Python Data Science Essentials

Third Edition

A practitioner's guide covering essential data science principles, tools, and techniques

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Alberto Boschetti and Luca Massaron

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> *I would like to thank my family, my friends, and my colleagues. Also, big thanks to the open source community.*

Luca Massaron is a data scientist and marketing research director specialized in multivariate statistical analysis, machine learning, and customer insight, with over a decade of experience of solving real-world problems and generating value for stakeholders by applying reasoning, statistics, data mining, and algorithms. From being a pioneer of web audience analysis in Italy to achieving the rank of a top-10 Kaggler, he has always been very passionate about every aspect of data and its analysis, and also about demonstrating the potential of data-driven knowledge discovery to both experts and non-experts. Favoring simplicity over unnecessary sophistication, Luca believes that a lot can be achieved in data science just by doing the essentials.

> *To Yukiko and Amelia, for their loving patience.*
>
> *"Roads go ever ever on, under cloud and under star, yet feet that wandering have gone turn at last to home afar."*

About the reviewers

Pietro Marinelli has been working with artificial intelligence, text analytics and many other data science techniques, and has more than 10 years of experience in designing products based on data for different industries.

He produced a variety of algorithms, ranging from predictive modeling to advanced simulation algorithm to support top management's business decisions for different multinational companies.

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Preface

"A journey of a thousand miles begins with a single step."

– Laozi (604 BC - 531 BC)

Data science is a relatively new knowledge domain that requires the successful integration of linear algebra, statistical modeling, visualization, computational linguistics, graph analysis, machine learning, business intelligence, and data storage and retrieval.

The Python programming language, having conquered the scientific community during the last decade, is now an indispensable tool for the data science practitioner and a must-have tool for every aspiring data scientist. Python will offer you a fast, reliable, cross-platform, and mature environment for data analysis, machine learning, and algorithmic problem solving. Whatever stopped you before from mastering Python for data science applications will be easily overcome by our easy, step-by-step, and example-oriented approach, which will help you apply the most straightforward and effective Python tools to both demonstrative and real-world datasets.

As the third edition of *Python Data Science Essentials*, this book offers updated and expanded content. Based on the recent Jupyter Notebook and JupyterLab interface (incorporating interchangeable kernels, a truly polyglot data science system), this book incorporates all the main recent improvements in NumPy, `pandas`, and scikit-learn. Additionally, it offers new content in the form of new GBM algorithms (XGBoost, LightGBM, and CatBoost), deep learning (by presenting Keras solutions based on TensorFlow), beautiful visualizations (mostly due to seaborn), and web deployment (using bottle).

This book starts by showing you how to set up your essential data science toolbox in Python's latest version (3.6), using a single-source approach (implying that the book's code will be easily reusable on Python 2.7 as well). Then, it will guide you across all the data munging and preprocessing phases in a manner that explains all the core data science activities related to loading data, transforming, and fixing it for analysis, and exploring/processing it. Finally, the book will complete its overview by presenting you with the principal machine learning algorithms, graph analysis techniques, and all the visualization and deployment instruments that make it easier to present your results to an audience of both data science experts and business users.

Who this book is for

If you are an aspiring data scientist and you have at least a working knowledge of data analysis and Python, this book will get you started in data science. Data analysis with experience of R or MATLAB/GNU Octave will also find the book to be a comprehensive reference to enhance their data manipulation and machine learning skills.

What this book covers

`Chapter 1`, *First Steps*, introduces Jupyter Notebook and demonstrates how you can have access to the data run in the tutorials.

`Chapter 2`, *Data Munging*, presents all the key data manipulation and transformation techniques, highlighting best practices for munging activities.

`Chapter 3`, *The Data Pipeline*, discusses all the operations that can potentially improve data science project results, rendering the reader capable of advanced data operations.

`Chapter 4`, *Machine Learning*, presents the most important learning algorithms available through the scikit-learn library. The reader will be shown practical applications and what is important to check and what parameters to tune for getting the best from each learning technique.

`Chapter 5`, *Visualization, Insights, and Results*, offers you basic and upper-intermediate graphical representations, indispensable for representing and visually understanding complex data structures and results obtained from machine learning.

`Chapter 6`, *Social Network Analysis*, provides the reader with practical and effective skills for handling data representing social relations and interactions.

`Chapter 7`, *Deep Learning Beyond the Basics*, demonstrates how to build a convolutional neural network from scratch, introduces all the tools of the trade to enhance your deep learning models, and explains how *transfer learning* works, as well as how to use recurrent neural networks for classifying text and predicting series.

`Chapter 8`, *Spark for Big Data*, introduces a new way to process data: scaling big data horizontally. This means running a cluster of machines, having installed the Hadoop and Spark frameworks.

`Appendix`, *Strengthening Your Python Foundations*, covers a few Python examples and tutorials that are focused on the key features of the language that are indispensable in order to work on data science projects.

To get the most out of this book

In order to get the most out of this book, you will need the following:

- A familiarity with the basic Python syntax and data structures (for example, lists and dictionaries)
- Some knowledge about data analysis, especially regarding descriptive statistics

You can build up both these skills as you are reading the book, though the book does not go too much into the details, instead providing only the essentials for most of the techniques that a data scientist has to know in order to be successful on her/his projects.

You will also need the following:

- A computer with a Windows, macOS, or Linux operating system and at least 8 GB of memory (if you have just 4 GB on your machine, you should be fine with most examples anyway)
- A GPU installed on your computer if you want to speed up the computations you will find in `Chapter 7`, *Deep Learning Beyond the Basics*.
- A Python 3.6 installation, preferably from Anaconda (`https://www.anaconda.com/download/`)

Download the example code files

You can download the example code files for this book from your account at `www.packt.com`. If you purchased this book elsewhere, you can visit `www.packt.com/support` and register to have the files emailed directly to you.

You can download the code files by following these steps:

1. Log in or register at `www.packt.com`.
2. Select the **SUPPORT** tab.
3. Click on **Code Downloads & Errata**.
4. Enter the name of the book in the **Search** box and follow the onscreen instructions.

Once the file is downloaded, please make sure that you unzip or extract the folder using the latest version of:

- WinRAR/7-Zip for Windows
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The code bundle for the book is also hosted on GitHub at `https://github.com/PacktPublishing/Python-Data-Science-Essentials-Third-Edition`. In case there's an update to the code, it will be updated on the existing GitHub repository.

We also have other code bundles from our rich catalog of books and videos available at `https://github.com/PacktPublishing/`. Check them out!

Download the color images

We also provide a PDF file that has color images of the screenshots/diagrams used in this book. You can download it here: `http://www.packtpub.com/sites/default/files/downloads/9781789537864_ColorImages.pdf`.

Conventions used

There are a number of text conventions used throughout this book.

`CodeInText`: Indicates code words in the text, database table names, folder names, filenames, file extensions, pathnames, dummy URLs, user input, and Twitter handles. Here is an example: "Mount the downloaded `WebStorm-10*.dmg` disk image file as another disk in your system."

A block of code is set as follows:

```
In: G.add_edge(3,4)
    G.add_edges_from([(2, 3), (4, 1)])
    nx.draw_networkx(G)
    plt.show()
```

Bold: Indicates a new term, an important word, or words that you see onscreen. For example, words in menus or dialog boxes appear in the text like this. Here is an example: "Select **System info** from the **Administration** panel."

Warnings or important notes appear like this.

Tips and tricks appear like this.

Get in touch

Feedback from our readers is always welcome.

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Reviews

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1
First Steps

Whether you are an eager learner of data science or a well-grounded data science practitioner, you can take advantage of this essential introduction to Python for data science. You can use it to the fullest if you already have at least some previous experience in basic coding, in writing general-purpose computer programs in Python, or in some other data-analysis-specific language such as MATLAB or R.

This book will delve directly into Python for data science, providing you with a straight and fast route to solving various data science problems using Python and its powerful data analysis and machine learning packages. The code examples that are provided in this book don't require you to be a master of Python. However, they will assume that you at least know the basics of Python scripting, including data structures such as lists and dictionaries, and the workings of class objects. If you don't feel confident about these subjects or have minimal knowledge of the Python language, before reading this book, we suggest that you take an online tutorial. There are good online tutorials that you may take, such as the one offered by the Code Academy course at `https://www.codecademy.com/learn/learn-python`, the one by Google's Python class at `https://developers.google.com/edu/python/`, or even the *Whirlwind tour of Python* by Jake Vanderplas (`https://github.com/jakevdp/WhirlwindTourOfPython`). All the courses are free, and, in a matter of a few hours of study, they should provide you with all the building blocks that will ensure you enjoy this book to the fullest. In order to provide an integration of the two aforementioned free courses, we have also prepared a tutorial of our own, which can be found in the appendix of this book.

In any case, don't be intimidated by our starting requirements; mastering Python enough for data science applications isn't as arduous as you may think. It's just that we have to assume some basic knowledge on the reader's part because our intention is to go straight to the point of doing data science without having to explain too much about the general aspects of the Python language that we will be using.

Are you ready, then? Let's get started!

In this short introductory chapter, we will work through the basics to set off in full swing and go through the following topics:

- How to set up a Python data science toolbox
- Using Jupyter
- An overview of the data that we are going to study in this book

Introducing data science and Python

Data science is a relatively new knowledge domain, though its core components have been studied and researched for many years by the computer science community. Its components include linear algebra, statistical modeling, visualization, computational linguistics, graph analysis, machine learning, business intelligence, and data storage and retrieval.

Data science is a new domain, and you have to take into consideration that, currently, its frontiers are still somewhat blurred and dynamic. Since data science is made of various constituent sets of disciplines, please also keep in mind that there are different profiles of data scientists depending on their competencies and areas of expertise (for instance, you may read the illustrative *There's More Than One Kind of Data Scientist* by Harlan D Harris at `radar.oreilly.com/2013/06/theres-more-than-one-kind-of-data-scientist.html`, or delve into the discussion about type A or B data scientists and other interesting taxonomies at `https://stats.stackexchange.com/questions/195034/what-is-a-data-scientist`).

In such a situation, what can be the best tool of the trade that you can learn and effectively use in your career as a data scientist? We believe that the best tool is Python, and we intend to provide you with all the essential information that you will need for a quick start.

In addition, other programming languages such as R and MATLAB provide data scientists with specialized tools to solve specific problems in statistical analysis and matrix manipulation in data science. However, only Python really completes your data scientist skill set with all the key techniques in a scalable and effective way. This multipurpose language is suitable for both development and production alike; it can handle small- to large-scale data problems and it is easy to learn and grasp, no matter what your background or experience is.

Created in 1991 as a general-purpose, interpreted, and object-oriented language, Python has slowly and steadily conquered the scientific community and grown into a mature ecosystem of specialized packages for data processing and analysis. It allows you to have uncountable and fast experimentations, easy theory development, and prompt deployment of scientific applications.

At present, the core Python characteristics that render it an indispensable data science tool are as follows:

- It offers a large, mature system of packages for data analysis and machine learning. It guarantees that you will get all that you may need in the course of a data analysis, and sometimes even more.
- Python can easily integrate different tools and offers a truly unifying ground for different languages, data strategies, and learning algorithms that can be fitted together easily and which can concretely help data scientists forge powerful solutions. There are packages that allow you to call code in other languages (in Java, C, Fortran, R, or Julia), outsourcing some of the computations to them and improving your script performance.
- It is very versatile. No matter what your programming background or style is (object-oriented, procedural, or even functional), you will enjoy programming with Python.
- It is cross-platform; your solutions will work perfectly and smoothly on Windows, Linux, and macOS systems. You won't have to worry all that much about portability.
- Although interpreted, it is undoubtedly fast compared to other mainstream data analysis languages such as R and MATLAB (though it is not comparable to C, Java, and the newly emerged Julia language). Moreover, there are also static compilers such as *Cython* or just-in-time compilers such as *PyPy* that can transform Python code into C for higher performance.
- It can work with large in-memory data because of its minimal memory footprint and excellent memory management. The memory garbage collector will often save the day when you load, transform, dice, slice, save, or discard data using various iterations and reiterations of data wrangling.
- It is very simple to learn and use. After you grasp the basics, there's no better way to learn more than by immediately starting with the coding.
- Moreover, the number of data scientists using Python is continuously growing: new packages and improvements have been released by the community every day, making the Python ecosystem an increasingly prolific and rich language for data science.

Installing Python

First, let's proceed and introduce all the settings you need in order to create a fully working data science environment to test the examples and experiment with the code that we are going to provide you with.

Python is an open source, object-oriented, and cross-platform programming language. Compared to some of its direct competitors (for instance, C++ or Java), Python is very concise. It allows you to build a working software prototype in a very short time, and yet it has become the most used language in the data scientist's toolbox not just because of that. It is also a general-purpose language, and it is very flexible due to a variety of available packages that solve a wide spectrum of problems and necessities.

Python 2 or Python 3?

