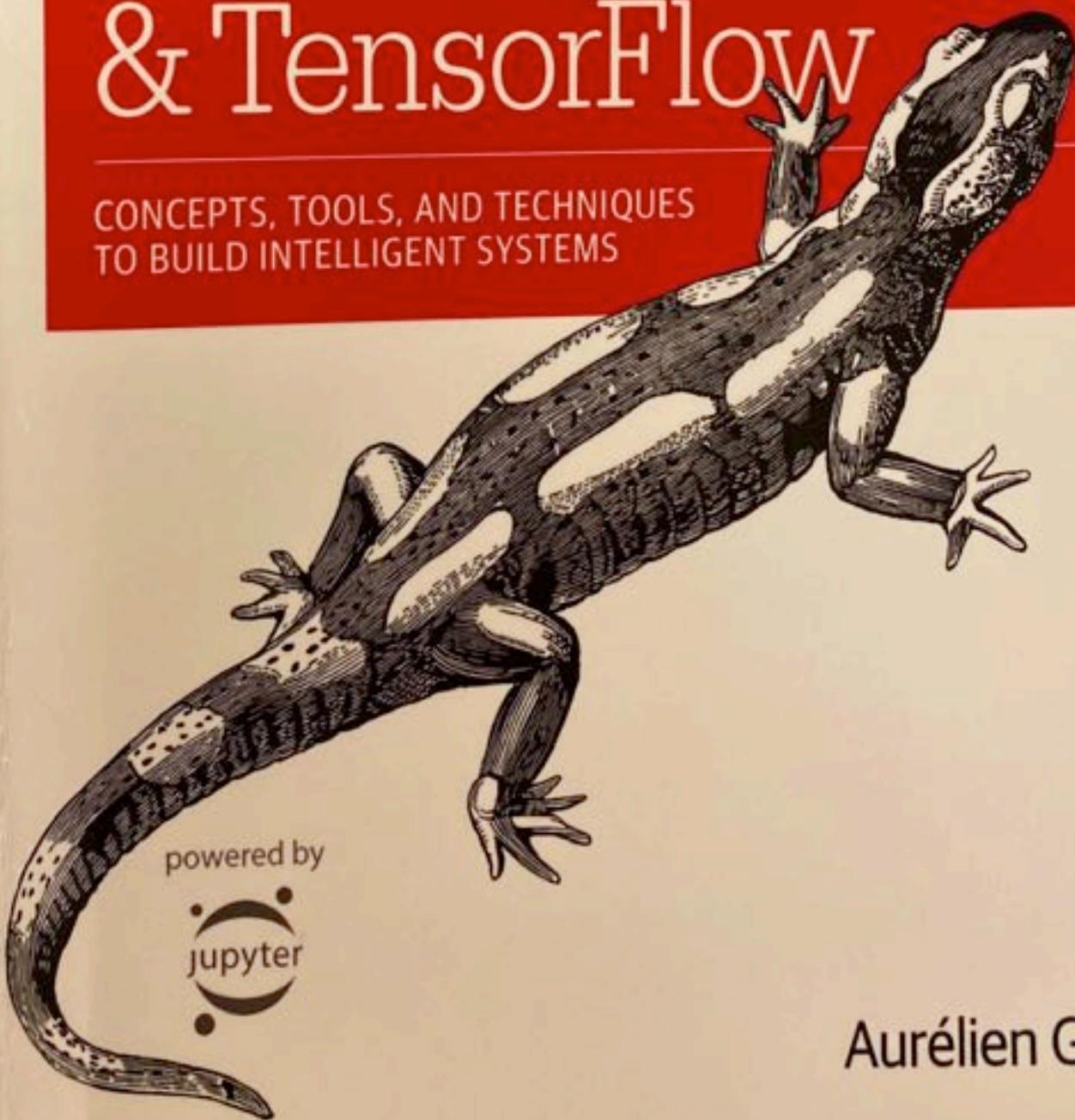


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# Hands-On Machine Learning with Scikit-Learn & TensorFlow

CONCEPTS, TOOLS, AND TECHNIQUES  
TO BUILD INTELLIGENT SYSTEMS



powered by



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# End-to-End Machine Learning Project

In this chapter, you will go through an example project end to end, pretending to be a recently hired data scientist in a real estate company.<sup>1</sup> Here are the main steps you will go through:

1. Look at the big picture.
2. Get the data.
3. Discover and visualize the data to gain insights.
4. Prepare the data for Machine Learning algorithms.
5. Select a model and train it.
6. Fine-tune your model.
7. Present your solution.
8. Launch, monitor, and maintain your system.

## 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:

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<sup>1</sup> The example project is completely fictitious; the goal is just to illustrate the main steps of a Machine Learning project, not to learn anything about the real estate business.

- UC Irvine Machine Learning Repository (<http://archive.ics.uci.edu/ml/>)
- Kaggle datasets (<https://www.kaggle.com/datasets>)
- Amazon's AWS datasets (<http://aws.amazon.com/fr/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 (<https://goo.gl/SJHN2k>)
  - Quora.com question (<http://goo.gl/zDR78y>)
  - Datasets subreddit (<https://www.reddit.com/r/datasets>)

In this chapter we chose the California Housing Prices dataset from the StatLib repository<sup>2</sup> (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.

