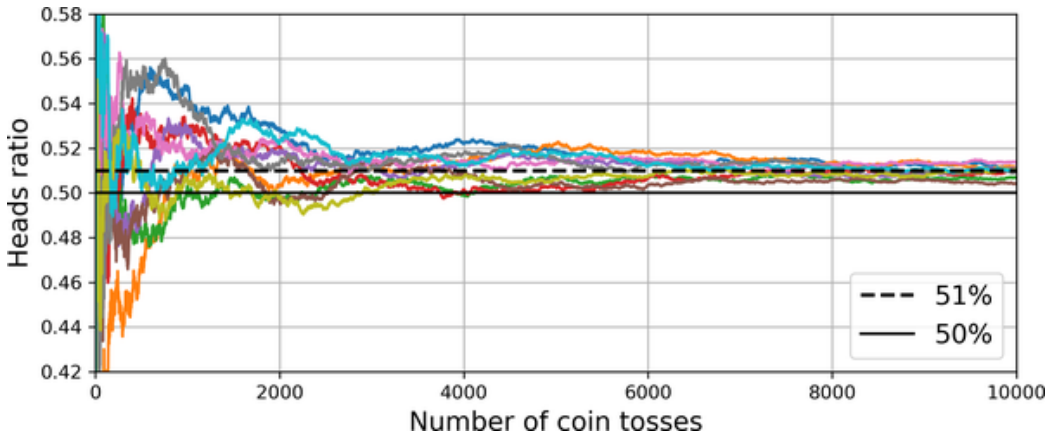

Figure 7-3. The law of large numbers

Similarly, suppose you build an ensemble containing 1,000 classifiers that are individually correct only 51% of the time (barely better than random guessing). If you predict the majority voted class, you can hope for up to 75% accuracy! However, this is only true if all classifiers are perfectly independent, making uncorrelated errors, which is clearly not the case because they are trained on the same data. They are likely to make the same types of errors, so there will be many majority votes for the wrong class, reducing the ensemble's accuracy.

> **TIP**
>
> Ensemble methods work best when the predictors are as independent from one another as possible. One way to get diverse classifiers is to train them using very different algorithms. This increases the chance that they will make very different types of errors, improving the ensemble's accuracy.

Scikit-Learn provides a `VotingClassifier` class that's quite easy to use: just give it a list of name/predictor pairs, and use it like a normal classifier. Let's try it on the moons

dataset (introduced in Chapter 5). We will load and split the moons dataset into a training set and a test set, then we'll create and train a voting classifier composed of three diverse classifiers:

```
from sklearn.datasets import make_moons
from sklearn.ensemble import RandomForestClassifier, VotingClassifier
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import train_test_split
from sklearn.svm import SVC

X, y = make_moons(n_samples=500, noise=0.30, random_state=42)
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=42)

voting_clf = VotingClassifier(
    estimators=[
        ('lr', LogisticRegression(random_state=42)),
        ('rf', RandomForestClassifier(random_state=42)),
        ('svc', SVC(random_state=42))
    ]
)
voting_clf.fit(X_train, y_train)
```

When you fit a `VotingClassifier`, it clones every estimator and fits the clones. The original estimators are available via the `estimators` attribute, while the fitted clones are available via the `estimators_` attribute. If you prefer a dict rather than a list, you can use `named_estimators` or `named_estimators_` instead. To begin, let's look at each fitted classifier's accuracy on the test set:

```
>>> for name, clf in voting_clf.named_estimators_.items():
...     print(name, "=", clf.score(X_test, y_test))
...
lr = 0.864
rf = 0.896
svc = 0.896
```

When you call the voting classifier's `predict()` method, it performs hard voting. For example, the voting classifier predicts class 1 for the first instance of the test set, because two out of three classifiers predict that class:

```
>>> voting_clf.predict(X_test[:1])
array([1])
>>> [clf.predict(X_test[:1]) for clf in voting_clf.estimators_]
[array([1]), array([1]), array([0])]
```

Now let's look at the performance of the voting classifier on the test set:

```
>>> voting_clf.score(X_test, y_test)
0.912
```

There you have it! The voting classifier outperforms all the individual classifiers.

If all classifiers are able to estimate class probabilities (i.e., if they all have a `predict_proba()` method), then you can tell Scikit-Learn to predict the class with the highest class probability, averaged over all the individual classifiers. This is called *soft voting*. It often achieves higher performance than hard voting because it gives more weight to highly confident votes. All you need to do is set the voting classifier's `voting` hyperparameter to `"soft"`, and ensure that all classifiers can estimate class probabilities. This is not the case for the `SVC` class by default, so you need to set its `probability` hyperparameter to `True` (this will make the `SVC` class use cross-validation to estimate class probabilities, slowing down training, and it will add a `predict_proba()` method). Let's try that:

```
>>> voting_clf.voting = "soft"
>>> voting_clf.named_estimators["svc"].probability = True
>>> voting_clf.fit(X_train, y_train)
>>> voting_clf.score(X_test, y_test)
0.92
```

We reach 92% accuracy simply by using soft voting—not bad!

Bagging and Pasting

One way to get a diverse set of classifiers is to use very different training algorithms, as just discussed. Another approach is to use the same training algorithm for every predictor but train them on different random subsets of the training set. When sampling is performed *with* replacement,[1] this method is called *bagging*[2] (short for *bootstrap aggregating*[3]). When sampling is performed *without* replacement, it is called *pasting*.[4]

In other words, both bagging and pasting allow training instances to be sampled several times across multiple predictors, but only bagging allows training instances to be sampled several times for the same predictor. This sampling and training process is represented in Figure 7-4.

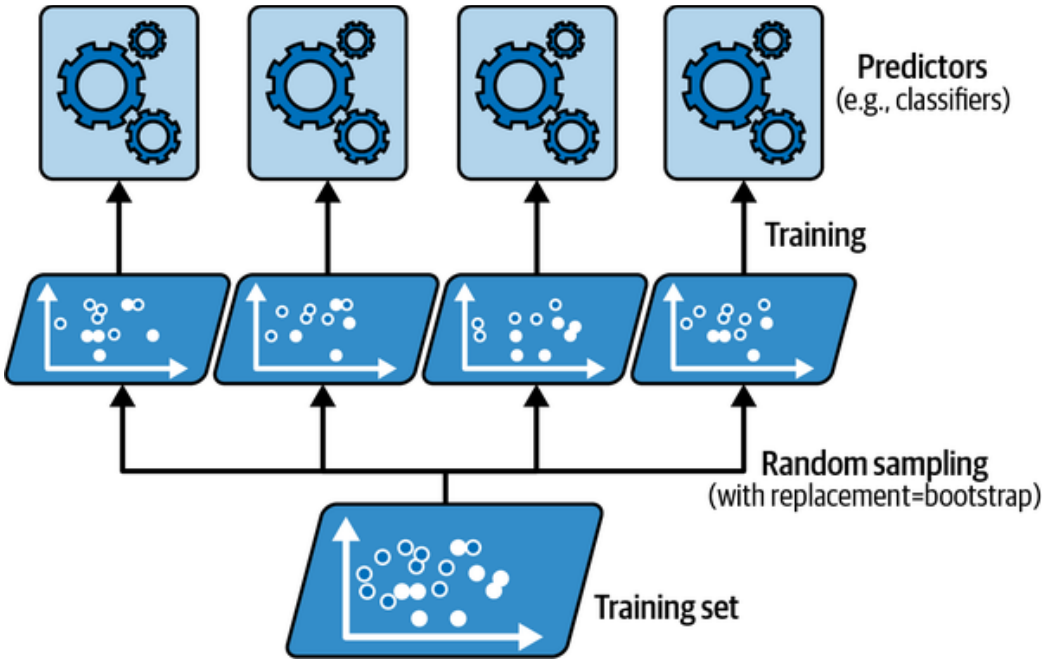

Figure 7-4. Bagging and pasting involve training several predictors on different random samples of the training set

