6 Decision trees and ensemble learning

This chapter covers

- Decision trees and the decision tree learning algorithm
- Random forests: putting multiple trees together into one model
- Gradient boosting as an alternative way of combining decision trees

In chapter 3, we described the binary classification problem and used the logistic regression model to predict if a customer is going to churn.

In this chapter, we also solve a binary classification problem, but we use a different family of machine learning models: tree-based models. Decision trees, the simplest tree-based model, are nothing but a sequence of if-then-else rules put together. We can combine multiple decision trees into an ensemble to achieve better performance. We cover two tree-based ensemble models: random forest and gradient boosting.

The project we prepared for this chapter is default prediction: we predict whether or not a customer will fail to pay back a loan. We learn how to train decision trees and random forest models with Scikit-learn and explore XGBoost—a library for implementing gradient boosting models.

6.1 Credit risk scoring project

Imagine that we work at a bank. When we receive a loan application, we need to make sure that if we give the money, the customer will be able to

pay it back. Every application carries a risk of *default*—the failure to return the money.

We'd like to minimize this risk: before agreeing to give a loan, we want to score the customer and assess the chances of default. If it's too high, we reject the application. This process is called "credit risk scoring."

Machine learning can be used for calculating the risk. For that, we need a dataset with loans, where for each application, we know whether or not it was paid back successfully. Using this data, we can build a model for predicting the probability of default, and we can use this model to assess the risk of future borrowers not repaying the money.

This is what we do in this chapter: use machine learning to calculate the risk of default. The plan for the project is the following:

- First, we get the data and do some initial preprocessing.
- Next, we train a decision tree model from Scikit-learn for predicting the probability of default.
- After that, we explain how decision trees work and which parameters the model has and show how to adjust these parameters to get the best performance.
- Then we combine multiple decision trees into one model—a random forest. We look at its parameters and tune them to achieve the best predictive performance.
- Finally, we explore a different way of combining decision trees—gradient boosting. We use XGBoost, a highly efficient library that implements gradient boosting. We'll train a model and tune its parameters.

Credit risk scoring is a binary classification problem: the target is positive ("1") if the customer defaults and negative ("0") otherwise. For evaluating

our solution, we'll use AUC (area under the ROC curve), which we covered in chapter 4. AUC describes how well our model can separate the cases into positive and negative ones.

The code for this project is available in the book's GitHub repository at **https://github.com/alexeygrigorev/mlbookcamp-code** (in the chapter-06-trees folder).

6.1.1 Credit scoring dataset

For this project, we use a dataset from a data mining course at the Polytechnic University of Catalonia (**https://www.cs.upc.edu/~belanche/Docencia/mineria/mineria.html**). The dataset describes the customers (seniority, age, marital status, income, and other characteristics), the loan (the requested amount, the price of the item), and its status (paid back or not).

We use a copy of this dataset available on GitHub at **https://github.com/gastonstat/ CreditScoring/**. Let's download it.

First, create a folder for our project (e.g., chapter-06-credit-risk), and then use `wget` to get it:

```
wget https://github.com/gastonstat/CreditScoring/raw/master/CreditScoring.csv
```

Alternatively, you can enter the link to your browser and save it to the project folder.

Next, start a Jupyter Notebook server if it's not started yet:

```
jupyter notebook
```

Go to the project folder, and create a new notebook (e.g., chapter-06-credit-risk).

As usual, we begin by importing Pandas, NumPy, Seaborn, and Matplotlib:

```
import pandas as pd
import numpy as np

import seaborn as sns
from matplotlib import pyplot as plt
%matplotlib inline
```

After we press Ctrl-Enter, the libraries are imported and we're ready to read the data with Pandas:

```
df = pd.read_csv('CreditScoring.csv')
```

Now the data is loaded, so let's take an initial look at it and see if we need to do any preprocessing before we can use it.

6.1.2 Data cleaning

To use a dataset for our task, we need to look for any issues in the data and fix them.

Let's start by looking at the first rows of the DataFrame, generated by the `df.head()` function (figure 6.1).

```
df.head()
```

	Status	Seniority	Home	Time	Age	Marital	Records	Job	Expenses	Income	Assets	Debt	Amount	Price
0	1	9	1	60	30	2	1	3	73	129	0	0	800	846
1	1	17	1	60	58	3	1	1	48	131	0	0	1000	1658
2	2	10	2	36	46	2	2	3	90	200	3000	0	2000	2985
3	1	0	1	60	24	1	1	1	63	182	2500	0	900	1325
4	1	0	1	36	26	1	1	1	46	107	0	0	310	910

Figure 6.1 The first five rows of the credit scoring dataset

First, we can see that all the column names start with a capital letter. Before doing anything else, let's lowercase all the column names and make it consistent with other projects (figure 6.2):

```
df.columns = df.columns.str.lower()
```

```
df.columns = df.columns.str.lower()
df.head()
```

	status	seniority	home	time	age	marital	records	job	expenses	income	assets	debt	amount	price
0	1	9	1	60	30	2	1	3	73	129	0	0	800	846
1	1	17	1	60	58	3	1	1	48	131	0	0	1000	1658
2	2	10	2	36	46	2	2	3	90	200	3000	0	2000	2985
3	1	0	1	60	24	1	1	1	63	182	2500	0	900	1325
4	1	0	1	36	26	1	1	1	46	107	0	0	310	910

Figure 6.2 The DataFrame with lowercase column names

We can see that the DataFrame has the following columns:

- status: whether the customer managed to pay back the loan (1) or not (2)
- seniority: job experience in years

- home: type of homeownership: renting (1), a homeowner (2), and others
- time: period planned for the loan (in months)
- age: age of the client
- marital [status]: single (1), married (2), and others
- records: whether the client has any previous records: no (1), yes (2) (It's not clear from the dataset description what kind of records we have in this column. For the purposes of this project, we may assume that it's about records in the bank's database.)
- job: type of job: full-time (1), part-time (2), and others
- expenses: how much the client spends per month
- income: how much the client earns per month
- assets: total worth of all the assets of the client
- debt: amount of credit debt
- amount: requested amount of the loan
- price: price of an item the client wants to buy

Although most of the columns are numerical, some are categorical: status, home, marital [status], records, and job. The values we see in the DataFrame, however, are numbers, not strings. This means that we need to translate them to their actual names. In the GitHub repository with the dataset is a script that decodes the numbers to categories (**https://github.-com/gastonstat/CreditScoring/blob/master/Part1_CredScoring_Processing.R**). Originally, this script was written in R, so we need to translate it to Pandas.

We start with the status column. The value "1" means "OK," the value "2" means "default," and "0" means that the value is missing—let's replace it with "unk" (short for "unknown").

In Pandas, we can use `map` for converting the numbers to strings. For that, we first define the dictionary with mapping from the current value (number) to the desired value (string):

```
status_values = {
    1: 'ok',
    2: 'default',
    0: 'unk'
}
```

Now we can use this dictionary to do the mapping:

```
df.status = df.status.map(status_values)
```

It creates a new series, which we immediately write back to the DataFrame. As a result, the values in the status column are overwritten and look more meaningful (figure 6.3).

```
status_values = {
    1: 'ok',
    2: 'default',
    0: 'unk'
}

df.status = df.status.map(status_values)
df.head()
```

	status	seniority	home	time	age	marital	records	job	expenses	income	assets	debt	amount	price
0	ok	9	1	60	30	2	1	3	73	129	0	0	800	846
1	ok	17	1	60	58	3	1	1	48	131	0	0	1000	1658
2	default	10	2	36	46	2	2	3	90	200	3000	0	2000	2985
3	ok	0	1	60	24	1	1	1	63	182	2500	0	900	1325
4	ok	0	1	36	26	1	1	1	46	107	0	0	310	910

Figure 6.3 To translate the original values in the status column (numbers) to a more meaningful representation (strings), we use the `map` method.

We repeat the same procedure for all the other columns. First, we'll do it for the home column:

```
home_values = {
    1: 'rent',
    2: 'owner',
    3: 'private',
    4: 'ignore',
    5: 'parents',
    6: 'other',
    0: 'unk'
}

df.home = df.home.map(home_values)
```

Next, let's do it for the marital, records, and job columns:

```
marital_values = {
    1: 'single',
    2: 'married',
    3: 'widow',
    4: 'separated',
    5: 'divorced',
    0: 'unk'
}

df.marital = df.marital.map(marital_values)


records_values = {
    1: 'no',
    2: 'yes',
    0: 'unk'
```

```
}

df.records = df.records.map(records_values)


job_values = {
    1: 'fixed',
    2: 'parttime',
    3: 'freelance',
    4: 'others',
    0: 'unk'
}

df.job = df.job.map(job_values)
```

After these transformations, the columns with categorical variables contain the actual values, not numbers (figure 6.4).

```
df.head()
```

	status	seniority	home	time	age	marital	records	job	expenses	income	assets	debt	amount	price
0	ok	9	rent	60	30	married	no	freelance	73	129	0	0	800	846
1	ok	17	rent	60	58	widow	no	fixed	48	131	0	0	1000	1658
2	default	10	owner	36	46	married	yes	freelance	90	200	3000	0	2000	2985
3	ok	0	rent	60	24	single	no	fixed	63	182	2500	0	900	1325
4	ok	0	rent	36	26	single	no	fixed	46	107	0	0	310	910

Figure 6.4 The values of categorical variables are translated from integers to strings.

As the next step, let's take a look at numerical columns. First, let's check the summary statistics for each of the columns: min, mean, max, and others. To do so, we can use the `describe` method of the DataFrame:

```
df.describe().round()
```

NOTE The output of `describe` may be confusing. In our case, there are values in scientific notation like 1.000000e+08 or 8.703625e+06. To force Pandas to use a different notation, we use `round`: it removes the fractional part of a number and rounds it to the closest integer.

It gives us an idea of how the distribution of the values in each column looks (figure 6.5).

```
df.describe().round()
```

	seniority	time	age	expenses	income	assets	debt	amount	price
count	4455.0	4455.0	4455.0	4455.0	4455.0	4455.0	4455.0	4455.0	4455.0
mean	8.0	46.0	37.0	56.0	763317.0	1060341.0	404382.0	1039.0	1463.0
std	8.0	15.0	11.0	20.0	8703625.0	10217569.0	6344253.0	475.0	628.0
min	0.0	6.0	18.0	35.0	0.0	0.0	0.0	100.0	105.0
25%	2.0	36.0	28.0	35.0	80.0	0.0	0.0	700.0	1118.0
50%	5.0	48.0	36.0	51.0	120.0	3500.0	0.0	1000.0	1400.0
75%	12.0	60.0	45.0	72.0	166.0	6000.0	0.0	1300.0	1692.0
max	48.0	72.0	68.0	180.0	99999999.0	99999999.0	99999999.0	5000.0	11140.0

Figure 6.5 The summary of all numerical columns of the dataframe. We notice that some of them have 99999999 as the max value.

One thing we notice immediately is that the max value is `99999999` in some cases. This is quite suspicious. As it turns out, it's an artificial value —this is how missing values are encoded in this dataset.

Three columns have this problem: income, assets, and debt. Let's replace this big number with NaN for these columns:

```
for c in ['income', 'assets', 'debt']:
    df[c] = df[c].replace(to_replace=99999999, value=np.nan)
```

We use the `replace` method, which takes two values:

- `to_replace:` the original value ("99999999," in our case)
- `value:` the target value ("NaN," in our case)

After this transformation, no more suspicious numbers appear in the summary (figure 6.6).

```
df.describe().round()
```

	seniority	time	age	expenses	income	assets	debt	amount	price
count	4455.0	4455.0	4455.0	4455.0	4421.0	4408.0	4437.0	4455.0	4455.0
mean	8.0	46.0	37.0	56.0	131.0	5403.0	343.0	1039.0	1463.0
std	8.0	15.0	11.0	20.0	86.0	11573.0	1246.0	475.0	628.0
min	0.0	6.0	18.0	35.0	0.0	0.0	0.0	100.0	105.0
25%	2.0	36.0	28.0	35.0	80.0	0.0	0.0	700.0	1118.0
50%	5.0	48.0	36.0	51.0	120.0	3000.0	0.0	1000.0	1400.0
75%	12.0	60.0	45.0	72.0	165.0	6000.0	0.0	1300.0	1692.0
max	48.0	72.0	68.0	180.0	959.0	300000.0	30000.0	5000.0	11140.0

Figure 6.6 The summary statistics after replacing large values with NaN

Before we finish with the dataset preparation, let's look at our target variable `status`:

```
df.status.value_counts()
```

The output of `value_counts` shows the count of each value:

```
ok          3200
default     1254
unk            1
Name: status, dtype: int64
```

Notice that there's one row with "unknown" status: we don't know whether or not this client managed to pay back the loan. For our project, this row is not useful, so let's remove it from the dataset:

```
df = df[df.status != 'unk']
```

In this case, we don't really "remove" it: we create a new DataFrame where we don't have records with "unknown" status.