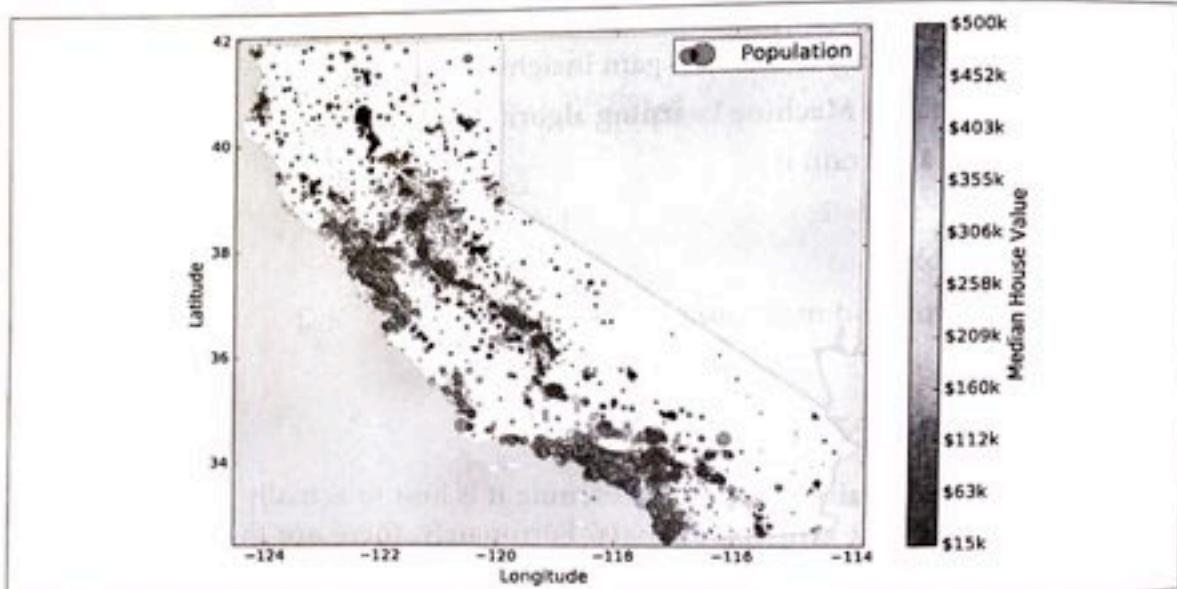


Figure 2-1. California housing prices

<sup>2</sup> The original dataset appeared in R. Kelley Pace and Ronald Barry, "Sparse Spatial Autoregressions," *Statistics & Probability Letters* 33, no. 3 (1997): 291–297.

# 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 Appendix B; 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*.<sup>3</sup> 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.

<sup>3</sup> A piece of information fed to a Machine Learning system is often called a *signal* in reference to Shannon’s information theory: you want a high signal/noise ratio.

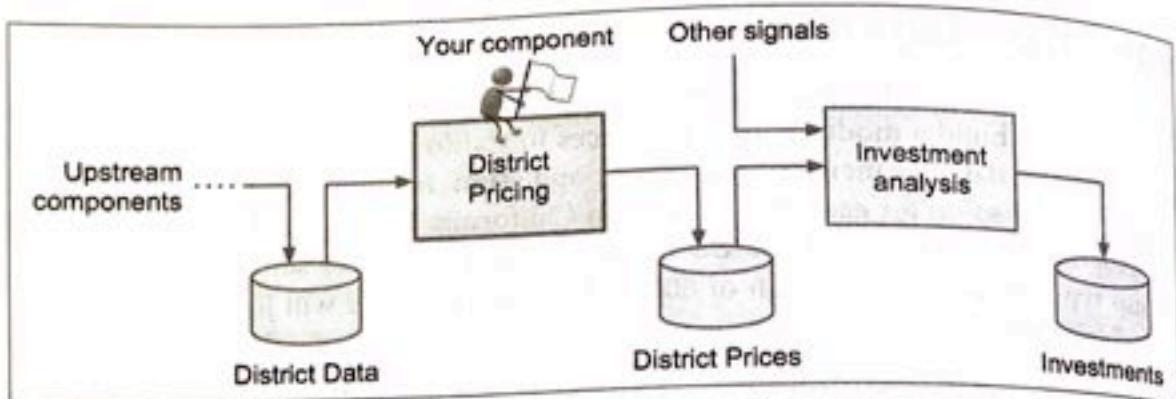


Figure 2-2. A Machine Learning pipeline for real estate investments

## 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 10%. 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 pur-

pose, 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 *multivariate regression* problem since the system will use multiple features to make a prediction (it will use the district's population, the median income, etc.). In the first chapter, you predicted life satisfaction based on just one feature, the GDP per capita, so it was a *univariate 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)

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

## 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  $i^{\text{th}}$  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  $-118.29^{\circ}$ , latitude  $33.91^{\circ}$ , 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  $i^{\text{th}}$  row is equal to the transpose of  $\mathbf{x}^{(i)}$ , noted  $(\mathbf{x}^{(i)})^T$ .<sup>4</sup>
  - For example, if the first district is as just described, then the matrix  $\mathbf{X}$  looks like this:

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

<sup>4</sup> 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  $\hat{y}^{(1)} - y^{(1)} = 2,000$ .
- $\text{RMSE}(\mathbf{X}, h)$  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*

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

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  $\ell_2$  norm, noted  $\|\cdot\|_2$  (or just  $\|\cdot\|$ ).
- Computing the sum of absolutes (MAE) corresponds to the  $\ell_1$  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  $\ell_k$  norm of a vector  $\mathbf{v}$  containing  $n$  elements is defined as 
$$\|\mathbf{v}\|_k = \left( |v_0|^k + |v_1|^k + \cdots + |v_n|^k \right)^{\frac{1}{k}}$$
.  $\ell_0$  just gives the number of non-zero elements in the vector, and  $\ell_\infty$  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-ml>.

## 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/>.<sup>5</sup>

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 43. If you don’t have them yet,

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<sup>5</sup> The latest version of Python 3 is recommended. Python 2.7+ should work fine too, but it is deprecated. If you use Python 2, you must add `from __future__ import division, print_function, unicode_literals` at the beginning of your code.

there are many ways to install them (and their dependencies). You can use your system'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).<sup>6</sup> You can check to see if pip is installed by typing the following command:

```
$ pip3 --version  
pip 9.0.1 from [...]/lib/python3.5/site-packages (python 3.5)
```

You should make sure you have a recent version of pip installed, at the very least >1.4 to support binary module installation (a.k.a. wheels). To upgrade the pip module, type:<sup>7</sup>

```
$ pip3 install --upgrade pip  
Collecting pip  
[...]  
Successfully installed pip-9.0.1
```

## 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 by running the following pip command:

```
$ pip3 install --user --upgrade 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/python3.5  
Also creating executable in [...]/ml/env/bin/python  
Installing setuptools, pip, wheel...done.
```

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

```
$ cd $ML_PATH  
$ source env/bin/activate
```

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

<sup>6</sup> 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.

<sup>7</sup> You may need to have administrator rights to run this command; if so, try prefixing it with sudo.