Once all predictors are trained, the ensemble can make a prediction for a new instance by simply aggregating the predictions of all predictors. The aggregation function is typically the *statistical mode* for classification (i.e., the most frequent prediction, just like with a hard voting classifier), or the average for regression. Each individual predictor has a higher bias than if it were trained on the original training set, but aggregation reduces both bias and variance.[5] Generally, the net result is that the ensemble has a similar bias but a lower variance than a single predictor trained on the original training set.

As you can see in Figure 7-4, predictors can all be trained in parallel, via different CPU cores or even different servers. Similarly, predictions can be made in parallel. This is one of the reasons bagging and pasting are such popular methods: they scale very well.

Bagging and Pasting in Scikit-Learn

Scikit-Learn offers a simple API for both bagging and pasting: `BaggingClassifier` class (or `BaggingRegressor` for regression). The following code trains an ensemble of 500 decision tree classifiers:[6] each is trained on 100 training instances randomly sampled from the training set with replacement (this is an example of bagging, but if you want to use pasting instead, just set `bootstrap=False`). The `n_jobs` parameter tells Scikit-Learn the number of CPU cores to use for training and predictions, and `-1` tells Scikit-Learn to use all available cores:

```
from sklearn.ensemble import BaggingClassifier
from sklearn.tree import DecisionTreeClassifier

bag_clf = BaggingClassifier(DecisionTreeClassifier(), n_estimators=500,
                            max_samples=100, n_jobs=-1, random_state=42)
bag_clf.fit(X_train, y_train)
```

> **NOTE**
>
> A `BaggingClassifier` automatically performs soft voting instead of hard voting if the base classifier can estimate class probabilities (i.e., if it has a `predict_proba()` method), which is the case with decision tree classifiers.

Figure 7-5 compares the decision boundary of a single decision tree with the decision boundary of a bagging ensemble of 500 trees (from the preceding code), both trained on the moons dataset. As you can see, the ensemble's predictions will likely generalize much better than the single decision tree's predictions: the ensemble has a comparable bias but a smaller variance (it makes roughly the same number of errors on the training set, but the decision boundary is less irregular).

Bagging introduces a bit more diversity in the subsets that each predictor is trained on, so bagging ends up with a slightly higher bias than pasting; but the extra diversity also means that the predictors end up being less correlated, so the ensemble's variance is reduced. Overall, bagging often results in better models, which explains why it's generally preferred. But if you have spare time and CPU power, you can use cross-validation to evaluate both bagging and pasting and select the one that works best.

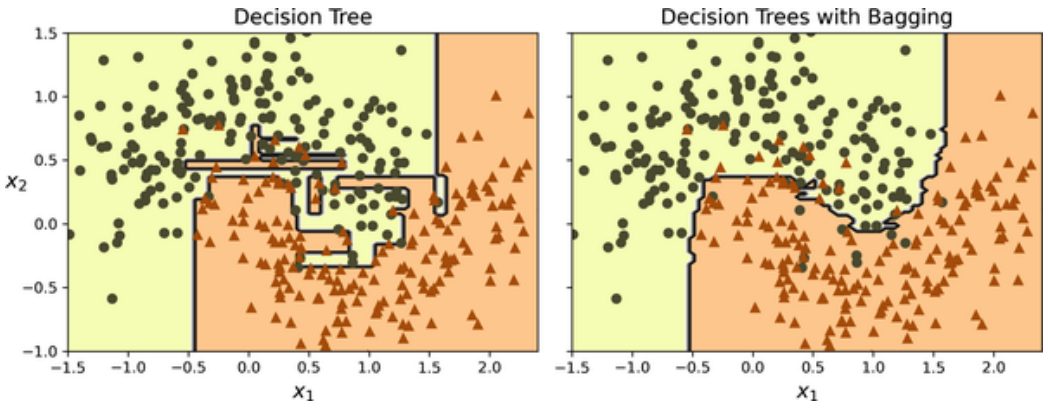

Figure 7-5. A single decision tree (left) versus a bagging ensemble of 500 trees (right)

Out-of-Bag Evaluation

With bagging, some training instances may be sampled several times for any given predictor, while others may not be sampled at all. By default a `BaggingClassifier`

samples *m* training instances with replacement (`bootstrap=True`), where *m* is the size of the training set. With this process, it can be shown mathematically that only about 63% of the training instances are sampled on average for each predictor.[7] The remaining 37% of the training instances that are not sampled are called *out-of-bag* (OOB) instances. Note that they are not the same 37% for all predictors.

A bagging ensemble can be evaluated using OOB instances, without the need for a separate validation set: indeed, if there are enough estimators, then each instance in the training set will likely be an OOB instance of several estimators, so these estimators can be used to make a fair ensemble prediction for that instance. Once you have a prediction for each instance, you can compute the ensemble's prediction accuracy (or any other metric).

In Scikit-Learn, you can set `oob_score=True` when creating a `BaggingClassifier` to request an automatic OOB evaluation after training. The following code demonstrates this. The resulting evaluation score is available in the `oob_score_` attribute:

```
>>> bag_clf = BaggingClassifier(DecisionTreeClassifier(), n_estimators=500,
...                             oob_score=True, n_jobs=-1, random_state=42)
...
>>> bag_clf.fit(X_train, y_train)
>>> bag_clf.oob_score_
0.896
```

According to this OOB evaluation, this `BaggingClassifier` is likely to achieve about 89.6% accuracy on the test set. Let's verify this:

```
>>> from sklearn.metrics import accuracy_score
>>> y_pred = bag_clf.predict(X_test)
>>> accuracy_score(y_test, y_pred)
0.92
```

We get 92% accuracy on the test. The OOB evaluation was a bit too pessimistic, just over 2% too low.

The OOB decision function for each training instance is also available through the `oob_decision_function_` attribute. Since the base estimator has a `predict_proba()` method, the decision function returns the class probabilities for each training instance. For example, the OOB evaluation estimates that the first training instance has a 67.6% probability of belonging to the positive class and a 32.4% probability of belonging to the negative class:

```
>>> bag_clf.oob_decision_function_[:3]  # probas for the first 3 instances
array([[0.32352941, 0.67647059],
```

```
       [0.3375    , 0.6625    ],
       [1.        , 0.        ]])
```

Random Patches and Random Subspaces

The `BaggingClassifier` class supports sampling the features as well. Sampling is controlled by two hyperparameters: `max_features` and `bootstrap_features`. They work the same way as `max_samples` and `bootstrap`, but for feature sampling instead of instance sampling. Thus, each predictor will be trained on a random subset of the input features.

