Working with Real Data

When you are learning about Machine Learning it is best to actually experiment with real-world data, not just artificial datasets. Fortunately, there are thousands of open datasets to choose from, ranging across all sorts of domains. Here are a few places you can look to get data:

- Popular open data repositories:
  - UC Irvine Machine Learning Repository
  - Kaggle datasets
  - Amazon's AWS datasets
- Meta portals (they list open data repositories):
  - *http://dataportals.org/*
  - *http://opendatamonitor.eu/*
  - *http://quandl.com/*
- Other pages listing many popular open data repositories:
  - Wikipedia's list of Machine Learning datasets
  - Quora.com question
  - Datasets subreddit

In this chapter we chose the California Housing Prices dataset from the StatLib repository[2] (see Figure 2-1). This dataset was based on data from the 1990 California census. It is not exactly recent (you could still afford a nice house in the Bay Area at the time), but it has many qualities for learning, so we will pretend it is recent data. We also added a categorical attribute and removed a few features for teaching purposes.

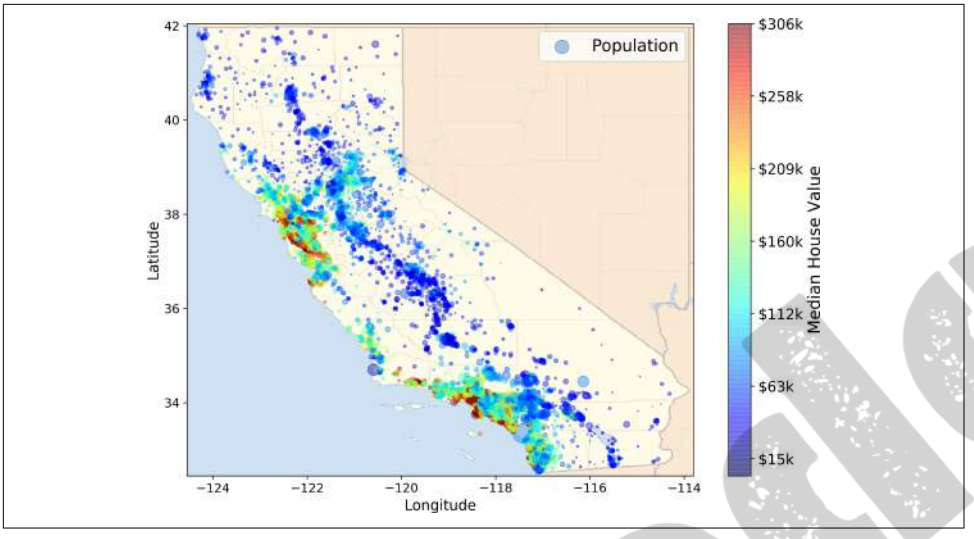


Figure 2-1. California housing prices

Look at the Big Picture

Welcome to Machine Learning Housing Corporation! The first task you are asked to perform is to build a model of housing prices in California using the California census data. This data has metrics such as the population, median income, median housing price, and so on for each block group in California. Block groups are the smallest geographical unit for which the US Census Bureau publishes sample data (a block group typically has a population of 600 to 3,000 people). We will just call them "districts" for short.

Your model should learn from this data and be able to predict the median housing price in any district, given all the other metrics.

Since you are a well-organized data scientist, the first thing you do is to pull out your Machine Learning project checklist. You can start with the one in ???; it should work reasonably well for most Machine Learning projects but make sure to adapt it to your needs. In this chapter we will go through many checklist items, but we will also skip a few, either because they are self-explanatory or because they will be discussed in later chapters.

Frame the Problem

The first question to ask your boss is what exactly is the business objective; building a model is probably not the end goal. How does the company expect to use and benefit

from this model? This is important because it will determine how you frame the problem, what algorithms you will select, what performance measure you will use to evaluate your model, and how much effort you should spend tweaking it.

Your boss answers that your model's output (a prediction of a district's median housing price) will be fed to another Machine Learning system (see Figure 2-2), along with many other *signals*.[3] This downstream system will determine whether it is worth investing in a given area or not. Getting this right is critical, as it directly affects revenue.

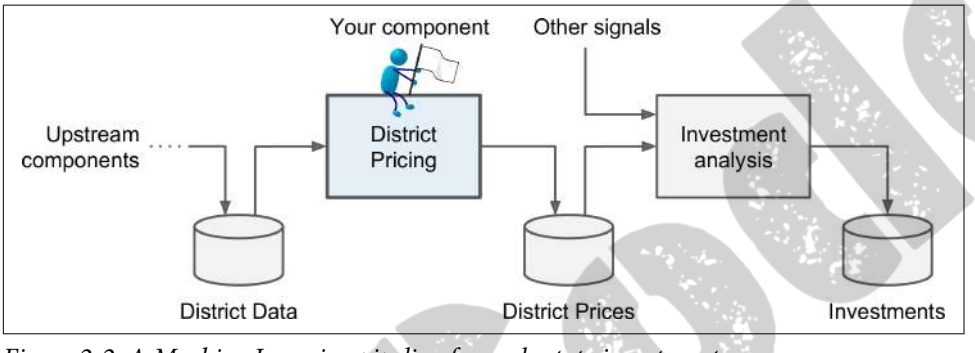


Figure 2-2. A Machine Learning pipeline for real estate investments

Pipelines

A sequence of data processing *components* is called a data *pipeline*. Pipelines are very common in Machine Learning systems, since there is a lot of data to manipulate and many data transformations to apply.

Components typically run asynchronously. Each component pulls in a large amount of data, processes it, and spits out the result in another data store, and then some time later the next component in the pipeline pulls this data and spits out its own output, and so on. Each component is fairly self-contained: the interface between components is simply the data store. This makes the system quite simple to grasp (with the help of a data flow graph), and different teams can focus on different components. Moreover, if a component breaks down, the downstream components can often continue to run normally (at least for a while) by just using the last output from the broken component. This makes the architecture quite robust.

On the other hand, a broken component can go unnoticed for some time if proper monitoring is not implemented. The data gets stale and the overall system's performance drops.

The next question to ask is what the current solution looks like (if any). It will often give you a reference performance, as well as insights on how to solve the problem. Your boss answers that the district housing prices are currently estimated manually by experts: a team gathers up-to-date information about a district, and when they cannot get the median housing price, they estimate it using complex rules.

This is costly and time-consuming, and their estimates are not great; in cases where they manage to find out the actual median housing price, they often realize that their estimates were off by more than 20%. This is why the company thinks that it would be useful to train a model to predict a district's median housing price given other data about that district. The census data looks like a great dataset to exploit for this purpose, since it includes the median housing prices of thousands of districts, as well as other data.

Okay, with all this information you are now ready to start designing your system. First, you need to frame the problem: is it supervised, unsupervised, or Reinforcement Learning? Is it a classification task, a regression task, or something else? Should you use batch learning or online learning techniques? Before you read on, pause and try to answer these questions for yourself.

Have you found the answers? Let's see: it is clearly a typical supervised learning task since you are given *labeled* training examples (each instance comes with the expected output, i.e., the district's median housing price). Moreover, it is also a typical regression task, since you are asked to predict a value. More specifically, this is a *multiple regression* problem since the system will use multiple features to make a prediction (it will use the district's population, the median income, etc.). It is also a *univariate regression* problem since we are only trying to predict a single value for each district. If we were trying to predict multiple values per district, it would be a *multivariate regression* problem. Finally, there is no continuous flow of data coming in the system, there is no particular need to adjust to changing data rapidly, and the data is small enough to fit in memory, so plain batch learning should do just fine.

If the data was huge, you could either split your batch learning work across multiple servers (using the *MapReduce* technique), or you could use an online learning technique instead.

Select a Performance Measure

Your next step is to select a performance measure. A typical performance measure for regression problems is the Root Mean Square Error (RMSE). It gives an idea of how much error the system typically makes in its predictions, with a higher weight for large errors. Equation 2-1 shows the mathematical formula to compute the RMSE.

Equation 2-1. Root Mean Square Error (RMSE)

$$\text{RMSE}(\mathbf{X}, h) = \sqrt{\frac{1}{m}\sum_{i=1}^{m}\left(h\left(\mathbf{x}^{(i)}\right) - y^{(i)}\right)^2}$$

Notations

This equation introduces several very common Machine Learning notations that we will use throughout this book:

- m is the number of instances in the dataset you are measuring the RMSE on.
  - For example, if you are evaluating the RMSE on a validation set of 2,000 districts, then $m = 2{,}000$.
- $\mathbf{x}^{(i)}$ is a vector of all the feature values (excluding the label) of the i^{th} instance in the dataset, and $y^{(i)}$ is its label (the desired output value for that instance).
  - For example, if the first district in the dataset is located at longitude –118.29°, latitude 33.91°, and it has 1,416 inhabitants with a median income of $38,372, and the median house value is $156,400 (ignoring the other features for now), then:

$$\mathbf{x}^{(1)} = \begin{pmatrix} -118.29 \\ 33.91 \\ 1{,}416 \\ 38{,}372 \end{pmatrix}$$

  and:

$$y^{(1)} = 156{,}400$$

- $\mathbf{X}$ is a matrix containing all the feature values (excluding labels) of all instances in the dataset. There is one row per instance and the i^{th} row is equal to the transpose of $\mathbf{x}^{(i)}$, noted $(\mathbf{x}^{(i)})^T$.[4]
  - For example, if the first district is as just described, then the matrix $\mathbf{X}$ looks like this:

$$\mathbf{X} = \begin{pmatrix} \left(\mathbf{x}^{(1)}\right)^T \\ \left(\mathbf{x}^{(2)}\right)^T \\ \vdots \\ \left(\mathbf{x}^{(1999)}\right)^T \\ \left(\mathbf{x}^{(2000)}\right)^T \end{pmatrix} = \begin{pmatrix} -118.29 & 33.91 & 1{,}416 & 38{,}372 \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

4 Recall that the transpose operator flips a column vector into a row vector (and vice versa).

- h is your system's prediction function, also called a *hypothesis*. When your system is given an instance's feature vector $\mathbf{x}^{(i)}$, it outputs a predicted value $\hat{y}^{(i)} = h(\mathbf{x}^{(i)})$ for that instance ($\hat{y}$ is pronounced "y-hat").
  - For example, if your system predicts that the median housing price in the first district is \$158,400, then $\hat{y}^{(1)} = h(\mathbf{x}^{(1)}) = 158{,}400$. The prediction error for this district is $\hat{y}^{(1)} - y^{(1)} = 2{,}000$.
- RMSE($\mathbf{X}$,h) is the cost function measured on the set of examples using your hypothesis h.

We use lowercase italic font for scalar values (such as m or $y^{(i)}$) and function names (such as h), lowercase bold font for vectors (such as $\mathbf{x}^{(i)}$), and uppercase bold font for matrices (such as $\mathbf{X}$).

Even though the RMSE is generally the preferred performance measure for regression tasks, in some contexts you may prefer to use another function. For example, suppose that there are many outlier districts. In that case, you may consider using the *Mean Absolute Error* (also called the Average Absolute Deviation; see Equation 2-2):

Equation 2-2. Mean Absolute Error

$$\text{MAE}(\mathbf{X}, h) = \frac{1}{m}\sum_{i=1}^{m}\left|h\left(\mathbf{x}^{(i)}\right) - y^{(i)}\right|$$

Both the RMSE and the MAE are ways to measure the distance between two vectors: the vector of predictions and the vector of target values. Various distance measures, or *norms*, are possible:

- Computing the root of a sum of squares (RMSE) corresponds to the *Euclidean norm*: it is the notion of distance you are familiar with. It is also called the ℓ_2 *norm*, noted $\|\cdot\|_2$ (or just $\|\cdot\|$).
- Computing the sum of absolutes (MAE) corresponds to the ℓ_1 *norm*, noted $\|\cdot\|_1$. It is sometimes called the *Manhattan norm* because it measures the distance between two points in a city if you can only travel along orthogonal city blocks.
- More generally, the ℓ_k *norm* of a vector $\mathbf{v}$ containing n elements is defined as $\|\mathbf{v}\|_k = \left(|v_0|^k + |v_1|^k + \cdots + |v_n|^k\right)^{\frac{1}{k}}$. ℓ_0 just gives the number of non-zero elements in the vector, and ℓ_∞ gives the maximum absolute value in the vector.
- The higher the norm index, the more it focuses on large values and neglects small ones. This is why the RMSE is more sensitive to outliers than the MAE. But when

outliers are exponentially rare (like in a bell-shaped curve), the RMSE performs very well and is generally preferred.

Check the Assumptions

Lastly, it is good practice to list and verify the assumptions that were made so far (by you or others); this can catch serious issues early on. For example, the district prices that your system outputs are going to be fed into a downstream Machine Learning system, and we assume that these prices are going to be used as such. But what if the downstream system actually converts the prices into categories (e.g., "cheap," "medium," or "expensive") and then uses those categories instead of the prices themselves? In this case, getting the price perfectly right is not important at all; your system just needs to get the category right. If that's so, then the problem should have been framed as a classification task, not a regression task. You don't want to find this out after working on a regression system for months.

Fortunately, after talking with the team in charge of the downstream system, you are confident that they do indeed need the actual prices, not just categories. Great! You're all set, the lights are green, and you can start coding now!

Get the Data

It's time to get your hands dirty. Don't hesitate to pick up your laptop and walk through the following code examples in a Jupyter notebook. The full Jupyter notebook is available at *https://github.com/ageron/handson-ml2*.

Create the Workspace

First you will need to have Python installed. It is probably already installed on your system. If not, you can get it at *https://www.python.org/*.[5]

Next you need to create a workspace directory for your Machine Learning code and datasets. Open a terminal and type the following commands (after the `$` prompts):

```
$ export ML_PATH="$HOME/ml"      # You can change the path if you prefer
$ mkdir -p $ML_PATH
```

You will need a number of Python modules: Jupyter, NumPy, Pandas, Matplotlib, and Scikit-Learn. If you already have Jupyter running with all these modules installed, you can safely skip to "Download the Data" on page 49. If you don't have them yet, there are many ways to install them (and their dependencies). You can use your sys-

tem's packaging system (e.g., apt-get on Ubuntu, or MacPorts or HomeBrew on MacOS), install a Scientific Python distribution such as Anaconda and use its packaging system, or just use Python's own packaging system, pip, which is included by default with the Python binary installers (since Python 2.7.9).[6] You can check to see if pip is installed by typing the following command:

```
$ python3 -m pip --version
pip 19.0.2 from [...]/lib/python3.6/site-packages (python 3.6)
```

You should make sure you have a recent version of pip installed. To upgrade the pip module, type:[7]

```
$ python3 -m pip install --user -U pip
Collecting pip
[...]
Successfully installed pip-19.0.2
```

Creating an Isolated Environment

If you would like to work in an isolated environment (which is strongly recommended so you can work on different projects without having conflicting library versions), install virtualenv[8] by running the following pip command (again, if you want virtualenv to be installed for all users on your machine, remove `--user` and run this command with administrator rights):

```
$ python3 -m pip install --user -U virtualenv
Collecting virtualenv
[...]
Successfully installed virtualenv
```

Now you can create an isolated Python environment by typing:

```
$ cd $ML_PATH
$ virtualenv env
Using base prefix '[...]'
New python executable in [...]/ml/env/bin/python3.6
Also creating executable in [...]/ml/env/bin/python
Installing setuptools, pip, wheel...done.
```

6 We will show the installation steps using pip in a bash shell on a Linux or MacOS system. You may need to adapt these commands to your own system. On Windows, we recommend installing Anaconda instead.

7 If you want to upgrade pip for all users on your machine rather than just your own user, you should remove the `--user` option and make sure you have administrator rights (e.g., by adding `sudo` before the whole command on Linux or MacOSX).

8 Alternative tools include venv (very similar to virtualenv and included in the standard library), virtualenvwrapper (provides extra functionalities on top of virtualenv), pyenv (allows easy switching between Python versions), and pipenv (a great packaging tool by the same author as the popular `requests` library, built on top of pip, virtualenv and more).

Now every time you want to activate this environment, just open a terminal and type:

```
$ cd $ML_PATH
$ source env/bin/activate # on Linux or MacOSX
$ .\env\Scripts\activate  # on Windows
```

To deactivate this environment, just type `deactivate`. While the environment is active, any package you install using pip will be installed in this isolated environment, and Python will only have access to these packages (if you also want access to the system's packages, you should create the environment using virtualenv's `--system-site-packages` option). Check out virtualenv's documentation for more information.

Now you can install all the required modules and their dependencies using this simple pip command (if you are not using a virtualenv, you will need the `--user` option or administrator rights):

```
$ python3 -m pip install -U jupyter matplotlib numpy pandas scipy scikit-learn
Collecting jupyter
  Downloading jupyter-1.0.0-py2.py3-none-any.whl
Collecting matplotlib
  [...]
```

To check your installation, try to import every module like this:

```
$ python3 -c "import jupyter, matplotlib, numpy, pandas, scipy, sklearn"
```

There should be no output and no error. Now you can fire up Jupyter by typing:

```
$ jupyter notebook
[I 15:24 NotebookApp] Serving notebooks from local directory: [...]/ml
[I 15:24 NotebookApp] 0 active kernels
[I 15:24 NotebookApp] The Jupyter Notebook is running at: http://localhost:8888/
[I 15:24 NotebookApp] Use Control-C to stop this server and shut down all
kernels (twice to skip confirmation).
```

A Jupyter server is now running in your terminal, listening to port 8888. You can visit this server by opening your web browser to *http://localhost:8888/* (this usually happens automatically when the server starts). You should see your empty workspace directory (containing only the *env* directory if you followed the preceding virtualenv instructions).

Now create a new Python notebook by clicking on the New button and selecting the appropriate Python version[9] (see Figure 2-3).

This does three things: first, it creates a new notebook file called *Untitled.ipynb* in your workspace; second, it starts a Jupyter Python kernel to run this notebook; and

third, it opens this notebook in a new tab. You should start by renaming this notebook to "Housing" (this will automatically rename the file to *Housing.ipynb*) by clicking Untitled and typing the new name.