also want access to the system's site 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 administrator rights, or to add the `--user` option):

```
$ pip3 install --upgrade 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<sup>8</sup> (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.

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<sup>8</sup> Note that Jupyter can handle multiple versions of Python, and even many other languages such as R or Octave.

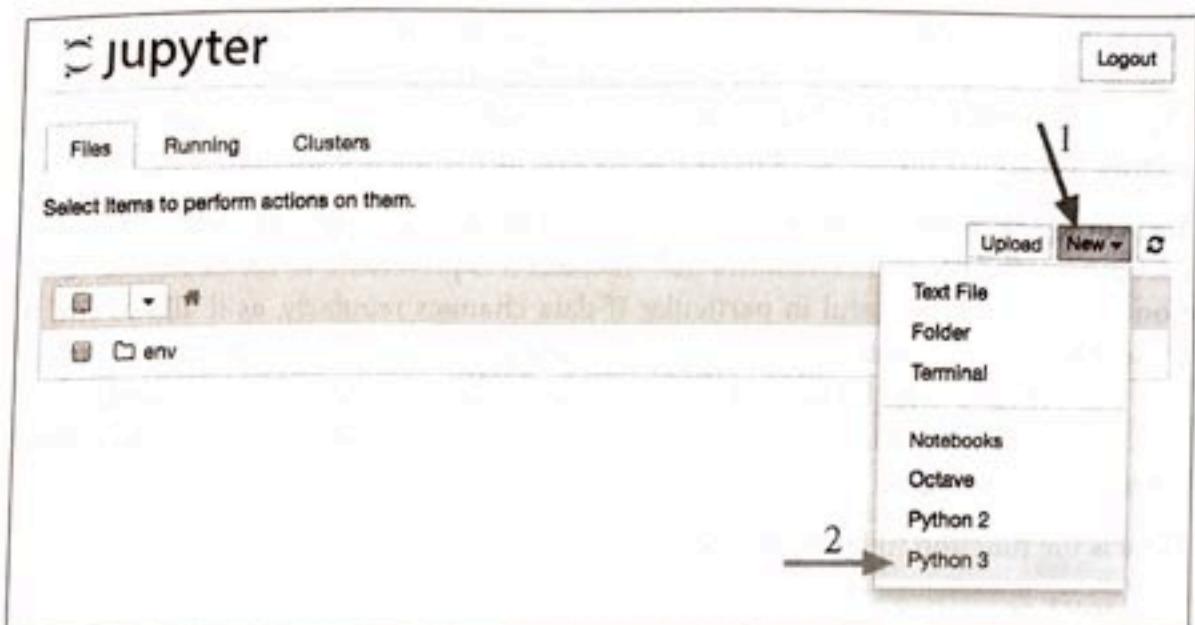


Figure 2-3. Your workspace in Jupyter

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.

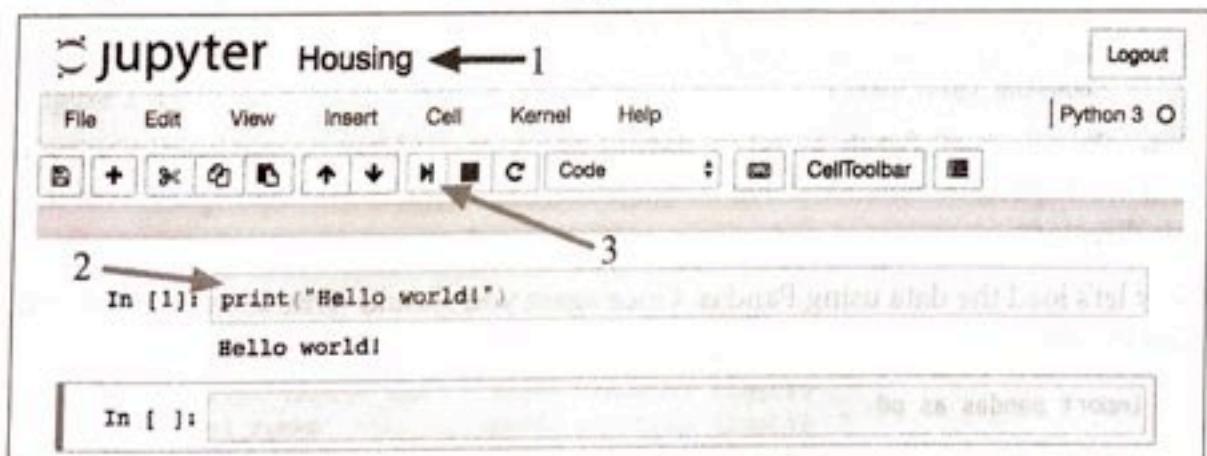


Figure 2-4. Hello world Python notebook

## 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,<sup>9</sup> 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:<sup>10</sup>

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

DOWNLOAD_ROOT = "https://raw.githubusercontent.com/ageron/handson-ml/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)
```

---

<sup>9</sup> You might also need to check legal constraints, such as private fields that should never be copied to unsafe datastores.

<sup>10</sup> In a real project you would save this code in a Python file, but for now you can just write it in your Jupyter notebook.

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	population	households
0	-122.23	37.88	41.0	880.0	129.0	322.0	88.0
1	-122.22	37.88	21.0	7099.0	1106.0	2401.0	367.0
2	-122.24	37.85	52.0	1467.0	190.0	496.0	142.0
3	-122.25	37.85	52.0	1274.0	235.0	558.0	127.0
4	-122.25	37.85	52.0	1627.0	280.0	585.0	143.0

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_bedrooms
	count	20640.000000	20640.000000	20640.000000	20640.000000	20433.000000
	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	8445.000000

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.<sup>11</sup> 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 25<sup>th</sup> percentile (or 1<sup>st</sup> quartile), the median, and the 75<sup>th</sup> percentile (or 3<sup>rd</sup> 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.

<sup>11</sup> The standard deviation is generally denoted  $\sigma$  (the Greek letter sigma), and it is the square root of the variance, which is the average of the squared deviation from the mean. When a feature has a bell-shaped *normal distribution* (also called a *Gaussian distribution*), which is very common, the "68-95-99.7" rule applies: about 68% of the values fall within  $1\sigma$  of the mean, 95% within  $2\sigma$ , and 99.7% within  $3\sigma$ .