By looking at the data, we have identified a few important issues in the data and addressed them.

For this project, we skip a more detailed exploratory data analysis like we did for chapter 2 (the car-price prediction project) and chapter 3 (churn prediction project), but you're free to repeat the steps we covered there for this project as well.

6.1.3 Dataset preparation

Now our dataset is cleaned, and we're almost ready to use it for model training. Before we can do that, we need to do a few more steps:

- Split the dataset into train, validation, and test.
- Handle missing values.
- Use one-hot encoding to encode categorical variables.

- Create the feature matrix X and the target variable y .

Let's start by splitting the data. We will split the data into three parts:

- Training data (60% of the original dataset)
- Validation data (20%)
- Test data (20%)

Like previously, we'll use `train_test_split` from Scikit-learn for that. Because we cannot split it into three datasets at once, we'll need to split two times (figure 6.7). First we'll hold out 20% of data for testing, and then split the remaining 80% into training and validation:

```
from sklearn.model_selection import train_test_split

df_train_full, df_test = train_test_split(df, test_size=0.2, random_state=11)
df_train, df_val = train_test_split(df_train_full, test_size=0.25, random_state=11)
```

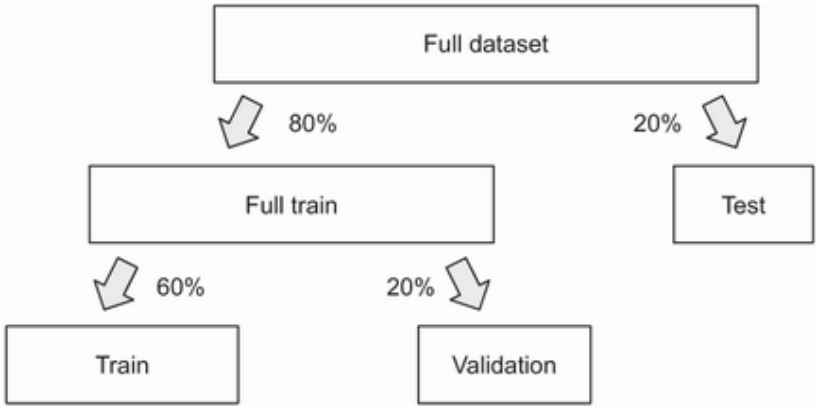


Figure 6.7 Because `train_test_split` can split a dataset into only two parts, but we need three, we perform the split two times.

When splitting for the second time, we put aside 25% of data instead of 20% (`test_ size=0.25`). Because `df_train_full` contains 80% of records, one-quarter (i.e., 25%) of 80% corresponds to 20% of the original dataset.

To check the size of our datasets, we can use the `len` function:

```
len(df_train), len(df_val), len(df_test)
```

When running it, we get the following output:

```
(2672, 891, 891)
```

So, for training, we will use approximately 2,700 examples and almost 900 for validation and testing.

The outcome we want to predict is `status`. We will use it to train a model, so it's our y—the target variable. Because our objective is to determine if somebody fails to pay back their loan, the positive class is `default`. This means that y is "1" if the client defaulted and "0" otherwise. It's quite simple to implement:

```
y_train = (df_train.status == 'default').values
y_val = (df_val.status == 'default').values
```

Now we need to remove `status` from the DataFrames. If we don't do it, we may accidentally use this variable for training. For that, we use the `del` operator:

```
del df_train['status']
del df_val['status']
```

Next, we'll take care of X—the feature matrix.

From the initial analysis, we know our data contains missing values—we added these NaNs ourselves. We can replace the missing values with zero:

```
df_train = df_train.fillna(0)
df_val = df_val.fillna(0)
```

To use categorical variables, we need to encode them. In chapter 3, we applied the one-hot encoding technique for that. In one-hot encoding, each value is encoded as "1" if it's present ("hot") or "0" if it's absent ("cold"). To implement it, we used `DictVectorizer` from Scikit-learn.

`DictVectorizer` needs a list of dictionaries, so we first need to convert the DataFrames into this format:

```
dict_train = df_train.to_dict(orient='records')
dict_val = df_val.to_dict(orient='records')
```

Each dictionary in the result represents a row from the DataFrame. For example, the first record in `dict_train` looks like this:

```
{'seniority': 10,
 'home': 'owner',
 'time': 36,
 'age': 36,
 'marital': 'married',
```

```
 'records': 'no',
 'job': 'freelance',
 'expenses': 75,
 'income': 0.0,
 'assets': 10000.0,
 'debt': 0.0,
 'amount': 1000,
 'price': 1400}
```

This list of dictionaries now can be used as input to `DictVectorizer`:

```
from sklearn.feature_extraction import DictVectorizer

dv = DictVectorizer(sparse=False)

X_train = dv.fit_transform(dict_train)
X_val = dv.transform(dict_val)
```

As a result, we have feature matrices for both train and validation datasets. Please refer to chapter 3 for more details on doing one-hot encoding with Scikit-learn.

Now we're ready to train a model! In the next section, we cover the simplest tree model: decision tree.

6.2 Decision trees

A *decision tree* is a data structure that encodes a series of if-then-else rules. Each node in a tree contains a condition. If the condition is satisfied, we go to the right side of the tree; otherwise, we go to the left. In the end we arrive at the final decision (figure 6.8).

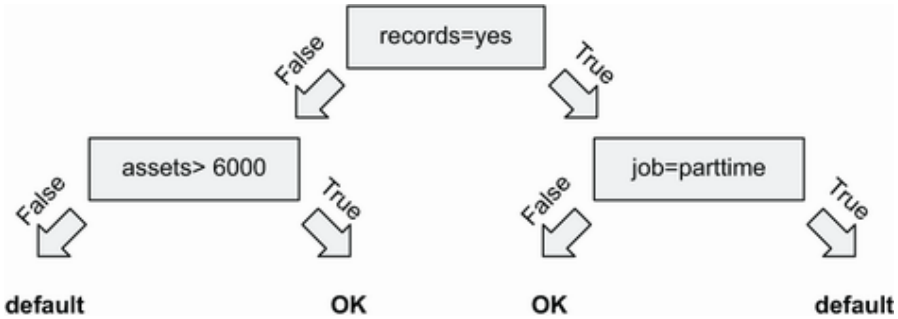


Figure 6.8 A decision tree consists of nodes with conditions. If the condition in a node is satisfied, we go right; otherwise, we go left.

It's quite easy to represent a decision tree as a set of `if-else` statements in Python. For example:

```
def assess_risk(client):
    if client['records'] == 'yes':
        if client['job'] == 'parttime':
            return 'default'
        else:
            return 'ok'
    else:
        if client['assets'] > 6000:
            return 'ok'
        else:
            return 'default'
```

With machine learning, we can extract these rules from data automatically. Let's see how we can do it.

6.2.1 Decision tree classifier

We'll use Scikit-learn for training a decision tree. Because we're solving a classification problem, we need to use `DecisionTreeClassifier` from the `tree` package. Let's import it:

```
from sklearn.tree import DecisionTreeClassifier
```

Training the model is as simple as invoking the `fit` method:

```
dt = DecisionTreeClassifier()
dt.fit(X_train, y_train)
```

To check if the result is good, we need to evaluate the predictive performance of the model on the validation set. Let's use AUC (area under the ROC curve) for that.

Credit risk scoring is a binary classification problem, and for cases like that, AUC is one of the best evaluation metrics. As you may recall from our discussion in chapter 4, AUC shows how well a model separates positive examples from negative examples. It has a nice interpretation: it describes the probability that a randomly chosen positive example ("default") has a higher score than a randomly chosen negative example ("OK"). This is a relevant metric for the project: we want risky clients to have higher scores than nonrisky ones. For more details on AUC, refer to chapter 4.

Like previously, we'll use an implementation from Scikit-learn, so let's import it:

```
from sklearn.metrics import roc_auc_score
```

First, we evaluate the performance on the training set. Because we chose AUC as the evaluation metric, we need scores, not hard predictions. As we know from chapter 3, we need to use the `predict_proba` method for that:

```
y_pred = dt.predict_proba(X_train)[:, 1]
roc_auc_score(y_train, y_pred)
```

When we execute it, we see that the score is 100%—the perfect score. Does it mean that we can predict default without errors? Let's check the score on validation before jumping to conclusions:

```
y_pred = dt.predict_proba(X_val)[:, 1]
roc_auc_score(y_val, y_pred)
```

After running, we see that AUC on validation is only 65%.

We just observed a case of *overfitting*. The tree learned the training data so well that it simply memorized the outcome for each customer. However, when we applied it to the validation set, the model failed. The rules it extracted from the data turned out to be too specific to the training set, so it worked poorly for customers it didn't see during training. In such cases, we say that the model cannot *generalize*.

Overfitting happens when we have a complex model with enough power to remember all the training data. If we force the model to be simpler, we can make it less powerful and improve the model's ability to generalize.

We have multiple ways to control the complexity of a tree. One option is to restrict its size: we can specify the `max_depth` parameter, which controls the maximum number of levels. The more levels a tree has, the more complex rules it can learn (figure 6.9).

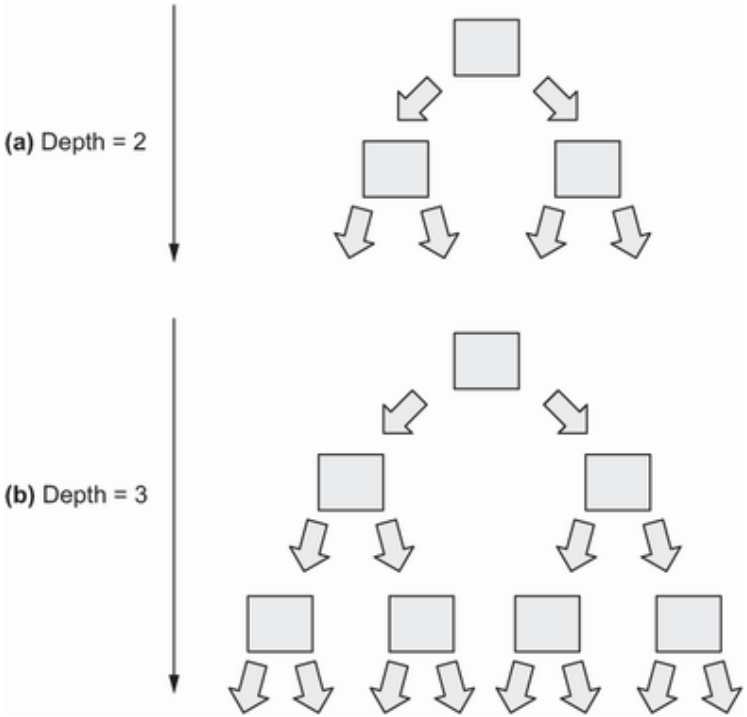


Figure 6.9 A tree with more levels can learn more complex rules. A tree with two levels is less complex than a tree with three levels and, thus, less prone to overfitting.

The default value for the `max_depth` parameter is `None`, which means that the tree can grow as large as possible. We can try a smaller value and compare the results.