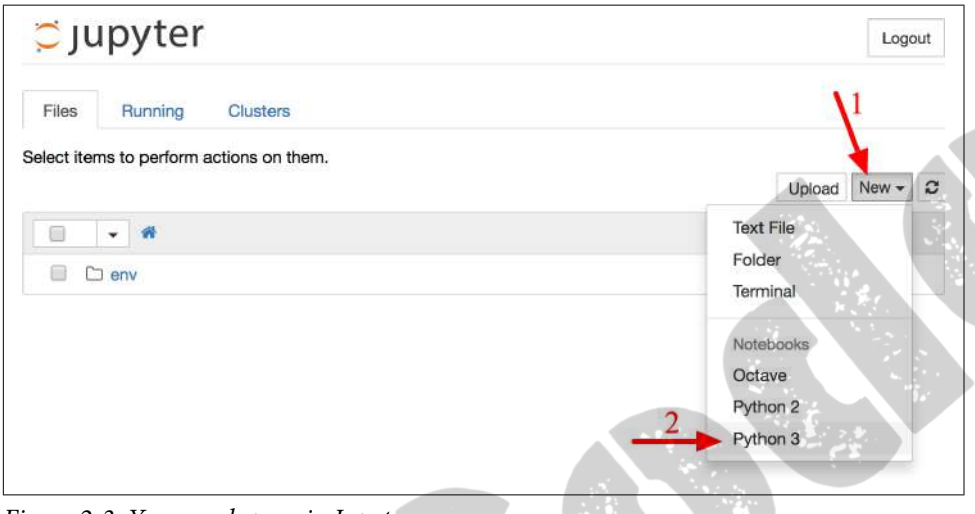


Figure 2-3. Your workspace in Jupyter

A notebook contains a list of cells. Each cell can contain executable code or formatted text. Right now the notebook contains only one empty code cell, labeled "In [1]:". Try typing **`print("Hello world!")`** in the cell, and click on the play button (see Figure 2-4) or press Shift-Enter. This sends the current cell to this notebook's Python kernel, which runs it and returns the output. The result is displayed below the cell, and since we reached the end of the notebook, a new cell is automatically created. Go through the User Interface Tour from Jupyter's Help menu to learn the basics.

Figure 2-4. Hello world Python notebook

Download the Data

In typical environments your data would be available in a relational database (or some other common datastore) and spread across multiple tables/documents/files. To access it, you would first need to get your credentials and access authorizations,[10] and familiarize yourself with the data schema. In this project, however, things are much simpler: you will just download a single compressed file, *housing.tgz*, which contains a comma-separated value (CSV) file called *housing.csv* with all the data.

You could use your web browser to download it, and run `tar xzf housing.tgz` to decompress the file and extract the CSV file, but it is preferable to create a small function to do that. It is useful in particular if data changes regularly, as it allows you to write a small script that you can run whenever you need to fetch the latest data (or you can set up a scheduled job to do that automatically at regular intervals). Automating the process of fetching the data is also useful if you need to install the dataset on multiple machines.

Here is the function to fetch the data:[11]

```
import os
import tarfile
from six.moves import urllib

DOWNLOAD_ROOT = "https://raw.githubusercontent.com/ageron/handson-ml2/master/"
HOUSING_PATH = os.path.join("datasets", "housing")
HOUSING_URL = DOWNLOAD_ROOT + "datasets/housing/housing.tgz"

def fetch_housing_data(housing_url=HOUSING_URL, housing_path=HOUSING_PATH):
    if not os.path.isdir(housing_path):
        os.makedirs(housing_path)
    tgz_path = os.path.join(housing_path, "housing.tgz")
    urllib.request.urlretrieve(housing_url, tgz_path)
    housing_tgz = tarfile.open(tgz_path)
    housing_tgz.extractall(path=housing_path)
    housing_tgz.close()
```

Now when you call `fetch_housing_data()`, it creates a *datasets/housing* directory in your workspace, downloads the *housing.tgz* file, and extracts the *housing.csv* from it in this directory.

Now let's load the data using Pandas. Once again you should write a small function to load the data:

```
import pandas as pd

def load_housing_data(housing_path=HOUSING_PATH):
    csv_path = os.path.join(housing_path, "housing.csv")
    return pd.read_csv(csv_path)
```

This function returns a Pandas DataFrame object containing all the data.

Take a Quick Look at the Data Structure

Let's take a look at the top five rows using the DataFrame's `head()` method (see Figure 2-5).

```
In [5]: housing = load_housing_data()
        housing.head()
```

Out[5]:

	longitude	latitude	housing_median_age	total_rooms	total_bedrooms	populatio
0	-122.23	37.88	41.0	880.0	129.0	322.0
1	-122.22	37.86	21.0	7099.0	1106.0	2401.0
2	-122.24	37.85	52.0	1467.0	190.0	496.0
3	-122.25	37.85	52.0	1274.0	235.0	558.0
4	-122.25	37.85	52.0	1627.0	280.0	565.0

Figure 2-5. Top five rows in the dataset

Each row represents one district. There are 10 attributes (you can see the first 6 in the screenshot): `longitude`, `latitude`, `housing_median_age`, `total_rooms`, `total_bedrooms`, `population`, `households`, `median_income`, `median_house_value`, and `ocean_proximity`.

The `info()` method is useful to get a quick description of the data, in particular the total number of rows, and each attribute's type and number of non-null values (see Figure 2-6).

```
In [6]: housing.info()
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 20640 entries, 0 to 20639
Data columns (total 10 columns):
longitude             20640 non-null float64
latitude              20640 non-null float64
housing_median_age    20640 non-null float64
total_rooms           20640 non-null float64
total_bedrooms        20433 non-null float64
population            20640 non-null float64
households            20640 non-null float64
median_income         20640 non-null float64
median_house_value    20640 non-null float64
ocean_proximity       20640 non-null object
dtypes: float64(9), object(1)
memory usage: 1.6+ MB
```

Figure 2-6. Housing info

There are 20,640 instances in the dataset, which means that it is fairly small by Machine Learning standards, but it's perfect to get started. Notice that the `total_bedrooms` attribute has only 20,433 non-null values, meaning that 207 districts are missing this feature. We will need to take care of this later.

All attributes are numerical, except the `ocean_proximity` field. Its type is `object`, so it could hold any kind of Python object, but since you loaded this data from a CSV file you know that it must be a text attribute. When you looked at the top five rows, you probably noticed that the values in the `ocean_proximity` column were repetitive, which means that it is probably a categorical attribute. You can find out what categories exist and how many districts belong to each category by using the `value_counts()` method:

```
>>> housing["ocean_proximity"].value_counts()
<1H OCEAN     9136
INLAND        6551
NEAR OCEAN    2658
NEAR BAY      2290
ISLAND           5
Name: ocean_proximity, dtype: int64
```

Let's look at the other fields. The `describe()` method shows a summary of the numerical attributes (Figure 2-7).

```
In [8]: housing.describe()
```

Out[8]:

	longitude	latitude	housing_median_age	total_rooms	total_bedrc
count	20640.000000	20640.000000	20640.000000	20640.000000	20433.0000
mean	-119.569704	35.631861	28.639486	2635.763081	537.870553
std	2.003532	2.135952	12.585558	2181.615252	421.385070
min	-124.350000	32.540000	1.000000	2.000000	1.000000
25%	-121.800000	33.930000	18.000000	1447.750000	296.000000
50%	-118.490000	34.260000	29.000000	2127.000000	435.000000
75%	-118.010000	37.710000	37.000000	3148.000000	647.000000
max	-114.310000	41.950000	52.000000	39320.000000	6445.00000

Figure 2-7. Summary of each numerical attribute

The `count`, `mean`, `min`, and `max` rows are self-explanatory. Note that the null values are ignored (so, for example, `count` of `total_bedrooms` is 20,433, not 20,640). The `std` row shows the *standard deviation*, which measures how dispersed the values are.[12] The 25%, 50%, and 75% rows show the corresponding *percentiles*: a percentile indicates the value below which a given percentage of observations in a group of observations falls. For example, 25% of the districts have a `housing_median_age` lower than 18, while 50% are lower than 29 and 75% are lower than 37. These are often called the 25th percentile (or 1st *quartile*), the median, and the 75th percentile (or 3rd quartile).

Another quick way to get a feel of the type of data you are dealing with is to plot a histogram for each numerical attribute. A histogram shows the number of instances (on the vertical axis) that have a given value range (on the horizontal axis). You can either plot this one attribute at a time, or you can call the `hist()` method on the whole dataset, and it will plot a histogram for each numerical attribute (see Figure 2-8). For example, you can see that slightly over 800 districts have a `median_house_value` equal to about $100,000.

```
%matplotlib inline   # only in a Jupyter notebook
import matplotlib.pyplot as plt
housing.hist(bins=50, figsize=(20,15))
plt.show()
```

The `hist()` method relies on Matplotlib, which in turn relies on a user-specified graphical backend to draw on your screen. So before you can plot anything, you need to specify which backend Matplotlib should use. The simplest option is to use Jupyter's magic command `%matplotlib inline`. This tells Jupyter to set up Matplotlib so it uses Jupyter's own backend. Plots are then rendered within the notebook itself. Note that calling `show()` is optional in a Jupyter notebook, as Jupyter will automatically display plots when a cell is executed.

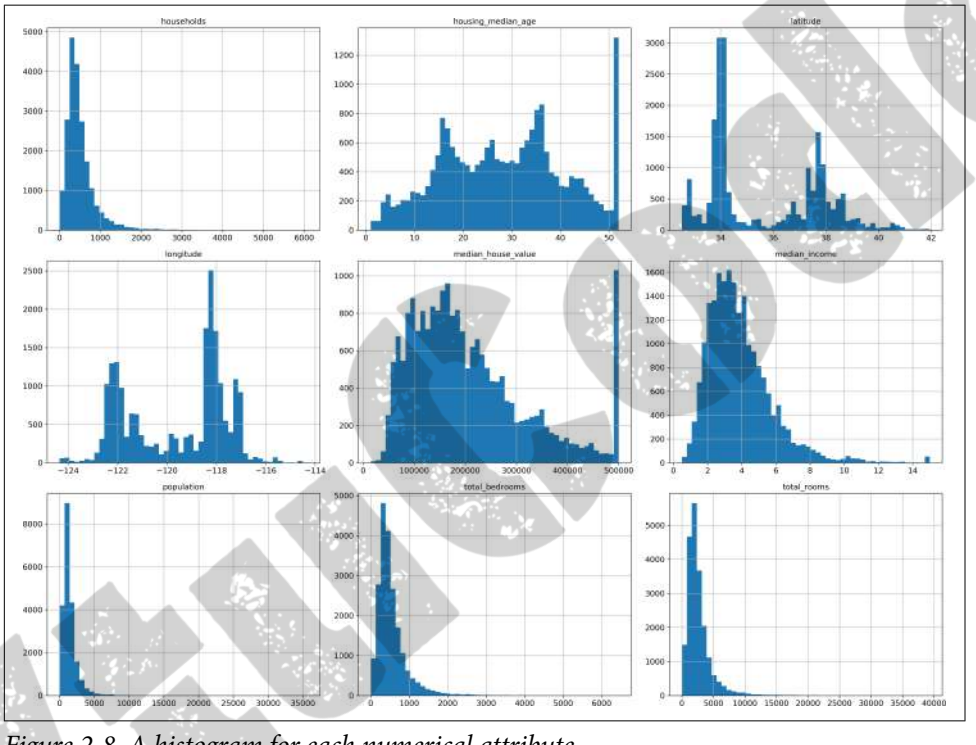


Figure 2-8. A histogram for each numerical attribute

Notice a few things in these histograms:

1. First, the median income attribute does not look like it is expressed in US dollars (USD). After checking with the team that collected the data, you are told that the data has been scaled and capped at 15 (actually 15.0001) for higher median incomes, and at 0.5 (actually 0.4999) for lower median incomes. The numbers represent roughly tens of thousands of dollars (e.g., 3 actually means about $30,000). Working with preprocessed attributes is common in Machine Learning,

and it is not necessarily a problem, but you should try to understand how the data was computed.

2. The housing median age and the median house value were also capped. The latter may be a serious problem since it is your target attribute (your labels). Your Machine Learning algorithms may learn that prices never go beyond that limit. You need to check with your client team (the team that will use your system's output) to see if this is a problem or not. If they tell you that they need precise predictions even beyond $500,000, then you have mainly two options:
   a. Collect proper labels for the districts whose labels were capped.
   b. Remove those districts from the training set (and also from the test set, since your system should not be evaluated poorly if it predicts values beyond $500,000).
3. These attributes have very different scales. We will discuss this later in this chapter when we explore feature scaling.
4. Finally, many histograms are *tail heavy*: they extend much farther to the right of the median than to the left. This may make it a bit harder for some Machine Learning algorithms to detect patterns. We will try transforming these attributes later on to have more bell-shaped distributions.

Hopefully you now have a better understanding of the kind of data you are dealing with.

Wait! Before you look at the data any further, you need to create a test set, put it aside, and never look at it.

Create a Test Set

It may sound strange to voluntarily set aside part of the data at this stage. After all, you have only taken a quick glance at the data, and surely you should learn a whole lot more about it before you decide what algorithms to use, right? This is true, but your brain is an amazing pattern detection system, which means that it is highly prone to overfitting: if you look at the test set, you may stumble upon some seemingly interesting pattern in the test data that leads you to select a particular kind of Machine Learning model. When you estimate the generalization error using the test set, your estimate will be too optimistic and you will launch a system that will not perform as well as expected. This is called *data snooping* bias.

Creating a test set is theoretically quite simple: just pick some instances randomly, typically 20% of the dataset (or less if your dataset is very large), and set them aside:

```
import numpy as np

def split_train_test(data, test_ratio):
    shuffled_indices = np.random.permutation(len(data))
    test_set_size = int(len(data) * test_ratio)
    test_indices = shuffled_indices[:test_set_size]
    train_indices = shuffled_indices[test_set_size:]
    return data.iloc[train_indices], data.iloc[test_indices]
```

You can then use this function like this:[13]

```
>>> train_set, test_set = split_train_test(housing, 0.2)
>>> len(train_set)
16512
>>> len(test_set)
4128
```

Well, this works, but it is not perfect: if you run the program again, it will generate a different test set! Over time, you (or your Machine Learning algorithms) will get to see the whole dataset, which is what you want to avoid.

One solution is to save the test set on the first run and then load it in subsequent runs. Another option is to set the random number generator's seed (e.g., `np.random.seed(42)`)[14] before calling `np.random.permutation()`, so that it always generates the same shuffled indices.

But both these solutions will break next time you fetch an updated dataset. A common solution is to use each instance's identifier to decide whether or not it should go in the test set (assuming instances have a unique and immutable identifier). For example, you could compute a hash of each instance's identifier and put that instance in the test set if the hash is lower or equal to 20% of the maximum hash value. This ensures that the test set will remain consistent across multiple runs, even if you refresh the dataset. The new test set will contain 20% of the new instances, but it will not contain any instance that was previously in the training set. Here is a possible implementation:

```
from zlib import crc32

def test_set_check(identifier, test_ratio):
    return crc32(np.int64(identifier)) & 0xffffffff < test_ratio * 2**32

def split_train_test_by_id(data, test_ratio, id_column):
    ids = data[id_column]
```

```
    in_test_set = ids.apply(lambda id_: test_set_check(id_, test_ratio))
    return data.loc[~in_test_set], data.loc[in_test_set]
```

Unfortunately, the housing dataset does not have an identifier column. The simplest solution is to use the row index as the ID:

```
housing_with_id = housing.reset_index()   # adds an `index` column
train_set, test_set = split_train_test_by_id(housing_with_id, 0.2, "index")
```

If you use the row index as a unique identifier, you need to make sure that new data gets appended to the end of the dataset, and no row ever gets deleted. If this is not possible, then you can try to use the most stable features to build a unique identifier. For example, a district's latitude and longitude are guaranteed to be stable for a few million years, so you could combine them into an ID like so:[15]

```
housing_with_id["id"] = housing["longitude"] * 1000 + housing["latitude"]
train_set, test_set = split_train_test_by_id(housing_with_id, 0.2, "id")
```

Scikit-Learn provides a few functions to split datasets into multiple subsets in various ways. The simplest function is `train_test_split`, which does pretty much the same thing as the function `split_train_test` defined earlier, with a couple of additional features. First there is a `random_state` parameter that allows you to set the random generator seed as explained previously, and second you can pass it multiple datasets with an identical number of rows, and it will split them on the same indices (this is very useful, for example, if you have a separate DataFrame for labels):

```
from sklearn.model_selection import train_test_split

train_set, test_set = train_test_split(housing, test_size=0.2, random_state=42)
```

So far we have considered purely random sampling methods. This is generally fine if your dataset is large enough (especially relative to the number of attributes), but if it is not, you run the risk of introducing a significant sampling bias. When a survey company decides to call 1,000 people to ask them a few questions, they don't just pick 1,000 people randomly in a phone book. They try to ensure that these 1,000 people are representative of the whole population. For example, the US population is composed of 51.3% female and 48.7% male, so a well-conducted survey in the US would try to maintain this ratio in the sample: 513 female and 487 male. This is called *stratified sampling*: the population is divided into homogeneous subgroups called *strata*, and the right number of instances is sampled from each stratum to guarantee that the test set is representative of the overall population. If they used purely random sampling, there would be about 12% chance of sampling a skewed test set with either less than 49% female or more than 54% female. Either way, the survey results would be significantly biased.