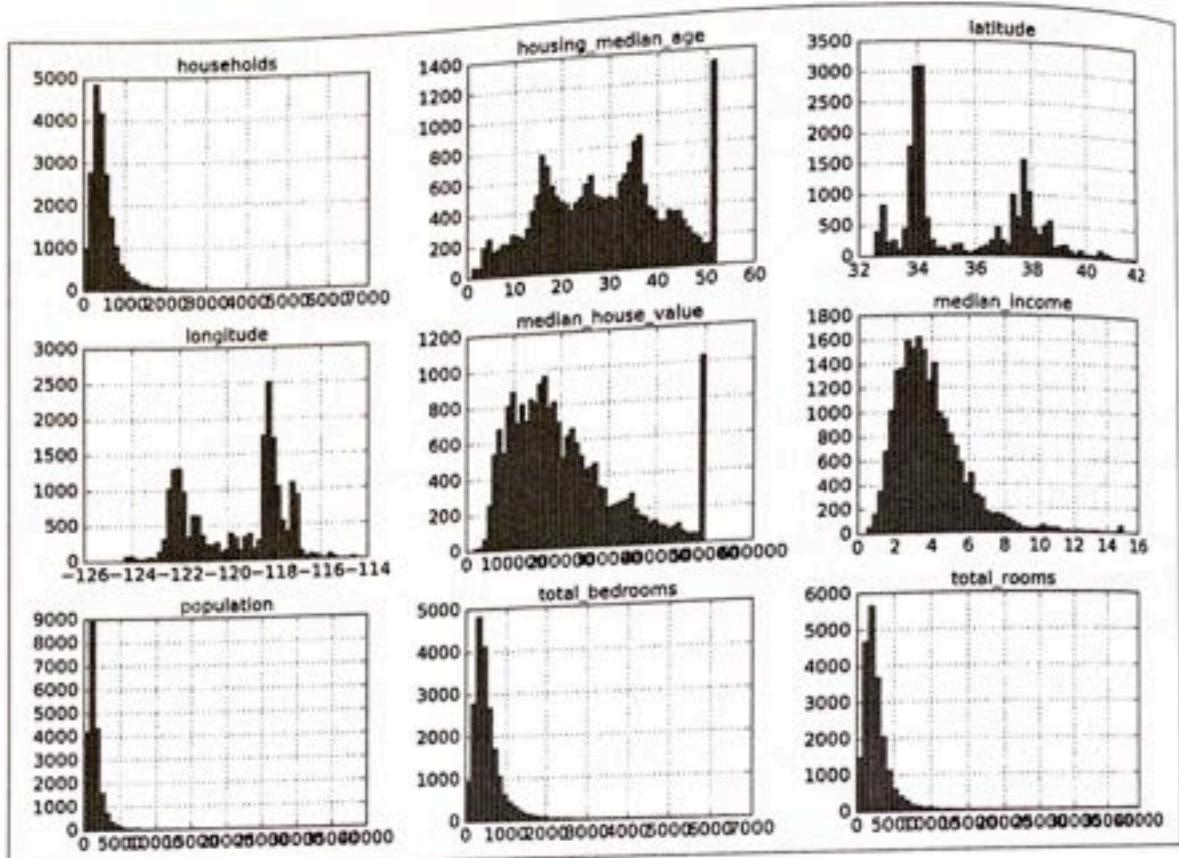


Figure 2-8. A histogram for each numerical attribute

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. 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, 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:

```
>>> train_set, test_set = split_train_test(housing, 0.2)
>>> print(len(train_set), "train +", len(test_set), "test")
16512 train + 4128 test
```

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)`)<sup>12</sup> 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, keep only the last byte of the hash, and put the instance in the test set if this value is lower or equal to 51 (~20% of 256). 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:

```
import hashlib

def test_set_check(identifier, test_ratio, hash):
    return hash(np.int64(identifier)).digest()[-1] < 256 * test_ratio

def split_train_test_by_id(data, test_ratio, id_column, hash=hashlib.md5):
    ids = data[id_column]
    in_test_set = ids.apply(lambda id_: test_set_check(id_, test_ratio, hash))
    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:<sup>13</sup>

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

---

<sup>12</sup> You will often see people set the random seed to 42. This number has no special property, other than to be The Answer to the Ultimate Question of Life, the Universe, and Everything.

<sup>13</sup> The location information is actually quite coarse, and as a result many districts will have the exact same ID,<sup>14</sup> so they will end up in the same set (test or train). This introduces some unfortunate sampling bias.

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 \$20,000–\$50,000, but some median incomes go far beyond \$60,000. 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 creates an income category attribute by dividing the median income by 1.5 (to limit the number of income categories), and rounding up using `ceil` (to have discrete categories), and then merging all the categories greater than 5 into category 5:

```
housing["income_cat"] = np.ceil(housing["median_income"] / 1.5)
housing["income_cat"].where(housing["income_cat"] < 5, 5.0, inplace=True)
```

These income categories are represented on Figure 2-9):

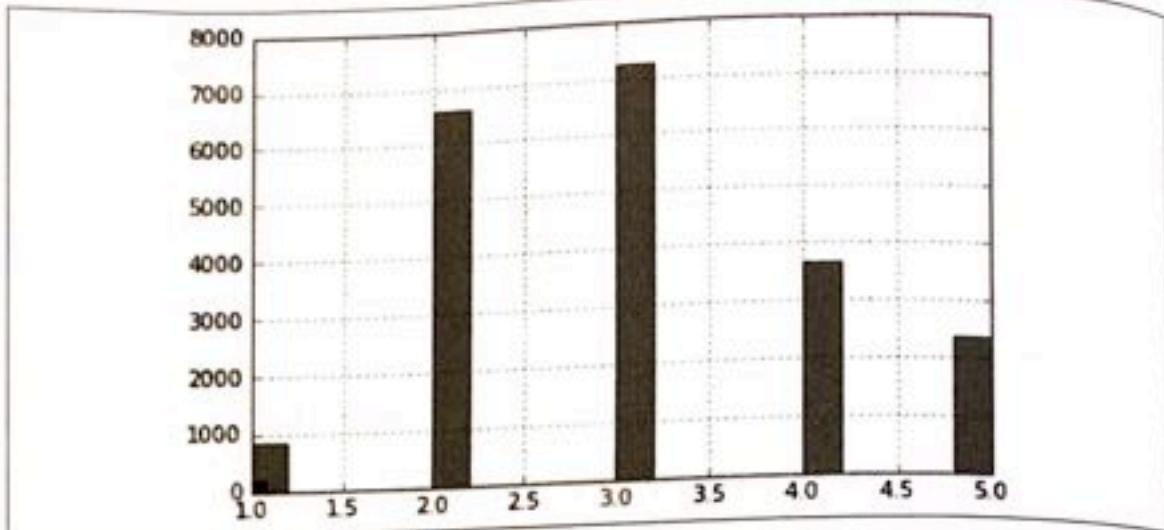


Figure 2-9. Histogram of income categories

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    0.350533  
2.0    0.318798  
4.0    0.176357  
5.0    0.114583  
1.0    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")
```