This technique is particularly useful when you are dealing with high-dimensional inputs (such as images), as it can considerably speed up training. Sampling both training instances and features is called the *random patches* method.[8] Keeping all training instances (by setting `bootstrap=False` and `max_samples=1.0`) but sampling features (by setting `bootstrap_features` to `True` and/or `max_features` to a value smaller than `1.0`) is called the *random subspaces* method.[9]

Sampling features results in even more predictor diversity, trading a bit more bias for a lower variance.

Random Forests

As we have discussed, a random forest[10] is an ensemble of decision trees, generally trained via the bagging method (or sometimes pasting), typically with `max_samples` set to the size of the training set. Instead of building a `BaggingClassifier` and passing it a `DecisionTreeClassifier`, you can use the `RandomForestClassifier` class, which is more convenient and optimized for decision trees[11] (similarly, there is a `RandomForestRegressor` class for regression tasks). The following code trains a random forest classifier with 500 trees, each limited to maximum 16 leaf nodes, using all available CPU cores:

```
from sklearn.ensemble import RandomForestClassifier

rnd_clf = RandomForestClassifier(n_estimators=500, max_leaf_nodes=16,
                                 n_jobs=-1, random_state=42)
rnd_clf.fit(X_train, y_train)

y_pred_rf = rnd_clf.predict(X_test)
```

With a few exceptions, a `RandomForestClassifier` has all the hyperparameters of a `DecisionTreeClassifier` (to control how trees are grown), plus all the hyperparameters of a `BaggingClassifier` to control the ensemble itself.

The random forest algorithm introduces extra randomness when growing trees; instead of searching for the very best feature when splitting a node (see Chapter 6), it searches for the best feature among a random subset of features. By default, it samples $\sqrt{n}$ features (where n is the total number of features). The algorithm results in greater tree diversity, which (again) trades a higher bias for a lower variance, generally yielding an overall better model. So, the following `BaggingClassifier` is equivalent to the previous `RandomForestClassifier`:

```
bag_clf = BaggingClassifier(
    DecisionTreeClassifier(max_features="sqrt", max_leaf_nodes=16),
    n_estimators=500, n_jobs=-1, random_state=42)
```

Extra-Trees

When you are growing a tree in a random forest, at each node only a random subset of the features is considered for splitting (as discussed earlier). It is possible to make trees even more random by also using random thresholds for each feature rather than searching for the best possible thresholds (like regular decision trees do). For this, simply set `splitter="random"` when creating a `DecisionTreeClassifier`.

A forest of such extremely random trees is called an *extremely randomized trees*[12] (or *extra-trees* for short) ensemble. Once again, this technique trades more bias for a lower variance. It also makes extra-trees classifiers much faster to train than regular random forests, because finding the best possible threshold for each feature at every node is one of the most time-consuming tasks of growing a tree.

You can create an extra-trees classifier using Scikit-Learn's `ExtraTreesClassifier` class. Its API is identical to the `RandomForestClassifier` class, except `bootstrap` defaults to `False`. Similarly, the `ExtraTreesRegressor` class has the same API as the `RandomForestRegressor` class, except `bootstrap` defaults to `False`.

> **TIP**
>
> It is hard to tell in advance whether a `RandomForestClassifier` will perform better or worse than an `ExtraTreesClassifier`. Generally, the only way to know is to try both and compare them using cross-validation.

Feature Importance

Yet another great quality of random forests is that they make it easy to measure the relative importance of each feature. Scikit-Learn measures a feature's importance by looking at how much the tree nodes that use that feature reduce impurity on average,

across all trees in the forest. More precisely, it is a weighted average, where each node's weight is equal to the number of training samples that are associated with it (see Chapter 6).

Scikit-Learn computes this score automatically for each feature after training, then it scales the results so that the sum of all importances is equal to 1. You can access the result using the `feature_importances_` variable. For example, the following code trains a `RandomForestClassifier` on the iris dataset (introduced in Chapter 4) and outputs each feature's importance. It seems that the most important features are the petal length (44%) and width (42%), while sepal length and width are rather unimportant in comparison (11% and 2%, respectively):

```
>>> from sklearn.datasets import load_iris
>>> iris = load_iris(as_frame=True)
>>> rnd_clf = RandomForestClassifier(n_estimators=500, random_state=42)
>>> rnd_clf.fit(iris.data, iris.target)
>>> for score, name in zip(rnd_clf.feature_importances_, iris.data.columns):
...     print(round(score, 2), name)
...
0.11 sepal length (cm)
0.02 sepal width (cm)
0.44 petal length (cm)
0.42 petal width (cm)
```

Similarly, if you train a random forest classifier on the MNIST dataset (introduced in Chapter 3) and plot each pixel's importance, you get the image represented in Figure 7-6.

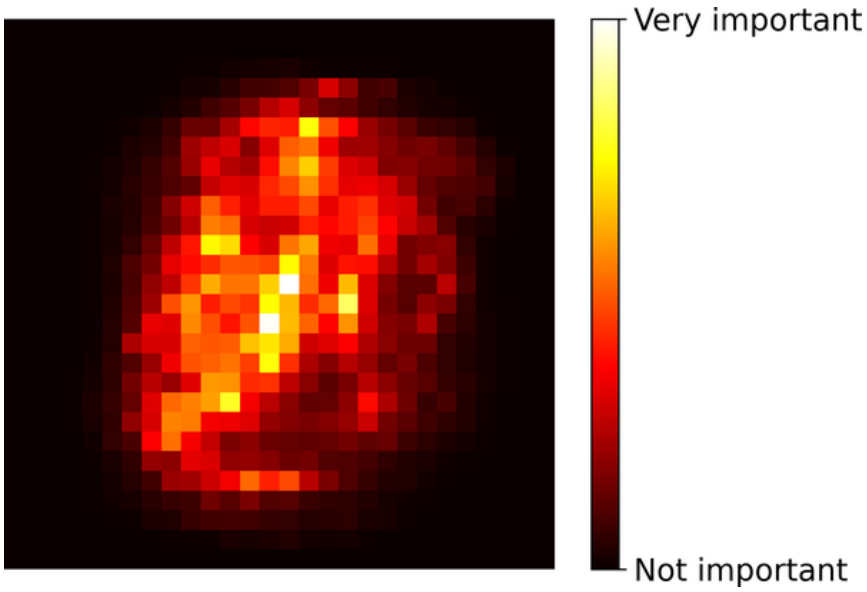

Figure 7-6. MNIST pixel importance (according to a random forest classifier)

Random forests are very handy to get a quick understanding of what features actually matter, in particular if you need to perform feature selection.

Boosting

Boosting (originally called *hypothesis boosting*) refers to any ensemble method that can combine several weak learners into a strong learner. The general idea of most boosting methods is to train predictors sequentially, each trying to correct its predecessor. There are many boosting methods available, but by far the most popular are *AdaBoost*[13] (short for *adaptive boosting*) and *gradient boosting*. Let's start with AdaBoost.

AdaBoost

One way for a new predictor to correct its predecessor is to pay a bit more attention to the training instances that the predecessor underfit. This results in new predictors focusing more and more on the hard cases. This is the technique used by AdaBoost.