Suppose you chatted with experts who told you that the median income is a very important attribute to predict median housing prices. You may want to ensure that the test set is representative of the various categories of incomes in the whole dataset. Since the median income is a continuous numerical attribute, you first need to create an income category attribute. Let's look at the median income histogram more closely (back in Figure 2-8): most median income values are clustered around 1.5 to 6 (i.e., $15,000–$60,000), but some median incomes go far beyond 6. It is important to have a sufficient number of instances in your dataset for each stratum, or else the estimate of the stratum's importance may be biased. This means that you should not have too many strata, and each stratum should be large enough. The following code uses the `pd.cut()` function to create an income category attribute with 5 categories (labeled from 1 to 5): category 1 ranges from 0 to 1.5 (i.e., less than $15,000), category 2 from 1.5 to 3, and so on:

```
housing["income_cat"] = pd.cut(housing["median_income"],
                               bins=[0., 1.5, 3.0, 4.5, 6., np.inf],
                               labels=[1, 2, 3, 4, 5])
```

These income categories are represented in Figure 2-9:

```
housing["income_cat"].hist()
```

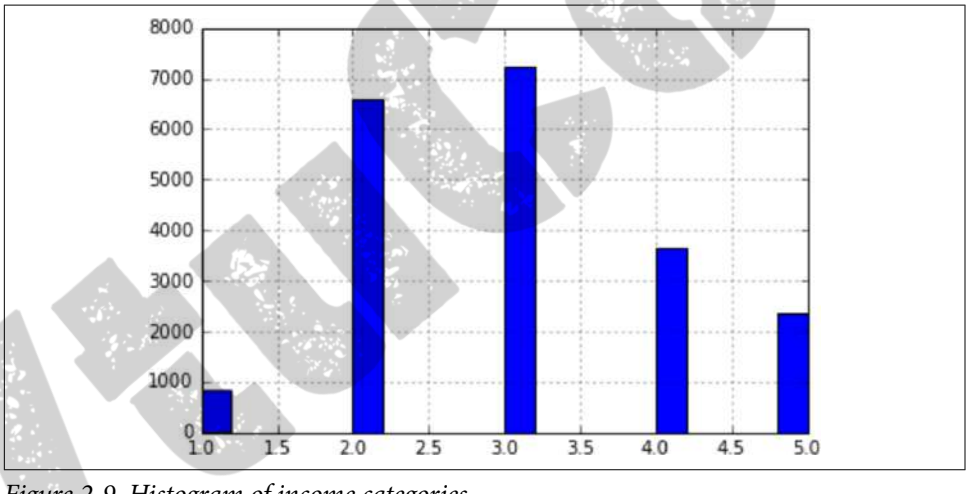


Figure 2-9. Histogram of income categories

Now you are ready to do stratified sampling based on the income category. For this you can use Scikit-Learn's `StratifiedShuffleSplit` class:

```
from sklearn.model_selection import StratifiedShuffleSplit

split = StratifiedShuffleSplit(n_splits=1, test_size=0.2, random_state=42)
for train_index, test_index in split.split(housing, housing["income_cat"]):
    strat_train_set = housing.loc[train_index]
    strat_test_set = housing.loc[test_index]
```

Let's see if this worked as expected. You can start by looking at the income category proportions in the test set:

```
>>> strat_test_set["income_cat"].value_counts() / len(strat_test_set)
3    0.350533
2    0.318798
4    0.176357
5    0.114583
1    0.039729
Name: income_cat, dtype: float64
```

With similar code you can measure the income category proportions in the full dataset. Figure 2-10 compares the income category proportions in the overall dataset, in the test set generated with stratified sampling, and in a test set generated using purely random sampling. As you can see, the test set generated using stratified sampling has income category proportions almost identical to those in the full dataset, whereas the test set generated using purely random sampling is quite skewed.

	Overall	Random	Stratified	Rand. %error	Strat. %error
1.0	0.039826	0.040213	0.039738	0.973236	-0.219137
2.0	0.318847	0.324370	0.318876	1.732260	0.009032
3.0	0.350581	0.358527	0.350618	2.266446	0.010408
4.0	0.176308	0.167393	0.176399	-5.056334	0.051717
5.0	0.114438	0.109496	0.114369	-4.318374	-0.060464

Figure 2-10. Sampling bias comparison of stratified versus purely random sampling

Now you should remove the `income_cat` attribute so the data is back to its original state:

```
for set_ in (strat_train_set, strat_test_set):
    set_.drop("income_cat", axis=1, inplace=True)
```

We spent quite a bit of time on test set generation for a good reason: this is an often neglected but critical part of a Machine Learning project. Moreover, many of these ideas will be useful later when we discuss cross-validation. Now it's time to move on to the next stage: exploring the data.

Discover and Visualize the Data to Gain Insights

So far you have only taken a quick glance at the data to get a general understanding of the kind of data you are manipulating. Now the goal is to go a little bit more in depth.

First, make sure you have put the test set aside and you are only exploring the training set. Also, if the training set is very large, you may want to sample an exploration

set, to make manipulations easy and fast. In our case, the set is quite small so you can just work directly on the full set. Let's create a copy so you can play with it without harming the training set:

```
housing = strat_train_set.copy()
```

Visualizing Geographical Data

Since there is geographical information (latitude and longitude), it is a good idea to create a scatterplot of all districts to visualize the data (Figure 2-11):

```
housing.plot(kind="scatter", x="longitude", y="latitude")
```

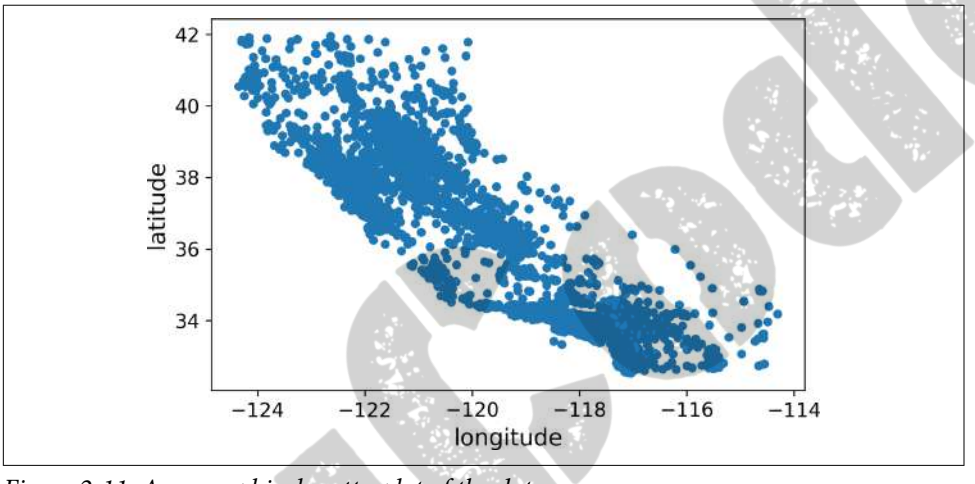


Figure 2-11. A geographical scatterplot of the data

This looks like California all right, but other than that it is hard to see any particular pattern. Setting the `alpha` option to `0.1` makes it much easier to visualize the places where there is a high density of data points (Figure 2-12):

```
housing.plot(kind="scatter", x="longitude", y="latitude", alpha=0.1)
```

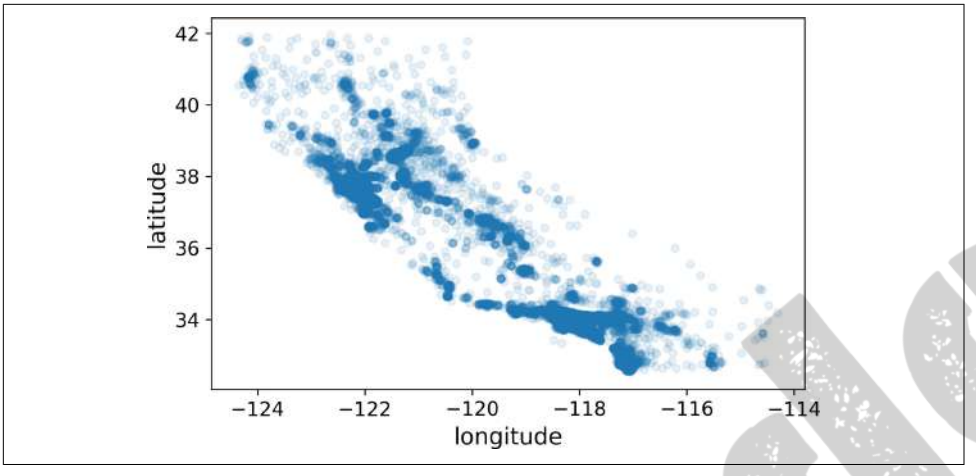


Figure 2-12. A better visualization highlighting high-density areas

Now that's much better: you can clearly see the high-density areas, namely the Bay Area and around Los Angeles and San Diego, plus a long line of fairly high density in the Central Valley, in particular around Sacramento and Fresno.

More generally, our brains are very good at spotting patterns on pictures, but you may need to play around with visualization parameters to make the patterns stand out.

Now let's look at the housing prices (Figure 2-13). The radius of each circle represents the district's population (option `s`), and the color represents the price (option `c`). We will use a predefined color map (option `cmap`) called `jet`, which ranges from blue (low values) to red (high prices):[16]

```
housing.plot(kind="scatter", x="longitude", y="latitude", alpha=0.4,
    s=housing["population"]/100, label="population", figsize=(10,7),
    c="median_house_value", cmap=plt.get_cmap("jet"), colorbar=True,
)
plt.legend()
```

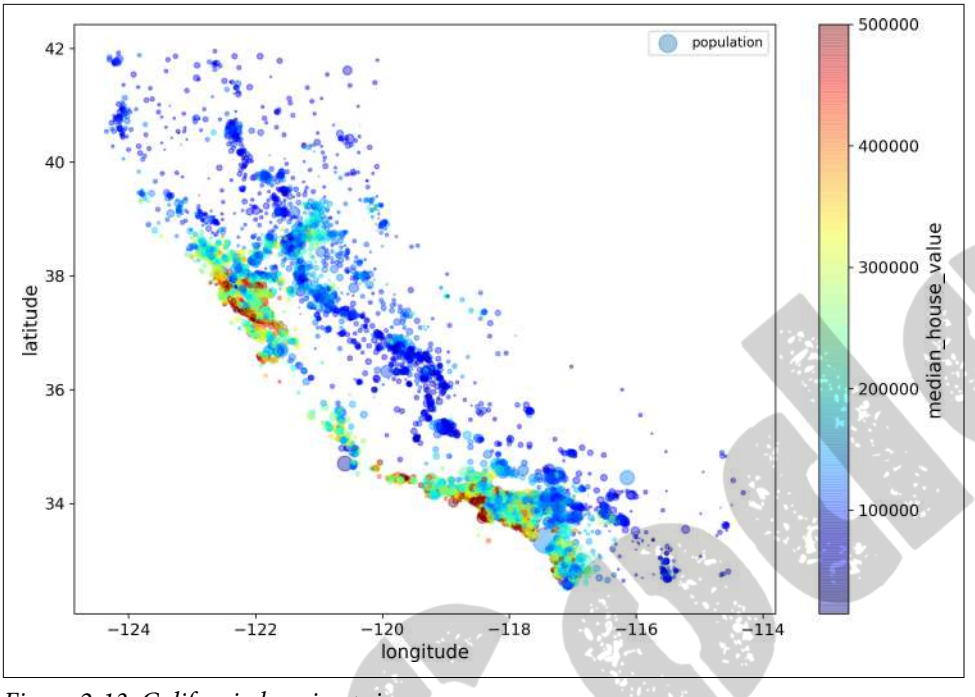


Figure 2-13. California housing prices

This image tells you that the housing prices are very much related to the location (e.g., close to the ocean) and to the population density, as you probably knew already. It will probably be useful to use a clustering algorithm to detect the main clusters, and add new features that measure the proximity to the cluster centers. The ocean proximity attribute may be useful as well, although in Northern California the housing prices in coastal districts are not too high, so it is not a simple rule.

Looking for Correlations

Since the dataset is not too large, you can easily compute the *standard correlation coefficient* (also called *Pearson's r*) between every pair of attributes using the `corr()` method:

```
corr_matrix = housing.corr()
```

Now let's look at how much each attribute correlates with the median house value:

```
>>> corr_matrix["median_house_value"].sort_values(ascending=False)
median_house_value    1.000000
median_income         0.687170
total_rooms           0.135231
housing_median_age    0.114220
households            0.064702
total_bedrooms        0.047865
population           -0.026699
longitude            -0.047279
latitude             -0.142826
Name: median_house_value, dtype: float64
```

The correlation coefficient ranges from –1 to 1. When it is close to 1, it means that there is a strong positive correlation; for example, the median house value tends to go up when the median income goes up. When the coefficient is close to –1, it means that there is a strong negative correlation; you can see a small negative correlation between the latitude and the median house value (i.e., prices have a slight tendency to go down when you go north). Finally, coefficients close to zero mean that there is no linear correlation. Figure 2-14 shows various plots along with the correlation coefficient between their horizontal and vertical axes.

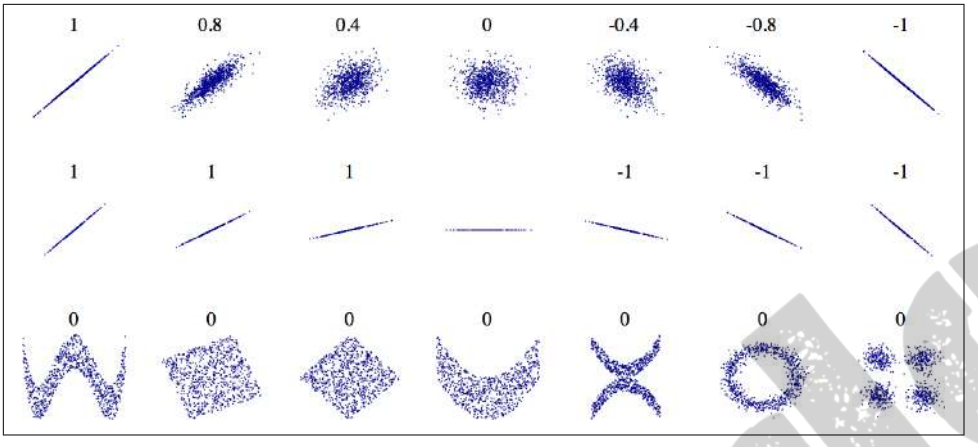


Figure 2-14. Standard correlation coefficient of various datasets (source: Wikipedia; public domain image)

The correlation coefficient only measures linear correlations ("if *x* goes up, then *y* generally goes up/down"). It may completely miss out on nonlinear relationships (e.g., "if *x* is close to zero then *y* generally goes up"). Note how all the plots of the bottom row have a correlation coefficient equal to zero despite the fact that their axes are clearly not independent: these are examples of nonlinear relationships. Also, the second row shows examples where the correlation coefficient is equal to 1 or –1; notice that this has nothing to do with the slope. For example, your height in inches has a correlation coefficient of 1 with your height in feet or in nanometers.

Another way to check for correlation between attributes is to use Pandas' `scatter_matrix` function, which plots every numerical attribute against every other numerical attribute. Since there are now 11 numerical attributes, you would get $11^2 = 121$ plots, which would not fit on a page, so let's just focus on a few promising attributes that seem most correlated with the median housing value (Figure 2-15):

```
from pandas.plotting import scatter_matrix

attributes = ["median_house_value", "median_income", "total_rooms",
              "housing_median_age"]
scatter_matrix(housing[attributes], figsize=(12, 8))
```

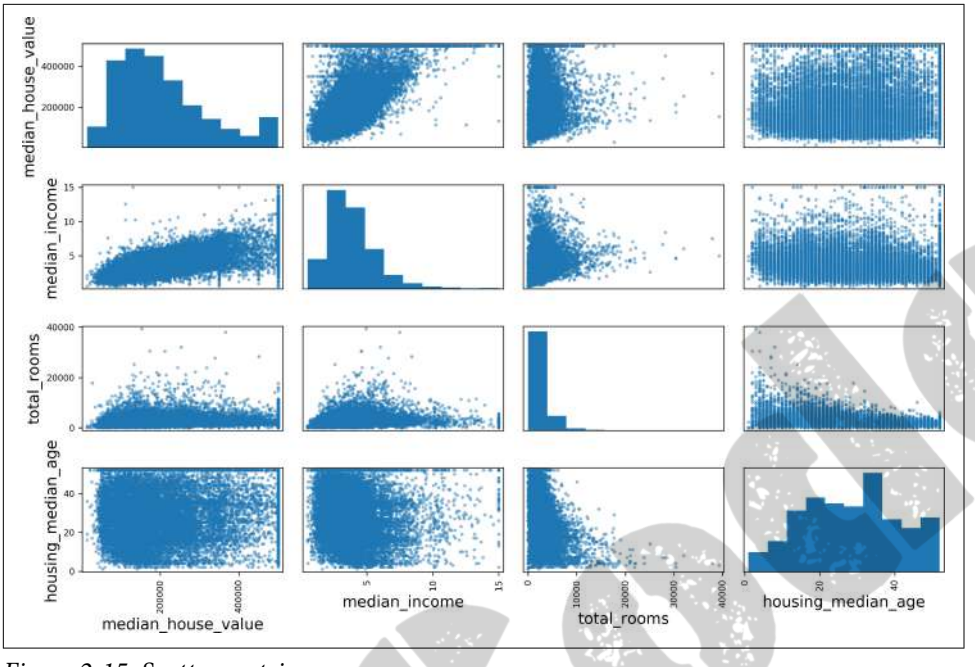


Figure 2-15. Scatter matrix

The main diagonal (top left to bottom right) would be full of straight lines if Pandas plotted each variable against itself, which would not be very useful. So instead Pandas displays a histogram of each attribute (other options are available; see Pandas' documentation for more details).