For example, we can change it to 2:

```
dt = DecisionTreeClassifier(max_depth=2)
dt.fit(X_train, y_train)
```

To visualize the tree we just learned, we can use the `export_text` function from the `tree` package:

```
from sklearn.tree import export_text

tree_text = export_text(dt, feature_names=dv.feature_names_)
print(tree_text)
```

We only need to specify the names of features using the `feature_names` parameter. We can get it from the `DictVectorizer`. When we print it, we get the following:

```
|--- records=no <= 0.50
|   |--- seniority <= 6.50
|   |   |--- class: True
|   |--- seniority >  6.50
|   |   |--- class: False
|--- records=no >  0.50
|   |--- job=parttime <= 0.50
|   |   |--- class: False
|   |--- job=parttime >  0.50
|   |   |--- class: True
```

Each line in the output corresponds to a node with a condition. If the condition is true, we go inside and repeat the process until we arrive at the final decision. At the end, if class is `True`, then the decision is "default," and otherwise it's "OK."

The condition `records=no > 0.50` means that a customer has no records. Recall that we use one-hot encoding to represent `records` with two features: `records=yes` and `records=no`. For a customer with no records, `records=no` is set to "1" and `records=yes` to "0." Thus, "`records=no > 0.50` is true when the value for `records` is `no` (figure 6.10).

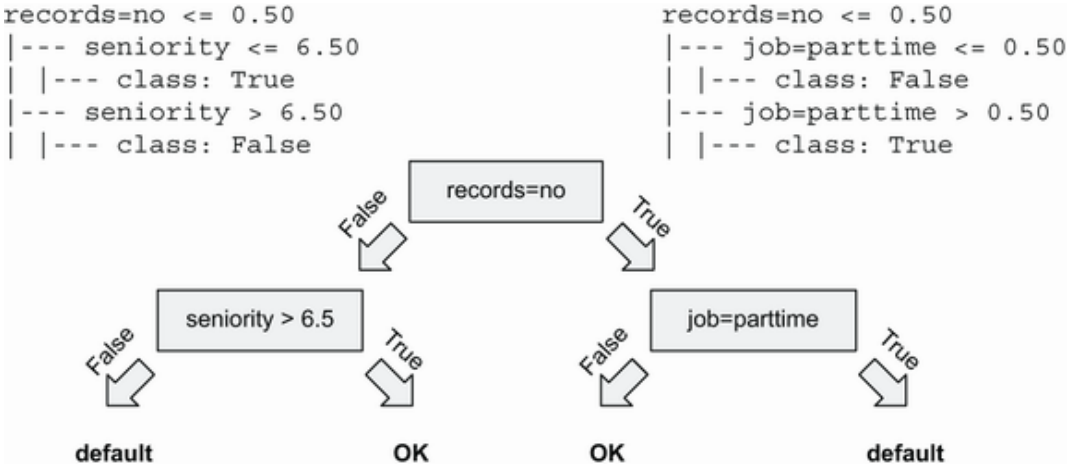


Figure 6.10 The tree we learned with `max_depth` set to 2

Let's check the score:

```
y_pred = dt.predict_proba(X_train)[:, 1]
auc = roc_auc_score(y_train, y_pred)
print('train auc', auc)

y_pred = dt.predict_proba(X_val)[:, 1]
auc = roc_auc_score(y_val, y_pred)
print('validation auc', auc)
```

We see that the score on train dropped:

```
train auc: 0.705
val auc: 0.669
```

Previously, the performance on the training set was 100%, but now it's only 70.5%. It means that the model can no longer memorize all the outcomes from the training set.

However, the score on the validation set is better: it's 66.9%, which is an improvement over the previous result (65%). By making it less complex, we improved the ability of our model to generalize. Now it's better at predicting the outcomes for customers it hasn't seen previously.

However, this tree has another problem—it's too simple. To make it better, we need to tune the model: try different parameters, and see which ones lead to the best AUC. In addition to `max_depth`, we can control other parameters. To understand what these parameters mean and how they influence the model, let's take a step back and look at how decision trees learn rules from data.

6.2.2 Decision tree learning algorithm

To understand how a decision tree learns from data, let's simplify the problem. First, we'll use a much smaller dataset with just one feature: `assets` (figure 6.11).

	assets	status
0	8000	default
1	2000	OK
2	0	OK
3	6000	OK
4	6000	default
5	9000	default

Figure 6.11 A smaller dataset with one feature: `assets`. The target variable is `status`.

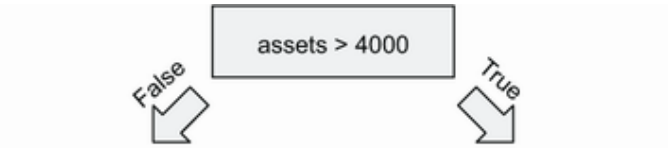
Second, we'll grow a very small tree, with a single node.

The only feature we have in the dataset is `assets`. This is why the condition in the node will be `assets > T`, where *T* is a threshold value that we need to determine. If the condition is true, we'll predict "OK," and if it's false, our prediction will be "default" (figure 6.12).

Figure 6.12 A simple decision tree with only one node. The node contains a condition `assets > T`. We need to find the best value for *T*.

The condition `assets > T` is called a *split*. It splits the dataset into two groups: the data points that satisfy the condition and the data points that do not.

If `T` is 4000, then we have customers with more than $4,000 in assets (on the right) and the customers with less than $4,000 in assets (on the left) (figure 6.13).



	assets	status
1	2000	default
2	0	default
5	4000	OK
7	3000	default

	assets	status
0	8000	default
3	5000	OK
4	5000	OK
6	9000	OK

Figure 6.13 The condition in a node splits the dataset into two parts: data points that satisfy the condition (on the right) and data points that don't (on the left).

Now we turn these groups into *leaves*—the decision nodes—by taking the most frequent status in each group and using it as the final decision. In our example, "default" is the most frequent outcome in the left group and "OK" in the right (figure 6.14).

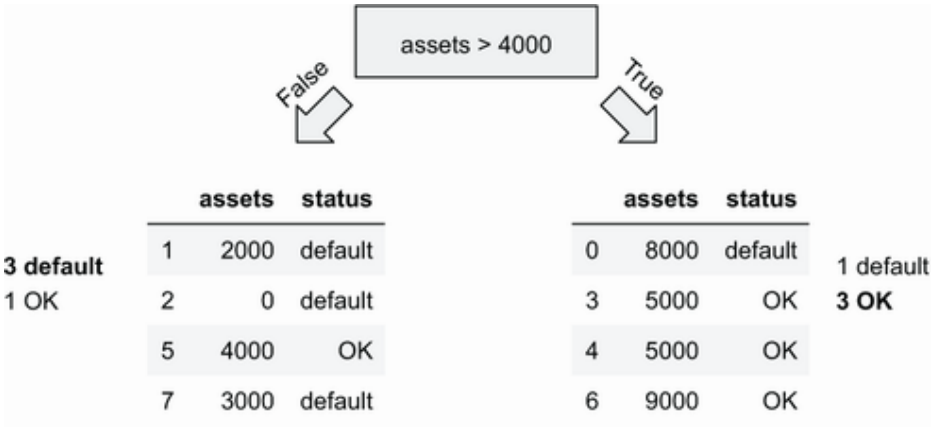


Figure 6.14 The most frequent outcome on the left is “default.” For the group on the right, it’s “OK.”

Thus, if a customer has more than $4,000 in assets, our decision is “OK,” and, otherwise, it’s “default” `assets > 4000` (figure 6.15).

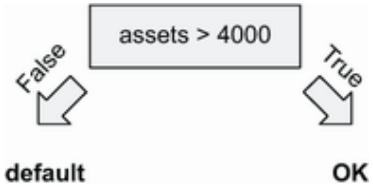


Figure 6.15 By taking the most frequent outcome in each group and assigning it to leaves, we get the final decision tree

IMPURITY

These groups should be as homogeneous as possible. Ideally, each group should contain only observations of one class. In this case, we call these groups *pure*.

For example, if we have a group of four customers with outcomes [“default,” “default,” “default,” “default”], it’s pure: it contains only customers

who defaulted. But a group [“default,” “default,” “default,” “OK”] is impure: there’s one customer who didn’t default.

When training a decision tree model, we want to find such T that the *impurity* of both groups is minimal.

So, the algorithm for finding T is quite simple:

- Try all possible values of T.
- For each T, split the dataset into left and right groups and measure their impurity.
- Select T that has the lowest degree of impurity.

We can use different criteria for measuring impurity. The easiest one to understand is the *misclassification rate*, which says how many observations in a group don’t belong to the majority class.

NOTE Scikit-learn uses more advanced split criteria such as entropy and the Gini impurity. We do not cover them in this book, but the idea is the same: they measure the degree of impurity of the split.

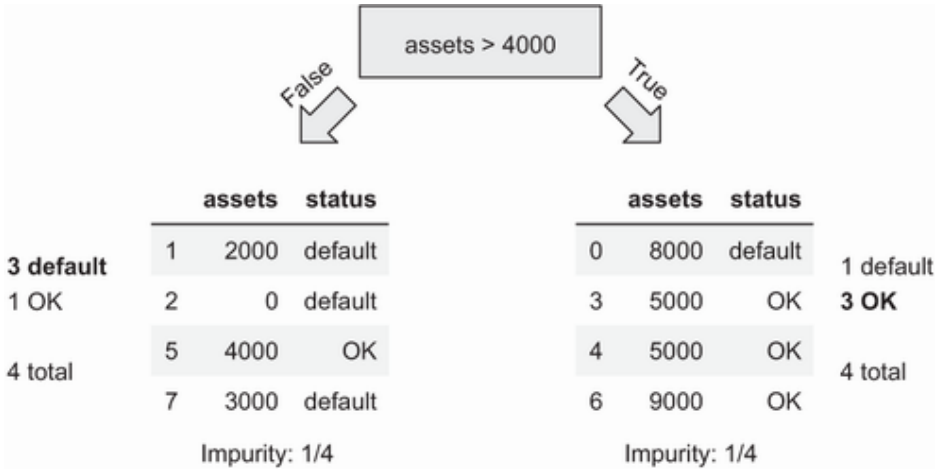


Figure 6.16 For `assets > 4000`, the misclassification rate for both groups is one-quarter.

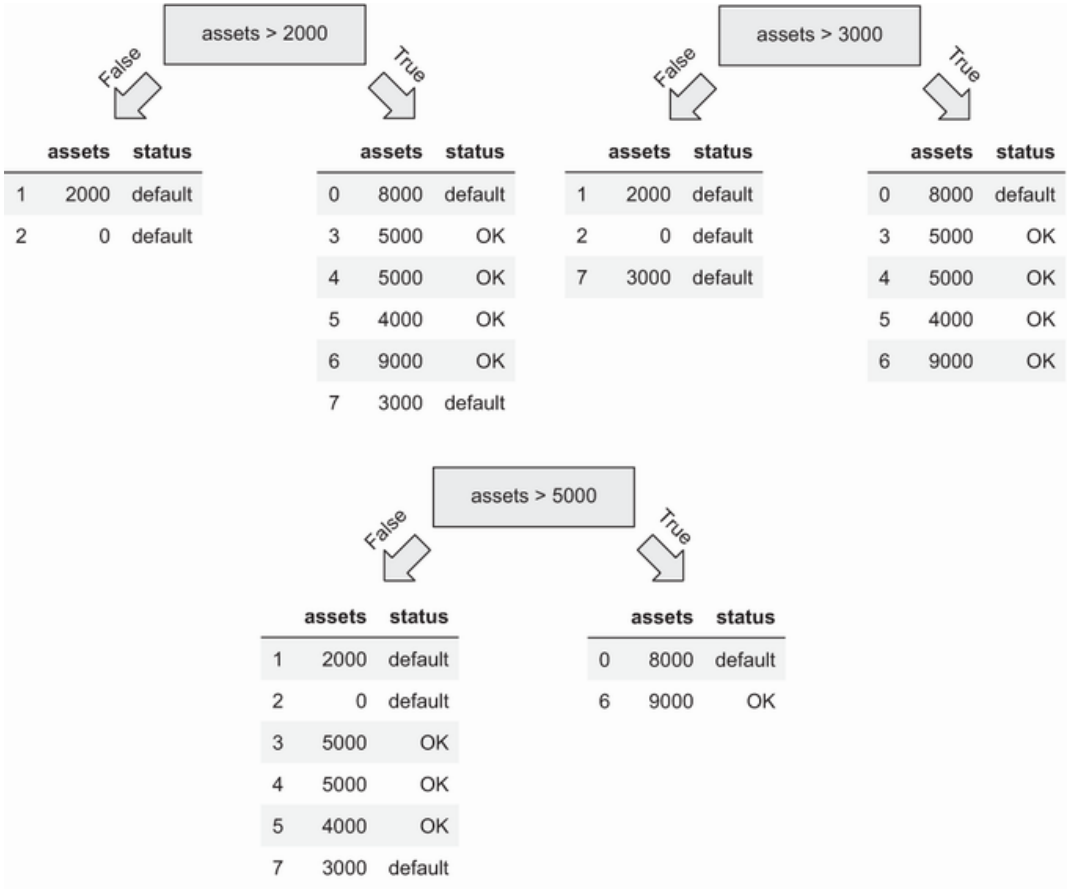
Let's calculate the misclassification rate for the split $T = 4000$ (figure 6.16):

- For the left group, the majority class is "default." There are four data points in total, and one doesn't belong to "default." The misclassification rate is 25% (1/4).
- For the right group, "OK" is the majority class, and there's one "default." Thus, the misclassification rate is also 25% (1/4).
- To calculate the overall impurity of the split, we can take the average across both groups. In this case, the average is 25%.