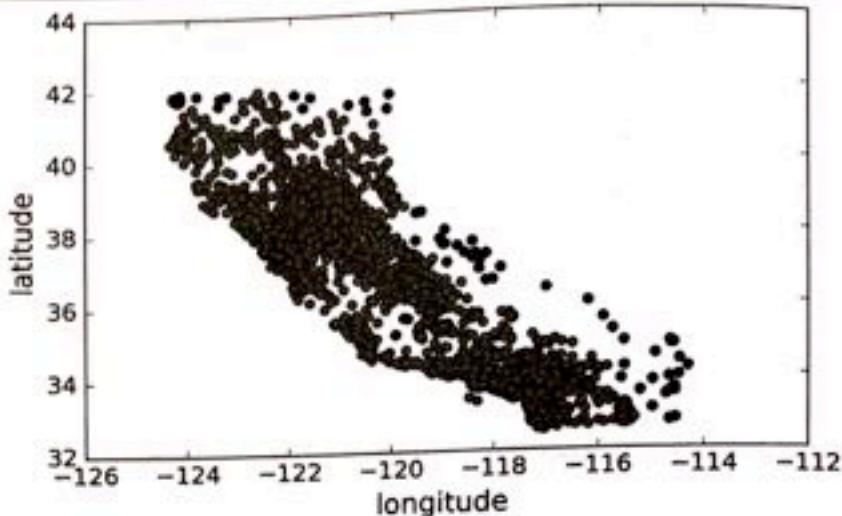


Figure 2-11. A geographical scatterplot of the data

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)
```

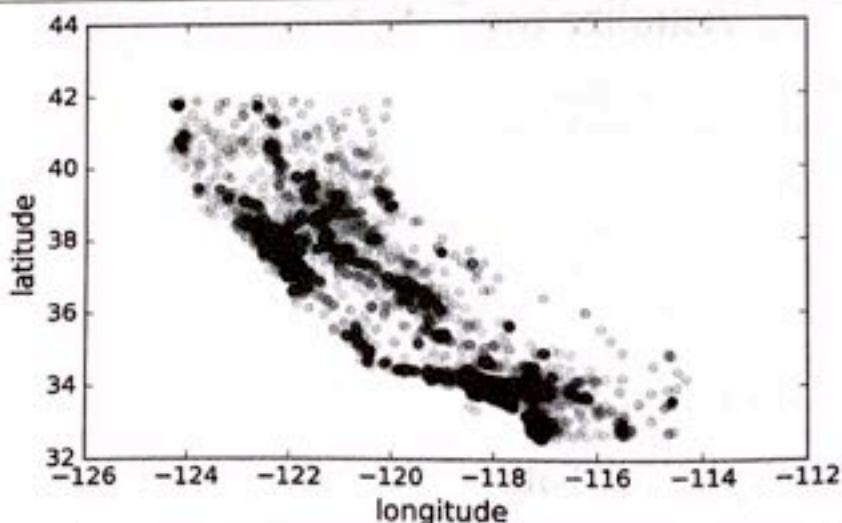


Figure 2-12. A better visualization highlighting high-density areas

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).<sup>14</sup>

```
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()
```

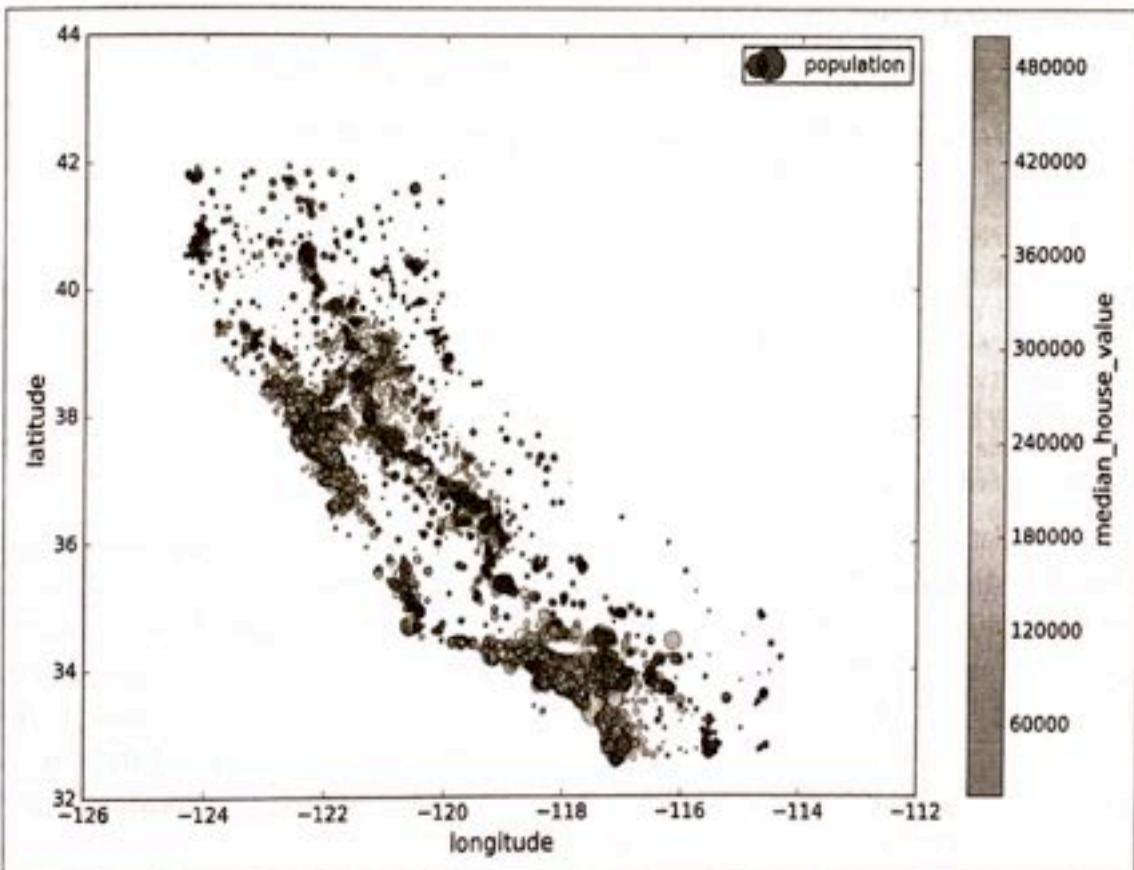


Figure 2-13. California housing prices

<sup>14</sup> If you are reading this in grayscale, grab a red pen and scribble over most of the coastline from the Bay Area down to San Diego (as you might expect). You can add a patch of yellow around Sacramento as well.

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

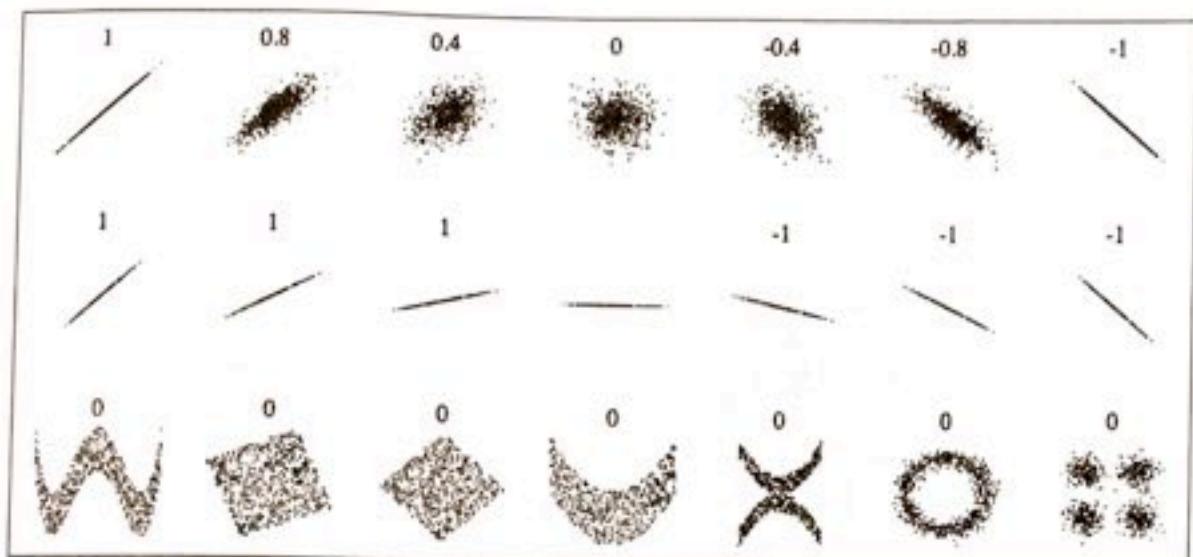
Since the dataset is not too large, you can easily compute the *standard correlation coefficient* (also called *Pearson's r*) between every pair of attributes using the `corr()` method:

```
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)*

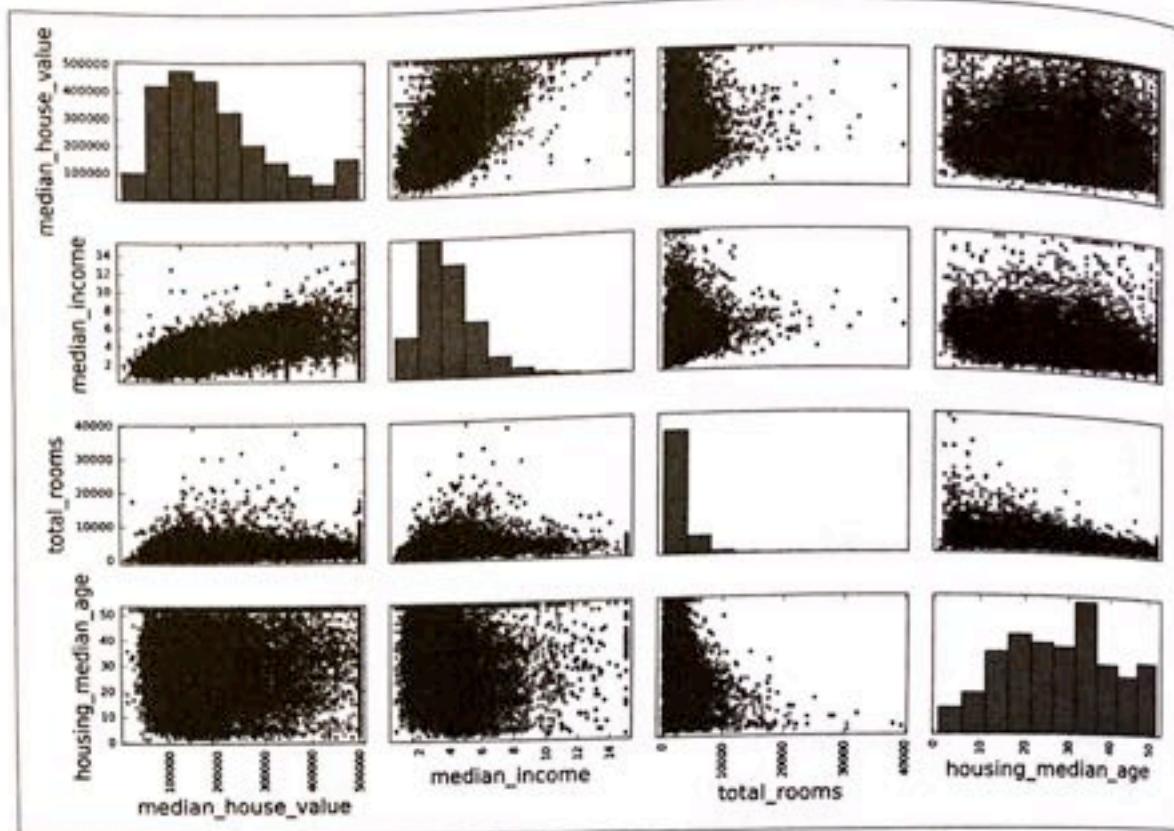


The correlation coefficient only measures linear correlations ("if  $x$  goes up, then  $y$  generally goes up/down"). It may completely miss out on nonlinear relationships (e.g., "if  $x$  is close to zero then  $y$  generally goes up"). Note how all the plots of the bottom row have a correlation coefficient 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.