The most promising attribute to predict the median house value is the median income, so let's zoom in on their correlation scatterplot (Figure 2-16):

```
housing.plot(kind="scatter", x="median_income", y="median_house_value",
             alpha=0.1)
```

This plot reveals a few things. First, the correlation is indeed very strong; you can clearly see the upward trend and the points are not too dispersed. Second, the price cap that we noticed earlier is clearly visible as a horizontal line at $500,000. But this plot reveals other less obvious straight lines: a horizontal line around $450,000, another around $350,000, perhaps one around $280,000, and a few more below that. You may want to try removing the corresponding districts to prevent your algorithms from learning to reproduce these data quirks.

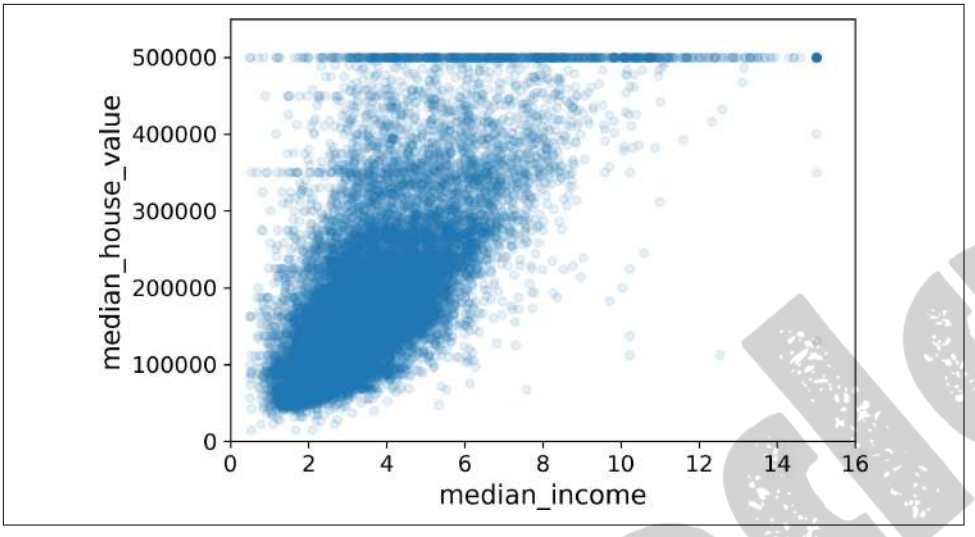


Figure 2-16. Median income versus median house value

Experimenting with Attribute Combinations

Hopefully the previous sections gave you an idea of a few ways you can explore the data and gain insights. You identified a few data quirks that you may want to clean up before feeding the data to a Machine Learning algorithm, and you found interesting correlations between attributes, in particular with the target attribute. You also noticed that some attributes have a tail-heavy distribution, so you may want to transform them (e.g., by computing their logarithm). Of course, your mileage will vary considerably with each project, but the general ideas are similar.

One last thing you may want to do before actually preparing the data for Machine Learning algorithms is to try out various attribute combinations. For example, the total number of rooms in a district is not very useful if you don't know how many households there are. What you really want is the number of rooms per household. Similarly, the total number of bedrooms by itself is not very useful: you probably want to compare it to the number of rooms. And the population per household also seems like an interesting attribute combination to look at. Let's create these new attributes:

```
housing["rooms_per_household"] = housing["total_rooms"]/housing["households"]
housing["bedrooms_per_room"] = housing["total_bedrooms"]/housing["total_rooms"]
housing["population_per_household"]=housing["population"]/housing["households"]
```

And now let's look at the correlation matrix again:

```
>>> corr_matrix = housing.corr()
>>> corr_matrix["median_house_value"].sort_values(ascending=False)
median_house_value          1.000000
```

```
median_income               0.687160
rooms_per_household         0.146285
total_rooms                 0.135097
housing_median_age          0.114110
households                  0.064506
total_bedrooms              0.047689
population_per_household   -0.021985
population                 -0.026920
longitude                  -0.047432
latitude                   -0.142724
bedrooms_per_room          -0.259984
Name: median_house_value, dtype: float64
```

Hey, not bad! The new `bedrooms_per_room` attribute is much more correlated with the median house value than the total number of rooms or bedrooms. Apparently houses with a lower bedroom/room ratio tend to be more expensive. The number of rooms per household is also more informative than the total number of rooms in a district—obviously the larger the houses, the more expensive they are.

This round of exploration does not have to be absolutely thorough; the point is to start off on the right foot and quickly gain insights that will help you get a first reasonably good prototype. But this is an iterative process: once you get a prototype up and running, you can analyze its output to gain more insights and come back to this exploration step.

Prepare the Data for Machine Learning Algorithms

It's time to prepare the data for your Machine Learning algorithms. Instead of just doing this manually, you should write functions to do that, for several good reasons:

- This will allow you to reproduce these transformations easily on any dataset (e.g., the next time you get a fresh dataset).
- You will gradually build a library of transformation functions that you can reuse in future projects.
- You can use these functions in your live system to transform the new data before feeding it to your algorithms.
- This will make it possible for you to easily try various transformations and see which combination of transformations works best.

But first let's revert to a clean training set (by copying `strat_train_set` once again), and let's separate the predictors and the labels since we don't necessarily want to apply the same transformations to the predictors and the target values (note that `drop()` creates a copy of the data and does not affect `strat_train_set`):

```
housing = strat_train_set.drop("median_house_value", axis=1)
housing_labels = strat_train_set["median_house_value"].copy()
```

Data Cleaning

Most Machine Learning algorithms cannot work with missing features, so let's create a few functions to take care of them. You noticed earlier that the `total_bedrooms` attribute has some missing values, so let's fix this. You have three options:

- Get rid of the corresponding districts.
- Get rid of the whole attribute.
- Set the values to some value (zero, the mean, the median, etc.).

You can accomplish these easily using DataFrame's `dropna()`, `drop()`, and `fillna()` methods:

```
housing.dropna(subset=["total_bedrooms"])    # option 1
housing.drop("total_bedrooms", axis=1)       # option 2
median = housing["total_bedrooms"].median()  # option 3
housing["total_bedrooms"].fillna(median, inplace=True)
```

If you choose option 3, you should compute the median value on the training set, and use it to fill the missing values in the training set, but also don't forget to save the median value that you have computed. You will need it later to replace missing values in the test set when you want to evaluate your system, and also once the system goes live to replace missing values in new data.

Scikit-Learn provides a handy class to take care of missing values: `SimpleImputer`. Here is how to use it. First, you need to create a `SimpleImputer` instance, specifying that you want to replace each attribute's missing values with the median of that attribute:

```
from sklearn.impute import SimpleImputer

imputer = SimpleImputer(strategy="median")
```

Since the median can only be computed on numerical attributes, we need to create a copy of the data without the text attribute `ocean_proximity`:

```
housing_num = housing.drop("ocean_proximity", axis=1)
```

Now you can fit the `imputer` instance to the training data using the `fit()` method:

```
imputer.fit(housing_num)
```

The `imputer` has simply computed the median of each attribute and stored the result in its `statistics_` instance variable. Only the `total_bedrooms` attribute had missing values, but we cannot be sure that there won't be any missing values in new data after the system goes live, so it is safer to apply the `imputer` to all the numerical attributes:

```
>>> imputer.statistics_
array([ -118.51 , 34.26 , 29. , 2119.5 , 433. , 1164. , 408. , 3.5409])
```

```
>>> housing_num.median().values
array([ -118.51 , 34.26 , 29. , 2119.5 , 433. , 1164. , 408. , 3.5409])
```

Now you can use this "trained" `imputer` to transform the training set by replacing missing values by the learned medians:

```
X = imputer.transform(housing_num)
```

The result is a plain NumPy array containing the transformed features. If you want to put it back into a Pandas DataFrame, it's simple:

```
housing_tr = pd.DataFrame(X, columns=housing_num.columns)
```

Scikit-Learn Design

Scikit-Learn's API is remarkably well designed. The main design principles are:[17]

- **Consistency**. All objects share a consistent and simple interface:
  - — *Estimators*. Any object that can estimate some parameters based on a dataset is called an *estimator* (e.g., an `imputer` is an estimator). The estimation itself is performed by the `fit()` method, and it takes only a dataset as a parameter (or two for supervised learning algorithms; the second dataset contains the labels). Any other parameter needed to guide the estimation process is considered a hyperparameter (such as an `imputer`'s `strategy`), and it must be set as an instance variable (generally via a constructor parameter).
  - — *Transformers*. Some estimators (such as an `imputer`) can also transform a dataset; these are called *transformers*. Once again, the API is quite simple: the transformation is performed by the `transform()` method with the dataset to transform as a parameter. It returns the transformed dataset. This transformation generally relies on the learned parameters, as is the case for an `imputer`. All transformers also have a convenience method called `fit_transform()` that is equivalent to calling `fit()` and then `transform()` (but sometimes `fit_transform()` is optimized and runs much faster).
  - — *Predictors*. Finally, some estimators are capable of making predictions given a dataset; they are called *predictors*. For example, the `LinearRegression` model in the previous chapter was a predictor: it predicted life satisfaction given a country's GDP per capita. A predictor has a `predict()` method that takes a dataset of new instances and returns a dataset of corresponding predictions. It also has a `score()` method that measures the quality of the predictions given

a test set (and the corresponding labels in the case of supervised learning algorithms).[18]

- **Inspection**. All the estimator's hyperparameters are accessible directly via public instance variables (e.g., `imputer.strategy`), and all the estimator's learned parameters are also accessible via public instance variables with an underscore suffix (e.g., `imputer.statistics_`).
- **Nonproliferation of classes**. Datasets are represented as NumPy arrays or SciPy sparse matrices, instead of homemade classes. Hyperparameters are just regular Python strings or numbers.
- **Composition**. Existing building blocks are reused as much as possible. For example, it is easy to create a `Pipeline` estimator from an arbitrary sequence of transformers followed by a final estimator, as we will see.
- **Sensible defaults**. Scikit-Learn provides reasonable default values for most parameters, making it easy to create a baseline working system quickly.

Handling Text and Categorical Attributes

Earlier we left out the categorical attribute `ocean_proximity` because it is a text attribute so we cannot compute its median:

```
>>> housing_cat = housing[["ocean_proximity"]]
>>> housing_cat.head(10)
       ocean_proximity
17606        <1H OCEAN
18632        <1H OCEAN
14650       NEAR OCEAN
3230            INLAND
3555         <1H OCEAN
19480           INLAND
8879         <1H OCEAN
13685           INLAND
4937         <1H OCEAN
4861         <1H OCEAN
```

Most Machine Learning algorithms prefer to work with numbers anyway, so let's convert these categories from text to numbers. For this, we can use Scikit-Learn's `OrdinalEncoder` class[19]:

```
>>> from sklearn.preprocessing import OrdinalEncoder
>>> ordinal_encoder = OrdinalEncoder()
```

```
>>> housing_cat_encoded = ordinal_encoder.fit_transform(housing_cat)
>>> housing_cat_encoded[:10]
array([[0.],
       [0.],
       [4.],
       [1.],
       [0.],
       [1.],
       [0.],
       [1.],
       [0.],
       [0.]])
```

You can get the list of categories using the `categories_` instance variable. It is a list containing a 1D array of categories for each categorical attribute (in this case, a list containing a single array since there is just one categorical attribute):

```
>>> ordinal_encoder.categories_
[array(['<1H OCEAN', 'INLAND', 'ISLAND', 'NEAR BAY', 'NEAR OCEAN'],
       dtype=object)]
```

One issue with this representation is that ML algorithms will assume that two nearby values are more similar than two distant values. This may be fine in some cases (e.g., for ordered categories such as "bad", "average", "good", "excellent"), but it is obviously not the case for the `ocean_proximity` column (for example, categories 0 and 4 are clearly more similar than categories 0 and 1). To fix this issue, a common solution is to create one binary attribute per category: one attribute equal to 1 when the category is "<1H OCEAN" (and 0 otherwise), another attribute equal to 1 when the category is "INLAND" (and 0 otherwise), and so on. This is called *one-hot encoding*, because only one attribute will be equal to 1 (hot), while the others will be 0 (cold). The new attributes are sometimes called *dummy* attributes. Scikit-Learn provides a `OneHotEncoder` class to convert categorical values into one-hot vectors[20]:

```
>>> from sklearn.preprocessing import OneHotEncoder
>>> cat_encoder = OneHotEncoder()
>>> housing_cat_1hot = cat_encoder.fit_transform(housing_cat)
>>> housing_cat_1hot
<16512x5 sparse matrix of type '<class 'numpy.float64'>'
    with 16512 stored elements in Compressed Sparse Row format>
```

Notice that the output is a SciPy *sparse matrix*, instead of a NumPy array. This is very useful when you have categorical attributes with thousands of categories. After one-hot encoding we get a matrix with thousands of columns, and the matrix is full of zeros except for a single 1 per row. Using up tons of memory mostly to store zeros would be very wasteful, so instead a sparse matrix only stores the location of the non-

zero elements. You can use it mostly like a normal 2D array,[21] but if you really want to convert it to a (dense) NumPy array, just call the `toarray()` method:

```
>>> housing_cat_1hot.toarray()
array([[1., 0., 0., 0., 0.],
       [1., 0., 0., 0., 0.],
       [0., 0., 0., 0., 1.],
       ...,
       [0., 1., 0., 0., 0.],
       [1., 0., 0., 0., 0.],
       [0., 0., 0., 1., 0.]])
```

Once again, you can get the list of categories using the encoder's `categories_` instance variable:

```
>>> cat_encoder.categories_
[array(['<1H OCEAN', 'INLAND', 'ISLAND', 'NEAR BAY', 'NEAR OCEAN'],
       dtype=object)]
```

If a categorical attribute has a large number of possible categories (e.g., country code, profession, species, etc.), then one-hot encoding will result in a large number of input features. This may slow down training and degrade performance. If this happens, you may want to replace the categorical input with useful numerical features related to the categories: for example, you could replace the `ocean_proximity` feature with the distance to the ocean (similarly, a country code could be replaced with the country's population and GDP per capita). Alternatively, you could replace each category with a learnable low dimensional vector called an *embedding*. Each category's representation would be learned during training: this is an example of *representation learning* (see Chapter 13 and ??? for more details).

Custom Transformers

Although Scikit-Learn provides many useful transformers, you will need to write your own for tasks such as custom cleanup operations or combining specific attributes. You will want your transformer to work seamlessly with Scikit-Learn functionalities (such as pipelines), and since Scikit-Learn relies on duck typing (not inheritance), all you need is to create a class and implement three methods: `fit()` (returning `self`), `transform()`, and `fit_transform()`. You can get the last one for free by simply adding `TransformerMixin` as a base class. Also, if you add `BaseEstimator` as a base class (and avoid `*args` and `**kargs` in your constructor) you will get two extra methods (`get_params()` and `set_params()`) that will be useful for auto-

matic hyperparameter tuning. For example, here is a small transformer class that adds the combined attributes we discussed earlier:

```
from sklearn.base import BaseEstimator, TransformerMixin

rooms_ix, bedrooms_ix, population_ix, households_ix = 3, 4, 5, 6

class CombinedAttributesAdder(BaseEstimator, TransformerMixin):
    def __init__(self, add_bedrooms_per_room = True): # no *args or **kargs
        self.add_bedrooms_per_room = add_bedrooms_per_room
    def fit(self, X, y=None):
        return self  # nothing else to do
    def transform(self, X, y=None):
        rooms_per_household = X[:, rooms_ix] / X[:, households_ix]
        population_per_household = X[:, population_ix] / X[:, households_ix]
        if self.add_bedrooms_per_room:
            bedrooms_per_room = X[:, bedrooms_ix] / X[:, rooms_ix]
            return np.c_[X, rooms_per_household, population_per_household,
                         bedrooms_per_room]
        else:
            return np.c_[X, rooms_per_household, population_per_household]

attr_adder = CombinedAttributesAdder(add_bedrooms_per_room=False)
housing_extra_attribs = attr_adder.transform(housing.values)
```

In this example the transformer has one hyperparameter, `add_bedrooms_per_room`, set to `True` by default (it is often helpful to provide sensible defaults). This hyperparameter will allow you to easily find out whether adding this attribute helps the Machine Learning algorithms or not. More generally, you can add a hyperparameter to gate any data preparation step that you are not 100% sure about. The more you automate these data preparation steps, the more combinations you can automatically try out, making it much more likely that you will find a great combination (and saving you a lot of time).

Feature Scaling

One of the most important transformations you need to apply to your data is *feature scaling*. With few exceptions, Machine Learning algorithms don't perform well when the input numerical attributes have very different scales. This is the case for the housing data: the total number of rooms ranges from about 6 to 39,320, while the median incomes only range from 0 to 15. Note that scaling the target values is generally not required.

There are two common ways to get all attributes to have the same scale: *min-max scaling* and *standardization*.

Min-max scaling (many people call this *normalization*) is quite simple: values are shifted and rescaled so that they end up ranging from 0 to 1. We do this by subtracting the min value and dividing by the max minus the min. Scikit-Learn provides a

transformer called `MinMaxScaler` for this. It has a `feature_range` hyperparameter that lets you change the range if you don't want 0–1 for some reason.

Standardization is quite different: first it subtracts the mean value (so standardized values always have a zero mean), and then it divides by the standard deviation so that the resulting distribution has unit variance. Unlike min-max scaling, standardization does not bound values to a specific range, which may be a problem for some algorithms (e.g., neural networks often expect an input value ranging from 0 to 1). However, standardization is much less affected by outliers. For example, suppose a district had a median income equal to 100 (by mistake). Min-max scaling would then crush all the other values from 0–15 down to 0–0.15, whereas standardization would not be much affected. Scikit-Learn provides a transformer called `StandardScaler` for standardization.

As with all the transformations, it is important to fit the scalers to the training data only, not to the full dataset (including the test set). Only then can you use them to transform the training set and the test set (and new data).