For example, when training an AdaBoost classifier, the algorithm first trains a base classifier (such as a decision tree) and uses it to make predictions on the training set. The algorithm then increases the relative weight of misclassified training instances. Then it trains a second classifier, using the updated weights, and again makes predictions on the training set, updates the instance weights, and so on (see Figure 7-7).

Figure 7-8 shows the decision boundaries of five consecutive predictors on the moons dataset (in this example, each predictor is a highly regularized SVM classifier with an RBF kernel).[14] The first classifier gets many instances wrong, so their weights get boosted. The second classifier therefore does a better job on these instances, and so on. The plot on the right represents the same sequence of predictors, except that the learning rate is halved (i.e., the misclassified instance weights are boosted much less at every iteration). As you can see, this sequential learning technique has some similarities with gradient descent, except that instead of tweaking a single predictor's parameters to minimize a cost function, AdaBoost adds predictors to the ensemble, gradually making it better.

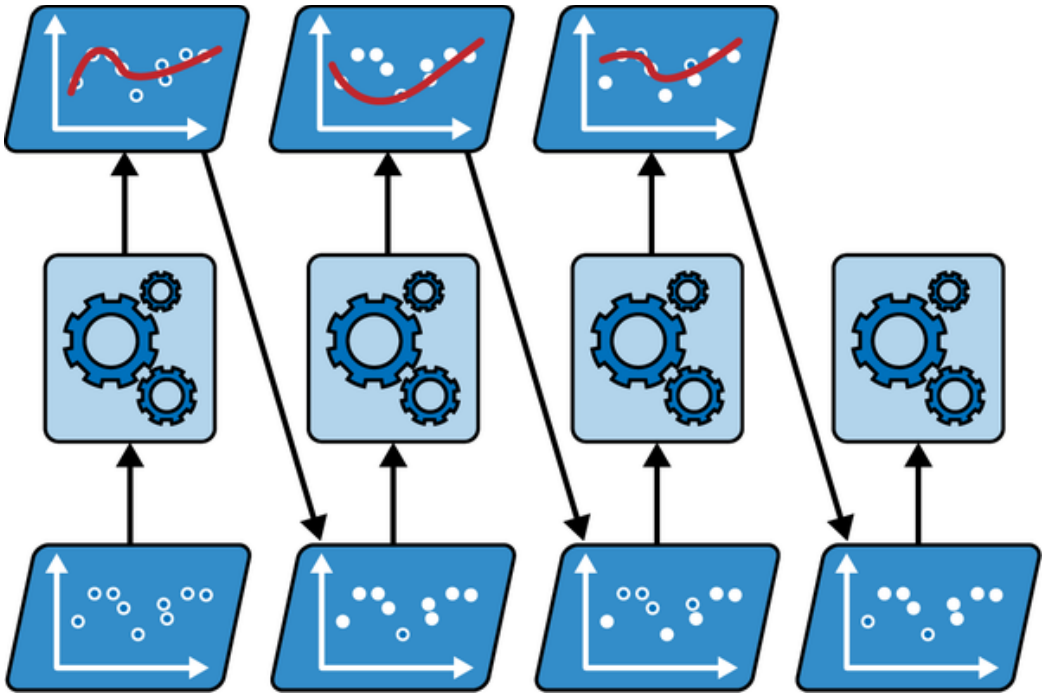

Figure 7-7. AdaBoost sequential training with instance weight updates

Once all predictors are trained, the ensemble makes predictions very much like bagging or pasting, except that predictors have different weights depending on their overall accuracy on the weighted training set.

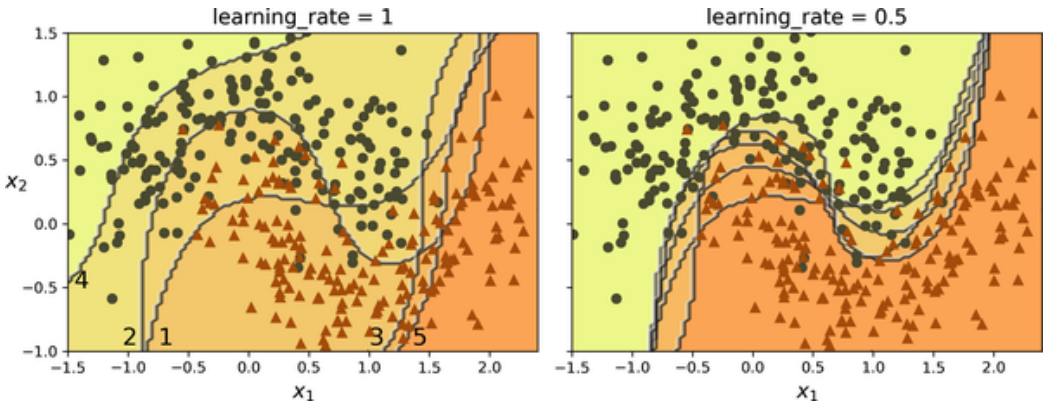

Figure 7-8. Decision boundaries of consecutive predictors

WARNING

There is one important drawback to this sequential learning technique: training cannot be parallelized since each predictor can only be trained after the previous predictor has been trained and evaluated. As a result, it does not scale as well as bagging or pasting.

Let's take a closer look at the AdaBoost algorithm. Each instance weight $w^{(i)}$ is initially set to $1/m$. A first predictor is trained, and its weighted error rate r_1 is computed on the training set; see Equation 7-1.

Equation 7-1. Weighted error rate of the j^{th} predictor

$$r_j = \sum_{\substack{i=1 \\ \hat{y}_j^{(i)} \neq y^{(i)}}}^{m} w^{(i)} \quad \text{where } \hat{y}_j^{(i)} \text{ is the } j^{\text{th}} \text{ predictor's prediction for the } i^{\text{th}} \text{ instance}$$

The predictor's weight α_j is then computed using Equation 7-2, where η is the learning rate hyperparameter (defaults to 1).[15] The more accurate the predictor is, the higher its weight will be. If it is just guessing randomly, then its weight will be close to zero. However, if it is most often wrong (i.e., less accurate than random guessing), then its weight will be negative.

Equation 7-2. Predictor weight

$$\alpha_j = \eta \log \frac{1 - r_j}{r_j}$$

Next, the AdaBoost algorithm updates the instance weights, using Equation 7-3, which boosts the weights of the misclassified instances.

Equation 7-3. Weight update rule

$$\begin{aligned} &\text{for } i = 1, 2, \cdots, m \\ &w^{(i)} \leftarrow \begin{cases} w^{(i)} & \text{if } \widehat{y_j}^{(i)} = y^{(i)} \\ w^{(i)} \exp\left(\alpha_j\right) & \text{if } \widehat{y_j}^{(i)} \neq y^{(i)} \end{cases} \end{aligned}$$

Then all the instance weights are normalized (i.e., divided by $\sum_{i=1}^{m} w^{(i)}$).

Finally, a new predictor is trained using the updated weights, and the whole process is repeated: the new predictor's weight is computed, the instance weights are updated, then another predictor is trained, and so on. The algorithm stops when the desired number of predictors is reached, or when a perfect predictor is found.

To make predictions, AdaBoost simply computes the predictions of all the predictors and weighs them using the predictor weights α_j. The predicted class is the one that receives the majority of weighted votes (see Equation 7-4).