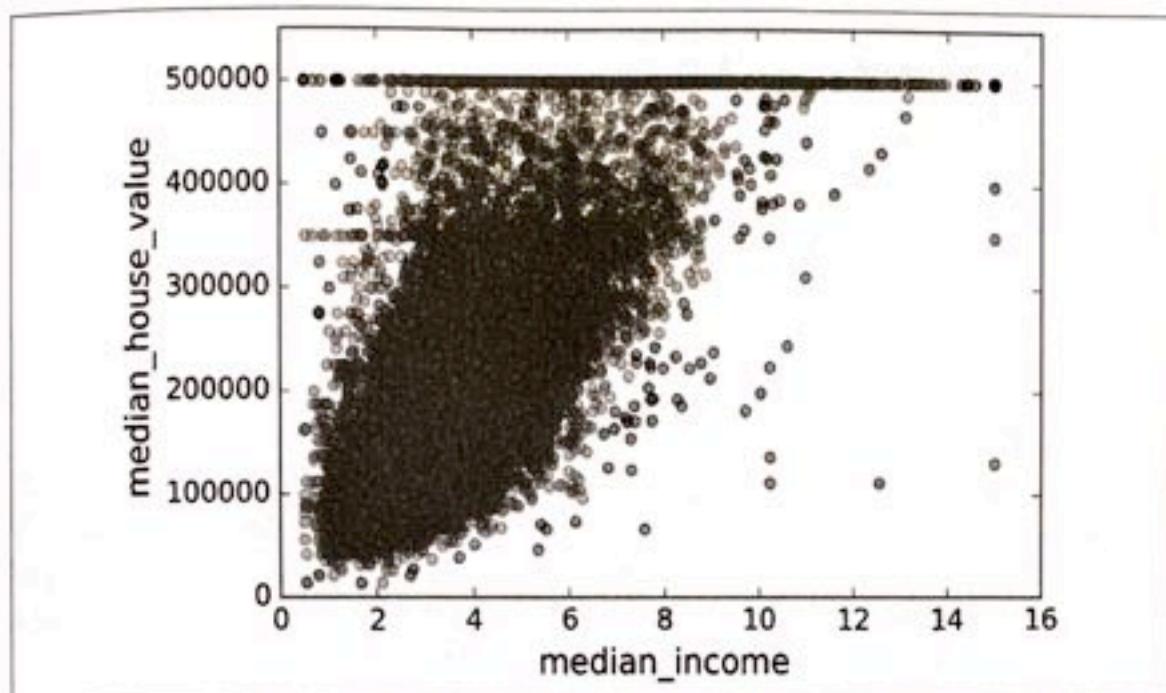


Figure 2-16. Median income versus median house value

## 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: `Imputer`. Here is how to use it. First, you need to create an `Imputer` instance, specifying that you want to replace each attribute's missing values with the median of that attribute:

```
from sklearn.preprocessing import Imputer
imputer = Imputer(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 (<http://goo.gl/wL10sI>) are:<sup>15</sup>

- **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).<sup>16</sup>

<sup>15</sup> For more details on the design principles, see “API design for machine learning software: experiences from the scikit-learn project,” L. Buitinck, G. Louppe, M. Blondel, F. Pedregosa, A. Müller, et al. (2013).

<sup>16</sup> Some predictors also provide methods to measure the confidence of their predictions.

- **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)
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
Name: ocean_proximity, dtype: object
```

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 Pandas' `factorize()` method which maps each category to a different integer:

```
>>> housing_cat_encoded, housing_categories = housing_cat.factorize()
>>> housing_cat_encoded[:10]
array([0, 0, 1, 2, 0, 2, 0, 2, 0, 0])
```

This is better: `housing_cat_encoded` is now purely numerical. The `factorize()` method also returns the list of categories ("`<1H OCEAN`" was mapped to 0, "`NEAR OCEAN`" was mapped to 1, etc.):

```
>>> housing_categories
Index(['<1H OCEAN', 'NEAR OCEAN', 'INLAND', 'NEAR BAY', 'ISLAND'], dtype='object')
```

One issue with this representation is that ML algorithms will assume that two nearby values are more similar than two distant values. Obviously this is not the case (for example, categories 0 and 4 are more similar than categories 0 and 2). 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 “*NEAR OCEAN*” (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*).

Scikit-Learn provides a `OneHotEncoder` encoder to convert integer categorical values into one-hot vectors. Let's encode the categories as one-hot vectors:

```
>>> from sklearn.preprocessing import OneHotEncoder  
>>> encoder = OneHotEncoder()  
>>> housing_cat_1hot = encoder.fit_transform(housing_cat_encoded.reshape(-1,1))  
>>> housing_cat_1hot  
<16512x5 sparse matrix of type '<class 'numpy.float64'>'  
with 16512 stored elements in Compressed Sparse Row format>
```

Note that `fit_transform()` expects a 2D array, but `housing_cat_encoded` is a 1D array, so we need to reshape it<sup>17</sup>. Also, 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 nonzero elements. You can use it mostly like a normal 2D array,<sup>18</sup> 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.,  1.,  0.,  0.,  0.],  
       ...,  
       [ 0.,  0.,  1.,  0.,  0.],  
       [ 1.,  0.,  0.,  0.,  0.],  
       [ 0.,  0.,  0.,  1.,  0.]])
```

You can apply both transformations (from text categories to integer categories, then from integer categories to one-hot vectors) in one shot using the `CategoricalEncoder` class. It is not part of Scikit-Learn 0.19.0 and earlier, but it will be added shortly, so it may already be available by the time you read this. If it is not, you can

<sup>17</sup> NumPy's `reshape()` function allows one dimension to be -1, which means “unspecified”: the value is inferred from the length of the array and the remaining dimensions.

<sup>18</sup> See SciPy's documentation for more details.

simply get it from the Jupyter notebook for this chapter (the code was copied from Pull Request #9151). Here is how to use it:

```
>>> from sklearn.preprocessing import CategoricalEncoder # or get from notebook
>>> cat_encoder = CategoricalEncoder()
>>> housing_cat_reshaped = housing_cat.values.reshape(-1, 1)
>>> housing_cat_1hot = cat_encoder.fit_transform(housing_cat_reshaped)
>>> housing_cat_1hot
<16512x5 sparse matrix of type '<class 'numpy.float64'>'>
    with 16512 stored elements in Compressed Sparse Row format>
```

By default, the `CategoricalEncoder` outputs a sparse matrix, but you can set the encoding to "onehot-dense" if you prefer a dense matrix:

```
>>> cat_encoder = CategoricalEncoder(encoding="onehot-dense")
>>> housing_cat_1hot = cat_encoder.fit_transform(housing_cat_reshaped)
>>> housing_cat_1hot
array([[ 1.,  0.,  0.,  0.],
       [ 1.,  0.,  0.,  0.],
       [ 0.,  0.,  0.,  1.],
       ...,
       [ 0.,  1.,  0.,  0.],
       [ 1.,  0.,  0.,  0.],
       [ 0.,  0.,  0.,  1.,  0.]])
```

You can get the list of categories using the encoder's `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):

```
>>> 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 will want to produce denser representations called *embeddings*, but this requires a good understanding of neural networks (see Chapter 14 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`

tor as a base class (and avoid `*args` and `**kwargs` in your constructor) you will get two extra methods (`get_params()` and `set_params()`) that will be useful for automatic 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, household_ix = 3, 4, 5, 6

class CombinedAttributesAdder(BaseEstimator, TransformerMixin):
    def __init__(self, add_bedrooms_per_room = True): # no *args or **kwargs
        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[:, household_ix]
        population_per_household = X[:, population_ix] / X[:, household_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 variance 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', Imputer(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 don't contain double underscores “`_`”).

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 (it also has a `fit_transform` method that we could have used instead of calling `fit()` and then `transform()`).

Now it would be nice if we could feed a Pandas DataFrame containing non-numerical columns directly into our pipeline, instead of having to first manually extract the numerical columns into a NumPy array. There is nothing in Scikit-Learn to handle Pandas DataFrames,<sup>19</sup> but we can write a custom transformer for this task:

```
from sklearn.base import BaseEstimator, TransformerMixin

class DataFrameSelector(BaseEstimator, TransformerMixin):
    def __init__(self, attribute_names):
        self.attribute_names = attribute_names
    def fit(self, X, y=None):
        return self
    def transform(self, X):
        return X[self.attribute_names].values
```

Our `DataFrameSelector` will transform the data by selecting the desired attributes, dropping the rest, and converting the resulting DataFrame to a NumPy array. With this, you can easily write a pipeline that will take a Pandas DataFrame and handle only the numerical values: the pipeline would just start with a `DataFrameSelector` to pick only the numerical attributes, followed by the other preprocessing steps we discussed earlier. And you can just as easily write another pipeline for the categorical attributes as well by simply selecting the categorical attributes using a `DataFrameSelector` and then applying a `CategoricalEncoder`.

