Download from finelybook www.finelybook.com 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 why 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 with the BaggingClas sifier class (or BaggingRegressor for regression). The following code trains an ensemble of 500 Decision Tree classifiers,⁵ each 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 (-1 tells Scikit-Learn to use all available cores):



The 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 Trees 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).

⁵ max_samples can alternatively be set to a float between 0.0 and 1.0, in which case the max number of instances to sample is equal to the size of the training set times max_samples.

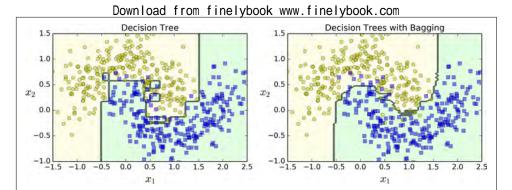


Figure 7-5. A single Decision Tree versus a bagging ensemble of 500 trees

Bootstrapping 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 this also means that predictors end up being less correlated so the ensemble's variance is reduced. Overall, bagging often results in better models, which explains why it is generally preferred. However, 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.

Out-of-Bag Evaluation

With bagging, some 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. This means that only about 63% of the training instances are sampled on average for each predictor.⁶ 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.

Since a predictor never sees the oob instances during training, it can be evaluated on these instances, without the need for a separate validation set or cross-validation. You can evaluate the ensemble itself by averaging out the oob evaluations of each predictor.

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 through the oob_score_ variable:

```
>>> bag_clf = BaggingClassifier(
>>> DecisionTreeClassifier(), n_estimators=500,
>>> bootstrap=True, n_jobs=-1, oob_score=True)
```

⁶ As m grows, this ratio approaches $1 - \exp(-1) \approx 63.212\%$.