There are two main branches of Python: 2.7.x and 3.x. At the time of the revision of this third edition of the book, the Python foundation (`www.python.org/`) is offering downloads for Python Version 2.7.15 (release date January 5, 2018) and 3.6.5 (release date January 3, 2018). Although the Python 3 version is the newest, the *older* Python 2 has still been in use in both scientific (20% adoption) and commercial (30% adoption) areas in 2017, as depicted in detail by this survey by JetBrains: `https://www.jetbrains.com/research/python-developers-survey-2017`. If you are still using Python 2, the situation could turn quite problematic soon, because in just one year's time Python 2 will be retired and maintenance will be ceased (`pythonclock.org/` will provide you with the countdown, but for an official statement about this, just read `https://www.python.org/dev/peps/pep-0373/`), and there are really only a handful of libraries still incompatible between the two versions (`py3readiness.org/`) that do not give enough reasons to stay with the older version.

In addition to all these reasons, there is no immediate backward compatibility between Python 3 and 2. In fact, if you try to run some code developed for Python 2 with a Python 3 interpreter, it may not work. Major changes have been made to the newest version, and that has affected past compatibility. Some data scientists, having built most of their work on Python 2 and its packages, are reluctant to switch to the new version.

In this third edition of the book, we will continue to address the larger audience of data scientists, data analysts, and developers, who do not have such a strong legacy with Python 2. Consequently, we will continue working with Python 3, and we suggest using a version such as the most recently available Python 3.6. After all, Python 3 is the present and the future of Python. It is the only version that will be further developed and improved by the Python foundation, and it will be the default version of the future on many operating systems.

Anyway, if you are currently working with version 2 and you prefer to keep on working with it, you can still use this book and all of its examples. In fact, for the most part, our code will simply work on Python 2 after having the code itself preceded by these imports:

```
from __future__ import (absolute_import, division,
                        print_function, unicode_literals)
from builtins import *
from future import standard_library
standard_library.install_aliases()
```

The `from __future__ import` commands should always occur at the beginning of your scripts, or else you may experience Python reporting an error.

As described in the Python-future website (`python-future.org`), these imports will help convert several Python 3-only constructs to a form that's compatible with both Python 3 and Python 2 (and in any case, most Python 3 code should just simply work on Python 2, even without the aforementioned imports).

In order to run the upward commands successfully, if the future package is not already available on your system, you should install it (version >= 0.15.2) by using the following command, which is to be executed from a shell:

```
$> pip install -U future
```

If you're interested in understanding the differences between Python 2 and Python 3 further, we recommend reading the wiki page offered by the Python foundation itself: `https://wiki.python.org/moin/Python2orPython3`.

Step-by-step installation

Novice data scientists who have never used Python (who likely don't have the language readily installed on their machines) need to first download the installer from the main website of the project, `www.python.org/downloads/`, and then install it on their local machine.

This section provides you with full control over what can be installed on your machine. This is very useful when you have to set up single machines to deal with different tasks in data science. Anyway, please be warned that a step-by-step installation really takes time and effort. Instead, installing a ready-made scientific distribution will lessen the burden of installation procedures and it may be well-suited for first starting and learning because it saves you time and sometimes even trouble, though it will put a large number of packages (and we won't use most of them) on your computer all at once. Therefore, if you want to start immediately with an easy installation procedure, just skip this part and proceed to the next section, *Scientific distributions*.

This being a multiplatform programming language, you'll find installers for machines that either run on Windows or Unix-like operating systems.

Remember that some of the latest versions of most Linux distributions (such as CentOS, Fedora, Red Hat Enterprise, and Ubuntu) have Python 2 packaged in the repository. In such a case, and in the case that you already have a Python version on your computer (since our examples run on Python 3), you first have to check what version you are exactly running. To do such a check, just follow these instructions:

1. Open a python shell, type `python` in the terminal, or click on any Python icon you find on your system.
2. Then, after starting Python, to test the installation, run the following code in the Python interactive shell or REPL:

```
>>> import sys
>>> print (sys.version_info)
```

3. If you can read that your Python version has the `major=2` attribute, it means that you are running a Python 2 instance. Otherwise, if the attribute is valued 3, or if the `print` statement reports back to you something like v3.x.x (for instance, v3.5.1), you are running the right version of Python, and you are ready to move forward.

To clarify the operations we have just mentioned, when a command is given in the terminal command line, we prefix the command with `$>`. Otherwise, if it's for the Python REPL, it's preceded by `>>>`.

Installing the necessary packages

Python won't come bundled with everything you need unless you take a specific pre-made distribution. Therefore, to install the packages you need, you can use either `pip` or `easy_install`. Both of these two tools run in the command line and make the process of installation, upgrading, and removing Python packages a breeze. To check which tools have been installed on your local machine, run the following command:

```
$> pip
```

To install `pip`, follow the instructions given at `https://pip.pypa.io/en/latest/installing/`.

Alternatively, you can also run the following command:

```
$> easy_install
```

If both of these commands end up with an error, you need to install any one of them. We recommend that you use `pip` because it is thought of as an improvement over `easy_install`. Moreover, `easy_install` is going to be dropped in the future and `pip` has important advantages over it. It is preferable to install everything using `pip` because of the following:

- It is the preferred package manager for Python 3. Starting with Python 2.7.9 and Python 3.4, it is included by default with the Python binary installers
- It provides an uninstall functionality
- It rolls back and leaves your system clear if, for whatever reason, the package's installation fails

Using easy_install in spite of the advantages of pip makes sense if you are working on Windows because pip won't always install pre-compiled binary packages. Sometimes, it will try to build the package's extensions directly from C source, thus requiring a properly configured compiler (and that's not an easy task on Windows). This depends on whether the package is running on eggs (and pip cannot directly use their binaries, but it needs to build from their source code) or wheels (in this case, pip can install binaries if available, as explained here: http://pythonwheels.com/). Instead, easy_install will always install available binaries from eggs and wheels. Therefore, if you are experiencing unexpected difficulties installing a package, easy_install can save your day (at some price, anyway, as we just mentioned in the list).

The most recent versions of Python should already have pip installed by default. Therefore, you may have it already installed on your system. If not, the safest way is to download the get-pi.py script from https://bootstrap.pypa.io/get-pip.py and then run it by using the following:

```
$> python get-pip.py
```

The script will also install the setup tool from pypi.org/project/setuptools, which also contains easy_install.

You're now ready to install the packages you need in order to run the examples provided in this book. To install the < package-name > generic package, you just need to run the following command:

```
$> pip install < package-name >
```

Alternatively, you can run the following command:

```
$> easy_install < package-name >
```

Note that, in some systems, pip might be named as pip3 and easy_install as easy_install-3 to stress the fact that both operate on packages for Python 3. If you're unsure, check the version of Python that pip is operating on with:

```
$> pip -V
```

For easy_install, the command is slightly different:

```
$> easy_install --version
```

After this, the `<pk>` package and all its dependencies will be downloaded and installed. If you're not certain whether a library has been installed or not, just try to import a module inside it. If the Python interpreter raises an `ImportError` error, it can be concluded that the package has not been installed.

This is what happens when the NumPy library has been installed:

```
>>> import numpy
```

This is what happens if it's not installed:

```
>>> import numpy

    Traceback (most recent call last):
    File "<stdin>", line 1, in <module>
    ImportError: No module named numpy
```

In the latter case, you'll need to first install it through `pip` or `easy_install`.

Take care that you don't confuse packages with modules. With `pip`, you install a package; in Python, you import a module. Sometimes, the package and the module have the same name, but in many cases, they don't match. For example, the sklearn module is included in the package named Scikit-learn.

Finally, to search and browse the Python packages available for Python, look at `pypi.org`.

Package upgrades

More often than not, you will find yourself in a situation where you have to upgrade a package because either the new version is required by a dependency or it has additional features that you would like to use. First, check the version of the library you have installed by glancing at the `__version__` attribute, as shown in the following example, `numpy`:

```
>>> import numpy
>>> numpy.__version__ # 2 underscores before and after
    '1.11.0'
```

Now, if you want to update it to a newer release, say the `1.12.1` version, you can run the following command from the command line:

```
$> pip install -U numpy==1.12.1
```

Alternatively, you can use the following command:

```
$> easy_install --upgrade numpy==1.12.1
```

Finally, if you're interested in upgrading it to the latest available version, simply run the following command:

```
$> pip install -U numpy
```

You can alternatively run the following command:

```
$> easy_install --upgrade numpy
```

Scientific distributions

As you've read so far, creating a working environment is a time-consuming operation for a data scientist. You first need to install Python, and then, one by one, you can install all the libraries that you will need (sometimes, the installation procedures may not go as smoothly as you'd hoped for earlier).

If you want to save time and effort and want to ensure that you have a fully working Python environment that is ready to use, you can just download, install, and use the scientific Python distribution. Apart from Python, they also include a variety of preinstalled packages, and sometimes, they even have additional tools and an IDE. A few of them are very well-known among data scientists, and in the sections that follow, you will find some of the key features of each of these packages.

We suggest that you first promptly download and install a scientific distribution, such as Anaconda (which is the most complete one), and after practicing the examples in this book, decide whether or not to fully uninstall the distribution and set up Python alone, which can be accompanied by just the packages you need for your projects.

Anaconda

Anaconda (`https://www.anaconda.com/download/`) is a Python distribution offered by Continuum Analytics that includes nearly 200 packages, which comprises NumPy, SciPy, pandas, Jupyter, Matplotlib, Scikit-learn, and NLTK. It's a cross-platform distribution (Windows, Linux, and macOS) that can be installed on machines with other existing Python distributions and versions. Its base version is free; instead, add-ons that contain advanced features are charged separately. Anaconda introduces `conda`, a binary package manager, as a command-line tool to manage your package installations.

As stated on the website, Anaconda's goal is to provide enterprise-ready Python distribution for large-scale processing, predictive analytics, and scientific computing.

Leveraging conda to install packages

If you've decided to install an Anaconda distribution, you can take advantage of the `conda` binary installer we mentioned previously. `conda` is an open source package management system, and consequently, it can be installed separately from an Anaconda distribution. The core difference from `pip` is that `conda` can be used to install any package (not just Python's ones) in a `conda` environment (that is, an environment where you have installed `conda` and you are using it for providing packages). There are many advantages in using `conda` over `pip`, as described by Jack VanderPlas in this famous blog post of his: `jakevdp.github.io/blog/2016/08/25/conda-myths-and-misconceptions`.

You can test immediately whether `conda` is available on your system. Open a shell and digit the following:

```
$> conda -V
```

If `conda` is available, your version will appear; otherwise, an error will be reported. If `conda` is not available, you can quickly install it on your system by going to `http://conda.pydata.org/miniconda.html` and installing the Miniconda software that's suitable for your computer. **Miniconda** is a minimal installation that only includes `conda` and its dependencies.

Conda can help you manage two tasks: installing packages and creating virtual environments. In this paragraph, we will explore how `conda` can help you easily install most of the packages you may need in your data science projects.

Before starting, please check that you have the latest version of `conda` at hand:

```
$> conda update conda
```

Now you can install any package you need. To install the `<package-name>` generic package, you just need to run the following command:

```
$> conda install <package-name>
```

You can also install a particular version of the package just by pointing it out:

```
$> conda install <package-name>=1.11.0
```

Similarly, you can install multiple packages at once by listing all their names:

```
$> conda install <package-name-1> <package-name-2>
```

If you just need to update a package that you previously installed, you can keep on using `conda`:

```
$> conda update <package-name>
```

You can update all the available packages simply by using the `--all` argument:

```
$> conda update --all
```

Finally, `conda` can also uninstall packages for you:

```
$> conda remove <package-name>
```

If you would like to know more about `conda`, you can read its documentation at `http://conda.pydata.org/docs/index.html`. In summary, as its main advantage, it handles binaries even better than `easy_install` (by always providing a successful installation on Windows without any need to compile the packages from source) but without its problems and limitations. With the use of `conda`, packages are easy to install (and installation is always successful), update, and even uninstall. On the other hand, `conda` cannot install directly from a `git` server (so it cannot access the latest version of many packages under development), and it doesn't cover all the packages available on PyPI like `pip` itself.

Enthought Canopy

Enthought Canopy (`https://www.enthought.com/products/canopy/`) is a Python distribution by Enthought Inc. It includes more than 200 preinstalled packages, such as NumPy, SciPy, Matplotlib, Jupyter, and pandas. This distribution is targeted at engineers, data scientists, quantitative and data analysts, and enterprises. Its base version is free (which is named Canopy Express), but if you need advanced features, you have to buy a front version. It's a multi-platform distribution, and its command-line installation tool is `canopy_cli`.

WinPython

WinPython (`http://winpython.github.io/`) is a free, open-source Python distribution that's maintained by the community. It is designed for scientists and includes many packages such as NumPy, SciPy, Matplotlib, and Jupyter. It also includes Spyder as an IDE. It is free and portable. You can put WinPython into any directory, or even into a USB flash drive, and at the same time maintain multiple copies and versions of it on your system. It only works on Microsoft Windows, and its command-line tool is the **WinPython Package Manager** (**WPPM**).