Equation 7-4. AdaBoost predictions

$$\hat{y}(\mathbf{x}) = \underset{k}{\operatorname{argmax}} \sum_{\substack{j=1 \\ \hat{y}_j(\mathbf{x})=k}}^{N} \alpha_j \quad \text{where } N \text{ is the number of predictors}$$

Scikit-Learn uses a multiclass version of AdaBoost called *SAMME*[16] (which stands for *Stagewise Additive Modeling using a Multiclass Exponential loss function*). When there are just two classes, SAMME is equivalent to AdaBoost. If the predictors can estimate class probabilities (i.e., if they have a `predict_proba()` method), Scikit-Learn can use a variant of SAMME called *SAMME.R* (the *R* stands for "Real"), which relies on class probabilities rather than predictions and generally performs better.

The following code trains an AdaBoost classifier based on 30 *decision stumps* using Scikit-Learn's `AdaBoostClassifier` class (as you might expect, there is also an `AdaBoostRegressor` class). A decision stump is a decision tree with `max_depth=1`—in other words, a tree composed of a single decision node plus two leaf nodes. This is the default base estimator for the `AdaBoostClassifier` class:

```
from sklearn.ensemble import AdaBoostClassifier

ada_clf = AdaBoostClassifier(
    DecisionTreeClassifier(max_depth=1), n_estimators=30,
    learning_rate=0.5, random_state=42)
ada_clf.fit(X_train, y_train)
```

> **TIP**
>
> If your AdaBoost ensemble is overfitting the training set, you can try reducing the number of estimators or more strongly regularizing the base estimator.

Gradient Boosting

Another very popular boosting algorithm is *gradient boosting*.[17] Just like AdaBoost, gradient boosting works by sequentially adding predictors to an ensemble, each one correcting its predecessor. However, instead of tweaking the instance weights at every iteration like AdaBoost does, this method tries to fit the new predictor to the *residual errors* made by the previous predictor.

Let's go through a simple regression example, using decision trees as the base predictors; this is called *gradient tree boosting*, or *gradient boosted regression trees* (GBRT). First, let's generate a noisy quadratic dataset and fit a `DecisionTreeRegressor` to it:

```
import numpy as np
from sklearn.tree import DecisionTreeRegressor

np.random.seed(42)
X = np.random.rand(100, 1) - 0.5
y = 3 * X[:, 0] ** 2 + 0.05 * np.random.randn(100)  # y = 3x² + Gaussian noise

tree_reg1 = DecisionTreeRegressor(max_depth=2, random_state=42)
tree_reg1.fit(X, y)
```

Next, we'll train a second `DecisionTreeRegressor` on the residual errors made by the first predictor:

```
y2 = y - tree_reg1.predict(X)
tree_reg2 = DecisionTreeRegressor(max_depth=2, random_state=43)
tree_reg2.fit(X, y2)
```

And then we'll train a third regressor on the residual errors made by the second predictor:

```
y3 = y2 - tree_reg2.predict(X)
tree_reg3 = DecisionTreeRegressor(max_depth=2, random_state=44)
tree_reg3.fit(X, y3)
```

Now we have an ensemble containing three trees. It can make predictions on a new instance simply by adding up the predictions of all the trees:

```
>>> X_new = np.array([[-0.4], [0.], [0.5]])
>>> sum(tree.predict(X_new) for tree in (tree_reg1, tree_reg2, tree_reg3))
array([0.49484029, 0.04021166, 0.75026781])
```

Figure 7-9 represents the predictions of these three trees in the left column, and the ensemble's predictions in the right column. In the first row, the ensemble has just one tree, so its predictions are exactly the same as the first tree's predictions. In the second row, a new tree is trained on the residual errors of the first tree. On the right you can see that the ensemble's predictions are equal to the sum of the predictions of the first two trees. Similarly, in the third row another tree is trained on the residual errors of the second tree. You can see that the ensemble's predictions gradually get better as trees are added to the ensemble.

You can use Scikit-Learn's `GradientBoostingRegressor` class to train GBRT ensembles more easily (there's also a `GradientBoostingClassifier` class for classification). Much like the `RandomForestRegressor` class, it has hyperparameters to control the growth of decision trees (e.g., `max_depth`, `min_samples_leaf`), as well as

hyperparameters to control the ensemble training, such as the number of trees (`n_estimators`). The following code creates the same ensemble as the previous one:

```
from sklearn.ensemble import GradientBoostingRegressor

gbrt = GradientBoostingRegressor(max_depth=2, n_estimators=3,
                                 learning_rate=1.0, random_state=42)
gbrt.fit(X, y)
```