NOTE In reality, instead of taking the simple average across both groups, we take a weighted average—we weight each group proportionally to its size. To simplify calculations, we use the simple average in this chapter.

$T = 4000$ is not the only possible split for `assets`. Let's try other values for T such as 2000, 3000, and 5000 (figure 6.17):

- For T = 2000, we have 0% impurity on the left (0/2, all are "default") and 33.3% impurity on the right (2/6, 2 out of 6 are "default," the rest are "OK"). The average is 16.6%.
- For T = 3000, 0% on the left and 20% (1/5) on the right. The average is 10%.
- For T = 5000, 50% (3/6) on the left and 50% (1/2) on the right. The average is 50%.



	assets	status
1	2000	default
2	0	default

	assets	status
0	8000	default
3	5000	OK
4	5000	OK
5	4000	OK
6	9000	OK
7	3000	default

	assets	status
1	2000	default
2	0	default
7	3000	default

	assets	status
0	8000	default
3	5000	OK
4	5000	OK
5	4000	OK
6	9000	OK

	assets	status
1	2000	default
2	0	default
3	5000	OK
4	5000	OK
5	4000	OK
7	3000	default

	assets	status
0	8000	default
6	9000	OK

Figure 6.17 In addition to `assets > 4000`, we can try other values of T, such as 2000, 3000, and 5000.

The best average impurity is 10% for $T = 3000$: we got zero mistakes for the left tree and only one (out of five rows) for the right. So, we should select 3000 as the threshold for our final model (figure 6.18).

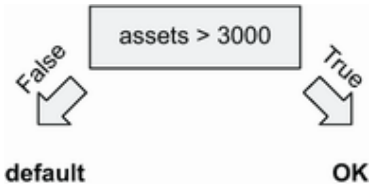


Figure 6.18 The best split for this dataset is `assets > 3000`.

SELECTING THE BEST FEATURE FOR SPLITTING

Now let's make the problem a bit more complex and add another feature to the dataset: `debt` (figure 6.19).

	assets	debt	status
0	8000	3000	default
1	2000	1000	default
2	0	1000	default
3	5000	1000	OK
4	5000	1000	OK
5	4000	1000	OK
6	9000	500	OK
7	3000	2000	default

Figure 6.19 A dataset with two features: `assets` and `debt`. The target variable is `status`.

Previously we had only one feature: `assets`. We knew for sure that it would be used for splitting the data. Now we have two features, so in ad-

dition to selecting the best threshold for splitting, we need to figure out which feature to use.

The solution is simple: we try all the features, and for each feature select the best threshold.

Let's modify the training algorithm to include this change:

- For each feature, try all possible thresholds.
- For each threshold value *T*, measure the impurity of the split.
- Select the feature and the threshold with the lowest impurity possible.

Let's apply this algorithm to our dataset:

- We already identified that for `assets`, the best *T* is 3000. The average impurity of this split is 10%.
- For `debt`, the best *T* is 1000. In this case, the average impurity is 17%.

So, the best split is `asset > 3000` (figure 6.20).

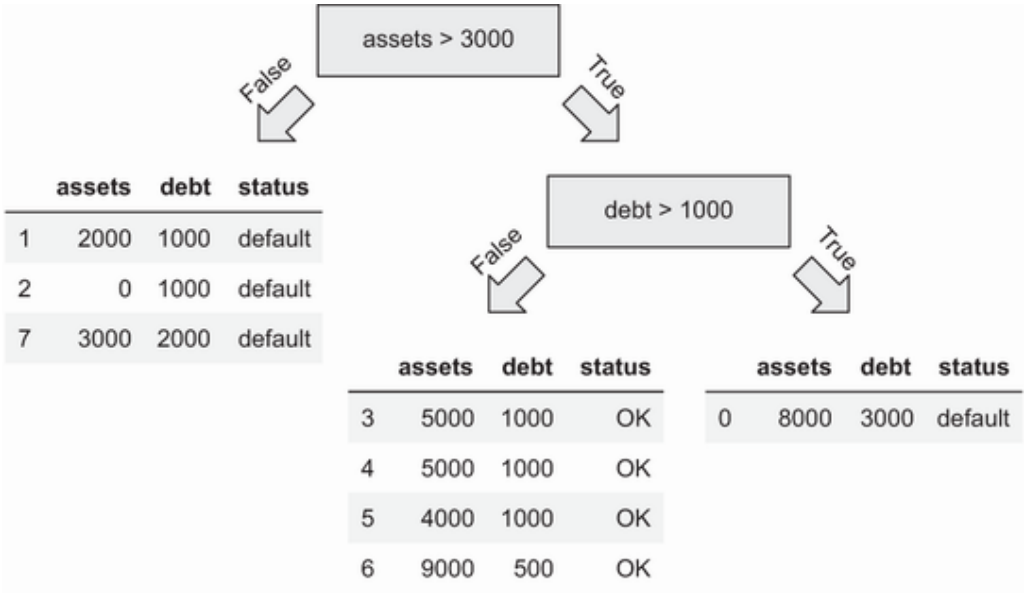
	assets	debt	status
1	2000	1000	default
2	0	1000	default
7	3000	2000	default

	assets	debt	status
0	8000	3000	default
3	5000	1000	OK
4	5000	1000	OK
5	4000	1000	OK
6	9000	500	OK

Figure 6.20 The best split is `assets > 3000`, which has the average impurity of 10%.

The group on the left is already pure, but the group on the right is not. We can make it less impure by repeating the process: split it again!

When we apply the same algorithm to the dataset on the right, we find that the best split condition is `debt > 1000`. We have two levels in the tree now—or we can say that the depth of this tree is 2 (figure 6.21).



	assets	debt	status
1	2000	1000	default
2	0	1000	default
7	3000	2000	default

	assets	debt	status
3	5000	1000	OK
4	5000	1000	OK
5	4000	1000	OK
6	9000	500	OK

	assets	debt	status
0	8000	3000	default

Figure 6.21 By repeating the algorithm recursively to the group on the right, we get a tree with two levels.

Before the decision tree is ready, we need to do the last step: convert the groups into decision nodes. For that, we take the most frequent status in each group. This way, we get a decision tree (figure 6.22).

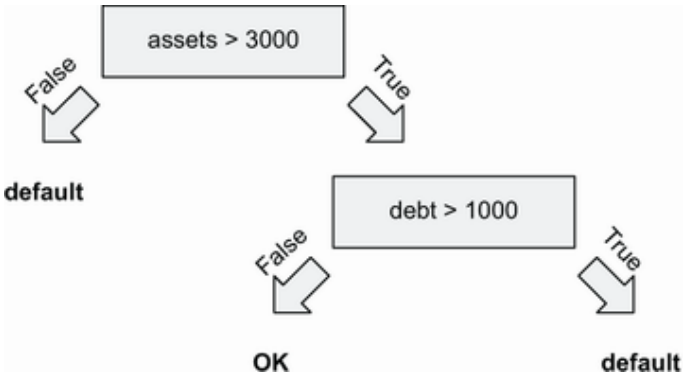


Figure 6.22 The groups are already pure, so the most frequent status is the only status each group has. We take this status as the final decision in each leaf.

STOPPING CRITERIA

When training a decision tree, we can keep splitting the data until all the groups are pure. This is exactly what happens when we don't put any restrictions on the trees in Scikit-learn. As we've seen, the resulting model becomes too complex, which leads to overfitting.

We solved this problem by using the `max_depth` parameter—we restricted the tree size and didn't let it grow too big.

To decide if we want to continue splitting the data, we use *stopping criteria*—criteria that describe if we should add another split in the tree or stop.

The most common stopping criteria are

- The group is already pure.
- The tree reached the depth limit (controlled by the `max_depth` parameter).
- The group is too small to continue splitting (controlled by the `min_samples_ leaf` parameter).

By using these criteria to stop earlier, we force our model to be less complex and, therefore, reduce the risk of overfitting.

Let's use this information to adjust the training algorithm:

- Find the best split:
  - For each feature try all possible threshold values.
  - Use the one with the lowest impurity.
- If the maximum allowed depth is reached, stop.

- If the group on the left is sufficiently large and it's not pure yet, repeat on the left.
- If the group on the right is sufficiently large and it's not pure yet, repeat on the right.

Even though this is a simplified version of the decision tree learning algorithm, it should provide you enough intuition about the internals of the learning process.

Most important, we know two parameters control the complexity of the model. By changing these parameters, we can improve the performance of the model.

Exercise 6.1

We have a dataset with 10 features and need to add another feature to this dataset. What happens with the speed of training?

a) With one more feature, training takes longer.

b) The number of features does not affect the speed of training.

6.2.3 Parameter tuning for decision tree

The process of finding the best set of parameters is called *parameter tuning*. We usually do it by changing the model and checking its score on the validation dataset. In the end, we use the model with the best validation score.

As we have just learned, we can tune two parameters:

- `max_depth`
- `min_leaf_size`

These two are the most important ones, so we will adjust only them. You can check the other parameters in the official documentation (**https://scikit-learn.org/stable/modules/generated/sklearn.tree.DecisionTreeClassifier.html**).

When we trained our model previously, we restricted the depth of the tree to 2, but we didn't touch `min_leaf_size`. With this, we got an AUC of 66% on the validation set.

Let's find the best parameters.

We start by tuning max_depth. For that, we iterate over a few reasonable values and see what works best:

```
for depth in [1, 2, 3, 4, 5, 6, 10, 15, 20, None]:
    dt = DecisionTreeClassifier(max_depth=depth)
    dt.fit(X_train, y_train)
    y_pred = dt.predict_proba(X_val)[:, 1]
    auc = roc_auc_score(y_val, y_pred)
    print('%4s -> %.3f' % (depth, auc))
```

The value `None` means that there's no restriction on depth, so the tree will grow as large as it can.

When we run this code, we see that `max_depth` of 5 gives the best AUC (76.6%), followed by 4 and 6 (figure 6.23).

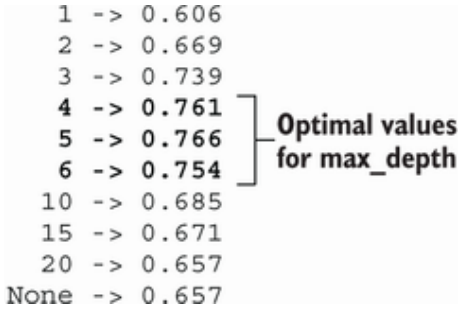


Figure 6.23 The optimal value for depth is 5 (76.6%) followed by 4 (76.1%) and 6 (75.4%).

Next, we tune `min_leaf_size`. For that, we iterate over the three best parameters of `max_depth`, and for each, go over different values of `min_leaf_size`:

```
for m in [4, 5, 6]:
    print('depth: %s' % m)

    for s in [1, 5, 10, 15, 20, 50, 100, 200]:
        dt = DecisionTreeClassifier(max_depth=m, min_samples_leaf=s)
        dt.fit(X_train, y_train)
        y_pred = dt.predict_proba(X_val)[:, 1]
        auc = roc_auc_score(y_val, y_pred)
        print('%s -> %.3f' % (s, auc))

    print()
```

After running it, we see that the best AUC is 78.5% with parameters `min_sample_ leaf=15` and `max_depth=6` (table 6.1).