Explaining virtual environments

No matter whether you have chosen to install a standalone Python or instead used a scientific distribution, you may have noticed that you are actually bound on your system to the Python version you have installed. The only exception, for Windows users, is to use a WinPython distribution, since it is a portable installation and you can have as many different installations as you need.

A simple solution to breaking free of such a limitation is to use `virtualenv`, which is a tool for creating isolated Python environments. That means, by using different Python environments, you can easily achieve the following things:

- Testing any new package installation or doing experimentation on your Python environment without any fear of breaking anything in an irreparable way. In this case, you need a version of Python that acts as a sandbox.
- Having at hand multiple Python versions (both Python 2 and Python 3), geared with different versions of installed packages. This can help you in dealing with different versions of Python for different purposes (for instance, some of the packages we are going to present on Windows OS only work when using Python 3.4, which is not the latest release).
- Taking a replicable snapshot of your Python environment easily and having your data science prototypes work smoothly on any other computer or in production. In this case, your main concern is the immutability and replicability of your working environment.

You can find documentation about `virtualenv` at `http://virtualenv.readthedocs.io/en/stable/`, though we are going to provide you with all the directions you need to start using it immediately. In order to take advantage of `virtualenv`, you first have to install it on your system:

```
$> pip install virtualenv
```

After the installation completes, you can start building your virtual environments. Before proceeding, you have to make a few decisions:

- If you have more versions of Python installed on your system, you have to decide which version to pick up. Otherwise, `virtualenv` will take the Python version that was used when `virtualenv` was installed on your system. In order to set a different Python version, you have to digit the argument `-p` followed by the version of Python you want, or insert the path of the Python executable to be used (for instance, by using `-p python2.7`, or by just pointing to a Python executable such as `-p c:Anaconda2python.exe`).
- With `virtualenv`, when required to install a certain package, it will install it from scratch, even if it is already available at a system level (on the python directory you created the virtual environment from). This default behavior makes sense because it allows you to create a completely separated empty environment. In order to save disk space and limit the time of installation of all the packages, you may instead decide to take advantage of already available packages on your system by using the argument `--system-site-packages`.
- You may want to be able to later move around your virtual environment across Python installations, even among different machines. Therefore, you may want to make the functionality of all of the environment's scripts relative to the path it is placed in by using the argument `--relocatable`.

After deciding on the Python version you wish to use, linking to existing global packages, and the virtual environment being relocatable or not, in order to start, you just need to launch the command from a shell. Declare the name you would like to assign to your new environment:

```
$> virtualenv clone
```

`virtualenv` will just create a new directory using the name you provided, in the path from which you actually launched the command. To start using it, you can just enter the directory and digit `activate`:

```
$> cd clone
$> activate
```

At this point, you can start working on your separated Python environment, installing packages, and working with code.

If you need to install multiple packages at once, you may need some special function from pip, `pip freeze`, which will enlist all the packages (and their versions) you have installed on your system. You can record the entire list in a text file by using the following command:

```
$> pip freeze > requirements.txt
```

After saving the list in a text file, just take it into your virtual environment and install all the packages in a breeze with a single command:

```
$> pip install -r requirements.txt
```

Each package will be installed according to the order in the list (packages are listed in a case-insensitive sorted order). If a package requires other packages that are later in the list, that's not a big deal because `pip` automatically manages such situations. So, if your package requires NumPy and NumPy is not yet installed, `pip` will install it first.

When you've finished installing packages and using your environment for scripting and experimenting, in order to return to your system defaults, just issue the following command:

```
$> deactivate
```

If you want to remove the virtual environment completely, after deactivating and getting out of the environment's directory, you just have to get rid of the environment's directory itself by performing a recursive deletion. For instance, on Windows, you just do the following:

```
$> rd /s /q clone
```

On Linux and macOS, the command will be as follows:

```
$> rm -r -f clone
```

If you are working extensively with virtual environments, you should consider using `virtualenvwrapper`, which is a set of wrappers for `virtualenv` in order to help you manage multiple virtual environments easily. It can be found at `bitbucket.org/dhellmann/virtualenvwrapper`. If you are operating on a Unix system (Linux or macOS), another solution we have to quote is `pyenv`, which can be found at `https://github.com/yyuu/pyenv`. It lets you set your main Python version, allows for the installation of multiple versions, and creates virtual environments. Its peculiarity is that it does not depend on Python to be installed and works perfectly at the user level (no need for `sudo` commands).

Conda for managing environments

If you have installed the Anaconda distribution, or you have tried `conda` by using a Miniconda installation, you can also take advantage of the `conda` command to run virtual environments as an alternative to `virtualenv`. Let's see how to use `conda` for that in practice. We can check what environments we have available like this:

```
>$ conda info -e
```

This command will report to you what environments you can use on your system based on `conda`. Most likely, your only environment will be `root`, pointing to your Anaconda `distribution` folder.

As an example, we can create an environment based on Python Version 3.6, having all the necessary Anaconda-packaged libraries installed. This makes sense, for instance, when installing a particular set of packages for a data science project. In order to create such an environment, just perform the following:

```
$> conda create -n python36 python=3.6 anaconda
```

The preceding command asks for a particular Python version, 3.6, and requires the installation of all packages that are available on the Anaconda distribution (the argument `anaconda`). It names the environment as `python36` using the argument `-n`. The complete installation should take a while, given a large number of packages in the Anaconda installation. After having completed all of the installations, you can activate the environment:

```
$> activate python36
```

If you need to install additional packages to your environment when activated, you just use the following:

```
$> conda install -n python36 <package-name1> <package-name2>
```

That is, you make the list of the required packages follow the name of your environment. Naturally, you can also use `pip` install, as you would do in a `virtualenv` environment.

You can also use a file instead of listing all the packages by name yourself. You can create a list in an environment using the list argument and pipe the output to a file:

```
$> conda list -e > requirements.txt
```

Then, in your target environment, you can install the entire list by using the following:

```
$> conda install --file requirements.txt
```

You can even create an environment, based on a requirements list:

```
$> conda create -n python36 python=3.6 --file requirements.txt
```

Finally, after having used the environment, to close the session, you simply use the following command:

```
$> deactivate
```

Contrary to `virtualenv`, there is a specialized argument in order to completely remove an environment from your system:

```
$> conda remove -n python36 --all
```

A glance at the essential packages

We mentioned previously that the two most relevant characteristics of Python are its ability to integrate with other languages and its mature package system, which is well embodied by PyPI (the Python Package Index: `pypi.org`), a common repository for the majority of Python open source packages that are constantly maintained and updated.

The packages that we are now going to introduce are strongly analytical and they will constitute a complete data science toolbox. All of the packages are made up of extensively tested and highly optimized functions for both memory usage and performance, ready to achieve any scripting operation with successful execution. A walkthrough on how to install them is provided in the following section.

Partially inspired by similar tools present in R and MATLAB environments, we will explore how a few selected Python commands can allow you to efficiently handle data and then explore, transform, experiment, and learn from the same without having to write too much code or reinvent the wheel.

NumPy

NumPy, which is Travis Oliphant's creation, is the true analytical workhorse of the Python language. It provides the user with multidimensional arrays, along with a large set of functions to operate a multiplicity of mathematical operations on these arrays. Arrays are blocks of data that are arranged along multiple dimensions, which implement mathematical vectors and matrices. Characterized by optimal memory allocation, arrays are useful—not just for storing data, but also for fast matrix operations (vectorization), which are indispensable when you wish to solve ad hoc data science problems:

- **Website**: `http://www.numpy.org/`
- **Version at the time of print**: 1.12.1
- **Suggested install command**: `pip install numpy`

As a convention largely adopted by the Python community, when importing NumPy, it is suggested that you alias it as `np`:

```
import numpy as np
```

We will be doing this throughout the course of this book.

SciPy

An original project by Travis Oliphant, Pearu Peterson, and Eric Jones, SciPy completes NumPy's functionalities, which offers a larger variety of scientific algorithms for linear algebra, sparse matrices, signal and image processing, optimization, fast Fourier transformation, and much more:

- **Website**: `http://www.scipy.org/`
- **Version at time of print**: 1.1.0
- **Suggested install command**: `pip install scipy`

pandas

The pandas package deals with everything that NumPy and SciPy cannot do. Thanks to its specific data structures, namely DataFrames and Series, pandas allows you to handle complex tables of data of different types (which is something that NumPy's arrays cannot do) and time series. Thanks to Wes McKinney's creation, you will be able to easily and smoothly load data from a variety of sources. You can then slice, dice, handle missing elements, add, rename, aggregate, reshape, and finally visualize your data at will:

- **Website**: `http://pandas.pydata.org/`
- **Version at the time of print**: 0.23.1
- **Suggested install command**: `pip install pandas`

Conventionally, the pandas package is imported as `pd`:

```
import pandas as pd
```

pandas-profiling

This is a GitHub project that easily allows you to create a report from a pandas DataFrame. The package will present the following measures in an interactive HTML report, which is used to evaluate the data at hand for a data science project:

- **Essentials**, such as type, unique values, and missing values
- **Quantile statistics**, such as minimum value, Q1, median, Q3, maximum, range, and interquartile range
- **Descriptive statistics** such as mean, mode, standard deviation, sum, median absolute deviation, the coefficient of variation, kurtosis, and skewness
- **Most frequent values**
- **Histograms**
- **Correlations** highlighting highly correlated variables, and Spearman and Pearson matrixes

Here is all the information about this package:

- **Website**: `https://github.com/pandas-profiling/pandas-profiling`
- **Version at the time of print**: 1.4.1
- **Suggested install command**: `pip install pandas-profiling`

Scikit-learn

Started as part of **SciKits** (**SciPy Toolkits**), Scikit-learn is the core of data science operations in Python. It offers all that you may need in terms of data preprocessing, supervised and unsupervised learning, model selection, validation, and error metrics. Expect us to talk at length about this package throughout this book. Scikit-learn started in 2007 as a Google Summer of Code project by David Cournapeau. Since 2013, it has been taken over by the researchers at **INRIA** (**Institut national de recherche en informatique et en automatique**, that is the French Institute for Research in Computer Science and Automation):

- **Website**: `http://Scikit-learn.org/stable`
- **Version at the time of print**: 0.19.1
- **Suggested install command**: `pip install Scikit-learn`

Note that the imported module is named `sklearn`.

Jupyter

A scientific approach requires the fast experimentation of different hypotheses in a reproducible fashion. Initially named IPython and limited to working only with the Python language, Jupyter was created by Fernando Perez in order to address the need for an interactive Python command shell (which is based on shell, web browser, and the application interface), with graphical integration, customizable commands, rich history (in the JSON format), and computational parallelism for an enhanced performance. Jupyter is our favored choice throughout this book; it is used to clearly and effectively illustrate operations with scripts and data, and the consequent results:

- **Website**: `http://jupyter.org/`
- **Version at the time of print**: 4.4.0 (ipykernel = 4.8.2)
- **Suggested install command**: `pip install jupyter`

JupyterLab

JupyterLab is the next user interface for the Jupyter project, which is currently in beta. It is an environment devised for interactive and reproducible computing which will offer all the usual notebook, terminal, text editor, file browser, rich outputs, and so on arranged in a more flexible and powerful user interface. JupyterLab will eventually replace the classic Jupyter Notebook after JupyterLab reaches Version 1.0. Therefore, we intend to introduce this package now in order to make you aware of it and of its functionalities:

- **Website**: `https://github.com/jupyterlab/jupyterlab`
- **Version at the time of print**: 0.32.0
- **Suggested install command**: `pip install jupyterlab`

Matplotlib

Originally developed by John Hunter, matplotlib is a library that contains all the building blocks that are required to create quality plots from arrays and to visualize them interactively.

You can find all the MATLAB-like plotting frameworks inside the PyLab module:

- **Website**: `http://matplotlib.org/`
- **Version at the time of print**: 2.2.2
- **Suggested install command**: `pip install matplotlib`

You can simply import what you need for your visualization purposes with the following command:

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

Seaborn

Working out beautiful graphics using matplotlib can be really time-consuming, for this reason, Michael Waskom (`http://www.cns.nyu.edu/~mwaskom/`) developed Seaborn, a high-level visualization package based on matplotlib and integrated with pandas data structures (such as Series and DataFrames) capable to produce informative and beautiful statistical visualizations.