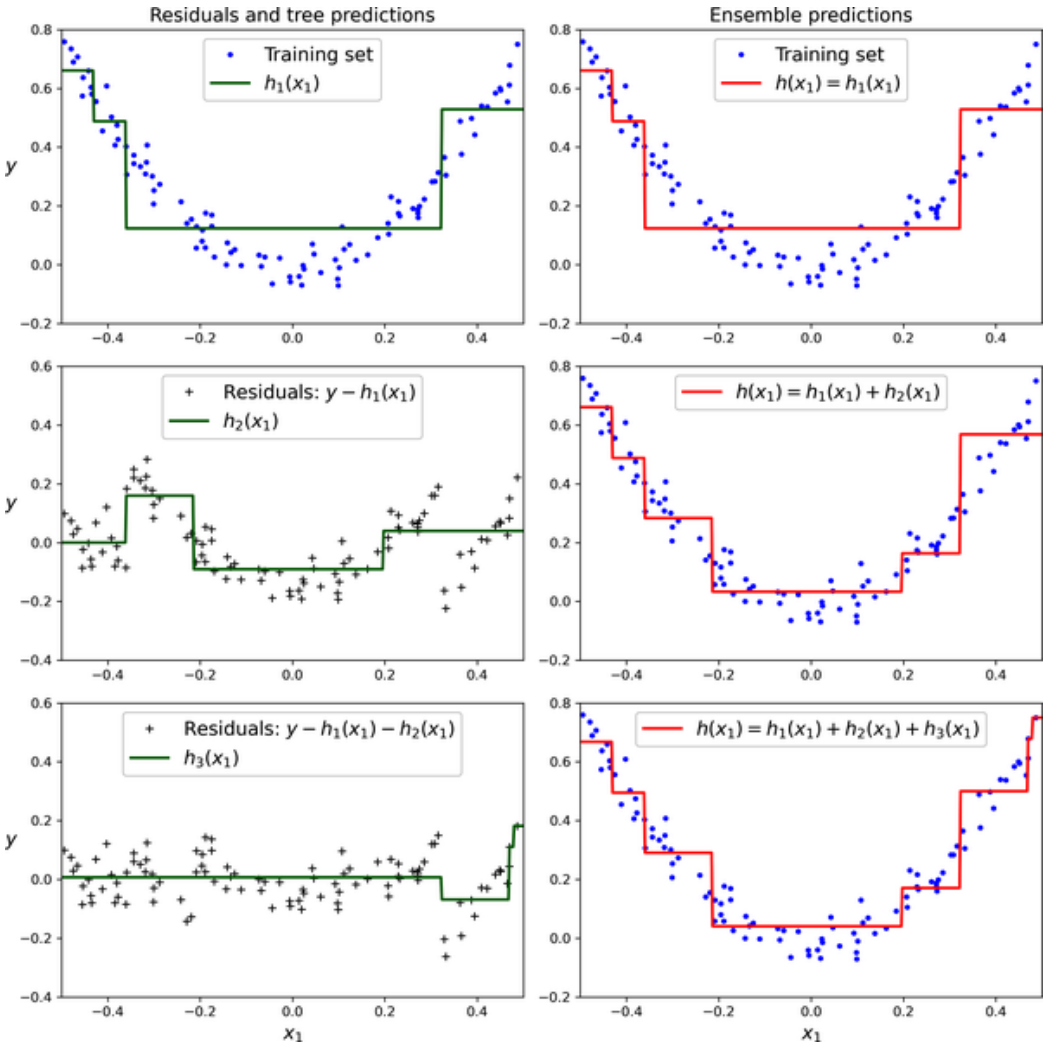

Figure 7-9. In this depiction of gradient boosting, the first predictor (top left) is trained normally, then each consecutive predictor (middle left and lower left) is trained on the previous predictor's residuals; the right column shows the resulting ensemble's predictions

The `learning_rate` hyperparameter scales the contribution of each tree. If you set it to a low value, such as `0.05`, you will need more trees in the ensemble to fit the training set, but the predictions will usually generalize better. This is a regularization technique called *shrinkage*. Figure 7-10 shows two GBRT ensembles trained with different hyperparameters: the one on the left does not have enough trees to fit the training set,

while the one on the right has about the right amount. If we added more trees, the GBRT would start to overfit the training set.

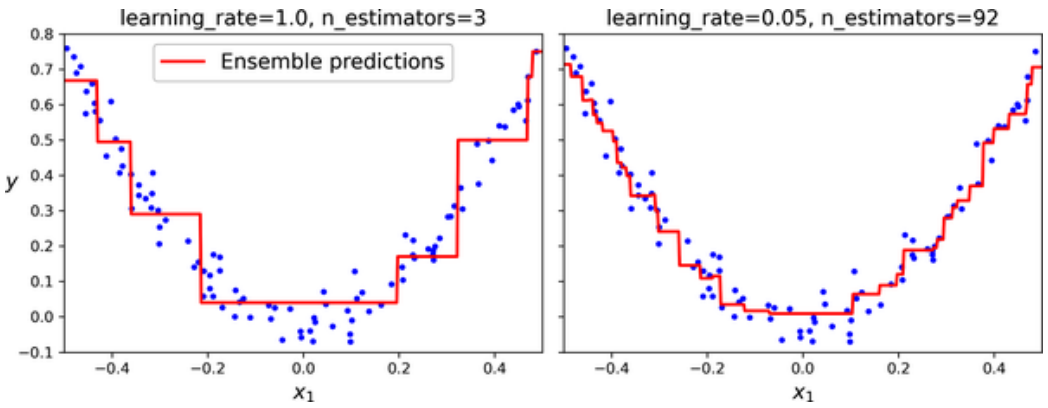

Figure 7-10. GBRT ensembles with not enough predictors (left) and just enough (right)

To find the optimal number of trees, you could perform cross-validation using `GridSearchCV` or `RandomizedSearchCV`, as usual, but there's a simpler way: if you set the `n_iter_no_change` hyperparameter to an integer value, say 10, then the `GradientBoostingRegressor` will automatically stop adding more trees during training if it sees that the last 10 trees didn't help. This is simply early stopping (introduced in Chapter 4), but with a little bit of patience: it tolerates having no progress for a few iterations before it stops. Let's train the ensemble using early stopping:

```
gbrt_best = GradientBoostingRegressor(
    max_depth=2, learning_rate=0.05, n_estimators=500,
    n_iter_no_change=10, random_state=42)
gbrt_best.fit(X, y)
```

If you set `n_iter_no_change` too low, training may stop too early and the model will underfit. But if you set it too high, it will overfit instead. We also set a fairly small learning rate and a high number of estimators, but the actual number of estimators in the trained ensemble is much lower, thanks to early stopping:

```
>>> gbrt_best.n_estimators_
92
```

When `n_iter_no_change` is set, the `fit()` method automatically splits the training set into a smaller training set and a validation set: this allows it to evaluate the model's performance each time it adds a new tree. The size of the validation set is controlled by the `validation_fraction` hyperparameter, which is 10% by default. The `tol` hyperparameter determines the maximum performance improvement that still counts as negligible. It defaults to 0.0001.

The `GradientBoostingRegressor` class also supports a `subsample` hyperparameter, which specifies the fraction of training instances to be used for training each tree. For example, if `subsample=0.25`, then each tree is trained on 25% of the training instances, selected randomly. As you can probably guess by now, this technique trades a higher bias for a lower variance. It also speeds up training considerably. This is called *stochastic gradient boosting*.

Histogram-Based Gradient Boosting

Scikit-Learn also provides another GBRT implementation, optimized for large datasets: *histogram-based gradient boosting* (HGB). It works by binning the input features, replacing them with integers. The number of bins is controlled by the `max_bins` hyperparameter, which defaults to 255 and cannot be set any higher than this. Binning can greatly reduce the number of possible thresholds that the training algorithm needs to evaluate. Moreover, working with integers makes it possible to use faster and more memory-efficient data structures. And the way the bins are built removes the need for sorting the features when training each tree.

As a result, this implementation has a computational complexity of $O(b \times m)$ instead of $O(n \times m \times \log(m))$, where b is the number of bins, m is the number of training instances, and n is the number of features. In practice, this means that HGB can train hundreds of times faster than regular GBRT on large datasets. However, binning causes a precision loss, which acts as a regularizer: depending on the dataset, this may help reduce overfitting, or it may cause underfitting.

Scikit-Learn provides two classes for HGB: `HistGradientBoostingRegressor` and `HistGradientBoostingClassifier`. They're similar to `GradientBoostingRegressor` and `GradientBoostingClassifier`, with a few notable differences:

- Early stopping is automatically activated if the number of instances is greater than 10,000. You can turn early stopping always on or always off by setting the `early_stopping` hyperparameter to `True` or `False`.
- Subsampling is not supported.
- `n_estimators` is renamed to `max_iter`.
- The only decision tree hyperparameters that can be tweaked are `max_leaf_nodes`, `min_samples_leaf`, and `max_depth`.

The HGB classes also have two nice features: they support both categorical features and missing values. This simplifies preprocessing quite a bit. However, the categorical

features must be represented as integers ranging from 0 to a number lower than `max_bins`. You can use an `OrdinalEncoder` for this. For example, here's how to build and train a complete pipeline for the California housing dataset introduced in Chapter 2:

```
from sklearn.pipeline import make_pipeline
from sklearn.compose import make_column_transformer
from sklearn.ensemble import HistGradientBoostingRegressor
from sklearn.preprocessing import OrdinalEncoder

hgb_reg = make_pipeline(
    make_column_transformer((OrdinalEncoder(), ["ocean_proximity"]),
                            remainder="passthrough"),
    HistGradientBoostingRegressor(categorical_features=[0], random_state=42)
)
hgb_reg.fit(housing, housing_labels)
```

The whole pipeline is just as short as the imports! No need for an imputer, scaler, or a one-hot encoder, so it's really convenient. Note that `categorical_features` must be set to the categorical column indices (or a Boolean array). Without any hyperparameter tuning, this model yields an RMSE of about 47,600, which is not too bad.