Transformation Pipelines

As you can see, there are many data transformation steps that need to be executed in the right order. Fortunately, Scikit-Learn provides the `Pipeline` class to help with such sequences of transformations. Here is a small pipeline for the numerical attributes:

```
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler

num_pipeline = Pipeline([
        ('imputer', SimpleImputer(strategy="median")),
        ('attribs_adder', CombinedAttributesAdder()),
        ('std_scaler', StandardScaler()),
    ])

housing_num_tr = num_pipeline.fit_transform(housing_num)
```

The `Pipeline` constructor takes a list of name/estimator pairs defining a sequence of steps. All but the last estimator must be transformers (i.e., they must have a `fit_transform()` method). The names can be anything you like (as long as they are unique and don't contain double underscores "__"): they will come in handy later for hyperparameter tuning.

When you call the pipeline's `fit()` method, it calls `fit_transform()` sequentially on all transformers, passing the output of each call as the parameter to the next call, until it reaches the final estimator, for which it just calls the `fit()` method.

The pipeline exposes the same methods as the final estimator. In this example, the last estimator is a `StandardScaler`, which is a transformer, so the pipeline has a `transform()` method that applies all the transforms to the data in sequence (and of course also a `fit_transform()` method, which is the one we used).

So far, we have handled the categorical columns and the numerical columns separately. It would be more convenient to have a single transformer able to handle all columns, applying the appropriate transformations to each column. In version 0.20, Scikit-Learn introduced the `ColumnTransformer` for this purpose, and the good news is that it works great with Pandas DataFrames. Let's use it to apply all the transformations to the housing data:

```
from sklearn.compose import ColumnTransformer

num_attribs = list(housing_num)
cat_attribs = ["ocean_proximity"]

full_pipeline = ColumnTransformer([
        ("num", num_pipeline, num_attribs),
        ("cat", OneHotEncoder(), cat_attribs),
    ])

housing_prepared = full_pipeline.fit_transform(housing)
```

Here is how this works: first we import the `ColumnTransformer` class, next we get the list of numerical column names and the list of categorical column names, and we construct a `ColumnTransformer`. The constructor requires a list of tuples, where each tuple contains a name[22], a transformer and a list of names (or indices) of columns that the transformer should be applied to. In this example, we specify that the numerical columns should be transformed using the `num_pipeline` that we defined earlier, and the categorical columns should be transformed using a `OneHotEncoder`. Finally, we apply this `ColumnTransformer` to the housing data: it applies each transformer to the appropriate columns and concatenates the outputs along the second axis (the transformers must return the same number of rows).

Note that the `OneHotEncoder` returns a sparse matrix, while the `num_pipeline` returns a dense matrix. When there is such a mix of sparse and dense matrices, the `ColumnTransformer` estimates the density of the final matrix (i.e., the ratio of non-zero cells), and it returns a sparse matrix if the density is lower than a given threshold (by default, `sparse_threshold=0.3`). In this example, it returns a dense matrix. And that's it! We have a preprocessing pipeline that takes the full housing data and applies the appropriate transformations to each column.

Instead of a transformer, you can specify the string `"drop"` if you want the columns to be dropped. Or you can specify `"passthrough"` if you want the columns to be left untouched. By default, the remaining columns (i.e., the ones that were not listed) will be dropped, but you can set the `remainder` hyperparameter to any transformer (or to `"passthrough"`) if you want these columns to be handled differently.

If you are using Scikit-Learn 0.19 or earlier, you can use a third-party library such as `sklearn-pandas`, or roll out your own custom transformer to get the same functionality as the `ColumnTransformer`. Alternatively, you can use the `FeatureUnion` class which can also apply different transformers and concatenate their outputs, but you cannot specify different columns for each transformer, they all apply to the whole data. It is possible to work around this limitation using a custom transformer for column selection (see the Jupyter notebook for an example).

Select and Train a Model

At last! You framed the problem, you got the data and explored it, you sampled a training set and a test set, and you wrote transformation pipelines to clean up and prepare your data for Machine Learning algorithms automatically. You are now ready to select and train a Machine Learning model.

Training and Evaluating on the Training Set

The good news is that thanks to all these previous steps, things are now going to be much simpler than you might think. Let's first train a Linear Regression model, like we did in the previous chapter:

```
from sklearn.linear_model import LinearRegression

lin_reg = LinearRegression()
lin_reg.fit(housing_prepared, housing_labels)
```

Done! You now have a working Linear Regression model. Let's try it out on a few instances from the training set:

```
>>> some_data = housing.iloc[:5]
>>> some_labels = housing_labels.iloc[:5]
>>> some_data_prepared = full_pipeline.transform(some_data)
>>> print("Predictions:", lin_reg.predict(some_data_prepared))
Predictions: [ 210644.6045  317768.8069  210956.4333  59218.9888  189747.5584]
>>> print("Labels:", list(some_labels))
Labels: [286600.0, 340600.0, 196900.0, 46300.0, 254500.0]
```

It works, although the predictions are not exactly accurate (e.g., the first prediction is off by close to 40%!). Let's measure this regression model's RMSE on the whole training set using Scikit-Learn's `mean_squared_error` function:

```
>>> from sklearn.metrics import mean_squared_error
>>> housing_predictions = lin_reg.predict(housing_prepared)
>>> lin_mse = mean_squared_error(housing_labels, housing_predictions)
>>> lin_rmse = np.sqrt(lin_mse)
>>> lin_rmse
68628.19819848922
```

Okay, this is better than nothing but clearly not a great score: most districts' `median_housing_values` range between $120,000 and $265,000, so a typical prediction error of $68,628 is not very satisfying. This is an example of a model underfitting the training data. When this happens it can mean that the features do not provide enough information to make good predictions, or that the model is not powerful enough. As we saw in the previous chapter, the main ways to fix underfitting are to select a more powerful model, to feed the training algorithm with better features, or to reduce the constraints on the model. This model is not regularized, so this rules out the last option. You could try to add more features (e.g., the log of the population), but first let's try a more complex model to see how it does.

Let's train a `DecisionTreeRegressor`. This is a powerful model, capable of finding complex nonlinear relationships in the data (Decision Trees are presented in more detail in Chapter 6). The code should look familiar by now:

```
from sklearn.tree import DecisionTreeRegressor

tree_reg = DecisionTreeRegressor()
tree_reg.fit(housing_prepared, housing_labels)
```

Now that the model is trained, let's evaluate it on the training set:

```
>>> housing_predictions = tree_reg.predict(housing_prepared)
>>> tree_mse = mean_squared_error(housing_labels, housing_predictions)
>>> tree_rmse = np.sqrt(tree_mse)
>>> tree_rmse
0.0
```

Wait, what!? No error at all? Could this model really be absolutely perfect? Of course, it is much more likely that the model has badly overfit the data. How can you be sure? As we saw earlier, you don't want to touch the test set until you are ready to launch a model you are confident about, so you need to use part of the training set for training, and part for model validation.

Better Evaluation Using Cross-Validation

One way to evaluate the Decision Tree model would be to use the `train_test_split` function to split the training set into a smaller training set and a validation set, then

train your models against the smaller training set and evaluate them against the validation set. It's a bit of work, but nothing too difficult and it would work fairly well.

A great alternative is to use Scikit-Learn's *K-fold cross-validation* feature. The following code randomly splits the training set into 10 distinct subsets called *folds*, then it trains and evaluates the Decision Tree model 10 times, picking a different fold for evaluation every time and training on the other 9 folds. The result is an array containing the 10 evaluation scores:

```
from sklearn.model_selection import cross_val_score
scores = cross_val_score(tree_reg, housing_prepared, housing_labels,
                         scoring="neg_mean_squared_error", cv=10)
tree_rmse_scores = np.sqrt(-scores)
```

Scikit-Learn's cross-validation features expect a utility function (greater is better) rather than a cost function (lower is better), so the scoring function is actually the opposite of the MSE (i.e., a negative value), which is why the preceding code computes `-scores` before calculating the square root.

Let's look at the results:

```
>>> def display_scores(scores):
...     print("Scores:", scores)
...     print("Mean:", scores.mean())
...     print("Standard deviation:", scores.std())
...
>>> display_scores(tree_rmse_scores)
Scores: [70194.33680785 66855.16363941 72432.58244769 70758.73896782
 71115.88230639 75585.14172901 70262.86139133 70273.6325285
 75366.87952553 71231.65726027]
Mean: 71407.68766037929
Standard deviation: 2439.4345041191004
```

Now the Decision Tree doesn't look as good as it did earlier. In fact, it seems to perform worse than the Linear Regression model! Notice that cross-validation allows you to get not only an estimate of the performance of your model, but also a measure of how precise this estimate is (i.e., its standard deviation). The Decision Tree has a score of approximately 71,407, generally ±2,439. You would not have this information if you just used one validation set. But cross-validation comes at the cost of training the model several times, so it is not always possible.

Let's compute the same scores for the Linear Regression model just to be sure:

```
>>> lin_scores = cross_val_score(lin_reg, housing_prepared, housing_labels,
...                              scoring="neg_mean_squared_error", cv=10)
...
>>> lin_rmse_scores = np.sqrt(-lin_scores)
>>> display_scores(lin_rmse_scores)
```

```
Scores: [66782.73843989 66960.118071   70347.95244419 74739.57052552
 68031.13388938 71193.84183426 64969.63056405 68281.61137997
 71552.91566558 67665.10082067]
Mean: 69052.46136345083
Standard deviation: 2731.674001798348
```

That's right: the Decision Tree model is overfitting so badly that it performs worse than the Linear Regression model.

Let's try one last model now: the `RandomForestRegressor`. As we will see in Chapter 7, Random Forests work by training many Decision Trees on random subsets of the features, then averaging out their predictions. Building a model on top of many other models is called *Ensemble Learning*, and it is often a great way to push ML algorithms even further. We will skip most of the code since it is essentially the same as for the other models:

```
>>> from sklearn.ensemble import RandomForestRegressor
>>> forest_reg = RandomForestRegressor()
>>> forest_reg.fit(housing_prepared, housing_labels)
>>> [...]
>>> forest_rmse
18603.515021376355
>>> display_scores(forest_rmse_scores)
Scores: [49519.80364233 47461.9115823  50029.02762854 52325.28068953
 49308.39426421 53446.37892622 48634.8036574  47585.73832311
 53490.10699751 50021.5852922 ]
Mean: 50182.303100336096
Standard deviation: 2097.0810550985693
```

Wow, this is much better: Random Forests look very promising. However, note that the score on the training set is still much lower than on the validation sets, meaning that the model is still overfitting the training set. Possible solutions for overfitting are to simplify the model, constrain it (i.e., regularize it), or get a lot more training data. However, before you dive much deeper in Random Forests, you should try out many other models from various categories of Machine Learning algorithms (several Support Vector Machines with different kernels, possibly a neural network, etc.), without spending too much time tweaking the hyperparameters. The goal is to shortlist a few (two to five) promising models.

You should save every model you experiment with, so you can come back easily to any model you want. Make sure you save both the hyperparameters and the trained parameters, as well as the cross-validation scores and perhaps the actual predictions as well. This will allow you to easily compare scores across model types, and compare the types of errors they make. You can easily save Scikit-Learn models by using Python's `pickle` module, or using `sklearn.externals.joblib`, which is more efficient at serializing large NumPy arrays:

```
from sklearn.externals import joblib

joblib.dump(my_model, "my_model.pkl")
# and later...
my_model_loaded = joblib.load("my_model.pkl")
```

Fine-Tune Your Model

Let's assume that you now have a shortlist of promising models. You now need to fine-tune them. Let's look at a few ways you can do that.

Grid Search

One way to do that would be to fiddle with the hyperparameters manually, until you find a great combination of hyperparameter values. This would be very tedious work, and you may not have time to explore many combinations.

Instead you should get Scikit-Learn's `GridSearchCV` to search for you. All you need to do is tell it which hyperparameters you want it to experiment with, and what values to try out, and it will evaluate all the possible combinations of hyperparameter values, using cross-validation. For example, the following code searches for the best combination of hyperparameter values for the `RandomForestRegressor`:

```
from sklearn.model_selection import GridSearchCV

param_grid = [
    {'n_estimators': [3, 10, 30], 'max_features': [2, 4, 6, 8]},
    {'bootstrap': [False], 'n_estimators': [3, 10], 'max_features': [2, 3, 4]},
  ]

forest_reg = RandomForestRegressor()

grid_search = GridSearchCV(forest_reg, param_grid, cv=5,
                           scoring='neg_mean_squared_error',
                           return_train_score=True)

grid_search.fit(housing_prepared, housing_labels)
```

When you have no idea what value a hyperparameter should have, a simple approach is to try out consecutive powers of 10 (or a smaller number if you want a more fine-grained search, as shown in this example with the `n_estimators` hyperparameter).

This `param_grid` tells Scikit-Learn to first evaluate all 3 × 4 = 12 combinations of `n_estimators` and `max_features` hyperparameter values specified in the first `dict` (don't worry about what these hyperparameters mean for now; they will be explained in Chapter 7), then try all 2 × 3 = 6 combinations of hyperparameter values in the second `dict`, but this time with the `bootstrap` hyperparameter set to `False` instead of `True` (which is the default value for this hyperparameter).

All in all, the grid search will explore 12 + 6 = 18 combinations of `RandomForestRegressor` hyperparameter values, and it will train each model five times (since we are using five-fold cross validation). In other words, all in all, there will be 18 × 5 = 90 rounds of training! It may take quite a long time, but when it is done you can get the best combination of parameters like this:

```
>>> grid_search.best_params_
{'max_features': 8, 'n_estimators': 30}
```

Since 8 and 30 are the maximum values that were evaluated, you should probably try searching again with higher values, since the score may continue to improve.

You can also get the best estimator directly:

```
>>> grid_search.best_estimator_
RandomForestRegressor(bootstrap=True, criterion='mse', max_depth=None,
           max_features=8, max_leaf_nodes=None, min_impurity_decrease=0.0,
           min_impurity_split=None, min_samples_leaf=1,
           min_samples_split=2, min_weight_fraction_leaf=0.0,
           n_estimators=30, n_jobs=None, oob_score=False, random_state=None,
           verbose=0, warm_start=False)
```

If `GridSearchCV` is initialized with `refit=True` (which is the default), then once it finds the best estimator using cross-validation, it retrains it on the whole training set. This is usually a good idea since feeding it more data will likely improve its performance.

And of course the evaluation scores are also available:

```
>>> cvres = grid_search.cv_results_
>>> for mean_score, params in zip(cvres["mean_test_score"], cvres["params"]):
```

```
...     print(np.sqrt(-mean_score), params)
...
63669.05791727153 {'max_features': 2, 'n_estimators': 3}
55627.16171305252 {'max_features': 2, 'n_estimators': 10}
53384.57867637289 {'max_features': 2, 'n_estimators': 30}
60965.99185930139 {'max_features': 4, 'n_estimators': 3}
52740.98248528835 {'max_features': 4, 'n_estimators': 10}
50377.344409590376 {'max_features': 4, 'n_estimators': 30}
58663.84733372485 {'max_features': 6, 'n_estimators': 3}
52006.15355973719 {'max_features': 6, 'n_estimators': 10}
50146.465964159885 {'max_features': 6, 'n_estimators': 30}
57869.25504027614 {'max_features': 8, 'n_estimators': 3}
51711.09443660957 {'max_features': 8, 'n_estimators': 10}
49682.25345942335 {'max_features': 8, 'n_estimators': 30}
62895.088889905004 {'bootstrap': False, 'max_features': 2, 'n_estimators': 3}
54658.14484390074 {'bootstrap': False, 'max_features': 2, 'n_estimators': 10}
59470.399594730654 {'bootstrap': False, 'max_features': 3, 'n_estimators': 3}
52725.01091081235 {'bootstrap': False, 'max_features': 3, 'n_estimators': 10}
57490.612956065226 {'bootstrap': False, 'max_features': 4, 'n_estimators': 3}
51009.51445842374 {'bootstrap': False, 'max_features': 4, 'n_estimators': 10}
```

In this example, we obtain the best solution by setting the `max_features` hyperparameter to `8`, and the `n_estimators` hyperparameter to `30`. The RMSE score for this combination is 49,682, which is slightly better than the score you got earlier using the default hyperparameter values (which was 50,182). Congratulations, you have successfully fine-tuned your best model!

Don't forget that you can treat some of the data preparation steps as hyperparameters. For example, the grid search will automatically find out whether or not to add a feature you were not sure about (e.g., using the `add_bedrooms_per_room` hyperparameter of your `CombinedAttributesAdder` transformer). It may similarly be used to automatically find the best way to handle outliers, missing features, feature selection, and more.

Randomized Search

The grid search approach is fine when you are exploring relatively few combinations, like in the previous example, but when the hyperparameter *search space* is large, it is often preferable to use `RandomizedSearchCV` instead. This class can be used in much the same way as the `GridSearchCV` class, but instead of trying out all possible combinations, it evaluates a given number of random combinations by selecting a random value for each hyperparameter at every iteration. This approach has two main benefits:

- If you let the randomized search run for, say, 1,000 iterations, this approach will explore 1,000 different values for each hyperparameter (instead of just a few values per hyperparameter with the grid search approach).
- You have more control over the computing budget you want to allocate to hyperparameter search, simply by setting the number of iterations.

Ensemble Methods

Another way to fine-tune your system is to try to combine the models that perform best. The group (or "ensemble") will often perform better than the best individual model (just like Random Forests perform better than the individual Decision Trees they rely on), especially if the individual models make very different types of errors. We will cover this topic in more detail in Chapter 7.