- **Website**: `http://seaborn.pydata.org/`
- **Version at the time of print**: 0.9.0
- **Suggested install command**: `pip install seaborn`

You can simply import what you need for your visualization purposes with the following command:

```
import seaborn as sns
```

Statsmodels

Previously a part of SciKits, `statsmodels` was thought to be a complement to SciPy's statistical functions. It features generalized linear models, discrete choice models, time series analysis, and a series of descriptive statistics, as well as parametric and non-parametric tests:

- **Website**: `http://statsmodels.sourceforge.net/`
- **Version at the time of print**: 0.9.0
- **Suggested install command**: `pip install statsmodels`

Beautiful Soup

Beautiful Soup, a creation of Leonard Richardson, is a great tool to scrap out data from HTML and XML files that are retrieved from the internet. It works incredibly well, even in the case of *tag soups* (hence the name), which are collections of malformed, contradictory, and incorrect tags. After choosing your parser (the HTML parser included in Python's standard library works fine), thanks to Beautiful Soup, you can navigate through the objects in the page and extract text, tables, and any other information that you may find useful:

- **Website**: `http://www.crummy.com/software/BeautifulSoup`
- **Version at the time of print**: 4.6.0
- **Suggested install command**: `pip install beautifulsoup4`

Note that the imported module is named `bs4`.

NetworkX

Developed by the Los Alamos National Laboratory, **NetworkX** is a package specialized in the creation, manipulation, analysis, and graphical representation of real-life network data (it can easily operate with graphs made up of a million nodes and edges). Besides specialized data structures for graphs and fine visualization methods (2D and 3D), it provides the user with many standard graph measures and algorithms, such as the shortest path, centrality, components, communities, clustering, and PageRank. We will mainly use this package in `Chapter 6`, *Social Network Analysis*:

- **Website**: `http://networkx.github.io/`
- **Version at the time of print**: 2.1
- **Suggested install command**: `pip install networkx`

Conventionally, NetworkX is imported as `nx`:

```
import networkx as nx
```

NLTK

The **Natural Language Toolkit** (**NLTK**) provides access to corpora and lexical resources, and to a complete suite of functions for **Natural Language Processing** (**NLP**), ranging from tokenizers to part-of-speech taggers and from tree models to named-entity recognition. Initially, Steven Bird and Edward Loper created the package as an NLP teaching infrastructure for their course at the University of Pennsylvania. Now it is a fantastic tool that you can use to prototype and build NLP systems:

- **Website**: `http://www.nltk.org/`
- **Version at the time of print**: 3.3
- **Suggested install command**: `pip install nltk`

Gensim

Gensim, programmed by Radim Řehůřek, is an open source package that is suitable for the analysis of large textual collections with the help of parallel distributable online algorithms. Among advanced functionalities, it implements **Latent Semantic Analysis** (**LSA**), topic modeling by **Latent Dirichlet Allocation** (**LDA**), and Google's *word2vec*, a powerful algorithm that transforms text into vector features that can be used in supervised and unsupervised machine learning:

- **Website**: `http://radimrehurek.com/gensim/`
- **Version at the time of print**: 3.4.0
- **Suggested install command**: `pip install gensim`

PyPy

PyPy is not a package; it is an alternative implementation of Python 3.5.3 that supports most of the commonly used Python standard packages (unfortunately, NumPy is currently not fully supported). As an advantage, it offers enhanced speed and memory handling. Thus, it is very useful for heavy-duty operations on large chunks of data, and it should be part of your big data handling strategies:

- **Website**: `http://pypy.org/`
- **Version at time of print**: 6.0
- **Download page**: `http://pypy.org/download.html`

XGBoost

XGBoost is a scalable, portable, and distributed gradient boosting library (a tree ensemble machine learning algorithm). Initially created by Tianqi Chen from Washington University, it has been enriched by a Python wrapper by Bing Xu and an R interface by Tong He (you can read the story behind XGBoost directly from its principal creator at `http://homes.cs.washington.edu/~tqchen/2016/03/10/story-and-lessons-behind-the-evolution-of-xgboost.html`). XGBoost is available for Python, R, Java, Scala, Julia, and C++, and it can work on a single machine (leveraging multithreading) in both Hadoop and Spark clusters:

- **Website:** `https://xgboost.readthedocs.io/en/latest/`
- **Version at the time of print:** 0.80
- **Download page**: `https://github.com/dmlc/xgboost`

Detailed instructions for installing XGBoost on your system can be found at `https://github.com/dmlc/xgboost/blob/master/doc/build.md`.

The installation of XGBoost on both Linux and macOS is quite straightforward, whereas it is a little bit trickier for Windows users, though the recent release of a pre-built binary wheel for Python has made the procedure a piece of cake for everyone. You simply have to type this on your shell:

```
$> pip install xgboost
```

If you want to install XGBoost from scratch because you need the most recent bug fixes or GPU support, you need to first build the shared library from C++ (`libxgboost.so` for Linux/macOS and `xgboost.dll` for Windows) and then install the Python package. On a Linux/macOS system, you just have to build the executable by the `make` command, but on Windows, things are a little bit more tricky.

Generally, refer to `https://xgboost.readthedocs.io/en/latest/build.html#`, which provides the most recent instructions for building from scratch. For a quick reference, here, we are going to provide specific installation steps to get XGBoost working on Windows:

1. First, download and install Git for Windows, (`https://git-for-windows.github.io/`).
2. Then, you need a MINGW compiler present on your system. You can download it from `http://www.mingw.org/` or `http://tdm-gcc.tdragon.net/`, according to the characteristics of your system.

3. From the command line, execute the following:

```
$> git clone --recursive https://github.com/dmlc/xgboost
$> cd xgboost
$> git submodule init
$> git submodule update
```

4. Then, always from the command line, copy the configuration for 64-byte systems to be the default one:

```
$> copy make\mingw64.mk config.mk
```

5. Alternatively, you just copy the plain 32-byte version:

```
$> copy make\mingw.mk config.mk
```

6. After copying the configuration file, you can run the compiler, setting it to use four threads in order to speed up the compiling procedure:

```
$> mingw32-make -j4
```

7. In MinGW, the `make` command comes with the name `mingw32-make`. If you are using a different compiler, the previous command may not work. If so, you can simply try this:

```
$> make -j4
```

8. Finally, if the compiler completes its work without errors, you can install the package in your Python by using the following:

```
$> cd python-package
$> python setup.py install
```

After following all the preceding instructions, if you try to import XGBoost in Python and it doesn't load and results in an error, it may well be that Python cannot find MinGW's g++ runtime libraries.
You just need to find the location on your computer of MinGW's binaries (in our case, it was in `C:\mingw-w64\mingw64\bin`; just modify the following code and put yours) and place the following code snippet before importing XGBoost:

```
import os
mingw_path = 'C:\mingw-w64\mingw64\bin'
os.environ['PATH']=mingw_path + ';' + os.environ['PATH']
import xgboost as xgb
```

LightGBM

LightGBM is a gradient boosting framework that was developed by Microsoft that uses the tree-based learning algorithm in a different fashion than other GBMs, favoring exploration of more promising leaves (leaf-wise) instead of developing level-wise.

In graph terminology, LightGBM is pursuing a depth-first search strategy than a breadth-first search one.

It has been designed to be distributed (Parallel and GPU learning supported), and its unique approach really achieves faster training speed with lower memory usage (thus allowing for the handling of the larger scale of data):

- **Website:** `https://github.com/Microsoft/LightGBM`
- **Version at the time of print:** 2.1.0

The installation of XGBoost requires some more actions on your side than usual Python packages. If you are operating on a Windows system, open a shell and issue the following commands:

```
$> git clone --recursive https://github.com/Microsoft/LightGBM
$> cd LightGBM
$> mkdir build
$> cd build
$> cmake -G "MinGW Makefiles" ..
$> mingw32-make.exe -j4
```

You may need to install CMake on your system first (`https://cmake.org`), and you also may need to run `cmake -G "MinGW Makefiles" ..` if a `sh.exe was found in your PATH` error is reported.

If you are instead operating on a Linux system, you just need to digit on a shell:

```
$> git clone --recursive https://github.com/Microsoft/LightGBM
$> cd LightGBM
$> mkdir build
$> cd build
$> cmake ..
$> make -j4
```

After you have completed compiling the package, no matter whether you are on Windows or Linux, you just import it on your Python command line:

```
import lightgbm as lgbm
```

You can also build the package using MPI for parallel computing architectures, HDFS, or GPU versions. You can find all the detailed instructions at `https://github.com/Microsoft/LightGBM/blob/master/docs/Installation-Guide.rst`.

CatBoost

Developed by Yandex researchers and engineers, **CatBoost** (which stands for **categorical boosting**) is a gradient boosting algorithm, based on decision trees, which is optimized in handling categorical features without much preprocessing (non-numeric features expressing a quality, such as a color, a brand, or a type). Since in most databases the majority of features are categorical, CatBoost can really boost your results on prediction:

- **Website:** `https://catboost.yandex`
- **Version at the time of print:** 0.8.1.1
- **Suggested install command**: `pip install catboost`
- **Download page**: `https://github.com/catboost/catboost`

CatBoost requires `msgpack`, which can be easily installed by using the `pip install msgpack` command.

TensorFlow

TensorFlow was initially developed by the Google Brain team to be used internally at Google, and was then to be released to the larger public. On November 9, 2015, it was distributed under the Apache 2.0 open source license, and since then it has become the most widespread open source software library for high-performance numerical computation (mostly used for deep learning). It is capable of computations across a variety of platforms (systems with multiple CPUs, GPUs, and TPUs), and from desktops to clusters of servers to mobile and edge devices.

In this book, we will use TensorFlow as the backend of Keras, that is, we won't use it directly, but we will need to have it running on our system:

- **Website:** `https://tensorflow.org/`
- **Version at the time of print:** 1.8.0

Installing TensorFlow on a CPU system is quite straightforward: just use `pip install tensorflow`. But if you have an NVIDIA GPU (you actually need a GPU card with CUDA Compute Capability 3.0 or higher) on your system, the requirements ramp up and you first have to install the following:

- CUDA Toolkit 9.0
- The NVIDIA drivers associated with CUDA Toolkit 9.0
- cuDNN v7.0

For each operation, you need to accomplish various steps depending on your system, as detailed on the NVIDIA website. You can find all the directions for installation depending on your system (Ubuntu, Windows, or macOS) at `https://www.tensorflow.org/install/`.

After having accomplished all the necessary steps, `pip install tensorflow-gpu` will install the TensorFlow package that's optimized for GPU computations.

Keras

Keras is a minimalist and highly modular neural networks library, written in Python and capable of running on top of TensorFlow (the source software library for numerical computation released by Google) as well as Microsoft Cognitive Toolkit (previously known as CNTK), Theano, or MXNet. Its primary developer and maintainer is François Chollet, a machine learning researcher working at Google:

- **Website:** `https://keras.io/`
- **Version at the time of print:** 2.2.0
- **Suggested install command**: `pip install keras`

As an alternative, you can install the latest available version (which is advisable since the package is in continuous development) by using the following command:

```
$> pip install git+git://github.com/fchollet/keras.git
```

Introducing Jupyter

Initially known as IPython, this project was initiated in 2001 as a free project by Fernando Perez. By his work, the author intended to address a lack in the Python stack and provide to the public a user programming interface for data investigations that could easily incorporate the scientific approach (mainly meaning experimenting and interactively discovering) in the process of data discovery and software development.

A scientific approach implies fast experimentation of different hypotheses in a reproducible fashion (as does data exploration and analysis in data science), and when using this interface, you will be able more naturally to implement an explorative, iterative, trial and error research strategy during your code writing.

Recently (during Spring 2015), a large part of the IPython project was moved to a new one called Jupyter. This new project extends the potential usability of the original IPython interface to a wide range of programming languages, such as these:

- R (`https://github.com/IRkernel/IRkernel`)
- Julia (`http://github.com/JuliaLang/IJulia.jl`)
- Scala (`https://github.com/mattpap/IScala`)

For a more complete list of available kernels for Jupyter, please visit `https://github.com/ipython/ipython/wiki/IPython-kernels-for-other-languages`.

For instance, once having installed Jupyter and its IPython kernel, you can easily add another useful kernel, such as the R kernel, in order to access the R language through the same interface. All you have to do is have an R installation, run your R interface, and enter the following commands:

```
install.packages(c('pbdZMQ', 'devtools'))
devtools::install_github('IRkernel/repr')
devtools::install_github('IRkernel/IRdisplay')
devtools::install_github('IRkernel/IRkernel')
IRkernel::installspec()
```

The commands will install the devtools library on your R, then pull and install all the necessary libraries from GitHub (you need to be connected to the internet while running the other commands), and finally register the R kernel both in your R installation and on Jupyter. After that, every time you call the Jupyter Notebook, you will have the choice of running either a Python or an R kernel, allowing you to use the same format and approach for all your data science projects.

You cannot mix the same notebook commands for different kernels; each notebook only refers to a single kernel, that is, the one it was initially created with.

Thanks to the powerful idea of kernels, programs that run the user's code that's communicated by the frontend interface and provide feedback on the results of the executed code to the interface itself, you can use the same interface and interactive programming style no matter what language you are using for development.

In such a context, IPython is the zero kernel, the original starting one, still existing but not intended to be used anymore to refer to the entire project.

Therefore, Jupyter can simply be described as a tool for interactive tasks that are operable by a console or by a web-based notebook, which offers special commands that help developers to better understand and build the code that is being currently written.