> **TIP**
>
> Several other optimized implementations of gradient boosting are available in the Python ML ecosystem: in particular, XGBoost, CatBoost, and LightGBM. These libraries have been around for several years. They are all specialized for gradient boosting, their APIs are very similar to Scikit-Learn's, and they provide many additional features, including GPU acceleration; you should definitely check them out! Moreover, the TensorFlow Random Forests library provides optimized implementations of a variety of random forest algorithms, including plain random forests, extra-trees, GBRT, and several more.

Stacking

The last ensemble method we will discuss in this chapter is called *stacking* (short for *stacked generalization*).[18] It is based on a simple idea: instead of using trivial functions (such as hard voting) to aggregate the predictions of all predictors in an ensemble, why don't we train a model to perform this aggregation? Figure 7-11 shows such an ensemble performing a regression task on a new instance. Each of the bottom three predictors predicts a different value (3.1, 2.7, and 2.9), and then the final predictor (called a *blender*, or a *meta learner*) takes these predictions as inputs and makes the final prediction (3.0).

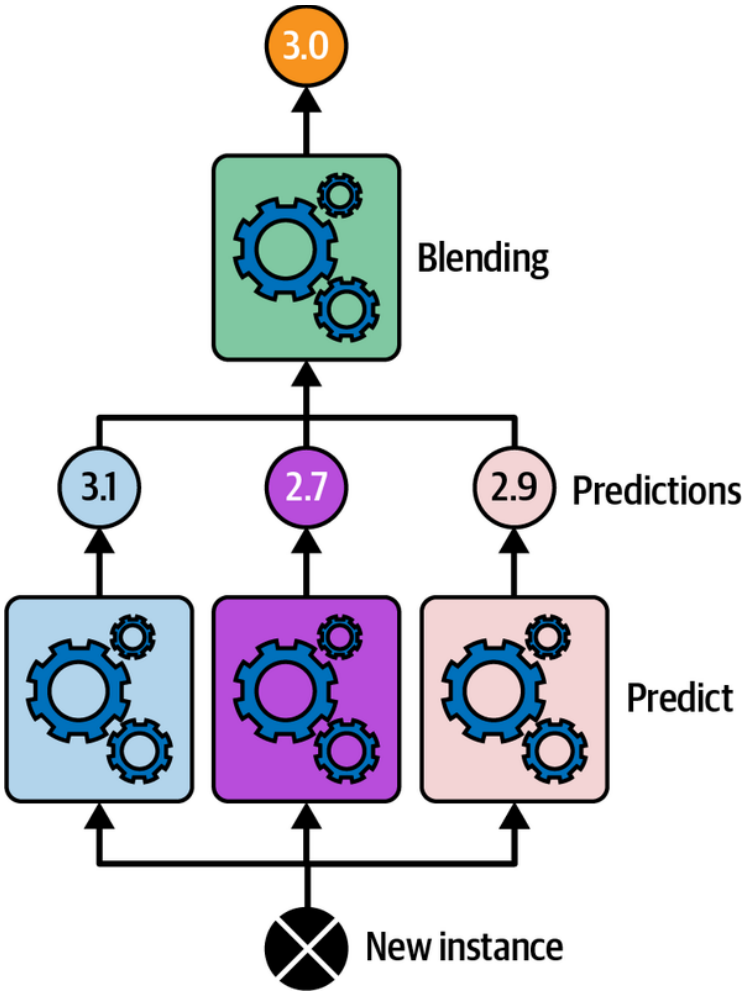

Figure 7-11. Aggregating predictions using a blending predictor

To train the blender, you first need to build the blending training set. You can use `cross_val_predict()` on every predictor in the ensemble to get out-of-sample predictions for each instance in the original training set (Figure 7-12), and use these can be used as the input features to train the blender; and the targets can simply be copied from the original training set. Note that regardless of the number of features in the original training set (just one in this example), the blending training set will contain one input feature per predictor (three in this example). Once the blender is trained, the base predictors are retrained one last time on the full original training set.

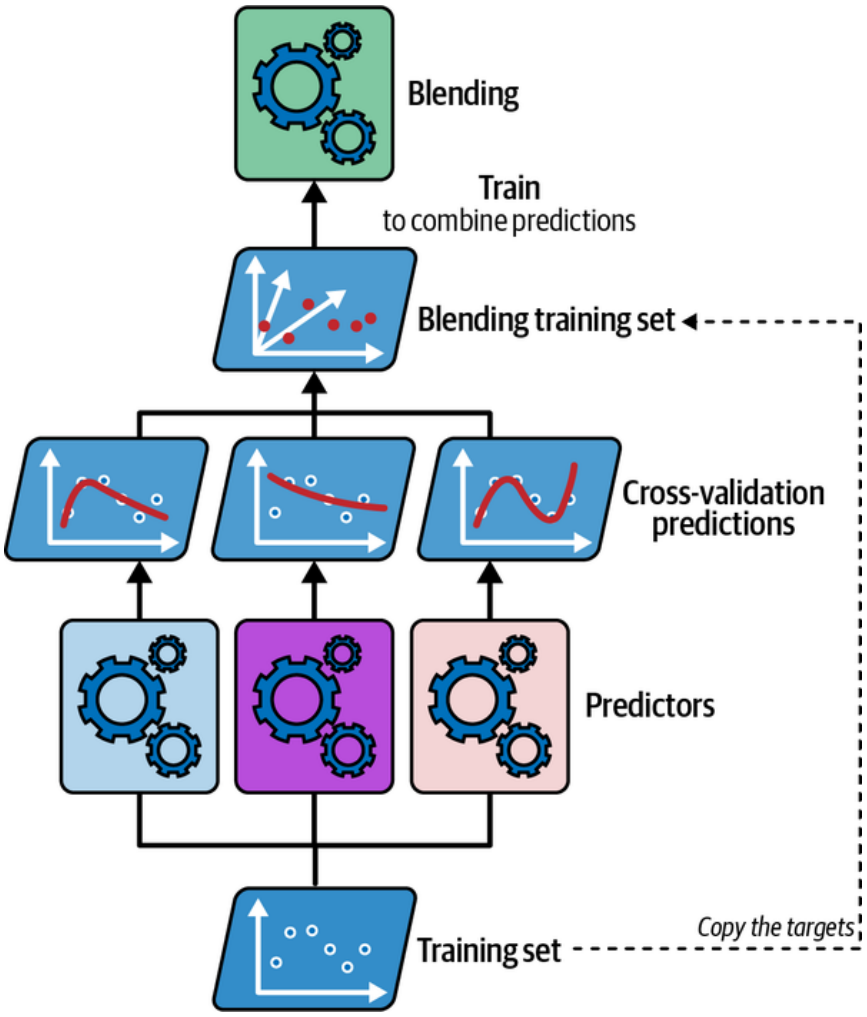

Figure 7-12. Training the blender in a stacking ensemble

It is actually possible to train several different blenders this way (e.g., one using linear regression, another using random forest regression) to get a whole layer of blenders, and then add another blender on top of that to produce the final prediction, as shown in Figure 7-13. You may be able to squeeze out a few more drops of performance by doing this, but it will cost you in both training time and system complexity.