NOTE As we see, the value we use for `min_leaf_size` influences the best value of `max_depth`. You can experiment with a wider range of val-

ues for `max_depth` to tweak the performance further.

Table 6.1 AUC on validation set for different values of `min_leaf_size` (rows) and `max_depth` (columns)

	depth=4	depth=5	depth=6
1	0.761	0.766	0.754
5	0.761	0.768	0.760
10	0.761	0.762	0.778
15	0.764	0.772	**0.785**
20	0.761	0.774	0.774
50	0.753	0.768	0.770
100	0.756	0.763	0.776
200	0.747	0.759	0.768

We have found the best parameters, so let's use them to train the final model:

```
dt = DecisionTreeClassifier(max_depth=6, min_samples_leaf=15)
dt.fit(X_train, y_train)
```

Decision trees are simple and effective models, but they become even more powerful when we combine many trees together. Next, we'll see how we can do it to achieve even better predictive performance.

6.3 Random forest

For a moment, let's suppose that we don't have a machine learning algorithm to help us with credit risk scoring. Instead, we have a group of experts.

Each expert can independently decide if we should approve a loan application or reject it. An individual expert may make a mistake. However, it's less likely that all the experts together decide to accept the application, but the customer fails to pay the money back.

Thus, we can ask all the experts independently and then combine their verdicts into the final decision, for example, by using the majority vote (figure 6.24).

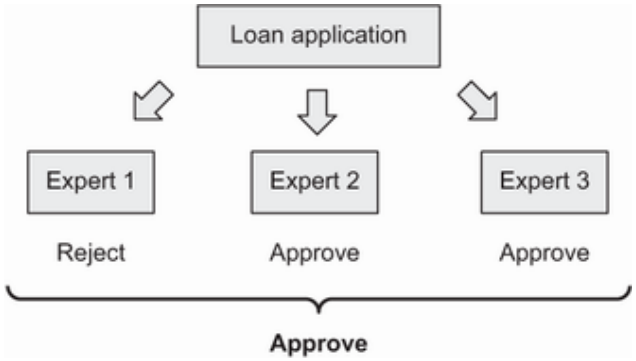


Figure 6.24 A group of experts can make a decision better than a single expert individually.

This idea also applies to machine learning. One model individually may be wrong, but if we combine the output of multiple models into one, the chance of an incorrect answer is smaller. This concept is called *ensemble learning*, and a combination of models is called an *ensemble*.

For this to work, the models need to be different. If we train the same decision tree model 10 times, they will all predict the same output, so it's not useful at all.

The easiest way to have different models is to train each tree on a different subset of features. For example, suppose we have three features: `assets`, `debts`, and `price`. We can train three models:

- The first will use `assets` and `debts`.
- The second will use `debts` and `price`.
- The last one will use `assets` and `price`.

With this approach, we'll have different trees, each making its own decisions (figure 6.25). But when we put their predictions together, their mistakes average out, and combined, they have more predictive power.

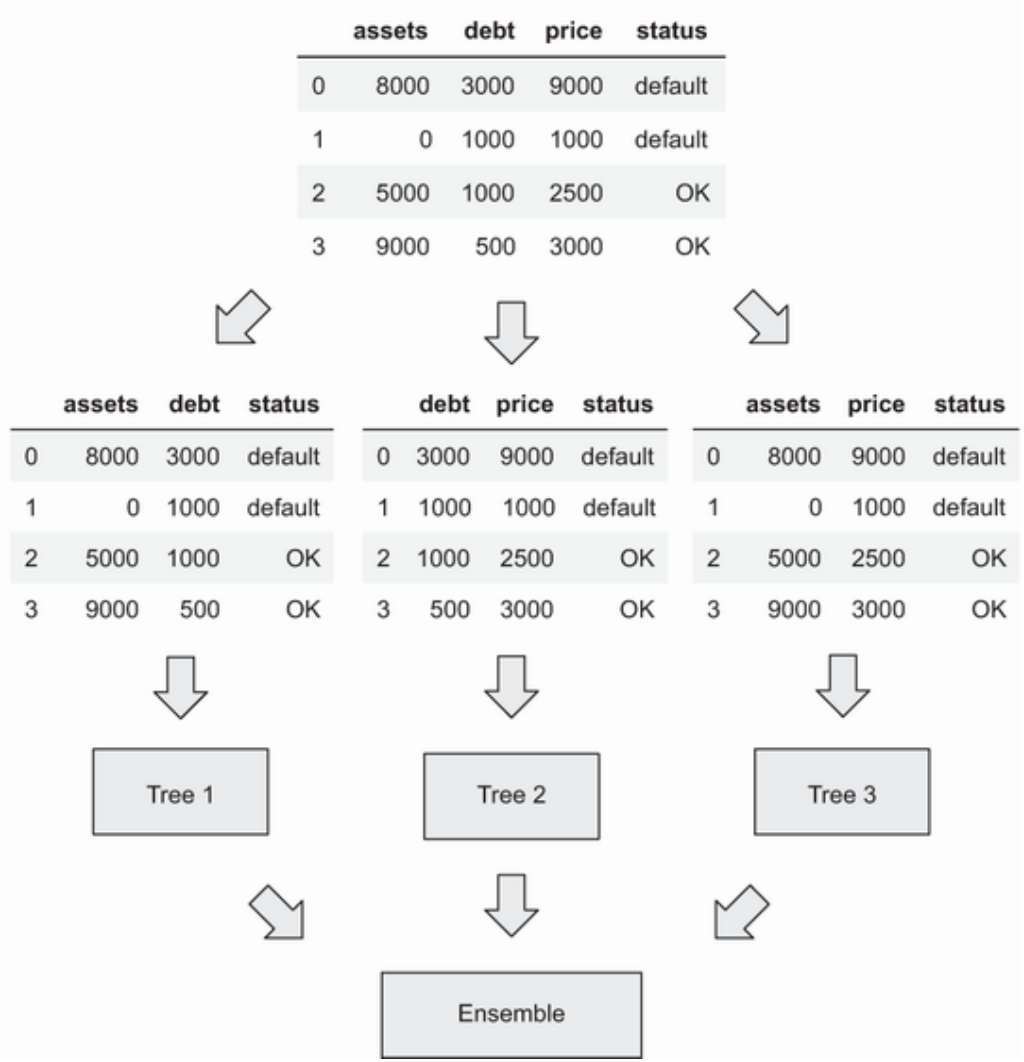


Figure 6.25 Models we want to combine in an ensemble should not be the same. We can make sure they are different by training each tree on a different subset of features.

This way of putting together multiple decision trees into an ensemble is called a *random forest*. To train a random forest, we can do this (figure 6.26):

- Train N independent decision tree models.

- For each model, select a random subset of features, and use only them for training.
- When predicting, combine the output of N models into one.

NOTE This is a very simplified version of the algorithm. It's enough to illustrate the main idea, but in reality, it's more complex.

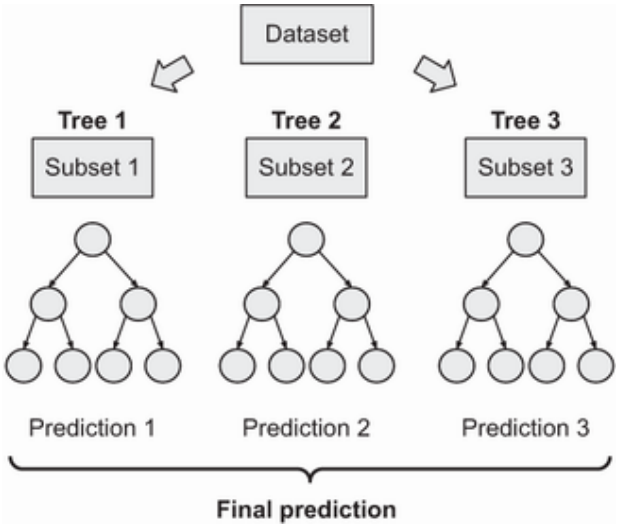


Figure 6.26 Training a random forest model: for training each tree, randomly select a subset of features. When making the final prediction, combine all the predictions into one.

Scikit-learn contains an implementation of a random forest, so we can use it for solving our problem. Let's do it.

6.3.1 Training a random forest

To use random forest in Scikit-learn, we need to import `RandomForestClassifier` from the `ensemble` package:

```
from sklearn.ensemble import RandomForestClassifier
```

When training a model, the first thing we need to specify is the number of trees we want to have in the ensemble. We do it with the `n_estimators` parameter:

```
rf = RandomForestClassifier(n_estimators=10)
rf.fit(X_train, y_train)
```

After training finishes, we can evaluate the performance of the result:

```
y_pred = rf.predict_proba(X_val)[:, 1]
roc_auc_score(y_val, y_pred)
```

It shows 77.9%. However, the number you see may be different. Every time we retrain the model, the score changes: it varies from 77% to 80%.

The reason for this is randomization: to train a tree, we randomly select a subset of features. To make the results consistent, we need to fix the seed for the random-number generator by assigning some value to the `random_state` parameter:

```
rf = RandomForestClassifier(n_estimators=10, random_state=3)
rf.fit(X_train, y_train)
```

Now we can evaluate it:

```
y_pred = rf.predict_proba(X_val)[:, 1]
```

```
roc_auc_score(y_val, y_pred)
```

This time, we get an AUC of 78%. This score doesn't change, no matter how many times we retrain the model.

The number of trees in the ensemble is an important parameter, and it influences the performance of the model. Usually, a model with more trees is better than a model with fewer trees. On the other hand, adding too many trees is not always helpful.

To see how many trees we need, we can iterate over different values for `n_estimators` and see its effect on AUC:

```
aucs = []                                                          ❶

for i in range(10, 201, 10):                                       ❷
    rf = RandomForestClassifier(n_estimators=i, random_state=3)    ❷
    rf.fit(X_train, y_train)                                       ❷

    y_pred = rf.predict_proba(X_val)[:, 1]                         ❸
    auc = roc_auc_score(y_val, y_pred)                             ❸
    print('%s -> %.3f' % (i, auc))                                 ❸

    aucs.append(auc)                                               ❹
```

❶ Creates a list with AUC results

❷ Trains progressively more trees in each iteration

❸ Evaluates the score

❹ Adds the score to the list with other scores

In this code, we try different numbers of trees: from 10 to 200, going by steps of 10 (10, 20, 30, ...). Each time we train a model, we calculate its AUC on the validation set and record it.

After we finish, we can plot the results:

```
plt.plot(range(10, 201, 10), aucs)
```

In figure 6.27, we can see the results.

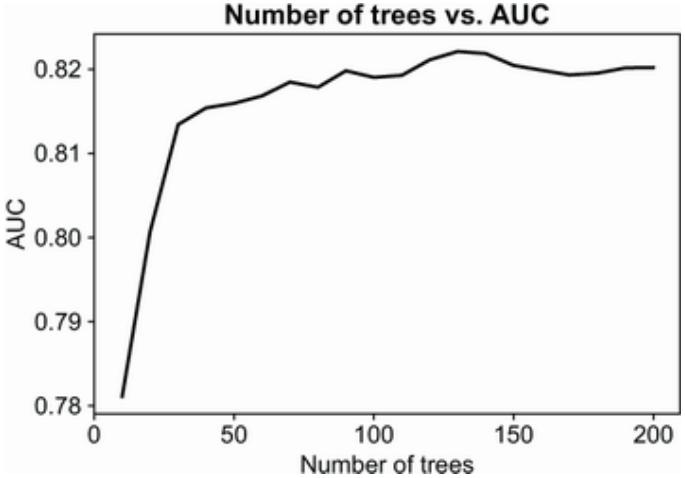


Figure 6.27 The performance of the random forest model with different values for the `n_estimators` parameter

The performance grows rapidly for the first 25–30 trees; then the growth slows down. After 130, adding more trees is not helpful anymore: the performance stays approximately at the level of 82%.

The number of trees is not the only parameter we can change to get better performance. Next, we see which other parameters we should also tune to improve the model.