Analyze the Best Models and Their Errors

You will often gain good insights on the problem by inspecting the best models. For example, the `RandomForestRegressor` can indicate the relative importance of each attribute for making accurate predictions:

```
>>> feature_importances = grid_search.best_estimator_.feature_importances_
>>> feature_importances
array([7.33442355e-02, 6.29090705e-02, 4.11437985e-02, 1.46726854e-02,
       1.41064835e-02, 1.48742809e-02, 1.42575993e-02, 3.66158981e-01,
       5.64191792e-02, 1.08792957e-01, 5.33510773e-02, 1.03114883e-02,
       1.64780994e-01, 6.02803867e-05, 1.96041560e-03, 2.85647464e-03])
```

Let's display these importance scores next to their corresponding attribute names:

```
>>> extra_attribs = ["rooms_per_hhold", "pop_per_hhold", "bedrooms_per_room"]
>>> cat_encoder = full_pipeline.named_transformers_["cat"]
>>> cat_one_hot_attribs = list(cat_encoder.categories_[0])
>>> attributes = num_attribs + extra_attribs + cat_one_hot_attribs
>>> sorted(zip(feature_importances, attributes), reverse=True)
[(0.3661589806181342, 'median_income'),
 (0.1647809935615905, 'INLAND'),
 (0.10879295677551573, 'pop_per_hhold'),
 (0.07334423551601242, 'longitude'),
 (0.0629090704826203, 'latitude'),
 (0.05641917918195401, 'rooms_per_hhold'),
 (0.05335107734767581, 'bedrooms_per_room'),
 (0.041143798478729635, 'housing_median_age'),
 (0.014874280890402767, 'population'),
 (0.014672685420543237, 'total_rooms'),
 (0.014257599323407807, 'households'),
 (0.014106483453584102, 'total_bedrooms'),
 (0.010311488326303787, '<1H OCEAN'),
 (0.002856474637320158, 'NEAR OCEAN'),
```

```
    (0.00196041559947807, 'NEAR BAY'),
    (6.028038672736599e-05, 'ISLAND')]
```

With this information, you may want to try dropping some of the less useful features (e.g., apparently only one `ocean_proximity` category is really useful, so you could try dropping the others).

You should also look at the specific errors that your system makes, then try to understand why it makes them and what could fix the problem (adding extra features or, on the contrary, getting rid of uninformative ones, cleaning up outliers, etc.).

Evaluate Your System on the Test Set

After tweaking your models for a while, you eventually have a system that performs sufficiently well. Now is the time to evaluate the final model on the test set. There is nothing special about this process; just get the predictors and the labels from your test set, run your `full_pipeline` to transform the data (call `transform()`, *not* `fit_transform()`, you do not want to fit the test set!), and evaluate the final model on the test set:

```
final_model = grid_search.best_estimator_

X_test = strat_test_set.drop("median_house_value", axis=1)
y_test = strat_test_set["median_house_value"].copy()

X_test_prepared = full_pipeline.transform(X_test)

final_predictions = final_model.predict(X_test_prepared)

final_mse = mean_squared_error(y_test, final_predictions)
final_rmse = np.sqrt(final_mse)  # => evaluates to 47,730.2
```

In some cases, such a point estimate of the generalization error will not be quite enough to convince you to launch: what if it is just 0.1% better than the model currently in production? You might want to have an idea of how precise this estimate is. For this, you can compute a 95% *confidence interval* for the generalization error using `scipy.stats.t.interval()`:

```
>>> from scipy import stats
>>> confidence = 0.95
>>> squared_errors = (final_predictions - y_test) ** 2
>>> np.sqrt(stats.t.interval(confidence, len(squared_errors) - 1,
...                          loc=squared_errors.mean(),
...                          scale=stats.sem(squared_errors)))
...
array([45685.10470776, 49691.25001878])
```

The performance will usually be slightly worse than what you measured using cross-validation if you did a lot of hyperparameter tuning (because your system ends up fine-tuned to perform well on the validation data, and will likely not perform as well

on unknown datasets). It is not the case in this example, but when this happens you must resist the temptation to tweak the hyperparameters to make the numbers look good on the test set; the improvements would be unlikely to generalize to new data.

Now comes the project prelaunch phase: you need to present your solution (highlighting what you have learned, what worked and what did not, what assumptions were made, and what your system's limitations are), document everything, and create nice presentations with clear visualizations and easy-to-remember statements (e.g., "the median income is the number one predictor of housing prices"). In this California housing example, the final performance of the system is not better than the experts', but it may still be a good idea to launch it, especially if this frees up some time for the experts so they can work on more interesting and productive tasks.

Launch, Monitor, and Maintain Your System

Perfect, you got approval to launch! You need to get your solution ready for production, in particular by plugging the production input data sources into your system and writing tests.

You also need to write monitoring code to check your system's live performance at regular intervals and trigger alerts when it drops. This is important to catch not only sudden breakage, but also performance degradation. This is quite common because models tend to "rot" as data evolves over time, unless the models are regularly trained on fresh data.

Evaluating your system's performance will require sampling the system's predictions and evaluating them. This will generally require a human analysis. These analysts may be field experts, or workers on a crowdsourcing platform (such as Amazon Mechanical Turk or CrowdFlower). Either way, you need to plug the human evaluation pipeline into your system.

You should also make sure you evaluate the system's input data quality. Sometimes performance will degrade slightly because of a poor quality signal (e.g., a malfunctioning sensor sending random values, or another team's output becoming stale), but it may take a while before your system's performance degrades enough to trigger an alert. If you monitor your system's inputs, you may catch this earlier. Monitoring the inputs is particularly important for online learning systems.

Finally, you will generally want to train your models on a regular basis using fresh data. You should automate this process as much as possible. If you don't, you are very likely to refresh your model only every six months (at best), and your system's performance may fluctuate severely over time. If your system is an online learning system, you should make sure you save snapshots of its state at regular intervals so you can easily roll back to a previously working state.

Classification

With Early Release ebooks, you get books in their earliest form—the author's raw and unedited content as he or she writes—so you can take advantage of these technologies long before the official release of these titles. The following will be Chapter 3 in the final release of the book.

In Chapter 1 we mentioned that the most common supervised learning tasks are regression (predicting values) and classification (predicting classes). In Chapter 2 we explored a regression task, predicting housing values, using various algorithms such as Linear Regression, Decision Trees, and Random Forests (which will be explained in further detail in later chapters). Now we will turn our attention to classification systems.

MNIST

In this chapter, we will be using the MNIST dataset, which is a set of 70,000 small images of digits handwritten by high school students and employees of the US Census Bureau. Each image is labeled with the digit it represents. This set has been studied so much that it is often called the "Hello World" of Machine Learning: whenever people come up with a new classification algorithm, they are curious to see how it will perform on MNIST. Whenever someone learns Machine Learning, sooner or later they tackle MNIST.

Scikit-Learn provides many helper functions to download popular datasets. MNIST is one of them. The following code fetches the MNIST dataset:[1]

```
>>> from sklearn.datasets import fetch_openml
>>> mnist = fetch_openml('mnist_784', version=1)
>>> mnist.keys()
dict_keys(['data', 'target', 'feature_names', 'DESCR', 'details',
           'categories', 'url'])
```

Datasets loaded by Scikit-Learn generally have a similar dictionary structure including:

- A `DESCR` key describing the dataset
- A `data` key containing an array with one row per instance and one column per feature
- A `target` key containing an array with the labels

Let's look at these arrays:

```
>>> X, y = mnist["data"], mnist["target"]
>>> X.shape
(70000, 784)
>>> y.shape
(70000,)
```

There are 70,000 images, and each image has 784 features. This is because each image is 28×28 pixels, and each feature simply represents one pixel's intensity, from 0 (white) to 255 (black). Let's take a peek at one digit from the dataset. All you need to do is grab an instance's feature vector, reshape it to a 28×28 array, and display it using Matplotlib's `imshow()` function:

```
import matplotlib as mpl
import matplotlib.pyplot as plt

some_digit = X[0]
some_digit_image = some_digit.reshape(28, 28)

plt.imshow(some_digit_image, cmap = mpl.cm.binary, interpolation="nearest")
plt.axis("off")
plt.show()
```

This looks like a 5, and indeed that's what the label tells us:

```
>>> y[0]
'5'
```

Note that the label is a string. We prefer numbers, so let's cast `y` to integers:

```
>>> y = y.astype(np.uint8)
```

Figure 3-1 shows a few more images from the MNIST dataset to give you a feel for the complexity of the classification task.

Figure 3-1. A few digits from the MNIST dataset

But wait! You should always create a test set and set it aside before inspecting the data closely. The MNIST dataset is actually already split into a training set (the first 60,000 images) and a test set (the last 10,000 images):

```
X_train, X_test, y_train, y_test = X[:60000], X[60000:], y[:60000], y[60000:]
```

The training set is already shuffled for us, which is good as this guarantees that all cross-validation folds will be similar (you don't want one fold to be missing some digits). Moreover, some learning algorithms are sensitive to the order of the training

instances, and they perform poorly if they get many similar instances in a row. Shuffling the dataset ensures that this won't happen.[2]

Training a Binary Classifier

Let's simplify the problem for now and only try to identify one digit—for example, the number 5. This "5-detector" will be an example of a *binary classifier*, capable of distinguishing between just two classes, 5 and not-5. Let's create the target vectors for this classification task:

```
y_train_5 = (y_train == 5)  # True for all 5s, False for all other digits.
y_test_5 = (y_test == 5)
```

Okay, now let's pick a classifier and train it. A good place to start is with a *Stochastic Gradient Descent* (SGD) classifier, using Scikit-Learn's `SGDClassifier` class. This classifier has the advantage of being capable of handling very large datasets efficiently. This is in part because SGD deals with training instances independently, one at a time (which also makes SGD well suited for *online learning*), as we will see later. Let's create an `SGDClassifier` and train it on the whole training set:

```
from sklearn.linear_model import SGDClassifier

sgd_clf = SGDClassifier(random_state=42)
sgd_clf.fit(X_train, y_train_5)
```

The `SGDClassifier` relies on randomness during training (hence the name "stochastic"). If you want reproducible results, you should set the `random_state` parameter.

Now you can use it to detect images of the number 5:

```
>>> sgd_clf.predict([some_digit])
array([ True])
```

The classifier guesses that this image represents a 5 (`True`). Looks like it guessed right in this particular case! Now, let's evaluate this model's performance.

Performance Measures

Evaluating a classifier is often significantly trickier than evaluating a regressor, so we will spend a large part of this chapter on this topic. There are many performance

measures available, so grab another coffee and get ready to learn many new concepts and acronyms!

Measuring Accuracy Using Cross-Validation

A good way to evaluate a model is to use cross-validation, just as you did in Chapter 2.

Implementing Cross-Validation

Occasionally you will need more control over the cross-validation process than what Scikit-Learn provides off-the-shelf. In these cases, you can implement cross-validation yourself; it is actually fairly straightforward. The following code does roughly the same thing as Scikit-Learn's `cross_val_score()` function, and prints the same result:

```
from sklearn.model_selection import StratifiedKFold
from sklearn.base import clone

skfolds = StratifiedKFold(n_splits=3, random_state=42)

for train_index, test_index in skfolds.split(X_train, y_train_5):
    clone_clf = clone(sgd_clf)
    X_train_folds = X_train[train_index]
    y_train_folds = y_train_5[train_index]
    X_test_fold = X_train[test_index]
    y_test_fold = y_train_5[test_index]

    clone_clf.fit(X_train_folds, y_train_folds)
    y_pred = clone_clf.predict(X_test_fold)
    n_correct = sum(y_pred == y_test_fold)
    print(n_correct / len(y_pred))  # prints 0.9502, 0.96565 and 0.96495
```

The `StratifiedKFold` class performs stratified sampling (as explained in Chapter 2) to produce folds that contain a representative ratio of each class. At each iteration the code creates a clone of the classifier, trains that clone on the training folds, and makes predictions on the test fold. Then it counts the number of correct predictions and outputs the ratio of correct predictions.

Let's use the `cross_val_score()` function to evaluate your `SGDClassifier` model using K-fold cross-validation, with three folds. Remember that K-fold cross-validation means splitting the training set into K-folds (in this case, three), then making predictions and evaluating them on each fold using a model trained on the remaining folds (see Chapter 2):

```
>>> from sklearn.model_selection import cross_val_score
>>> cross_val_score(sgd_clf, X_train, y_train_5, cv=3, scoring="accuracy")
array([0.96355, 0.93795, 0.95615])
```

Wow! Above 93% *accuracy* (ratio of correct predictions) on all cross-validation folds? This looks amazing, doesn't it? Well, before you get too excited, let's look at a very dumb classifier that just classifies every single image in the "not-5" class:

```
from sklearn.base import BaseEstimator

class Never5Classifier(BaseEstimator):
    def fit(self, X, y=None):
        pass
    def predict(self, X):
        return np.zeros((len(X), 1), dtype=bool)
```

Can you guess this model's accuracy? Let's find out:

```
>>> never_5_clf = Never5Classifier()
>>> cross_val_score(never_5_clf, X_train, y_train_5, cv=3, scoring="accuracy")
array([0.91125, 0.90855, 0.90915])
```

That's right, it has over 90% accuracy! This is simply because only about 10% of the images are 5s, so if you always guess that an image is *not* a 5, you will be right about 90% of the time. Beats Nostradamus.

This demonstrates why accuracy is generally not the preferred performance measure for classifiers, especially when you are dealing with *skewed datasets* (i.e., when some classes are much more frequent than others).

Confusion Matrix

A much better way to evaluate the performance of a classifier is to look at the *confusion matrix*. The general idea is to count the number of times instances of class A are classified as class B. For example, to know the number of times the classifier confused images of 5s with 3s, you would look in the 5th row and 3rd column of the confusion matrix.

To compute the confusion matrix, you first need to have a set of predictions, so they can be compared to the actual targets. You could make predictions on the test set, but let's keep it untouched for now (remember that you want to use the test set only at the very end of your project, once you have a classifier that you are ready to launch). Instead, you can use the `cross_val_predict()` function:

```
from sklearn.model_selection import cross_val_predict

y_train_pred = cross_val_predict(sgd_clf, X_train, y_train_5, cv=3)
```

Just like the `cross_val_score()` function, `cross_val_predict()` performs K-fold cross-validation, but instead of returning the evaluation scores, it returns the predic-

tions made on each test fold. This means that you get a clean prediction for each instance in the training set ("clean" meaning that the prediction is made by a model that never saw the data during training).

Now you are ready to get the confusion matrix using the `confusion_matrix()` function. Just pass it the target classes (`y_train_5`) and the predicted classes (`y_train_pred`):

```
>>> from sklearn.metrics import confusion_matrix
>>> confusion_matrix(y_train_5, y_train_pred)
array([[53057,  1522],
       [ 1325,  4096]])
```

Each row in a confusion matrix represents an *actual class*, while each column represents a *predicted class*. The first row of this matrix considers non-5 images (the *negative class*): 53,057 of them were correctly classified as non-5s (they are called *true negatives*), while the remaining 1,522 were wrongly classified as 5s (*false positives*). The second row considers the images of 5s (the *positive class*): 1,325 were wrongly classified as non-5s (*false negatives*), while the remaining 4,096 were correctly classified as 5s (*true positives*). A perfect classifier would have only true positives and true negatives, so its confusion matrix would have nonzero values only on its main diagonal (top left to bottom right):

```
>>> y_train_perfect_predictions = y_train_5  # pretend we reached perfection
>>> confusion_matrix(y_train_5, y_train_perfect_predictions)
array([[54579,     0],
       [    0,  5421]])
```

The confusion matrix gives you a lot of information, but sometimes you may prefer a more concise metric. An interesting one to look at is the accuracy of the positive predictions; this is called the *precision* of the classifier (Equation 3-1).

Equation 3-1. Precision

$$\text{precision} = \frac{TP}{TP + FP}$$

TP is the number of true positives, and FP is the number of false positives.

A trivial way to have perfect precision is to make one single positive prediction and ensure it is correct (precision = 1/1 = 100%). This would not be very useful since the classifier would ignore all but one positive instance. So precision is typically used along with another metric named *recall*, also called *sensitivity* or *true positive rate*

(*TPR*): this is the ratio of positive instances that are correctly detected by the classifier (Equation 3-2).

Equation 3-2. Recall

$$\text{recall} = \frac{TP}{TP + FN}$$

FN is of course the number of false negatives.

If you are confused about the confusion matrix, Figure 3-2 may help.

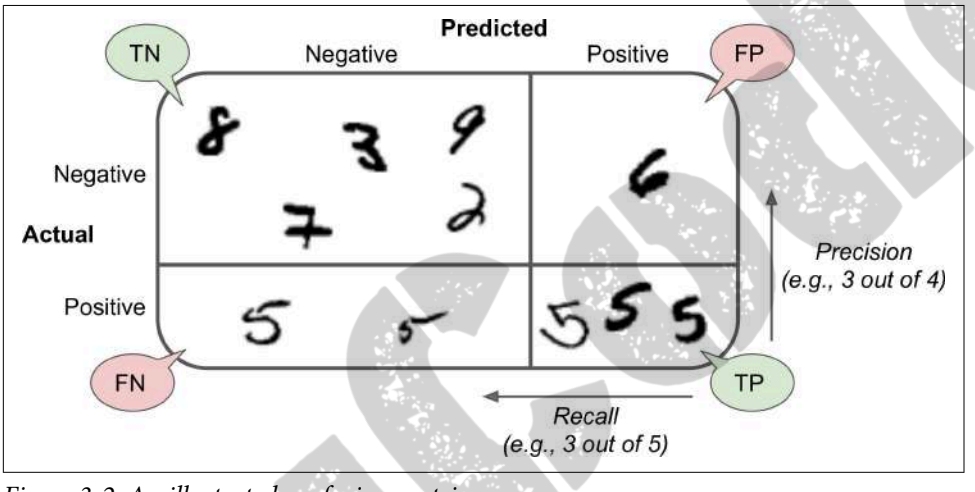


Figure 3-2. An illustrated confusion matrix

Precision and Recall

Scikit-Learn provides several functions to compute classifier metrics, including precision and recall:

```
>>> from sklearn.metrics import precision_score, recall_score
>>> precision_score(y_train_5, y_train_pred) # == 4096 / (4096 + 1522)
0.7290850836596654
>>> recall_score(y_train_5, y_train_pred) # == 4096 / (4096 + 1325)
0.7555801512636044
```

Now your 5-detector does not look as shiny as it did when you looked at its accuracy. When it claims an image represents a 5, it is correct only 72.9% of the time. Moreover, it only detects 75.6% of the 5s.