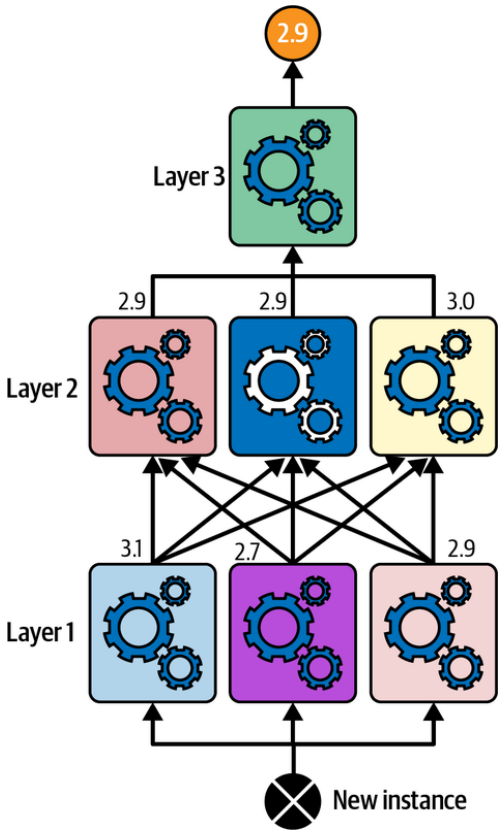

Figure 7-13. Predictions in a multilayer stacking ensemble

Scikit-Learn provides two classes for stacking ensembles: `StackingClassifier` and `StackingRegressor`. For example, we can replace the `VotingClassifier` we used at the beginning of this chapter on the moons dataset with a `StackingClassifier`:

```
from sklearn.ensemble import StackingClassifier

stacking_clf = StackingClassifier(
    estimators=[
        ('lr', LogisticRegression(random_state=42)),
        ('rf', RandomForestClassifier(random_state=42)),
        ('svc', SVC(probability=True, random_state=42))
    ],
    final_estimator=RandomForestClassifier(random_state=43),
    cv=5  # number of cross-validation folds
)
stacking_clf.fit(X_train, y_train)
```

For each predictor, the stacking classifier will call `predict_proba()` if available; if not it will fall back to `decision_function()` or, as a last resort, call `predict()`. If you don't provide a final estimator, `StackingClassifier` will use `LogisticRegression` and `StackingRegressor` will use `RidgeCV`.

If you evaluate this stacking model on the test set, you will find 92.8% accuracy, which is a bit better than the voting classifier using soft voting, which got 92%.

In conclusion, ensemble methods are versatile, powerful, and fairly simple to use. Random forests, AdaBoost, and GBRT are among the first models you should test for most machine learning tasks, and they particularly shine with heterogeneous tabular data. Moreover, as they require very little preprocessing, they're great for getting a prototype up and running quickly. Lastly, ensemble methods like voting classifiers and stacking classifiers can help push your system's performance to its limits.

Exercises

1. If you have trained five different models on the exact same training data, and they all achieve 95% precision, is there any chance that you can combine these models to get better results? If so, how? If not, why?
2. What is the difference between hard and soft voting classifiers?
3. Is it possible to speed up training of a bagging ensemble by distributing it across multiple servers? What about pasting ensembles, boosting ensembles, random forests, or stacking ensembles?
4. What is the benefit of out-of-bag evaluation?
5. What makes extra-trees ensembles more random than regular random forests? How can this extra randomness help? Are extra-trees classifiers slower or faster than regular random forests?
6. If your AdaBoost ensemble underfits the training data, which hyperparameters should you tweak, and how?
7. If your gradient boosting ensemble overfits the training set, should you increase or decrease the learning rate?
8. Load the MNIST dataset (introduced in Chapter 3), and split it into a training set, a validation set, and a test set (e.g., use 50,000 instances for training, 10,000 for validation, and 10,000 for testing). Then train various classifiers, such as a random forest classifier, an extra-trees classifier, and an SVM classifier. Next, try to combine them into an ensemble that outperforms each individual classifier on the validation set, using soft or hard voting. Once you have found one, try it on the test set. How much better does it perform compared to the individual classifiers?

9. Run the individual classifiers from the previous exercise to make predictions on the validation set, and create a new training set with the resulting predictions: each training instance is a vector containing the set of predictions from all your classifiers for an image, and the target is the image's class. Train a classifier on this new training set. Congratulations—you have just trained a blender, and together with the classifiers it forms a stacking ensemble! Now evaluate the ensemble on the test set. For each image in the test set, make predictions with all your classifiers, then feed the predictions to the blender to get the ensemble's predictions. How does it compare to the voting classifier you trained earlier? Now try again using a `StackingClassifier` instead. Do you get better performance? If so, why?

Solutions to these exercises are available at the end of this chapter's notebook, at *https://homl.info/colab3*.

---

1 Imagine picking a card randomly from a deck of cards, writing it down, then placing it back in the deck before picking the next card: the same card could be sampled multiple times.

2 Leo Breiman, "Bagging Predictors", *Machine Learning* 24, no. 2 (1996): 123–140.

3 In statistics, resampling with replacement is called *bootstrapping*.

4 Leo Breiman, "Pasting Small Votes for Classification in Large Databases and On-Line", *Machine Learning* 36, no. 1–2 (1999): 85–103.

5 Bias and variance were introduced in Chapter 4.

6 `max_samples` can alternatively be set to a float between 0.0 and 1.0, in which case the max number of sampled instances is equal to the size of the training set times `max_samples`.

7 As m grows, this ratio approaches $1 – \exp(–1) \approx 63\%$.

8 Gilles Louppe and Pierre Geurts, "Ensembles on Random Patches", *Lecture Notes in Computer Science* 7523 (2012): 346–361.

9 Tin Kam Ho, "The Random Subspace Method for Constructing Decision Forests", *IEEE Transactions on Pattern Analysis and Machine Intelligence* 20, no. 8 (1998): 832–844.

10 Tin Kam Ho, "Random Decision Forests", *Proceedings of the Third International Conference on Document Analysis and Recognition* 1 (1995): 278.

11 The `BaggingClassifier` class remains useful if you want a bag of something other than decision trees.

12 Pierre Geurts et al., "Extremely Randomized Trees", *Machine Learning* 63, no. 1 (2006): 3–42.

13 Yoav Freund and Robert E. Schapire, "A Decision-Theoretic Generalization of On-Line Learning and an Application to Boosting", *Journal of Computer and System Sciences* 55, no. 1 (1997): 119–139.

14 This is just for illustrative purposes. SVMs are generally not good base predictors for AdaBoost; they are slow and tend to be unstable with it.

15 The original AdaBoost algorithm does not use a learning rate hyperparameter.

16 For more details, see Ji Zhu et al., "Multi-Class AdaBoost", *Statistics and Its Interface* 2, no. 3 (2009): 349–360.

17 Gradient boosting was first introduced in Leo Breiman's 1997 paper "Arcing the Edge" and was further developed in the 1999 paper "Greedy Function Approximation: A Gradient Boosting Machine" by Jerome H. Friedman.

18 David H. Wolpert, "Stacked Generalization", *Neural Networks* 5, no. 2 (1992): 241–259.