6.3.2 Parameter tuning for random forest

A random forest ensemble consists of multiple decision trees, so the most important parameters we need to tune for random forest are the same:

- `max_depth`
- `min_leaf_size`

We can change other parameters, but we won't cover them in detail in this chapter. Refer to the official documentation for more information (**https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html**).

Let's start with `max_depth`. We already know that this parameter significantly affects the performance of a decision tree. This is also the case for random forest: larger trees tend to overfit more than smaller trees.

Let's test a few values for `max_depth` and see how AUC evolves as the number of trees grows:

```
all_aucs = {}                                          ❶

for depth in [5, 10, 20]:                              ❷
    print('depth: %s' % depth)
    aucs = []                                          ❸

    for i in range(10, 201, 10):                       ❸
        rf = RandomForestClassifier(n_estimators=i,
              max_depth=depth, random_state=1)         ❹
        rf.fit(X_train, y_train)
        y_pred = rf.predict_proba(X_val)[:, 1]
```

```
        auc = roc_auc_score(y_val, y_pred)          ❺
        print('%s -> %.3f' % (i, auc))              ❺
        aucs.append(auc)                            ❺

    all_aucs[depth] = aucs                          ❻
    print()
```

❶ Creates a dictionary with AUC results

❷ Iterates over different depth values

❸ Creates a list with AUC results for the current depth level

❹ Iterates over different n_estimator values

❺ Evaluates the model

❻ Save the AUCs for the current depth level in the dictionary

Now for each value of `max_depth`, we have a series of AUC scores. We can plot them now:

```
num_trees = list(range(10, 201, 10))
plt.plot(num_trees, all_aucs[5], label='depth=5')
plt.plot(num_trees, all_aucs[10], label='depth=10')
plt.plot(num_trees, all_aucs[20], label='depth=20')
plt.legend()
```

In figure 6.28 we see the result.

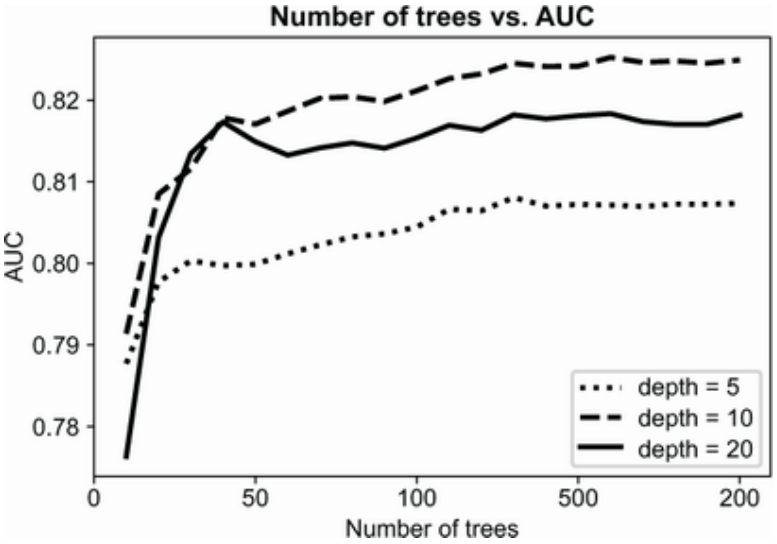


Figure 6.28 The performance of random forest with different values of the `max_depth` parameter

With `max_depth=10`, AUC goes over 82%, whereas for other values it performs worse.

Now let's tune `min_samples_leaf`. We set the value for the `max_depth` parameter from the previous step and then follow the same approach as previously for determining the best value for `min_samples_leaf`:

```
all_aucs = {}

for m in [3, 5, 10]:
    print('min_samples_leaf: %s' % m)
    aucs = []

    for i in range(10, 201, 20):
        rf = RandomForestClassifier(n_estimators=i, max_depth=10, min_samples_leaf=m, random_state
        rf.fit(X_train, y_train)
        y_pred = rf.predict_proba(X_val)[:, 1]
```

```
        auc = roc_auc_score(y_val, y_pred)
        print('%s -> %.3f' % (i, auc))
        aucs.append(auc)

    all_aucs[m] = aucs
    print()
```

Let's plot it:

```
num_trees = list(range(10, 201, 20))
plt.plot(num_trees, all_aucs[3], label='min_samples_leaf=3')
plt.plot(num_trees, all_aucs[5], label='min_samples_leaf=5')
plt.plot(num_trees, all_aucs[10], label='min_samples_leaf=10')
plt.legend()
```

Then review the results (figure 6.29).

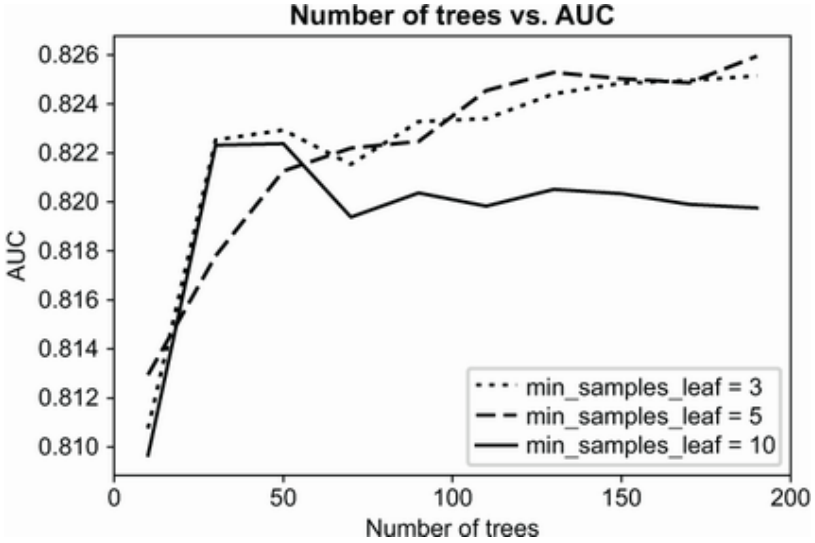


Figure 6.29 The performance of random forest with different values of `min_samples_leaf` (with `max_depth=10`)

We see that AUC is slightly better for small values of `min_samples_leaf` and the best value is 5.

Thus, the best parameters for random forest for our problem are

- `max_depth=10`
- `min_samples_leaf=5`

We achieved the best AUC with 200 trees, so we should set the `n_estimators` parameter to 200.

Let's train the final model:

```
rf = RandomForestClassifier(n_estimators=200, max_depth=10, min_samples_leaf=5, random_state=1)
```

Random forest is not the only way to combine multiple decision trees.
There's a different approach: gradient boosting. We cover that next.

Exercise 6.2

To make an ensemble useful, trees in a random forest should be different from each other. This is done by

a) Selecting different parameters for each individual tree

b) Randomly selecting a different subset of features for each tree

c) Randomly selecting values for splitting

6.4 Gradient boosting

In a random forest, each tree is independent: it's trained on a different set of features. After individual trees are trained, we combine all their decisions together to get the final decision.

It's not the only way to combine multiple models together in one ensemble, however. Alternatively, we can train models sequentially—each next model tries to fix errors from the previous one:

- Train the first model.
- Look at the errors it makes.
- Train another model that fixes these errors.
- Look at the errors again; repeat sequentially.

This way of combining models is called *boosting*. *Gradient boosting* is a particular variation of this approach that works especially well with trees (figure 6.30).

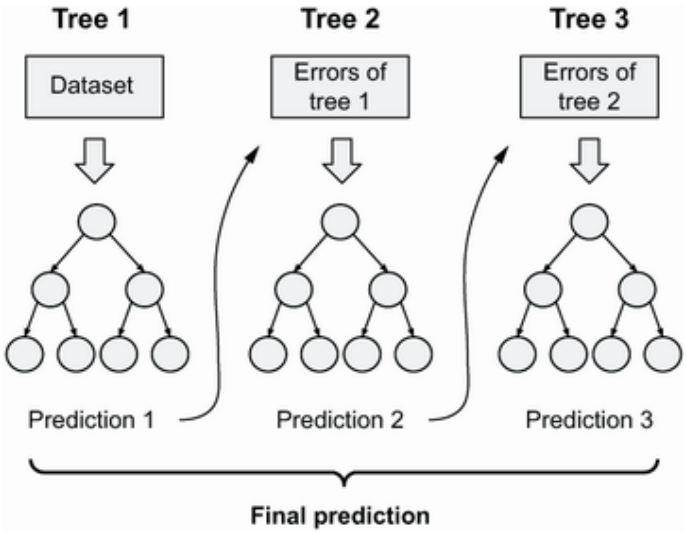


Figure 6.30 In gradient boosting, we train the models sequentially, and each next tree fixes the errors of the previous one.

Let's have a look at how we can use it for solving our problem.

6.4.1 XGBoost: Extreme gradient boosting

We have many good implementations of the gradient boosting model: `GradientBoostingClassifier` from Scikit-learn, XGBoost, LightGBM and CatBoost. In this chapter, we use XGBoost (short for "Extreme Gradient Boosting"), which is the most popular implementation.

XGBoost doesn't come with Anaconda, so to use it, we need to install it. The easiest way is to install it with `pip`:

```
pip install xgboost
```

Next, open the notebook with our project and import it:

```
import xgboost as xgb
```

NOTE In some cases, importing XGBoost may give you a warning like `YMLLoadWarning`. You shouldn't worry about it; the library will work without problems.

Using the alias `xgb` when importing XGBoost is a convention, just like with other popular machine learning packages in Python.

Before we can train an XGBoost model, we need to wrap our data into `DMatrix` —a special data structure for finding splits efficiently. Let's do it:

```
dtrain = xgb.DMatrix(X_train, label=y_train, feature_names=dv.feature_names_)
```

When creating an instance of `DMatrix`, we pass three parameters:

- `X_train`: the feature matrix
- `y_train`: the target variable
- `feature_names`: the names of features in `X_train`

Let's do the same for the validation dataset:

```
dval = xgb.DMatrix(X_val, label=y_val, feature_names=dv.feature_names_)
```

The next step is specifying the parameters for training. We're using only a small subset of the default parameters of XGBoost (check the official documentation for the entire list of parameter: **https://xgboost.readthedocs.io/en/latest/parameter.html**):

```
xgb_params = {
    'eta': 0.3,
    'max_depth': 6,
    'min_child_weight': 1,

    'objective': 'binary:logistic',
    'nthread': 8,
    'seed': 1,
    'silent': 1
}
```

For us, the most important parameter now is `objective`: it specifies the learning task. We're solving a binary classification problem—that's why we need to choose `binary :logistic`. We cover the rest of these parameters later in this section.

For training an XGBoost model, we use the `train` function. Let's start with 10 trees:

```
model = xgb.train(xgb_params, dtrain, num_boost_round=10)
```

We provide three arguments to `train`:

- `xgb_params`: the parameters for training
- `dtrain`: the dataset for training (an instance of `DMatrix`)
- `num_boost_round=10`: the number of trees to train

After a few seconds, we get a model. To evaluate it, we need to make a prediction on the validation dataset. For that, use the `predict` method with the validation data wrapped in `DMatrix`:

```
y_pred = model.predict(dval)
```

The result, `y_pred`, is a one-dimensional NumPy array with predictions: the risk score for each customer in the validation dataset (figure 6.31).

```
y_pred = model.predict(dval)
y_pred[:10]
```

```
array([0.08926772, 0.0468099 , 0.09692743, 0.17261842, 0.05435968,
       0.12576081, 0.08033007, 0.61870354, 0.486538  , 0.04056795],
      dtype=float32)
```

Figure 6.31 The predictions of XGBoost

Next, we calculate AUC using the same approach as previously:

```
roc_auc_score(y_val, y_pred)
```

After executing it, we get 81.5%. This is quite a good result, but it's still slightly worse than our best random forest model (82.5%).

Training an XGBoost model is simpler when we can see how its performance changes when the number of trees grows. We see how to do it next.

6.4.2 Model performance monitoring

To get an idea of how AUC changes as the number of trees grows, we can use a watchlist—a built-in feature in XGBoost for monitoring model performance.