Contrary to an IDE—which is built around the idea of writing a script, running it afterward, and finally evaluating its results—Jupyter lets you write your code in chunks, named cells, run each of them sequentially, and evaluate the results of each one separately, examining both textual and graphical outputs. Besides graphical integration, it provides you with further help, thanks to customizable commands, a rich history (in the JSON format), and computational parallelism for an enhanced performance when dealing with heavy numeric computations.

Such an approach is also particularly fruitful for tasks involving developing code based on data, since it automatically accomplishes the often neglected duty of documenting and illustrating how data analysis has been done, its premises and assumptions, and its intermediate and final results. If a part of your job is to also present your work and persuade an internal or external stakeholder in the project, Jupyter can really do the magic of storytelling for you with little additional effort.

You can easily combine code, comments, formulas, charts, interactive plots, and rich media such as images and videos, making each Jupyter Notebook a complete scientific sketchpad to find all your experimentations and their results together.

Jupyter works on your favorite browser (which could be Explorer, Firefox, or Chrome, for instance) and, when started, presents a cell waiting for code to be written in. Each block of code enclosed in a cell can be run, and its results are reported in the space just after the cell. Plots can be represented in the notebook (inline plot) or in a separate window. In our example, we decided to plot our chart inline.

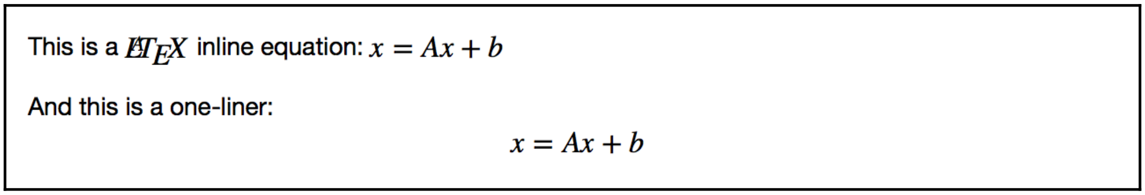
Moreover, written notes can be written easily using the Markdown language, a very easy and fast-to-grasp markup language (`http://daringfireball.net/projects/markdown/`). Math formulas can be handled using MathJax (`https://www.mathjax.org/`) to render any LaTeX script inside HTML/markdown.

There are several ways to insert LaTeX code in a cell. The easiest way is to simply use the Markdown syntax, wrapping the equations with a single dollar sign, `$`, for an inline LaTeX formula, or with a double dollar sign, `$$`, for a one-line central equation. Remember that to have a correct output, the cell should be set as Markdown. Here's an example:

In Markdown:

```
This is a $LaTeX$ inline equation: $x = Ax+b$

And this is a one-liner: $$x = Ax + b$$
```

This produces the following output:



This is a $LaTeX$ inline equation: $x = Ax + b$

And this is a one-liner:

$$x = Ax + b$$

If you're looking for something more elaborate, that is, a formula that spans for more than one line, a table, a series of equations that should be aligned, or simply the use of special LaTeX functions, then it's better to use the `%%latex` magic command offered by the Jupyter Notebook. In this case, the cell must be in code mode and contain the magic command as the first line. The following lines must define a complete LaTeX environment that can be compiled by the LaTeX interpreter.

Here are a couple of examples that show you what you can do:

```
In:%%latex
    [
     |u(t)| =
      begin{cases}
       u(t) & text{if } t geq 0 \
       -u(t)       & text{otherwise }
      end{cases}
    ]
```

Here is the output of the first example:

$$|u(t)| = \begin{cases} u(t) & if\ t \geq 0 \\ -u(t) & otherwise \end{cases}$$

```
In:%%latex
   begin{align}
   f(x) &= (a+b)^2 \
        &= a^2 + (a+b) + (a+b) + b^2 \
        &= a^2 + 2cdot (a+b) + b^2
   end{align}
```

The new output when the second example is run is:

$$\begin{aligned} f(x) &= (a+b)^2 \\ &= a^2 + (a+b) + (a+b) + b^2 \\ &= a^2 + 2.(a+b) + b^2 \end{aligned}$$

Remember that by using the `%%latex` magic command, the whole cell must comply with the LaTeX syntax. Therefore, if you just need to write a few simple equations in the text, we strongly advise that you use the Markdown method (a text-to-HTML conversion tool for web writers developed by John Gruber, with the help of Aaron Swartz: `https://daringfireball.net/projects/markdown/)`.

Being able to integrate technical formulas in markdown is particularly fruitful for tasks involving the development of code based on data since it automatically accomplishes the often neglected duty of documenting and illustrating how data analysis has been managed as well as its premises, assumptions, and intermediate and final results. If a part of your job is to also present your work and persuade internal or external stakeholders in the project, Jupyter can really do the magic of storytelling for you with little additional effort.

On the web page `https://github.com/ipython/ipython/wiki/A-gallery-of-interesting-IPython-Notebooks`, there are many examples, some of which you may find inspiring for your work, as it did for ours. Actually, we have to confess that keeping a clean, up-to-date Jupyter Notebook has saved us uncountable times when meeting with managers and stakeholders have suddenly popped up, requiring us to present the state of our work hastily.

In short, Jupyter allows you to do the following:

- See intermediate (debugging) results for each step of the analysis
- Run only some sections (or cells) of the code
- Store intermediate results in JSON format and have the ability to perform version control on them
- Present your work (this will be a combination of text, code, and images), share it via the Jupyter Notebook Viewer service (`http://nbviewer.jupyter.org/`), and easily export it into HTML, PDF, or even slideshows

In the next section, we will discuss Jupyter's installation in more detail and show an example of its usage in a data science task.

Fast installation and first test usage

Jupyter is our favored choice throughout this book. It is used to clearly and effectively illustrate and narrate operations using scripts and data, and their consequent results.

Though we strongly recommend using Jupyter, if you are using a REPL or an IDE, you can use the same instructions and expect identical results (except for the print formats and extensions of the returned results).

If you do not have Jupyter installed on your system, you can promptly set it up by using the following command:

```
$> pip install jupyter
```

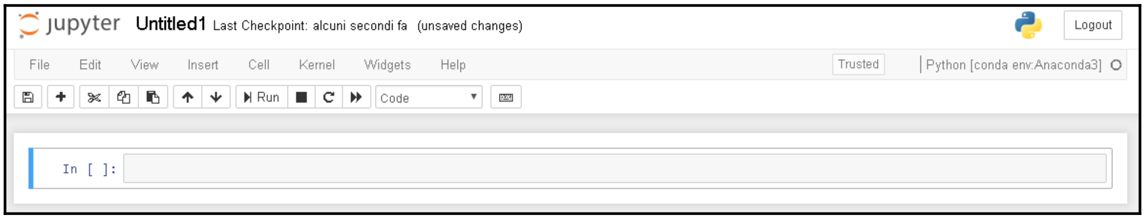
You can find complete instructions about Jupyter installation (covering different operating systems) at `http://jupyter.readthedocs.io/en/latest/install.html`.

After installation, you can immediately start using Jupyter by calling it from the command line:

```
$> jupyter notebook
```

Once the Jupyter instance has opened in the browser, click on the **New** button; in the Notebooks section, choose Python 3 (other kernels may be present in the section depending on what you installed).

At this point, your new empty notebook will look like the following image:


jupyter
Untitled1 Last Checkpoint: alcuni secondi fa (unsaved changes)
Logout
File
Edit
View
Insert
Cell
Kernel
Widgets
Help
Trusted
Python [conda env:Anaconda3]
Run
Code
In [ ]:

At this point, you can start entering the commands in the first cell. For instance, you may start trying typing the following into the cell where the cursor is flashing:

```
In: print ("This is a test")
```

After writing in the cell, you just press the **Play** button which is below the cell tab (or, as a keyboard hotkey, you can push shift and enter buttons at the same time) to run it and obtain an output. Then, another cell will appear for your input. As you are writing in a cell, if you press the plus button on the menu bar, you will get a new cell, and you can move from one cell to another using the arrows on the menu.

Most of the other functions are quite intuitive, and we invite you to try them. In order to learn how Jupyter works, you may use a quick start guide such as `http://jupyter-notebook-beginner-guide.readthedocs.io/en/latest/`, or buy a book specializing in Jupyter functionalities.

For a complete treatise of the full range of Jupyter functionalities when running the IPython kernel, refer to the following Packt Publishing books:

- IPython Interactive Computing and Visualization Cookbook by Cyrille Rossant, Packt Publishing, September 25, 2014
- *Learning IPython for Interactive Computing and Data Visualization* by Cyrille Rossant, Packt Publishing, April 25, 2013

For illustrative purposes, just consider that every Jupyter block of instructions has a numbered input statement and an output of one. Therefore, you will find the code presented in this book structured in two blocks, at least when the output is not trivial at all. Otherwise, expect only the input part:

```
In: <the code you have to enter> Out: <the output you should get>
```

As a rule, you just have to type the code after `In:` in your cells and run it. You can then compare your output with the output that we may provide using `Out:`, followed by the output that we actually obtained on our computers when we tested the code.

If you are using `conda` or `env` environments, it may happen that you cannot find your new environments in the Jupyter interface. If that happens, just issue `conda install ipykernel` from a command line and restart the Jupyter Notebook. Your kernels should appear among the notebook options under the **New** button.

Jupyter magic commands

As a special tool for interactive tasks, Jupyter offers special commands that help to better understand the code that you are currently writing.

For instance, some of the commands are as follows:

- `* <object>? and <object>??`: This prints a detailed description (with `??` being even more verbose) of `<object>`
- `%<function>`: This uses the special `<magic function>`

Let's demonstrate the usage of these commands with an example. We first start the interactive console with the `jupyter` command, which is used to run Jupyter from the command line, as shown here:

```
$> jupyter console
   Jupyter Console 4.1.1

In [1]: obj1 = range(10)
```

Then, in the first line of code, which is marked by Jupyter as `[1]`, we create a list of 10 numbers (from 0 to 9), assigning the output to an object named `obj1`:

```
In [2]: obj1?
        Type:        range
        String form: range(0, 10)
        Length:      10
        Docstring:
        range(stop) -> range object
        range(start, stop[, step]) -> range object
        Return an object that produces a sequence of integers from
        start (inclusive)
        to stop (exclusive) by step.  range(i, j) produces i, i+1, i+2,
        ..., j-1.
```

```
         start defaults to 0, and stop is omitted!  range(4) produces 0,
         1, 2, 3.
         These are exactly the valid indices for a list of 4 elements.
         When step is given, it specifies the increment (or decrement).

In [3]: %timeit x=100
         The slowest run took 184.61 times longer than the fastest.
         This could mean that an intermediate result is being cached.
         10000000 loops, best of 3: 24.6 ns per loop

In [4]: %quickref
```

In the next line of code, which is numbered `[2]`, we inspect the `obj1` object using the Jupyter command `?`. Jupyter introspects the object, prints its details (`obj` is a range object that can generate the values `[1, 2, 3..., 9]` and elements), and finally prints some general documentation on the range objects. For complex objects, the usage of `??` instead of `?` provides even more verbose output.

In line `[3]`, we use the `timeit` magic function with a Python assignment (`x=100`). The `timeit` function runs this instruction many times and stores the computational time needed to execute it. Finally, it prints the average time that was taken to run the Python function.

We complete the overview with a list of all the possible special Jupyter functions by running the `quickref` helper function, as shown in line `[4]`.

As you must have noticed, each time we use Jupyter, we have an input cell and, optionally, an output cell if there is something that has to be printed on `stdout`. Each input is numbered so it can be referenced inside the Jupyter environment itself. For our purposes, we don't need to provide such references in the code of this book. Therefore, we will just report inputs and outputs without their numbers. However, we'll use the generic `In:` and `Out:` notations to point out the input and output cells. Just copy the commands after `In:` to your own Jupyter cell and expect an output that will be reported on the following `Out:`.

Therefore, the basic notations will be as follows:

- The `In:` command
- The `Out:` output (wherever it is present and useful to be reported in this book)

Otherwise, if we expect you to operate directly on the Python console, we will use the following form:

```
>>> command
```

Wherever necessary, the command-line input and output will be written as follows:

```
$> command
```

Moreover, to run the `bash` command in the Jupyter console, prefix it with a `!` (exclamation mark):

```
In: !ls
    Applications    Google Drive    Public          Desktop
    Develop
    Pictures        env             temp
    ...

In: !pwd
    /Users/mycomputer
```

Installing packages directly from Jupyter Notebooks

Jupyter magic commands are really efficient in accomplishing different tasks, but you may sometimes find it difficult to achieve installing new packages during a Jupyter session (and it will happen often since you are using different environments based on `conda` or `env`). As Jake VanderPlas explained in his blog post **Installing Python Packages from a Jupyter Notebook** (`https://jakevdp.github.io/blog/2017/12/05/installing-python-packages-from-jupyter/`), it is a matter of fact that Jupyter kernels are different from the shell you started from, that is, you may be upgrading a wrong environment when you issue magic commands such as `!pip install numpy` or `!conda install --yes numpy`.