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

num_pipeline = Pipeline([
    ('selector', DataFrameSelector(num_attribs)),
    ('imputer', Imputer(strategy="median")),
    ('attribs_adder', CombinedAttributesAdder()),
    ('std_scaler', StandardScaler()),
])

```

---

<sup>19</sup> But check out Pull Request #3886, which may introduce a `ColumnTransformer` class making attribute-specific transformations easy. You could also run `pip3 install sklearn-pandas` to get a `DataFrameMapper` class with a similar objective.

```
cat_pipeline = Pipeline([
    ('selector', DataFrameSelector(cat_attributes)),
    ('cat_encoder', CategoricalEncoder(encoding="onehot-dense")),
])
```

But how can you join these two pipelines into a single pipeline? The answer is to use Scikit-Learn's `FeatureUnion` class. You give it a list of transformers (which can be entire transformer pipelines); when its `transform()` method is called, it runs each transformer's `transform()` method in parallel, waits for their output, and then concatenates them and returns the result (and of course calling its `fit()` method calls each transformer's `fit()` method). A full pipeline handling both numerical and categorical attributes may look like this:

```
from sklearn.pipeline import FeatureUnion

full_pipeline = FeatureUnion(transformer_list=[
    ("num_pipeline", num_pipeline),
    ("cat_pipeline", cat_pipeline),
])
```

And you can run the whole pipeline simply:

```
>>> housing_prepared = full_pipeline.fit_transform(housing)
>>> housing_prepared
array([[ -1.15604281,  0.77194962,  0.74333089, ...,  0.        ,
         0.        ,  0.        ],
       [-1.17602483,  0.6596948 , -1.1653172 , ...,  0.        ,
         0.        ,  0.        ],
       [...]
      ])
>>> housing_prepared.shape
(16512, 16)
```

## 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
68628.198198489219
```

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 *cross-validation* feature. The following code performs *K-fold cross-validation*: it 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 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: [ 70232.0136482  66828.46839892  72444.08721003  70761.50186201
         71125.52697653  75581.29319857  70169.59286164  70055.37863456
         75370.49116773  71222.39081244]
Mean: 71379.0744771
Standard deviation: 2458.31882043
```

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 71,379, generally  $\pm 2,458$ . 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: 69052.4613635
Standard deviation: 2731.6740018
```

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
21941.911027380233
>>> display_scores(forest_rmse_scores)
Scores: [ 51650.94405471  48920.80645498  52979.16096752  54412.74042021
         50861.29381163  56488.55699727  51866.90120786  49752.24599537
         55399.50713191  53309.74548294]
Mean: 52564.1902524
Standard deviation: 2301.87380392
```

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')

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  $3 \times 4 = 12$  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  $2 \times 3 = 6$  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  $18 \times 5 = 90$  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=1, oob_score=False, random_state=42,
                      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)
...
63647.854446 {'n_estimators': 3, 'max_features': 2}
55611.5015988 {'n_estimators': 10, 'max_features': 2}
53370.0640736 {'n_estimators': 30, 'max_features': 2}
60959.1388585 {'n_estimators': 3, 'max_features': 4}
52740.5841667 {'n_estimators': 10, 'max_features': 4}
50374.1421461 {'n_estimators': 30, 'max_features': 4}
58661.2866462 {'n_estimators': 3, 'max_features': 6}
52089.9739798 {'n_estimators': 10, 'max_features': 6}
50154.1177737 {'n_estimators': 30, 'max_features': 6}
57865.3616801 {'n_estimators': 3, 'max_features': 8}
51730.0755087 {'n_estimators': 10, 'max_features': 8}
49694.8514333 {'n_estimators': 30, 'max_features': 8}
62874.4073931 {'n_estimators': 3, 'bootstrap': False, 'max_features': 2}
54643.4998083 {'n_estimators': 10, 'bootstrap': False, 'max_features': 2}
59437.8922859 {'n_estimators': 3, 'bootstrap': False, 'max_features': 3}
52735.3582936 {'n_estimators': 10, 'bootstrap': False, 'max_features': 3}
57490.0168279 {'n_estimators': 3, 'bootstrap': False, 'max_features': 4}
51008.2615672 {'n_estimators': 10, 'bootstrap': False, 'max_features': 4}
```

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 49,694, which is slightly better than the score you got earlier using the default hyperparameter values (which was 52,564). 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 = cat_pipeline.named_steps["cat_encoder"]
>>> 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)
[(0.36615898061813418, 'median_income'),
 (0.16478099356159051, 'INLAND'),
 (0.10879295677551573, 'pop_per_hhold'),
 (0.073344235516012421, 'longitude'),
 (0.062909070482620302, 'latitude'),
 (0.056419179181954007, 'rooms_per_hhold'),
 (0.053351077347675809, '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'),  
(0.0028564746373201579, 'NEAR OCEAN'),  
(0.0019604155994780701, 'NEAR BAY'),  
(6.0280386727365991e-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()!`), 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 47,766.0
```

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").

## 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.

### Try It Out!

Hopefully this chapter gave you a good idea of what a Machine Learning project looks like, and showed you some of the tools you can use to train a great system. As you can see, much of the work is in the data preparation step, building monitoring tools, setting up human evaluation pipelines, and automating regular model training. The Machine Learning algorithms are also important, of course, but it is probably preferable to be comfortable with the overall process and know three or four algorithms well rather than to spend all your time exploring advanced algorithms and not enough time on the overall process.

So, if you have not already done so, now is a good time to pick up a laptop, select a dataset that you are interested in, and try to go through the whole process from A to

Z. A good place to start is on a competition website such as <http://kaggle.com/>: you will have a dataset to play with, a clear goal, and people to share the experience with.

## Exercises

Using this chapter's housing dataset:

1. Try a Support Vector Machine regressor (`sklearn.svm.SVR`), with various hyperparameters such as `kernel="linear"` (with various values for the `C` hyperparameter) or `kernel="rbf"` (with various values for the `C` and `gamma` hyperparameters). Don't worry about what these hyperparameters mean for now. How does the best SVR predictor perform?
2. Try replacing `GridSearchCV` with `RandomizedSearchCV`.
3. Try adding a transformer in the preparation pipeline to select only the most important attributes.
4. Try creating a single pipeline that does the full data preparation plus the final prediction.
5. Automatically explore some preparation options using `GridSearchCV`.

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

# Hands-On Machine Learning with Scikit-Learn & TensorFlow

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