A watchlist is a Python list with tuples. Each tuple contains a DMatrix and its name. This is how we typically do it:

```
watchlist = [(dtrain, 'train'), (dval, 'val')]
```

Additionally, we modify the list of parameters for training: we need to specify the metric we use for evaluation. In our case, it's the AUC:

```
xgb_params = {
    'eta': 0.3,
    'max_depth': 6,
    'min_child_weight': 1,

    'objective': 'binary:logistic',
    'eval_metric': 'auc',              ❶
    'nthread': 8,
    'seed': 1,
    'silent': 1
}
```

❶ Sets the evaluation metric to the AUC

To use the watchlist during training, we need to specify two extra arguments for the `train` function:

- `evals` : the watchlist.
- `verbose_eval` : how often we print the metric. If we set it to "10," we see the result after each 10th step.

Let's train it:

```
model = xgb.train(xgb_params, dtrain,
                  num_boost_round=100,
                  evals=watchlist, verbose_eval=10)
```

While training, XGBoost prints the scores to the output:

```
[0]  train-auc:0.862996  val-auc:0.768179
[10] train-auc:0.950021  val-auc:0.815577
[20] train-auc:0.973165  val-auc:0.817748
[30] train-auc:0.987718  val-auc:0.817875
[40] train-auc:0.994562  val-auc:0.813873
[50] train-auc:0.996881  val-auc:0.811282
[60] train-auc:0.998887  val-auc:0.808006
[70] train-auc:0.999439  val-auc:0.807316
[80] train-auc:0.999847  val-auc:0.806771
[90] train-auc:0.999915  val-auc:0.806371
[99] train-auc:0.999975  val-auc:0.805457
```

As the number of trees grows, the score on the training set goes up (figure 6.32).

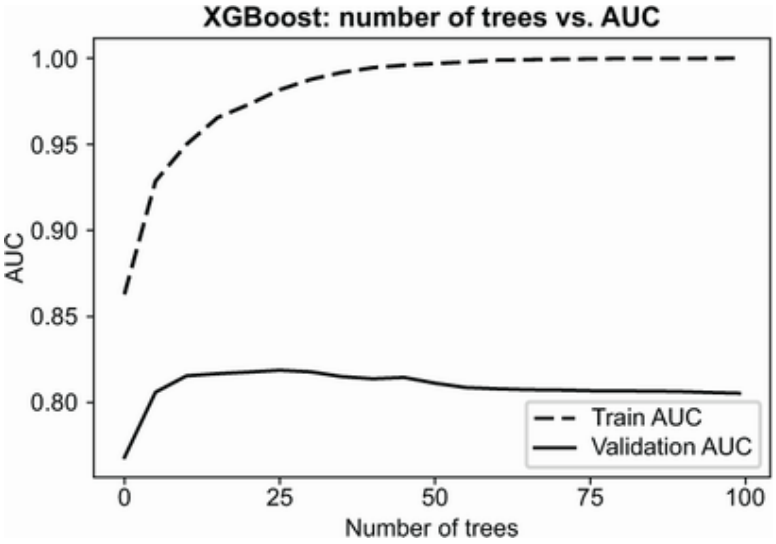


Figure 6.32 The effect of the number of trees on the AUC from train and validation sets. To see how to plot these values, check the notebook in the book's GitHub repository.

This behavior is expected: in boosting, every next model tries to fix the mistakes from the previous step, so the score is always improving.

For the validation score, however, this is not the case. It goes up initially but then starts to decrease. This is the effect of overfitting: our model becomes more and more complex until it simply memorizes the entire training set. It's not helpful for predicting the outcome for the customers outside of the training set, and the validation score reflects that.

We get the best AUC on the 30th iteration (81.7%), but it's not so different from the score we got on the 10th iteration (81.5%).

Next, we'll see how to get the best out of XGBoost by tuning its parameters.

6.4.3 Parameter tuning for XGBoost

Previously, we used a subset of default parameters for training a model:

```
xgb_params = {
    'eta': 0.3,
    'max_depth': 6,
    'min_child_weight': 1,
    'objective': 'binary:logistic',
    'eval_metric': 'auc',
    'nthread': 8,
    'seed': 1,
    'silent': 1
}
```

We're mostly interested in the first three parameters. These parameters control the training process:

- `eta` : Learning rate. Decision trees and random forest don't have this parameter. We cover it later in this section when we tune it.
- `max_depth` : The maximum allowed depth of each tree; the same as `max_depth` in `DecisionTreeClassifier` from Scikit-learn.
- `min_child_weight` : The minimal number of observations in each group; the same as `min_leaf_size` in `DecisionTreeClassifier` from Scikit-learn.

Other parameters:

- `objective` : The type of task we want to solve. For classification, it should be `binary:logistic` .

- `eval_metric` : The metric we use for evaluation. For this project, it's "AUC."
- `nthread` : The number of threads we use for training the model. XGBoost is very good at parallelizing training, so set it to the number of cores your computer has.
- `seed` : The seed for the random-number generator; we need to set it to make sure the results are reproducible.
- `silent` : The verbosity of the output. When we set it to "1," it outputs only warnings.

This is not the full list of parameters, only the basic ones. You can learn more about all the parameters in the official documentation (**https://xgboost.readthedocs.io/en/ latest/parameter.html**).

We already know `max_depth` and `min_child_weight` (`min_leaf_size`), but we haven't previously come across `eta` —the learning rate parameter. Let's talk about it and see how we can optimize it.

LEARNING RATE

In boosting, each tree tries to correct the mistakes from the previous iterations. Learning rate determines the weight of this correction. If we have a large value for `eta`, the correction overweights the previous predictions significantly. On the other hand, if the value is small, only a small fraction of this correction is used.

In practice it means

- If `eta` is too large, the model starts to overfit quite early without realizing its full potential.

- If it's too small, we need to train too many trees before it can produce good results.

The default value of 0.3 is reasonably good for large datasets, but for smaller datasets like ours, we should try smaller values like 0.1 or even 0.05.

Let's do it and see if it helps to improve the performance:

```
xgb_params = {
    'eta': 0.1,       ❶
    'max_depth': 6,
    'min_child_weight': 1,

    'objective': 'binary:logistic',
    'eval_metric': 'auc',
    'nthread': 8,
    'seed': 1,
    'silent': 1
}
```

❶ Changes eta from 0.3 to 0.1

Because now we can use a watchlist to monitor the performance of our model, we can train for as many iterations as we want. Previously we used 100 iterations, but this may be not enough for smaller `eta`. So let's use 500 rounds for training:

```
model = xgb.train(xgb_params, dtrain,
                  num_boost_round=500, verbose_eval=10,
                  evals=watchlist)
```

When running it, we see that the best validation score is 82.4%:

```
[60] train-auc:0.976407  val-auc:0.824456
```

Previously, we could achieve AUC of 81.7% when `eta` was set to the default value of 0.3. Let's compare these two models (figure 6.33).

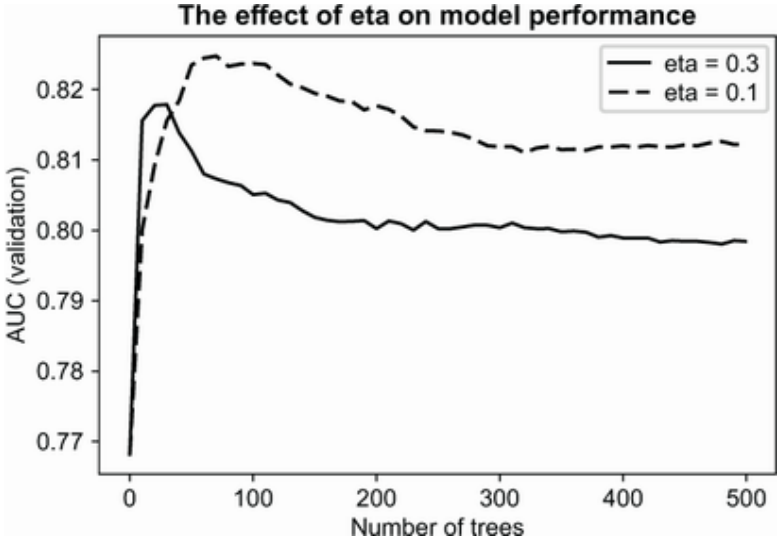


Figure 6.33 The effect of the `eta` parameter on the validation score

When `eta` is 0.3, we get the best AUC pretty quickly, but then it starts to overfit. After the 30th iteration, the performance on the validation set goes down.

When `eta` is 0.1, AUC grows more slowly but peaks at a higher value. For a smaller learning rate, it takes more trees to reach the peak, but we could achieve better performance.

For comparison, we can also try other values of `eta` (figure 6.34):

- For 0.05, the best AUC is 82.2% (after 120 iterations).
- For 0.01, the best AUC is 82.1% (after 500 iterations).

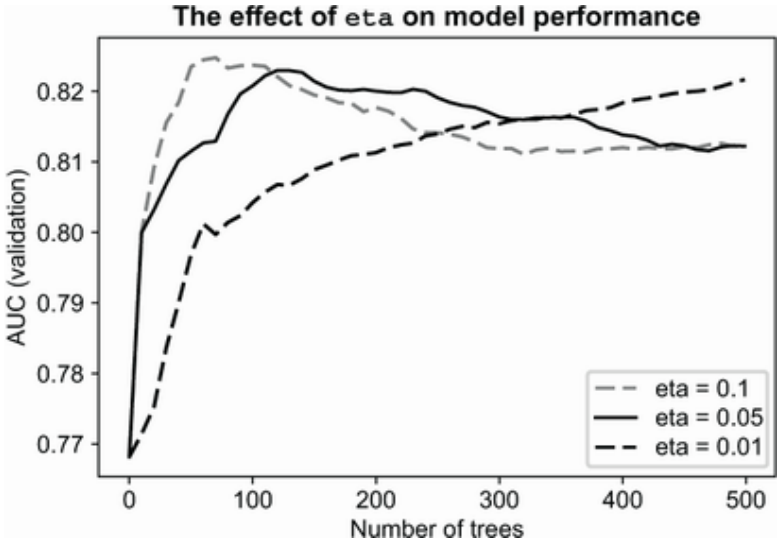


Figure 6.34 The model requires more trees when `eta` is small.

When `eta` is 0.05, the performance is similar to 0.1, but it takes 60 more iterations to reach the peak.

For `eta` of 0.01, it grows too slowly, and even after 500 iterations, it hasn't reached the peak. If we tried it for more iterations, it could potentially get to the same level of AUC as other values. Even if it was the case, it's not practical: it becomes computationally expensive to evaluate all these trees during prediction time.

Thus, we use the value of 0.1 for `eta` . Next, let's tune other parameters.

Exercise 6.3

We have a gradient boosting model with `eta=0.1` . It needs 60 trees to get the peak performance. If we increase `eta` to 0.5, what will happen?

a) The number of trees will not change.

b) The model will need more trees to reach its peak performance.

c) The model will need fewer trees to reach its peak performance.

TUNING OTHER PARAMETERS

The next parameter we tune is `max_depth`. The default value is 6, so we can try

- A lower value; for example, 3
- A higher value; for example, 10

The outcome should give us an idea if the best value for `max_depth` is between 3 and 6 or between 6 and 10.

First, check 3:

```
xgb_params = {
    'eta': 0.1,
    'max_depth': 3,          ❶
    'min_child_weight': 1,

    'objective': 'binary:logistic',
    'eval_metric': 'auc',
    'nthread': 8,
    'seed': 1,
    'silent': 1
}
```

❶ Changes max_depth from 6 to 3

The best AUC we get with it is 83.6%.

Next, try 10. In this case, the best value is 81.1%.

This means that the optimal parameter of `max_depth` should be between 3 and 6. When we try 4, however, we see that the best AUC is 83%, which is slightly worse than the AUC we got with the depth of 3 (figure 6.35).