Unless you are using the default Python kernel that's active on the shell on the notebook, you actually won't succeed because your Jupyter Notebook is pointing to a different kernel than the one operated by `pip` and `conda` at a shell level.

The correct approach for installing, let's say, NumPy, using `pip` under a Jupyter Notebook is by creating a cell like this:

```
In: import sys
    !"{sys.executable}" -m pip install numpy
```

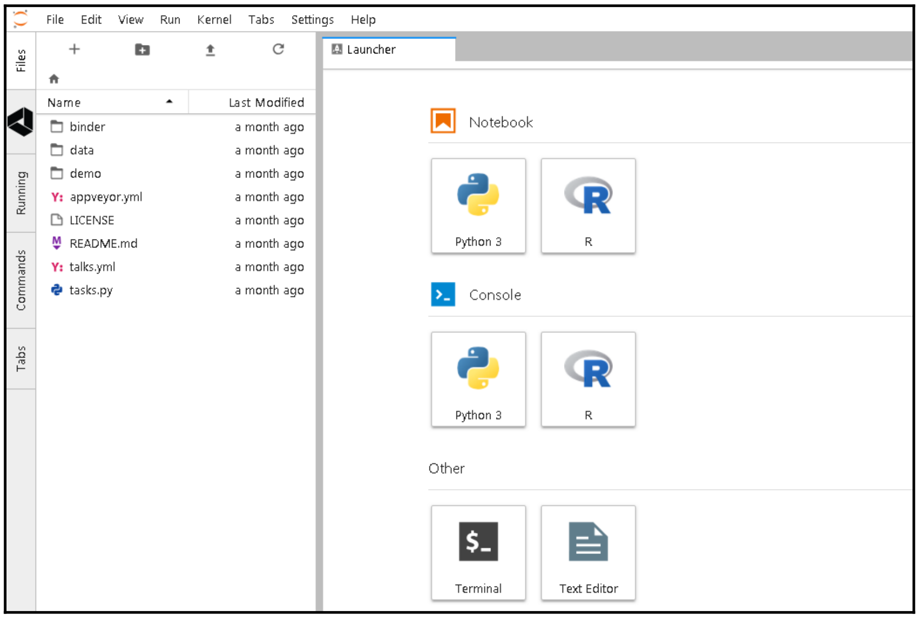
Instead, if you want to use `conda`, this is the cell you have to create:

```
In: import sys
    !conda install --yes --prefix "{sys.prefix}" numpy
```

Just replace `numpy` with any package you would like to install and then run, and the installation is guaranteed to succeed.

Checking the new JupyterLab environment

If you feel like using JupyterLab and want to be a precursor of using the interface that will become a standard in a short time, you can just switch from issuing `$> jupyter notebook` to `$> jupyter lab`. JupyterLab will start automatically on your browser at the `http://localhost:8888` address:



Name	Last Modified
binder	a month ago
data	a month ago
demo	a month ago
appveyor.yml	a month ago
LICENSE	a month ago
README.md	a month ago
talks.yml	a month ago
tasks.py	a month ago

You will be welcomed by a user interface composed of a launcher, where you can find many starting options represented as icons (in the original interface they were menu items), and a series of tabs offering direct access to files on disks, on Google Drive, showing the running kernels and notebooks, and commands for configuring the notebook and formatting the information in it.

Basically, it is an advanced and flexible interface, which is especially useful if you access all such resources on a remote server, allowing you to have everything at a glance on the very same workbench.

How Jupyter Notebooks can help data scientists

The main goal of the Jupyter Notebook is easy storytelling. Storytelling is essential in data science because you must have the power to do the following:

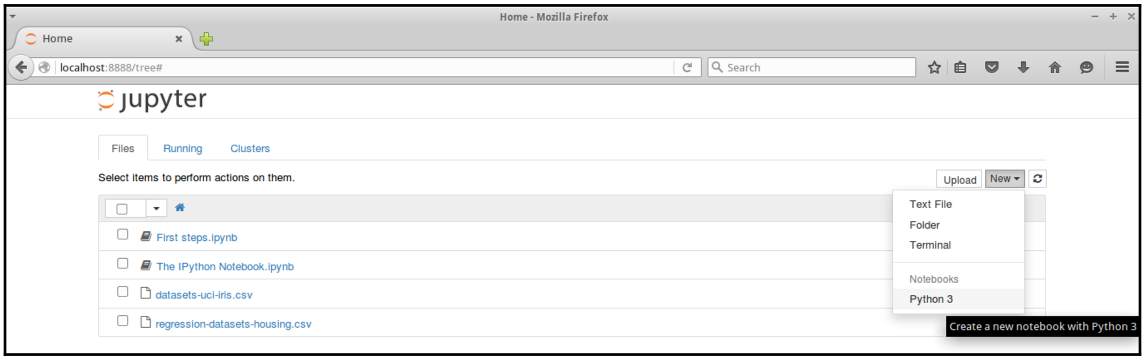
- See intermediate (debugging) results for each step of the algorithm you're developing
- Run only some sections (or cells) of the code
- Store intermediate results and have the ability to version them
- Present your work (this will be a combination of text, code, and images)

Here comes Jupyter; it actually implements all of the preceding actions:

1. To launch the Jupyter Notebook, run the following command:

```
$> jupyter notebook
```

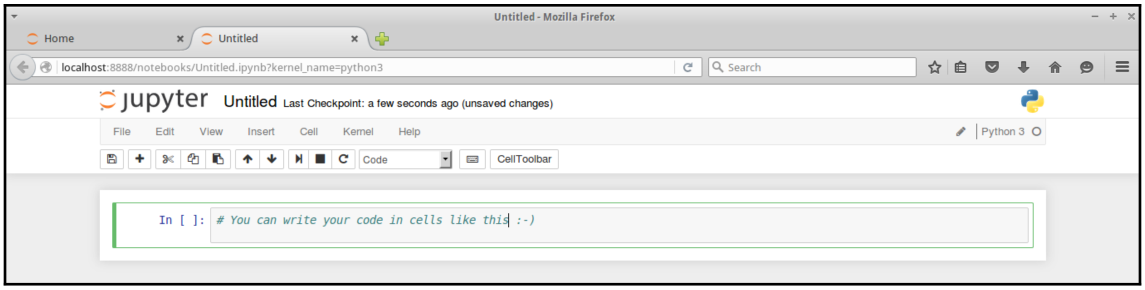
2. A web browser window will pop up on your desktop, backed by a Jupyter server instance. This is what the main window looks like:



Select items to perform actions on them.

First steps.ipynb
The IPython Notebook.ipynb
datasets-uci-iris.csv
regression-datasets-housing.csv

3. Then, click on **New Notebook**. A new window will open, as shown in the following screenshot. You can start using the notebook as soon as the kernel is ready. The small circle on the top right, below the Python icon, indicates the state of the kernel: if it's filled, it means that the kernel is busy working; if it's empty (like the one in the screenshot), it means that the kernel is in idle, that is, ready to run any code:


Untitled - Mozilla Firefox
Home
Untitled
localhost:8888/notebooks/Untitled.ipynb?kernel_name=python3
Search
jupyter
Untitled Last Checkpoint: a few seconds ago (unsaved changes)
File Edit View Insert Cell Kernel Help
Python 3
Code
CellToolbar
In [ ]:

```
# You can write your code in cells like this :-)
```

This is the web app that you'll use to compose your story. It's very similar to a Python IDE, with the bottom section (where you can write the code) composed of cells.

A cell can be either a piece of text (eventually formatted with a markup language) or a piece of code. In the second case, you have the ability to run the code, and any eventual output (the standard output) will be placed under the cell. The following is a very simple example of the same:

```
In: import random
    a = random.randint(0, 100)
    a

Out: 16

In: a*2

Out: 32
```

In the first cell, which is denoted by `In:`, we import the random module, assign a random value between `0` and `100` to the variable `a`, and print the value. When this cell is run, the output, which is denoted as `Out:`, is the random number. Then, in the next cell, we will just print the double of the value of the variable `a`.

As you can see, it's a great tool for debugging and deciding which parameter is best for a given operation. Now, what happens if we run the code in the first cell? Will the output of the second cell being modified since `a` is different? Actually, no, it won't. Each cell is independent and autonomous. In fact, after we run the code in the first cell, we end up with this inconsistent status:

```
In: import random
    a = random.randint(0, 100)
    a

Out: 56

In: a*2

Out: 32
```

Note that the number in the squared parentheses has changed (from 1 to 3) since it's the third executed command (and its output) from the time the notebook started. Since each cell is autonomous, by looking at these numbers, you can understand their order of execution.

Jupyter is a simple, flexible, and powerful tool. However, as seen in the preceding example, you must note that when you update a variable that is going to be used later on in your Notebook, remember to run all the cells following the updated code so that you have a consistent state.

When you save a Jupyter Notebook, the resulting `.ipynb` file is JSON formatted, and it contains all the cells and their content plus the output. This makes things easier because you don't need to run the code to see the notebook (actually, you also don't need to have Python and its set of toolkits installed). This is very handy, especially when you have pictures featured in the output and some very time-consuming routines in the code. A downside of using the Jupyter Notebook is that its file format, which is JSON structured, cannot be easily read by humans. In fact, it contains images, code, text, and so on.

Now, let's discuss a data science-related example (don't worry about understanding it completely):

```
In: %matplotlib inline
    import matplotlib.pyplot as plt
    from sklearn import datasets
    from sklearn.feature_selection import SelectKBest, f_regression
    from sklearn.linear_model import LinearRegression
    from sklearn.svm import SVR
    from sklearn.ensemble import RandomForestRegressor
```

In the following cell, some Python modules are imported:

```
In: boston_dataset = datasets.load_boston()
    X_full = boston_dataset.data
    Y = boston_dataset.target
    print (X_full.shape)
    print (Y.shape)

Out:(506, 13)
    (506,)
```

Then, in `cell [2]`, the dataset is loaded and an indication of its shape is shown. The dataset contains `506` house values that were sold in the suburbs of Boston, along with their respective data arranged in columns. Each column of the data represents a feature. A feature is a characteristic property of the observation. Machine learning uses features to establish models that can turn them into predictions. If you are from a statistical background, you can add features that can be intended as variables (values that vary with respect to the observations).

To see a complete description of the dataset, use `print boston_dataset.DESCR`.

After loading the observations and their features, in order to provide a demonstration of how Jupyter can effectively support the development of data science solutions, we will perform some transformations and analysis on the dataset. We will use classes, such as `SelectKBest`, and methods, such as `.getsupport()` or `.fit()`. Don't worry whether these are not clear to you now; they will all be covered extensively later in this book. Try to run the following code:

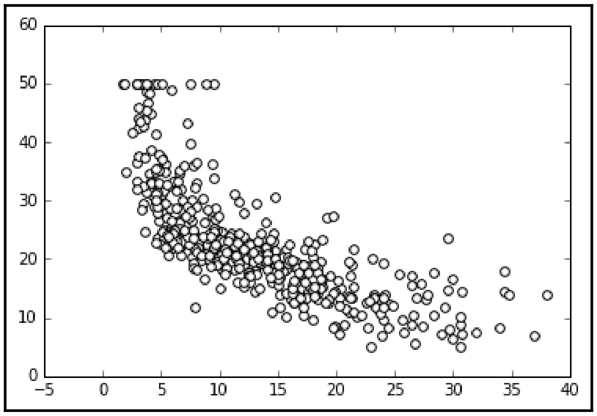
```
In: selector = SelectKBest(f_regression, k=1)
    selector.fit(X_full, Y)
    X = X_full[:, selector.get_support()]
    print (X.shape)

Out:(506, 1)
```

For `In:`, we select a feature (the most discriminative one) of the `SelectKBest` class that is fitted to the data by using the `.fit()` method. Thus, we reduce the dataset to a vector with the help of a selection operated by indexing on all the rows and on the selected feature, which can be retrieved by the `.get_support()` method.

Since the target value is a vector, we can, therefore, try to see whether there is a linear relationship between the input (the feature) and the output (the house value). When there is a linear relationship between two variables, the output will constantly react to changes in the input by the same proportional amount and direction:

```
In: def plot_scatter(X,Y,R=None):
        plt.scatter(X, Y, s=32, marker='o', facecolors='white')
        if R is not None:
                plt.scatter(X, R, color='red', linewidth=0.5)
        plt.show()

In: plot_scatter(X,Y)
```

The following is the output obtained after executing the preceding command:

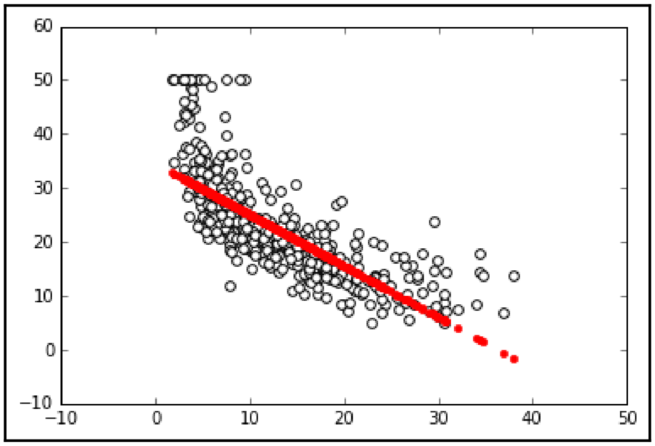


In our example, as *X* increases, *Y* decreases. However, this does not happen at a constant rate, because the rate of change is intense up to a certain *X* value, and then it decreases and becomes constant. This is a condition of nonlinearity, and we can further visualize it using a regression model. This model hypothesizes that the relationship between *X* and *Y* is linear in the form of *y=a+bX*. Its *a* and *b* parameters are estimated according to certain criteria.