It is often convenient to combine precision and recall into a single metric called the F_1 *score*, in particular if you need a simple way to compare two classifiers. The F_1 score is the *harmonic mean* of precision and recall (Equation 3-3). Whereas the regular mean

treats all values equally, the harmonic mean gives much more weight to low values. As a result, the classifier will only get a high F_1 score if both recall and precision are high.

Equation 3-3. F_1

$$F_1 = \frac{2}{\frac{1}{\text{precision}} + \frac{1}{\text{recall}}} = 2 \times \frac{\text{precision} \times \text{recall}}{\text{precision} + \text{recall}} = \frac{TP}{TP + \frac{FN + FP}{2}}$$

To compute the F_1 score, simply call the `f1_score()` function:

```
>>> from sklearn.metrics import f1_score
>>> f1_score(y_train_5, y_train_pred)
0.7420962043663375
```

The F_1 score favors classifiers that have similar precision and recall. This is not always what you want: in some contexts you mostly care about precision, and in other contexts you really care about recall. For example, if you trained a classifier to detect videos that are safe for kids, you would probably prefer a classifier that rejects many good videos (low recall) but keeps only safe ones (high precision), rather than a classifier that has a much higher recall but lets a few really bad videos show up in your product (in such cases, you may even want to add a human pipeline to check the classifier's video selection). On the other hand, suppose you train a classifier to detect shoplifters on surveillance images: it is probably fine if your classifier has only 30% precision as long as it has 99% recall (sure, the security guards will get a few false alerts, but almost all shoplifters will get caught).

Unfortunately, you can't have it both ways: increasing precision reduces recall, and vice versa. This is called the *precision/recall tradeoff*.

Precision/Recall Tradeoff

To understand this tradeoff, let's look at how the `SGDClassifier` makes its classification decisions. For each instance, it computes a score based on a *decision function*, and if that score is greater than a threshold, it assigns the instance to the positive class, or else it assigns it to the negative class. Figure 3-3 shows a few digits positioned from the lowest score on the left to the highest score on the right. Suppose the *decision threshold* is positioned at the central arrow (between the two 5s): you will find 4 true positives (actual 5s) on the right of that threshold, and one false positive (actually a 6). Therefore, with that threshold, the precision is 80% (4 out of 5). But out of 6 actual 5s, the classifier only detects 4, so the recall is 67% (4 out of 6). Now if you raise the threshold (move it to the arrow on the right), the false positive (the 6) becomes a true negative, thereby increasing precision (up to 100% in this case), but one true positive becomes a false negative, decreasing recall down to 50%. Conversely, lowering the threshold increases recall and reduces precision.

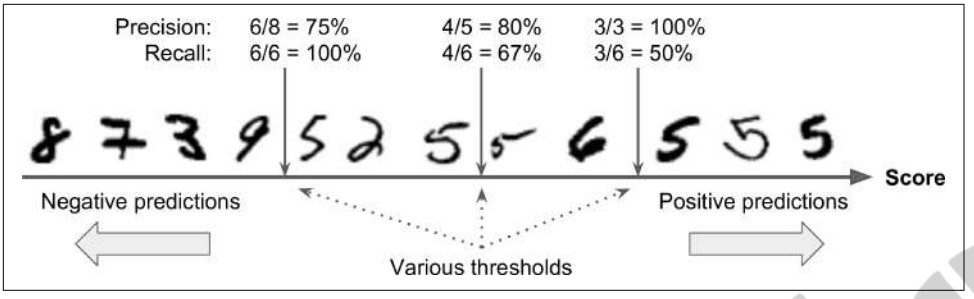


Figure 3-3. Decision threshold and precision/recall tradeoff

Scikit-Learn does not let you set the threshold directly, but it does give you access to the decision scores that it uses to make predictions. Instead of calling the classifier's `predict()` method, you can call its `decision_function()` method, which returns a score for each instance, and then make predictions based on those scores using any threshold you want:

```
>>> y_scores = sgd_clf.decision_function([some_digit])
>>> y_scores
array([2412.53175101])
>>> threshold = 0
>>> y_some_digit_pred = (y_scores > threshold)
array([ True])
```

The `SGDClassifier` uses a threshold equal to 0, so the previous code returns the same result as the `predict()` method (i.e., `True`). Let's raise the threshold:

```
>>> threshold = 8000
>>> y_some_digit_pred = (y_scores > threshold)
>>> y_some_digit_pred
array([False])
```

This confirms that raising the threshold decreases recall. The image actually represents a 5, and the classifier detects it when the threshold is 0, but it misses it when the threshold is increased to 8,000.

Now how do you decide which threshold to use? For this you will first need to get the scores of all instances in the training set using the `cross_val_predict()` function again, but this time specifying that you want it to return decision scores instead of predictions:

```
y_scores = cross_val_predict(sgd_clf, X_train, y_train_5, cv=3,
                             method="decision_function")
```

Now with these scores you can compute precision and recall for all possible thresholds using the `precision_recall_curve()` function:

```
from sklearn.metrics import precision_recall_curve

precisions, recalls, thresholds = precision_recall_curve(y_train_5, y_scores)
```

Finally, you can plot precision and recall as functions of the threshold value using Matplotlib (Figure 3-4):

```
def plot_precision_recall_vs_threshold(precisions, recalls, thresholds):
    plt.plot(thresholds, precisions[:-1], "b--", label="Precision")
    plt.plot(thresholds, recalls[:-1], "g-", label="Recall")
    [...] # highlight the threshold, add the legend, axis label and grid

plot_precision_recall_vs_threshold(precisions, recalls, thresholds)
plt.show()
```

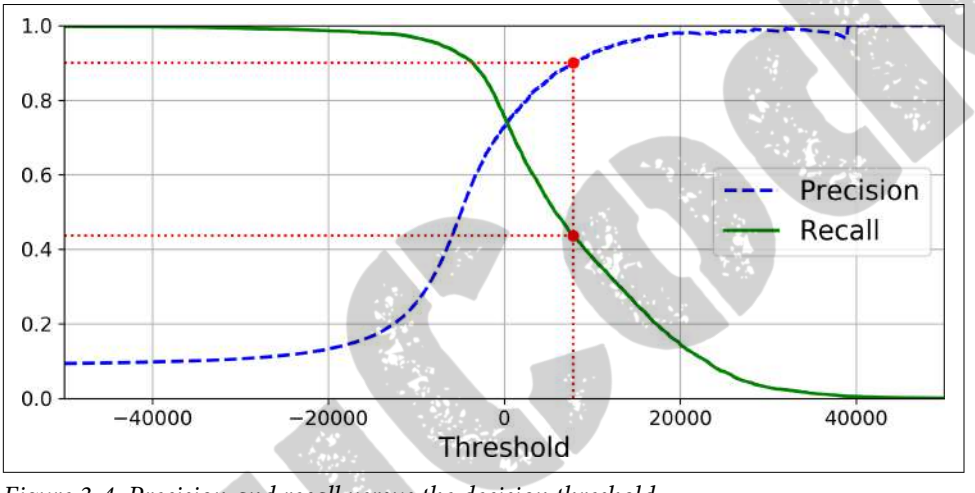


Figure 3-4. Precision and recall versus the decision threshold

You may wonder why the precision curve is bumpier than the recall curve in Figure 3-4. The reason is that precision may sometimes go down when you raise the threshold (although in general it will go up). To understand why, look back at Figure 3-3 and notice what happens when you start from the central threshold and move it just one digit to the right: precision goes from 4/5 (80%) down to 3/4 (75%). On the other hand, recall can only go down when the threshold is increased, which explains why its curve looks smooth.

Another way to select a good precision/recall tradeoff is to plot precision directly against recall, as shown in Figure 3-5 (the same threshold as earlier is highlighed).

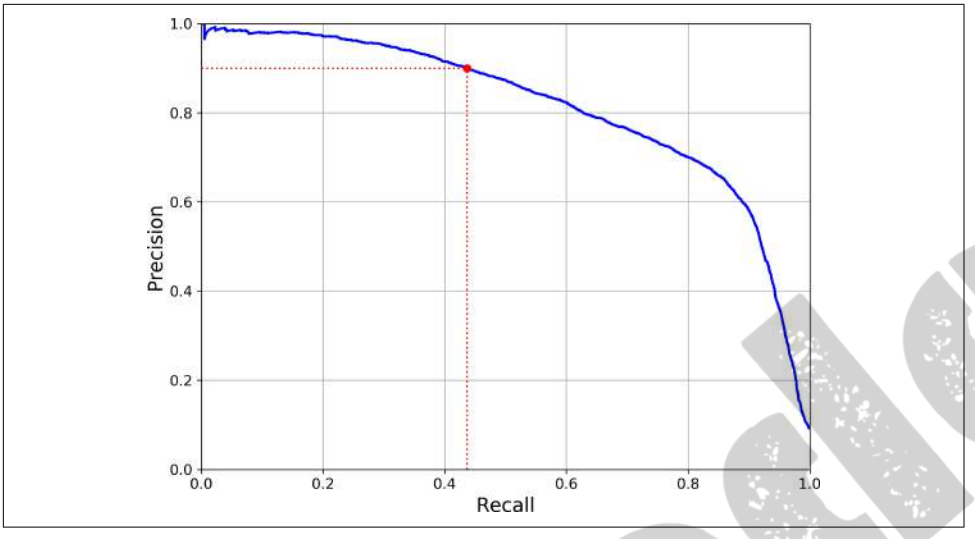


Figure 3-5. Precision versus recall

You can see that precision really starts to fall sharply around 80% recall. You will probably want to select a precision/recall tradeoff just before that drop—for example, at around 60% recall. But of course the choice depends on your project.

So let's suppose you decide to aim for 90% precision. You look up the first plot and find that you need to use a threshold of about 8,000. To be more precise you can search for the lowest threshold that gives you at least 90% precision (`np.argmax()` will give us the first index of the maximum value, which in this case means the first `True` value):

```
threshold_90_precision = thresholds[np.argmax(precisions >= 0.90)] # ~7816
```

To make predictions (on the training set for now), instead of calling the classifier's `predict()` method, you can just run this code:

```
y_train_pred_90 = (y_scores >= threshold_90_precision)
```

Let's check these predictions' precision and recall:

```
>>> precision_score(y_train_5, y_train_pred_90)
0.9000380083618396
>>> recall_score(y_train_5, y_train_pred_90)
0.4368197749492714
```

Great, you have a 90% precision classifier ! As you can see, it is fairly easy to create a classifier with virtually any precision you want: just set a high enough threshold, and you're done. Hmm, not so fast. A high-precision classifier is not very useful if its recall is too low!

If someone says "let's reach 99% precision," you should ask, "at what recall?"

The ROC Curve

The *receiver operating characteristic* (ROC) curve is another common tool used with binary classifiers. It is very similar to the precision/recall curve, but instead of plotting precision versus recall, the ROC curve plots the *true positive rate* (another name for recall) against the *false positive rate*. The FPR is the ratio of negative instances that are incorrectly classified as positive. It is equal to one minus the *true negative rate*, which is the ratio of negative instances that are correctly classified as negative. The TNR is also called *specificity*. Hence the ROC curve plots *sensitivity* (recall) versus 1 – *specificity*.

To plot the ROC curve, you first need to compute the TPR and FPR for various threshold values, using the `roc_curve()` function:

```
from sklearn.metrics import roc_curve

fpr, tpr, thresholds = roc_curve(y_train_5, y_scores)
```

Then you can plot the FPR against the TPR using Matplotlib. This code produces the plot in Figure 3-6:

```
def plot_roc_curve(fpr, tpr, label=None):
    plt.plot(fpr, tpr, linewidth=2, label=label)
    plt.plot([0, 1], [0, 1], 'k--') # dashed diagonal
    [...] # Add axis labels and grid

plot_roc_curve(fpr, tpr)
plt.show()
```

Figure 3-6. ROC curve

Once again there is a tradeoff: the higher the recall (TPR), the more false positives (FPR) the classifier produces. The dotted line represents the ROC curve of a purely random classifier; a good classifier stays as far away from that line as possible (toward the top-left corner).

One way to compare classifiers is to measure the *area under the curve* (AUC). A perfect classifier will have a *ROC AUC* equal to 1, whereas a purely random classifier will have a ROC AUC equal to 0.5. Scikit-Learn provides a function to compute the ROC AUC:

```
>>> from sklearn.metrics import roc_auc_score
>>> roc_auc_score(y_train_5, y_scores)
0.9611778893101814
```

Since the ROC curve is so similar to the precision/recall (or PR) curve, you may wonder how to decide which one to use. As a rule of thumb, you should prefer the PR curve whenever the positive class is rare or when you care more about the false positives than the false negatives, and the ROC curve otherwise. For example, looking at the previous ROC curve (and the ROC AUC score), you may think that the classifier is really good. But this is mostly because there are few positives (5s) compared to the negatives (non-5s). In contrast, the PR curve makes it clear that the classifier has room for improvement (the curve could be closer to the top-right corner).

Let's train a `RandomForestClassifier` and compare its ROC curve and ROC AUC score to the `SGDClassifier`. First, you need to get scores for each instance in the training set. But due to the way it works (see Chapter 7), the `RandomForestClassifier` class does not have a `decision_function()` method. Instead it has a `predict_proba()` method. Scikit-Learn classifiers generally have one or the other. The `predict_proba()` method returns an array containing a row per instance and a column per class, each containing the probability that the given instance belongs to the given class (e.g., 70% chance that the image represents a 5):

```
from sklearn.ensemble import RandomForestClassifier

forest_clf = RandomForestClassifier(random_state=42)
y_probas_forest = cross_val_predict(forest_clf, X_train, y_train_5, cv=3,
                                    method="predict_proba")
```

But to plot a ROC curve, you need scores, not probabilities. A simple solution is to use the positive class's probability as the score:

```
y_scores_forest = y_probas_forest[:, 1]   # score = proba of positive class
fpr_forest, tpr_forest, thresholds_forest = roc_curve(y_train_5,y_scores_forest)
```

Now you are ready to plot the ROC curve. It is useful to plot the first ROC curve as well to see how they compare (Figure 3-7):

```
plt.plot(fpr, tpr, "b:", label="SGD")
plot_roc_curve(fpr_forest, tpr_forest, "Random Forest")
plt.legend(loc="lower right")
plt.show()
```

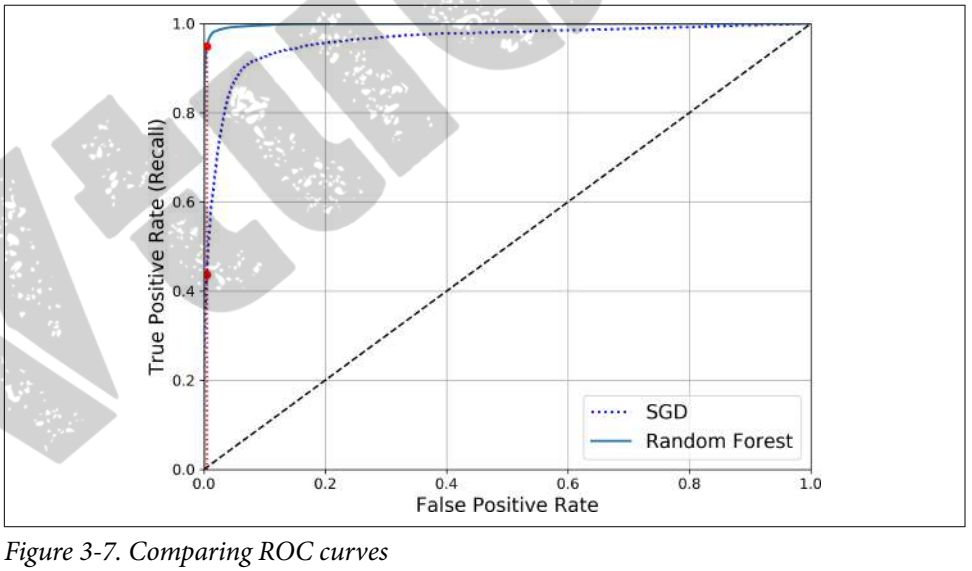


Figure 3-7. Comparing ROC curves

As you can see in Figure 3-7, the `RandomForestClassifier`'s ROC curve looks much better than the `SGDClassifier`'s: it comes much closer to the top-left corner. As a result, its ROC AUC score is also significantly better:

```
>>> roc_auc_score(y_train_5, y_scores_forest)
0.9983436731328145
```

Try measuring the precision and recall scores: you should find 99.0% precision and 86.6% recall. Not too bad!

Hopefully you now know how to train binary classifiers, choose the appropriate metric for your task, evaluate your classifiers using cross-validation, select the precision/recall tradeoff that fits your needs, and compare various models using ROC curves and ROC AUC scores. Now let's try to detect more than just the 5s.

Multiclass Classification

Whereas binary classifiers distinguish between two classes, *multiclass classifiers* (also called *multinomial classifiers*) can distinguish between more than two classes.

Some algorithms (such as Random Forest classifiers or naive Bayes classifiers) are capable of handling multiple classes directly. Others (such as Support Vector Machine classifiers or Linear classifiers) are strictly binary classifiers. However, there are various strategies that you can use to perform multiclass classification using multiple binary classifiers.

For example, one way to create a system that can classify the digit images into 10 classes (from 0 to 9) is to train 10 binary classifiers, one for each digit (a 0-detector, a 1-detector, a 2-detector, and so on). Then when you want to classify an image, you get the decision score from each classifier for that image and you select the class whose classifier outputs the highest score. This is called the *one-versus-all* (OvA) strategy (also called *one-versus-the-rest*).

Another strategy is to train a binary classifier for every pair of digits: one to distinguish 0s and 1s, another to distinguish 0s and 2s, another for 1s and 2s, and so on. This is called the *one-versus-one* (OvO) strategy. If there are N classes, you need to train $N \times (N - 1) / 2$ classifiers. For the MNIST problem, this means training 45 binary classifiers! When you want to classify an image, you have to run the image through all 45 classifiers and see which class wins the most duels. The main advantage of OvO is that each classifier only needs to be trained on the part of the training set for the two classes that it must distinguish.