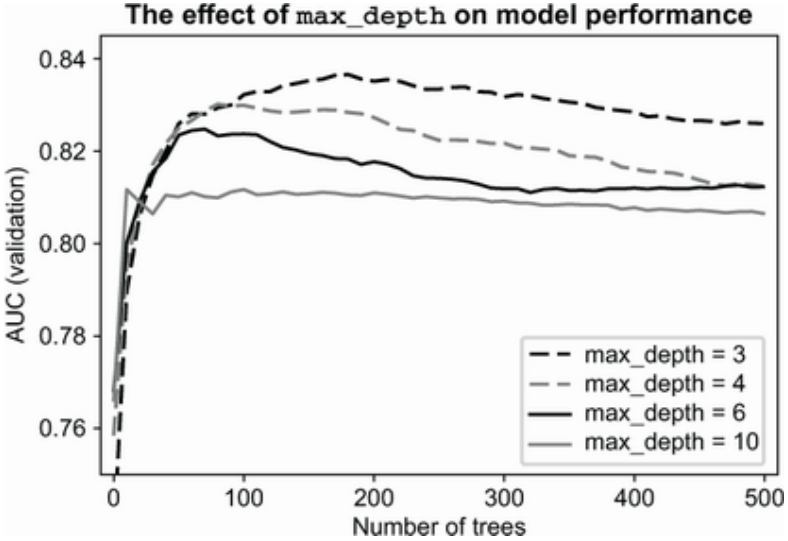


Figure 6.35 The optimal value for `max_depth` is 4: with it, we can achieve an AUC of 83.6%.

The next parameter we tune is `min_child_weight`. It's the same as `min_leaf_size` in decision trees from Scikit-learn: it controls the minimal number of observations a tree can have in a leaf.

Let's try a range of values and see which one works best. In addition to the default value (1), we can try 10 and 30 (figure 6.36).

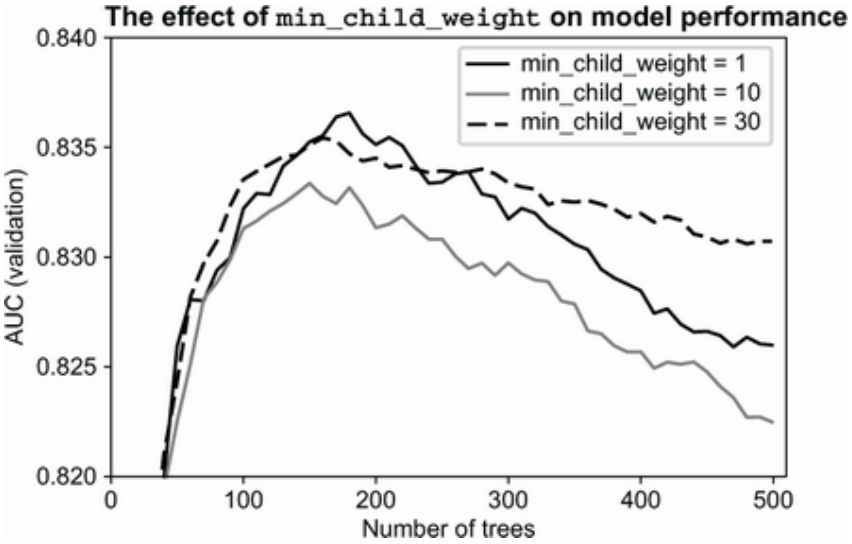


Figure 6.36 The optimal value for `min_child_weight` is 1, but it's not drastically different from other values for this parameter.

From figure 6.36 we see that

- For `min_child_weight=1` , AUC is 83.6%.
- For `min_child_weight=10` , AUC is 83.3%.
- For `min_child_weight=30` , AUC is 83.5%.

The difference between these options is not significant, so we'll leave the default value.

The parameters for our final model are

```
xgb_params = {
    'eta': 0.1,
    'max_depth': 3,
    'min_child_weight': 1,

    'objective': 'binary:logistic',
```

```
    'eval_metric': 'auc',
    'nthread': 8,
    'seed': 1,
    'silent': 1
}
```

We need to do one last step before we can finish the model: we need to select the optimal number of trees. It's quite simple: look at the iteration when the validation score peaked and use this number.

In our case, we need to train 180 trees for the final model (figure 6.37):

```
[160] train-auc:0.935513   val-auc:0.835536
[170] train-auc:0.937885   val-auc:0.836384
[180] train-auc:0.93971    val-auc:0.836565 <- best
[190] train-auc:0.942029   val-auc:0.835621
[200] train-auc:0.943343   val-auc:0.835124
```

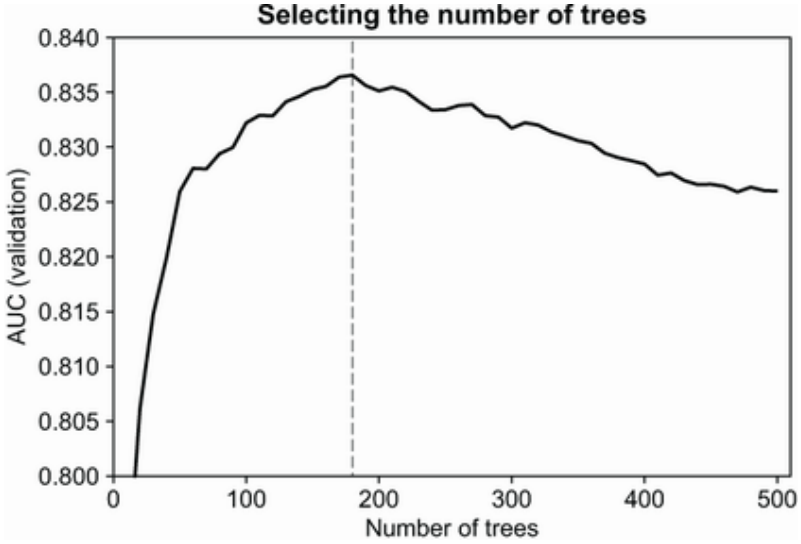


Figure 6.37 The optimal number of trees for the final model is 180.

The best the random forest model was able to get 82.5% AUC, whereas the best the gradient boosting model could get was 1% more (83.6%).

This is the best model, so let's use it as our final model—and we should use it for scoring loan applications.

6.4.4 Testing the final model

We're almost ready to use it for risk scoring. We still need to do two things before we can use it:

- Retrain the final model on both train and validation datasets combined. We no longer need the validation dataset, so we can use more data for training, which will make the model slightly better.
- Test the model on the test set. This is the part of data we kept aside from the beginning. Now we use it to make sure the model didn't overfit and performs well on completely unseen data.

The next steps are:

- Apply the same preprocessing to `df_full_train` and `df_test` as we did to `df_train` and `df_val`. As a result, we get the feature matrices `X_train` and `X_test` as well as our target variables `y_train` and `y_test`.
- Train a model on the combined dataset with the parameters we selected previously.
- Apply the model to the test data to get the test predictions.
- Verify that the model performs well and doesn't overfit.

Let's do it. First, create the target variable:

```
y_train = (df_train_full.status == 'default').values
y_test = (df_test.status == 'default').values
```

Because we use the entire DataFrame for creating the feature matrix, we need to remote the target variable:

```
del df_train_full['status']
del df_test['status']
```

Next, we convert DataFrames into lists of dictionaries and then use one-hot encoding to get the feature matrices:

```
dict_train = df_train_full.fillna(0).to_dict(orient='records')
dict_test = df_test.fillna(0).to_dict(orient='records')

dv = DictVectorizer(sparse=False)
X_train = dv.fit_transform(dict_train)
X_test = dv.transform(dict_test)
```

Finally, we train the XGBoost model using this data and the optimal parameters we determined previously:

```
dtrain = xgb.DMatrix(X_train, label=y_train, feature_names=dv.feature_names_)
dtest = xgb.DMatrix(X_test, label=y_test, feature_names=dv.feature_names_)

xgb_params = {
    'eta': 0.1,
    'max_depth': 3,
    'min_child_weight': 1,

    'objective': 'binary:logistic',
```

```
    'eval_metric': 'auc',
    'nthread': 8,
    'seed': 1,
    'silent': 1
}

num_trees = 160

model = xgb.train(xgb_params, dtrain, num_boost_round=num_trees)
```

Then evaluate its performance on the test set:

```
y_pred_xgb = model.predict(dtest)
roc_auc_score(y_test, y_pred_xgb)
```

The output is 83.2%, which is comparable to 83.6%—the performance on the validation set. It means that our model doesn't overfit and can work well with customers it hasn't seen.

Exercise 6.4

The main difference between random forest and gradient boosting is

a) Trees in gradient boosting are trained sequentially, and each next tree improves the previous one. In a random forest, all trees are trained independently.

b) Gradient boosting is a lot faster than using a random forest.

c) Trees in a random forest are trained sequentially, and each next tree improves the previous one. In gradient boosting, all trees are trained

independently.

6.5 Next steps

We've learned the basics about decision trees, random forest, and gradient boosting. We've learned a lot, but there's much more than we could fit in this chapter. You can explore this topic further by doing the exercises.

6.5.1 Exercises

- Feature engineering is the process of creating new features out of existing ones. For this project, we haven't created any features; we simply used the ones provided in the dataset. Adding more features should help improve the performance of our model. For example, we can add the ratio of requested money to the total price of the item. Experiment with engineering more features.
- When training a random forest, we get different models by selecting a random subset of features for each tree. To control the size of the subset, we use the `max_features` parameter. Try adjusting this parameter, and see if it changes the AUC on validation.
- Extreme randomized trees (or extra trees, for short) is a variation of a random forest where the idea of randomization is taken to the extreme. Instead of finding the best possible split, it picks a splitting condition randomly. This approach has a few advantages: extra trees are faster to train, and they are less prone to overfitting. On the other hand, they require more trees to have adequate performance. In Scikit-learn, `ExtraTreesClassifier` from the `ensemble` package implements it. Experiment with it for this project.

- In XGBoost, the `colsample_bytree` parameter controls the number of features we select for each tree—it's similar to `max_features` from the random forest. Experiment with this parameter, and see if it improves the performance: try values from 0.1 to 1.0 with a step of 0.1. Usually the optimal values are between 0.6 and 0.8, but sometimes 1.0 gives the best result.
- In addition to randomly selecting columns (features), we can also select a subset of rows (customers). This is called *subsampling*, and it helps to prevent overfitting. In XGBoost, the `subsample` parameter controls the fraction of examples we select for training each tree in the ensemble. Try values from 0.4 to 1.0 with a step of 0.1. Usually the optimal values are between 0.6 and 0.8.

6.5.2 Other projects

- All tree-based models can solve the regression problem—predict a number. In Scikit-learn, DecisionTreeRegressor, and RandomForestRegressor, implement the regression variation of the models. In XGBoost, we need to change the objective to `reg:squarederror`. Use these models for predicting the price of the car, and try to solve other regression problems as well.

Summary

- Decision tree is a model that represents a sequence of if-then-else decisions. It's easy to understand, and it also performs quite well in practice.
- We train decision trees by selecting the best split using impurity measures. The main parameters that we control are the depth of the tree and the maximum number of samples in each leaf.

- A random forest is a way to combine many decision trees into one model. Like a team of experts, individual trees can make mistakes, but together, they are less likely to reach an incorrect decision.
- A random forest should have a diverse set of models to make good predictions. That's why each tree in the model uses a different set of features for training.
- The main parameters we need to change for random forest are the same as for decision trees: the depth and the maximum number of samples in each leaf. Additionally, we need to select the number of trees we want to have in the ensemble.
- While in a random forest the trees are independent, in gradient boosting, the trees are sequential, and each next model corrects the mistakes of the previous one. In some cases, this leads to better predictive performance.
- The parameters we need to tune for gradient boosting are similar for a random forest: the depth, the maximum number of observations in the leaf, and the number of trees. In addition to that, we have `eta` — the learning rate. It specifies the contribution of each individual tree to the ensemble.

Tree-based models are easy to interpret and understand, and often they perform quite well. Gradient boosting is great and often achieves the best possible performance on structured data (data in tabular format).

In the next chapter, we look at neural nets: a different type of model, which, in contrast, achieves best performance on unstructured data, such as images.

Answers to exercises

- Exercise 6.1 A) With one more feature, training takes longer.
- Exercise 6.3 C) The model will need fewer trees to reach its peak performance.
- Exercise 6.2 B) Randomly selecting a different subset of features for each tree.
- Exercise 6.4 A) Trees in gradient boosting are trained sequentially. In a random forest, trees are trained independently.