In the fourth cell, we scatter the input and output values for this problem:

```
In: regressor = LinearRegression(normalize=True).fit(X, Y)
    plot_scatter(X, Y, regressor.predict(X))
```

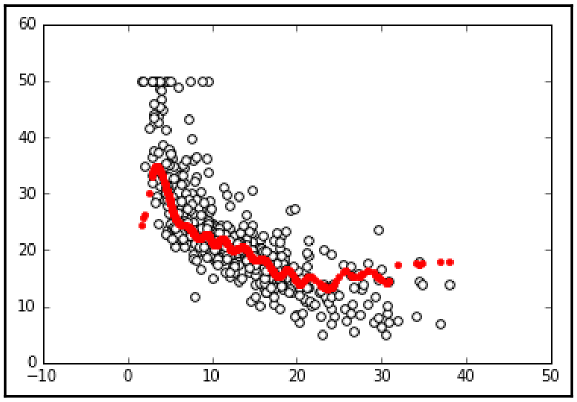
The following is the output obtained after executing the preceding code:



In the next cell, we create a regressor (a simple linear regression with feature normalization), train the regressor, and finally plot the best linear relation (that's the linear model of the regressor) between the input and output. Clearly, the linear model is an approximation that is not working well. We have two possible paths that we can follow at this point. We can transform the variables in order to make their relationship linear, or we can use a nonlinear model. **Support Vector Machine** (**SVM**) is a class of models that can easily solve nonlinearities. Also, **Random Forests** is another model for automatic solving of similar problems. Let's see them in action in Jupyter:

```
In: regressor = SVR().fit(X, Y)
    plot_scatter(X, Y, regressor.predict(X))
```

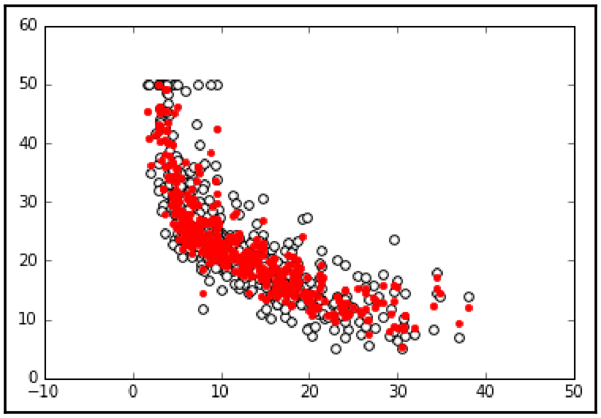
The following is the output obtained after executing the preceding code:



Now we proceed using the even more sophisticated algorithm, the Random Forests regressor:

```
In: regressor = RandomForestRegressor().fit(X, Y)
    plot_scatter(X, Y, regressor.predict(X))
```

The following is the output obtained after executing the preceding code:



Finally, in the last two cells, we will repeat the same procedure. This time, we will use two nonlinear approaches: an SVM and a Random Forest-based regressor.

This demonstrative code solves the nonlinearity problem. At this point, it is very easy to change the selected feature, regressor, and the number of features we use to train the model, and so on by simply modifying the cells where the script is. Everything can be done interactively, and according to the results we see, we can decide on both what should be kept or changed and what is to be done next.

Alternatives to Jupyter

If you don't like using Jupyter, there are actually a few alternatives that can help you test the code you will find in this book. If you have experience with R, the RStudio (`http://www.rstudio.com/`) layout may appeal more to you. In this case, Yhat, a company providing data science solutions for decision APIs, offers their data science IDE for Python free of charge, named Rodeo (`http://www.yhat.com/products/rodeo`). Rodeo works by using the IPython kernel of Jupyter under the hood, yet it is an interesting alternative given its different user interface.

The main advantages of using Rodeo are as follows:

- A video layout arranged in four Windows: editor, console, plots, and environment
- Autocomplete for the editor and console
- Plots are always visible inside the application in a specific Window
- You can easily inspect the working variables in the environment Window

Rodeo can be simply installed using the installer. You can download it from its website, or you can simply use the following in the command line:

```
$> pip install rodeo
```

After the installation, you can immediately run the Rodeo IDE with the following command:

```
$> rodeo .
```

Instead, if you have experience with MATLAB from Mathworks, you will find it easier to work with Spyder (`http://pythonhosted.org/spyder/`), a scientific IDE that can be found in major Scientific Python distributions (it is present in Anaconda, WinPython, and Python (x, y)—all distributions that we have suggested in this book). If you don't use a distribution, in order to install Spyder, you have to follow the instructions that can be found at `http://pythonhosted.org/spyder/installation.html`. Spyder allows for advanced editing, interactive editing, debugging, and introspection features, and your scripts can be run in a Jupyter console or in a shell-like environment.

Datasets and code used in this book

As we progress through the concepts presented in this book, in order to facilitate the reader's understanding, learning, and memorizing processes, we will illustrate practical and effective data science Python applications on various explicative datasets. The reader will always be able to immediately replicate, modify, and experiment with the proposed instructions and scripts on the data that we will use in this book.

As for the code that you are going to find in this book, we will limit our discussions to the most essential commands in order to inspire you from the beginning of your data science journey with Python to do more with less by leveraging key functions from the packages we presented beforehand.

Given our previous introduction, we will present the code to be run interactively as it appears on a Jupyter console or Notebook.

All the presented code will be offered in Notebooks, which is available on the Packt website (as pointed out in the *Preface*). As for the data, we will provide different examples of datasets.

Scikit-learn toy datasets

The Scikit-learn toy dataset module is embedded in the Scikit-learn package. Such datasets can easily be directly loaded into Python by the `import` command, and they don't require any download from any external internet repository. Some examples of this type of dataset are the Iris, Boston, and Digits datasets, to name the principal ones mentioned in uncountable publications and books, and a few other classic ones for classification and regression.

Structured in a dictionary-like object, besides the features and target variables, they offer complete descriptions and contextualization of the data itself.

For instance, to load the Iris dataset, enter the following commands:

```
In: from sklearn import datasets
    iris = datasets.load_iris()
```

After loading the dataset, we can explore the data description and understand how the features and targets are stored. All Scikit-learn datasets present the following methods:

- `.DESCR`: This provides a general description of the dataset
- `.data`: This contains all the features
- `.feature_names`: This reports the names of the features
- `.target`: This contains the target values, expressed as values or numbered classes
- `.target_names`: This reports the names of the classes in the target
- `.shape`: This is a method that you can apply to both `.data` and `.target`; it reports the number of observations (the first value) and features (the second value, if present) that are present

Now, let's just try to implement them (no output is reported, but the print commands will provide you with plenty of information):

```
In: print (iris.DESCR)
    print (iris.data)
    print (iris.data.shape)
    print (iris.feature_names)
    print (iris.target)
    print (iris.target.shape)
    print (iris.target_names)
```

You should know something else about the dataset—how many examples and variables are present, and what their names are. Notice that the main data structures that are enclosed in the iris object are the two arrays, data, and target:

```
In: print (type(iris.data))

Out: <class 'numpy.ndarray'>
```

`Iris.data` offers the numeric values of the variables named `sepal length`, `sepal width`, `petal length`, and `petal width`, arranged in a matrix form (150,4), where 150 is the number of observations and 4 is the number of features. The order of the variables is the order presented in `iris.feature_names`.

`Iris.target` is a vector of integer values, where each number represents a distinct class (refer to the content of `target_names`; each class name is related to its index number and *setosa*, which is the zero element of the list, is represented as `0` in the target vector).

The `Iris flower` dataset was first used in 1936 by Ronald Fisher, who was one of the fathers of modern statistical analysis, in order to demonstrate the functionality of linear discriminant analysis on a small set of empirically verifiable examples (each of the 150 data points represented iris flowers). These examples were arranged into tree-balanced species classes (each class consisted of one-third of the examples) and were provided with four metric descriptive variables that, when combined, were able to separate the classes.

The advantage of using such a dataset is that it is very easy to load, handle, and explore for different purposes, from supervised learning to a graphical representation. Modeling activities take almost no time on any computer, no matter what its specifications are. Moreover, the relationship between the classes and the role of the explicative variables are well-known. Therefore, the task is challenging, but it is not very arduous.

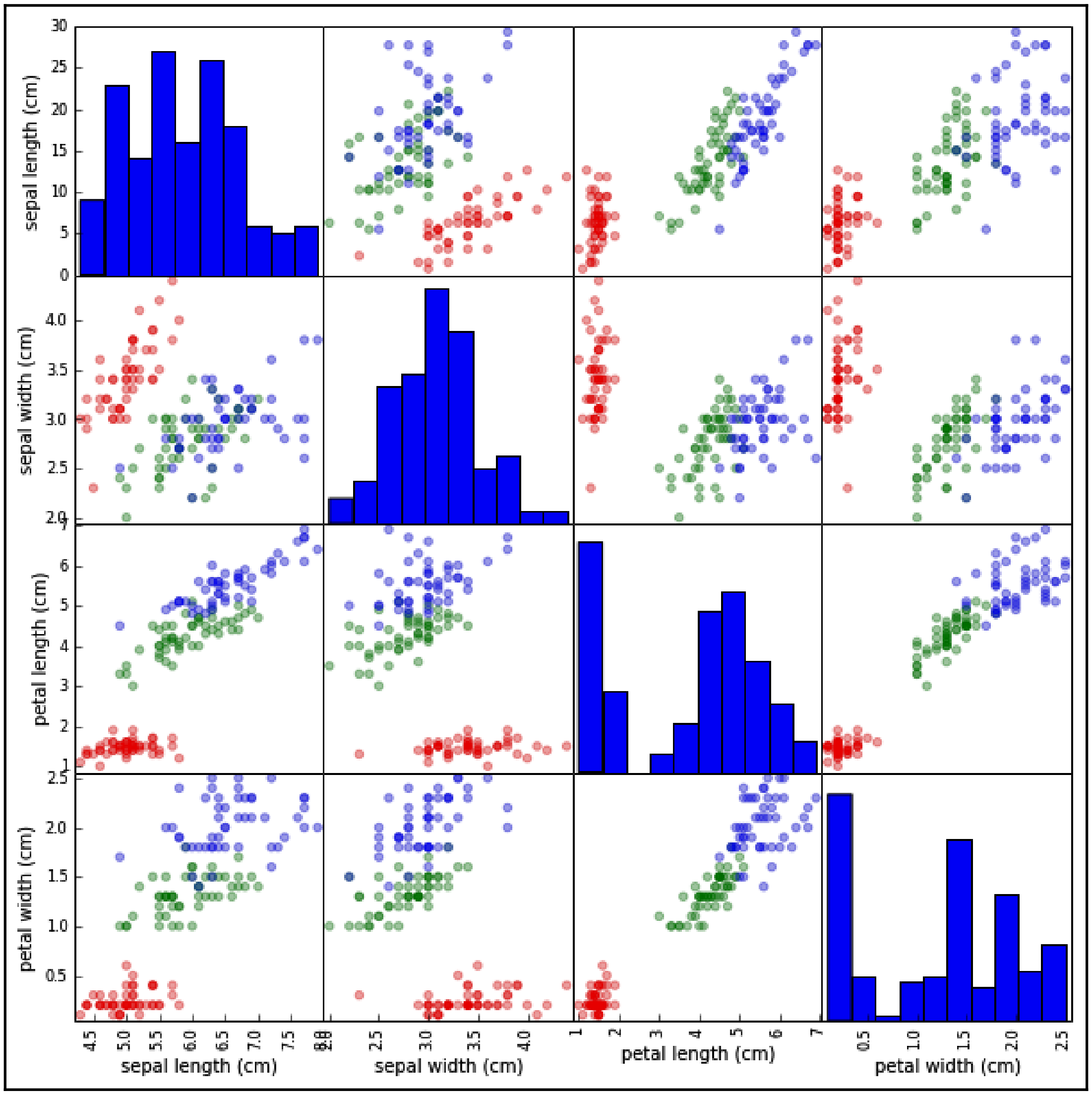
For example, let's just observe how classes can be easily separated when you wish to combine at least two of the four available variables by using a scatterplot matrix.