Some algorithms (such as Support Vector Machine classifiers) scale poorly with the size of the training set, so for these algorithms OvO is preferred since it is faster to train many classifiers on small training sets than training few classifiers on large training sets. For most binary classification algorithms, however, OvA is preferred.

Scikit-Learn detects when you try to use a binary classification algorithm for a multiclass classification task, and it automatically runs OvA (except for SVM classifiers for which it uses OvO). Let's try this with the `SGDClassifier`:

```
>>> sgd_clf.fit(X_train, y_train)  # y_train, not y_train_5
>>> sgd_clf.predict([some_digit])
array([5], dtype=uint8)
```

That was easy! This code trains the `SGDClassifier` on the training set using the original target classes from 0 to 9 (`y_train`), instead of the 5-versus-all target classes (`y_train_5`). Then it makes a prediction (a correct one in this case). Under the hood, Scikit-Learn actually trained 10 binary classifiers, got their decision scores for the image, and selected the class with the highest score.

To see that this is indeed the case, you can call the `decision_function()` method. Instead of returning just one score per instance, it now returns 10 scores, one per class:

```
>>> some_digit_scores = sgd_clf.decision_function([some_digit])
>>> some_digit_scores
array([[-15955.22627845, -38080.96296175, -13326.66694897,
          573.52692379, -17680.6846644 ,   2412.53175101,
        -25526.86498156, -12290.15704709,  -7946.05205023,
        -10631.35888549]])
```

The highest score is indeed the one corresponding to class 5:

```
>>> np.argmax(some_digit_scores)
5
>>> sgd_clf.classes_
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9], dtype=uint8)
>>> sgd_clf.classes_[5]
5
```

When a classifier is trained, it stores the list of target classes in its `classes_` attribute, ordered by value. In this case, the index of each class in the `classes_` array conveniently matches the class itself (e.g., the class at index 5 happens to be class 5), but in general you won't be so lucky.

If you want to force ScikitLearn to use one-versus-one or one-versus-all, you can use the `OneVsOneClassifier` or `OneVsRestClassifier` classes. Simply create an instance and pass a binary classifier to its constructor. For example, this code creates a multiclass classifier using the OvO strategy, based on a `SGDClassifier`:

```
>>> from sklearn.multiclass import OneVsOneClassifier
>>> ovo_clf = OneVsOneClassifier(SGDClassifier(random_state=42))
>>> ovo_clf.fit(X_train, y_train)
>>> ovo_clf.predict([some_digit])
```

```
array([5], dtype=uint8)
>>> len(ovo_clf.estimators_)
45
```

Training a `RandomForestClassifier` is just as easy:

```
>>> forest_clf.fit(X_train, y_train)
>>> forest_clf.predict([some_digit])
array([5], dtype=uint8)
```

This time Scikit-Learn did not have to run OvA or OvO because Random Forest classifiers can directly classify instances into multiple classes. You can call `predict_proba()` to get the list of probabilities that the classifier assigned to each instance for each class:

```
>>> forest_clf.predict_proba([some_digit])
array([[0.  , 0.  , 0.01, 0.08, 0.  , 0.9 , 0.  , 0.  , 0.  , 0.01]])
```

You can see that the classifier is fairly confident about its prediction: the 0.9 at the 5th index in the array means that the model estimates a 90% probability that the image represents a 5. It also thinks that the image could instead be a 2, a 3 or a 9, respectively with 1%, 8% and 1% probability.

Now of course you want to evaluate these classifiers. As usual, you want to use cross-validation. Let's evaluate the `SGDClassifier`'s accuracy using the `cross_val_score()` function:

```
>>> cross_val_score(sgd_clf, X_train, y_train, cv=3, scoring="accuracy")
array([0.8489802 , 0.87129356, 0.86988048])
```

It gets over 84% on all test folds. If you used a random classifier, you would get 10% accuracy, so this is not such a bad score, but you can still do much better. For example, simply scaling the inputs (as discussed in Chapter 2) increases accuracy above 89%:

```
>>> from sklearn.preprocessing import StandardScaler
>>> scaler = StandardScaler()
>>> X_train_scaled = scaler.fit_transform(X_train.astype(np.float64))
>>> cross_val_score(sgd_clf, X_train_scaled, y_train, cv=3, scoring="accuracy")
array([0.89707059, 0.8960948 , 0.90693604])
```

Error Analysis

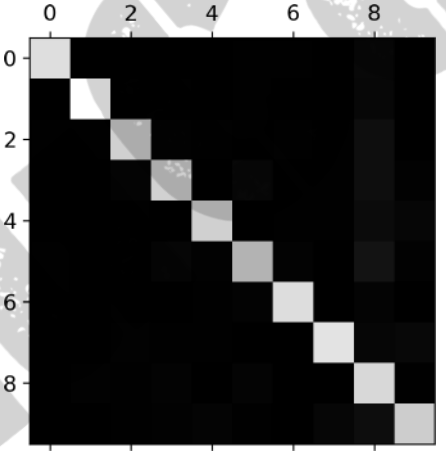
Of course, if this were a real project, you would follow the steps in your Machine Learning project checklist (see ???): exploring data preparation options, trying out multiple models, shortlisting the best ones and fine-tuning their hyperparameters using `GridSearchCV`, and automating as much as possible, as you did in the previous chapter. Here, we will assume that you have found a promising model and you want to find ways to improve it. One way to do this is to analyze the types of errors it makes.

First, you can look at the confusion matrix. You need to make predictions using the `cross_val_predict()` function, then call the `confusion_matrix()` function, just like you did earlier:

```
>>> y_train_pred = cross_val_predict(sgd_clf, X_train_scaled, y_train, cv=3)
>>> conf_mx = confusion_matrix(y_train, y_train_pred)
>>> conf_mx
array([[5578,    0,   22,    7,    8,   45,   35,    5,  222,    1],
       [   0, 6410,   35,   26,    4,   44,    4,    8,  198,   13],
       [  28,   27, 5232,  100,   74,   27,   68,   37,  354,   11],
       [  23,   18,  115, 5254,    2,  209,   26,   38,  373,   73],
       [  11,   14,   45,   12, 5219,   11,   33,   26,  299,  172],
       [  26,   16,   31,  173,   54, 4484,   76,   14,  482,   65],
       [  31,   17,   45,    2,   42,   98, 5556,    3,  123,    1],
       [  20,   10,   53,   27,   50,   13,    3, 5696,  173,  220],
       [  17,   64,   47,   91,    3,  125,   24,   11, 5421,   48],
       [  24,   18,   29,   67,  116,   39,    1,  174,  329, 5152]])
```

That's a lot of numbers. It's often more convenient to look at an image representation of the confusion matrix, using Matplotlib's `matshow()` function:

```
plt.matshow(conf_mx, cmap=plt.cm.gray)
plt.show()
```



This confusion matrix looks fairly good, since most images are on the main diagonal, which means that they were classified correctly. The 5s look slightly darker than the other digits, which could mean that there are fewer images of 5s in the dataset or that the classifier does not perform as well on 5s as on other digits. In fact, you can verify that both are the case.

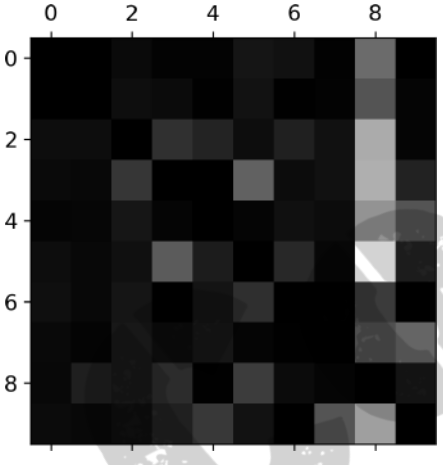
Let's focus the plot on the errors. First, you need to divide each value in the confusion matrix by the number of images in the corresponding class, so you can compare error

rates instead of absolute number of errors (which would make abundant classes look unfairly bad):

```
row_sums = conf_mx.sum(axis=1, keepdims=True)
norm_conf_mx = conf_mx / row_sums
```

Now let's fill the diagonal with zeros to keep only the errors, and let's plot the result:

```
np.fill_diagonal(norm_conf_mx, 0)
plt.matshow(norm_conf_mx, cmap=plt.cm.gray)
plt.show()
```



Now you can clearly see the kinds of errors the classifier makes. Remember that rows represent actual classes, while columns represent predicted classes. The column for class 8 is quite bright, which tells you that many images get misclassified as 8s. However, the row for class 8 is not that bad, telling you that actual 8s in general get properly classified as 8s. As you can see, the confusion matrix is not necessarily symmetrical. You can also see that 3s and 5s often get confused (in both directions).

Analyzing the confusion matrix can often give you insights on ways to improve your classifier. Looking at this plot, it seems that your efforts should be spent on reducing the false 8s. For example, you could try to gather more training data for digits that look like 8s (but are not) so the classifier can learn to distinguish them from real 8s. Or you could engineer new features that would help the classifier—for example, writing an algorithm to count the number of closed loops (e.g., 8 has two, 6 has one, 5 has none). Or you could preprocess the images (e.g., using Scikit-Image, Pillow, or OpenCV) to make some patterns stand out more, such as closed loops.

Analyzing individual errors can also be a good way to gain insights on what your classifier is doing and why it is failing, but it is more difficult and time-consuming.

For example, let's plot examples of 3s and 5s (the `plot_digits()` function just uses Matplotlib's `imshow()` function; see this chapter's Jupyter notebook for details):

```
cl_a, cl_b = 3, 5
X_aa = X_train[(y_train == cl_a) & (y_train_pred == cl_a)]
X_ab = X_train[(y_train == cl_a) & (y_train_pred == cl_b)]
X_ba = X_train[(y_train == cl_b) & (y_train_pred == cl_a)]
X_bb = X_train[(y_train == cl_b) & (y_train_pred == cl_b)]

plt.figure(figsize=(8,8))
plt.subplot(221); plot_digits(X_aa[:25], images_per_row=5)
plt.subplot(222); plot_digits(X_ab[:25], images_per_row=5)
plt.subplot(223); plot_digits(X_ba[:25], images_per_row=5)
plt.subplot(224); plot_digits(X_bb[:25], images_per_row=5)
plt.show()
```

The two 5×5 blocks on the left show digits classified as 3s, and the two 5×5 blocks on the right show images classified as 5s. Some of the digits that the classifier gets wrong (i.e., in the bottom-left and top-right blocks) are so badly written that even a human would have trouble classifying them (e.g., the 5 on the 1st row and 2nd column truly looks like a badly written 3). However, most misclassified images seem like obvious errors to us, and it's hard to understand why the classifier made the mistakes it did.[3] The reason is that we used a simple `SGDClassifier`, which is a linear model. All it does is assign a weight per class to each pixel, and when it sees a new image it just sums up the weighted pixel intensities to get a score for each class. So since 3s and 5s differ only by a few pixels, this model will easily confuse them.

The main difference between 3s and 5s is the position of the small line that joins the top line to the bottom arc. If you draw a 3 with the junction slightly shifted to the left, the classifier might classify it as a 5, and vice versa. In other words, this classifier is quite sensitive to image shifting and rotation. So one way to reduce the 3/5 confusion would be to preprocess the images to ensure that they are well centered and not too rotated. This will probably help reduce other errors as well.

Multilabel Classification

Until now each instance has always been assigned to just one class. In some cases you may want your classifier to output multiple classes for each instance. For example, consider a face-recognition classifier: what should it do if it recognizes several people on the same picture? Of course it should attach one tag per person it recognizes. Say the classifier has been trained to recognize three faces, Alice, Bob, and Charlie; then when it is shown a picture of Alice and Charlie, it should output [1, 0, 1] (meaning "Alice yes, Bob no, Charlie yes"). Such a classification system that outputs multiple binary tags is called a *multilabel classification* system.

We won't go into face recognition just yet, but let's look at a simpler example, just for illustration purposes:

```
from sklearn.neighbors import KNeighborsClassifier

y_train_large = (y_train >= 7)
y_train_odd = (y_train % 2 == 1)
y_multilabel = np.c_[y_train_large, y_train_odd]

knn_clf = KNeighborsClassifier()
knn_clf.fit(X_train, y_multilabel)
```

This code creates a `y_multilabel` array containing two target labels for each digit image: the first indicates whether or not the digit is large (7, 8, or 9) and the second indicates whether or not it is odd. The next lines create a `KNeighborsClassifier` instance (which supports multilabel classification, but not all classifiers do) and we train it using the multiple targets array. Now you can make a prediction, and notice that it outputs two labels:

```
>>> knn_clf.predict([some_digit])
array([[False,  True]])
```

And it gets it right! The digit 5 is indeed not large (`False`) and odd (`True`).

There are many ways to evaluate a multilabel classifier, and selecting the right metric really depends on your project. For example, one approach is to measure the F_1 score for each individual label (or any other binary classifier metric discussed earlier), then simply compute the average score. This code computes the average F_1 score across all labels:

```
>>> y_train_knn_pred = cross_val_predict(knn_clf, X_train, y_multilabel, cv=3)
>>> f1_score(y_multilabel, y_train_knn_pred, average="macro")
0.976410265560605
```

This assumes that all labels are equally important, which may not be the case. In particular, if you have many more pictures of Alice than of Bob or Charlie, you may want to give more weight to the classifier's score on pictures of Alice. One simple option is to give each label a weight equal to its *support* (i.e., the number of instances with that target label). To do this, simply set `average="weighted"` in the preceding code.[4]

Multioutput Classification

The last type of classification task we are going to discuss here is called *multioutput-multiclass classification* (or simply *multioutput classification*). It is simply a generalization of multilabel classification where each label can be multiclass (i.e., it can have more than two possible values).

To illustrate this, let's build a system that removes noise from images. It will take as input a noisy digit image, and it will (hopefully) output a clean digit image, represented as an array of pixel intensities, just like the MNIST images. Notice that the classifier's output is multilabel (one label per pixel) and each label can have multiple values (pixel intensity ranges from 0 to 255). It is thus an example of a multioutput classification system.

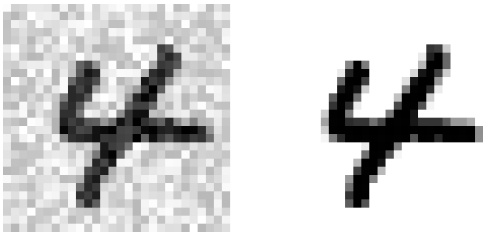
The line between classification and regression is sometimes blurry, such as in this example. Arguably, predicting pixel intensity is more akin to regression than to classification. Moreover, multioutput systems are not limited to classification tasks; you could even have a system that outputs multiple labels per instance, including both class labels and value labels.

Let's start by creating the training and test sets by taking the MNIST images and adding noise to their pixel intensities using NumPy's `randint()` function. The target images will be the original images:

```
noise = np.random.randint(0, 100, (len(X_train), 784))
X_train_mod = X_train + noise
noise = np.random.randint(0, 100, (len(X_test), 784))
X_test_mod = X_test + noise
y_train_mod = X_train
y_test_mod = X_test
```

4 Scikit-Learn offers a few other averaging options and multilabel classifier metrics; see the documentation for more details.

Let's take a peek at an image from the test set (yes, we're snooping on the test data, so you should be frowning right now):



On the left is the noisy input image, and on the right is the clean target image. Now let's train the classifier and make it clean this image:

```
knn_clf.fit(X_train_mod, y_train_mod)
clean_digit = knn_clf.predict([X_test_mod[some_index]])
plot_digit(clean_digit)
```

Looks close enough to the target! This concludes our tour of classification. Hopefully you should now know how to select good metrics for classification tasks, pick the appropriate precision/recall tradeoff, compare classifiers, and more generally build good classification systems for a variety of tasks.

Exercises

1. Try to build a classifier for the MNIST dataset that achieves over 97% accuracy on the test set. Hint: the `KNeighborsClassifier` works quite well for this task; you just need to find good hyperparameter values (try a grid search on the `weights` and `n_neighbors` hyperparameters).
2. Write a function that can shift an MNIST image in any direction (left, right, up, or down) by one pixel.[5] Then, for each image in the training set, create four shif-

5 You can use the `shift()` function from the `scipy.ndimage.interpolation` module. For example, `shift(image, [2, 1], cval=0)` shifts the image 2 pixels down and 1 pixel to the right.

ted copies (one per direction) and add them to the training set. Finally, train your best model on this expanded training set and measure its accuracy on the test set. You should observe that your model performs even better now! This technique of artificially growing the training set is called *data augmentation* or *training set expansion*.

3. Tackle the *Titanic* dataset. A great place to start is on Kaggle.
4. Build a spam classifier (a more challenging exercise):
   - Download examples of spam and ham from Apache SpamAssassin's public datasets.
   - Unzip the datasets and familiarize yourself with the data format.
   - Split the datasets into a training set and a test set.
   - Write a data preparation pipeline to convert each email into a feature vector. Your preparation pipeline should transform an email into a (sparse) vector indicating the presence or absence of each possible word. For example, if all emails only ever contain four words, "Hello," "how," "are," "you," then the email "Hello you Hello Hello you" would be converted into a vector [1, 0, 0, 1] (meaning ["Hello" is present, "how" is absent, "are" is absent, "you" is present]), or [3, 0, 0, 2] if you prefer to count the number of occurrences of each word.
   - You may want to add hyperparameters to your preparation pipeline to control whether or not to strip off email headers, convert each email to lowercase, remove punctuation, replace all URLs with "URL," replace all numbers with "NUMBER," or even perform *stemming* (i.e., trim off word endings; there are Python libraries available to do this).
   - Then try out several classifiers and see if you can build a great spam classifier, with both high recall and high precision.

Solutions to these exercises are available in the online Jupyter notebooks at *https://github.com/ageron/handson-ml2*.