Scatterplot matrices are arranged in a matrix format, whose columns and rows are the dataset variables. The elements of the matrix contain single scatterplots whose *x* values are determined by the row variable of the matrix and *y* values by the column variable. The diagonal elements of the matrix may contain a distribution histogram or some other univariate representation of the variable at the same time in its row and column.

The pandas library offers an off-the-shelf function to quickly build scatterplot matrices and start exploring relationships and distributions between the quantitative variables in a dataset:

```
In: import pandas as pd
    import numpy as np
    colors = list()
    palette = {0: "red", 1: "green", 2: "blue"}

In: for c in np.nditer(iris.target): colors.append(palette[int(c)])
        # using the palette dictionary, we convert
        # each numeric class into a color string
    dataframe = pd.DataFrame(iris.data,  columns=iris.feature_names)

In: sc = pd.scatter_matrix(dataframe, alpha=0.3, figsize=(10, 10),
    diagonal='hist', color=colors, marker='o', grid=True)
```

The following is the output obtained after executing the preceding code:



We encourage you to experiment a lot with this dataset and with similar ones before you work on other complex real data because the advantage of focusing on an accessible, non-trivial data problem is that it can help you to quickly build your foundations on data science.

After a while anyway, though they are useful and interesting for your learning activities, toy datasets will start limiting the variety of different experimentations that you can achieve. In spite of the insights provided, in order to progress, you'll need to gain access to complex and realistic data science topics. Consequently, we will have to resort to some external data.

The MLdata.org and other public repositories for open source data

The second type of example dataset that we will present can be downloaded directly from the machine learning dataset repository, or from the **LIBSVM** data website. Contrary to the previous dataset, in this case, you will need access to the internet.

First, `mldata.org` is a public repository for machine learning datasets that is hosted by the TU Berlin University and supported by **Pattern Analysis, Statistical Modelling, and Computational Learning** (**PASCAL**), a network funded by the European Union. You are free to download any dataset from this repository and experiment with it.

For example, if you need to download all the data related to earthquakes since 1972, as reported by the United States Geological Survey, in order to analyze the data to search for predictive patterns, you will find the data repository at `http://mldata.org/repository/data/viewslug/global-earthquakes/` (here, you will find a detailed description of the data).

Note that the directory that contains the dataset is `global-earthquakes`; you can directly obtain the data by using the following commands:

```
In: from sklearn.datasets import fetch_mldata
    earthquakes = fetch_mldata('global-earthquakes')
    print (earthquakes.data)
    print (earthquakes.data.shape)

Out: (59209L, 4L)
```

As in the case of the Scikit-learn package toy dataset, the obtained object is a complex dictionary-like structure, where your predictive variables are `earthquakes.data` and your target to be predicted is `earthquakes.target`. This being the real data, in this case, you will have quite a lot of examples and just a few variables available.

LIBSVM data examples

LIBSVM Data (`http://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/`) is a page that gathers data from many other collections. It is maintained by Chih-Jen Lin, one of the authors of LIBSVM, a support vector machines learning algorithm for predictions (*Chih-Chung Chang and Chih-Jen Lin,* LIBSVM : *a library for support vector machines. ACM Transactions on Intelligent Systems and Technology, 2:27:1--27:27, 2011*). This offers different regression, binary, and multilabel classification datasets that are stored in the LIBSVM format. This repository is quite interesting if you wish to experiment with the support vector machine's algorithm, and, again, it is free for you to download and use the data.

If you want to load a dataset, first go to the web page where you can visualize the data on your browser. In the case of our example, visit `http://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/binary/a1a` and note down the address (`a1a` is a dataset that's originally from the UC Irvine Machine Learning Repository, another open source data repository). Then, you can proceed by performing a direct download using that address:

```
In: import urllib2
    url =
    'http://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/binary/a1a'
    a2a = urllib2.urlopen(url)

In: from sklearn.datasets import load_svmlight_file
    X_train, y_train = load_svmlight_file(a2a)
    print (X_train.shape, y_train.shape)

Out: (1605, 119) (1605,)
```

In return, you will get two single objects: a set of training examples in a sparse matrix format and an array of responses.

Loading data directly from CSV or text files

Sometimes, you may have to download the datasets directly from their repository by using a web browser or a `wget` command (on Linux systems).

If you have already downloaded and unpacked the data (if necessary) into your working directory, the simplest way to load your data and start working is offered by the NumPy and the pandas library with their respective `loadtxt` and `read_csv` functions.

For instance, if you intend to analyze the Boston housing data and use the version present at `http://mldata.org/repository/data/viewslug/regression-datasets-housing`, you first have to download the `regression-datasets-housing.csv` file in your local directory.

You can use the following link for a direct download of the dataset: `http://mldata.org/repository/data/download/csv/regression-datasets-housing`.

Since the variables in the dataset are all numeric (13 continuous and one binary), the fastest way to load and start using it is by trying out the `loadtxt` NumPy function and directly loading all the data into an array.

Even in real-life datasets, you will often find mixed types of variables, which can be addressed by `pandas.read_table` or `pandas.read_csv`. Data can then be extracted by the `values` method; `loadtxt` can save a lot of memory if your data is already numeric. In fact, the `loadtxt` command doesn't require any in-memory duplication:

```
In: housing = np.loadtxt('regression-datasets-housing.csv',
    delimiter=',')
    print (type(housing))

Out: <class 'numpy.ndarray'>

In: print (housing.shape)

Out: (506, 14)
```

The `loadtxt` function expects, by default, tabulation as a separator between the values on a file. If the separator is a colon (`,`) or a semicolon(`;`), you have to make it explicit by using the parameter delimiter:

```
>>>  import numpy as np
>>> type(np.loadtxt)
    <type 'function'>
>>> help(np.loadtxt)
```

Help on the `loadtxt` function can be found in the `numpy.lib.npyio` module.

Another important default parameter is `dtype`, which is set to float.

This means that loadtxt will force all of the loaded data to be converted into a floating-point number.

If you need to determinate a different type (for example, int), you have to declare it beforehand.

For instance, if you want to convert numeric data to int, use the following code:

```
In: housing_int =housing.astype(int)
```

Printing the first three elements of the row of the housing and housing_int arrays can help you understand the difference:

```
In:  print (housing[0,:3], 'n', housing_int[0,:3])

Out: [  6.32000000e-03   1.80000000e+01   2.31000000e+00]
     [ 0 18  2]
```

Frequently, though not always the case in our example, the data on files feature in the first line of a textual header contains the name of the variables. In this situation, the parameter that is skipped will point out the row in the loadtxt file from where it will start reading the data. Being the header on row 0 (in Python, counting always starts from 0), the skip=1 parameter will save the day and allow you to avoid an error and fail to load your data.

The situation would be slightly different if you were to download the Iris dataset, which is present at http://mldata.org/repository/data/viewslug/datasets-uci-iris/. In fact, this dataset presents a qualitative target variable, class, which is a string that expresses the iris species. Specifically, it's a categorical variable with four levels.

Therefore, if you were to use the loadtxt function, you will get a value error because an array must have all its elements of the same type. The variable class is a string, whereas the other variables are constituted by floating-point values.

The pandas library offers the solution to this and many similar cases, thanks to its DataFrame data structure that can easily handle datasets in a matrix form (row per columns) that is made up of different types of variables.

First, just download the datasets-uci-iris.csv file and have it saved in your local directory.

The dataset can be downloaded from `http://archive.ics.uci.edu/ml/machine-learning-databases/iris/`. This archive is the UC Irvine Machine Learning Repository, which currently maintains 440 datasets as a service to the machine learning community. Apart from this Iris dataset, you are free to download and try any other dataset present in the repository.

At this point, using `read_csv` from pandas is quite straightforward:

```
In: iris_filename = 'datasets-uci-iris.csv'
    iris = pd.read_csv(iris_filename, sep=',', decimal='.',
    header=None, names= ['sepal_length', 'sepal_width', \
    'petal_length', 'petal_width', 'target'])
    print (type(iris))

Out: <class 'pandas.core.frame.DataFrame'>
```

In order to not make the snippets of code printed in this book too cumbersome, we often wrap it and make it nicely formatted. When necessary, in order to safely interrupt the code and wrap it to a new line, we use the backslash symbol `\` as in the preceding code example. When rendering the code of the book by yourself, you can ignore backslash symbols and go on writing all of the instructions on the same line, or you can digit the backslash and start a new line continuing with the code instructions. Please be warned that typing the backslash and then continuing the instruction on the same line will cause an execution error.

Apart from the filename, you can specify the separator (`sep`), the way the decimal points are expressed (decimal), whether there is a header (in this case, `header=None`; normally, if you have a header, then `header=0`), and the name of the variable where there is one (you can use a list; otherwise, pandas will provide some automatic naming).

Also, we have defined names that use single words (instead of spaces, we used underscores). Thus, we can later directly extract single variables by calling them as we do for methods; for instance, `iris.sepal_length` will extract the sepal length data.

At this point, if you need to convert the pandas `DataFrame` into a couple of NumPy arrays that contain the data and target values, this can be done easily in a couple of commands:

```
In: iris_data = iris.values[:,:4]
    iris_target, iris_target_labels = pd.factorize(iris.target)
    print (iris_data.shape, iris_target.shape)

Out: (150, 4) (150,)
```

Scikit-learn sample generators

As a last learning resource, the Scikit-learn package also offers the possibility to quickly create synthetic datasets for regression, binary and multilabel classification, cluster analysis, and dimensionality reduction.

The main advantage of recurring synthetic data lies in its instantaneous creation in the working memory of your Python console. It is, therefore, possible to create bigger data examples without having to engage in long downloading sessions from the internet (and saving a lot of stuff on your disk).

For example, you may need to work on a classification problem involving a million data points:

```
In: from sklearn import datasets
    X,y = datasets.make_classification(n_samples=10**6,
    n_features=10, random_state=101)
    print (X.shape,  y.shape)

Out: (1000000, 10) (1000000,)
```

After importing just the datasets module, we ask, using the `make_classification` command, for one million examples (the `n_samples` parameter) and 10 useful features (`n_features`). The `random_state` should be `101`, so we are assured that we can replicate the same datasets at a different time and in a different machine.

For instance, you can type the following command:

```
In: datasets.make_classification(1, n_features=4, random_state=101)
```

This will always give you the following output:

```
Out: (array([[-3.31994186, -2.39469384, -2.35882002,  1.40145585]]),
      array([0]))
```

No matter what the computer and the specific situation are, `random_state` assures deterministic results that make your experimentations perfectly replicable.

Defining the `random_state` parameter using a specific integer number (in this case, it's `101`, but it may be any number that you prefer or find useful) allows easy replication of the same dataset on your machine, the way it is set up, on different operating systems, and on different machines.

By the way, did it take too long?

On a i3-2330M CPU @ 2.20 GHz machine, it takes this:

```
In: %timeit X,y = datasets.make_classification(n_samples=10**6,
    n_features=10, random_state=101)

Out: 1 loops, best of 3: 1.17 s per loop
```

If it doesn't seem like it did take too long on your machine, and if you are ready, having set up and tested everything up to this point, we can start our data science journey.

Summary

In this introductory chapter, we installed everything that we will be using throughout this book, from Python packages to examples. They were installed either directly or by using a scientific distribution. We also introduced Jupyter Notebooks and demonstrated how you can have access to the data run in the tutorials.

In the next chapter, *Data Munging*, we will have an overview of the data science pipeline and explore all the key tools to handle and prepare data before you apply any learning algorithm and set up your hypothesis experimentation schedule.

2
Data Munging

We are just getting into the action with data! In this chapter, you'll learn how to munge data. What does data munging mean ?

The term **mung** is a technical term that was coined about half a century ago by students of at **Massachusetts Institute of Technology** (**MIT**). Munging means to change, in a series of well-specified and reversible steps, a piece of original data to a completely different (and hopefully more useful) one. Deep-rooted in hacker culture, munging is often described in the data science pipeline using other, almost synonymous, terms such as data wrangling or data preparation.

Given such premises, in this chapter, the following topics will be covered:

- The data science process (so that you'll know what is going on and what's next)
- Uploading data from a file
- Selecting the data you need
- Cleaning up any missing or wrong data
- Adding, inserting, and deleting data
- Grouping and transforming data to obtain new and meaningful information
- Managing to obtain a dataset matrix or an array to feed into the data science pipeline

The data science process

Although every data science project is different, for our illustrative purposes, we can partition an ideal data science project into a series of reduced and simplified phases.

The process starts by obtaining data (a phase known as data ingestion). Data ingestion implies a series of possible alternatives, from simply uploading data to assembling it from RDBMS or NoSQL repositories, or from synthetically generating it to scraping it from web APIs or HTML pages.

Especially when faced with novel challenges, uploading data can reveal itself as a critical part of a data scientist's work. Your data can arrive from multiple sources: databases, CSV or Excel files, raw HTML, images, sound recordings, APIs (if you are clueless about what an API is, you can read a good tutorial about APIs with Python here: `https://www.dataquest.io/blog/python-api-tutorial/`) providing **JavaScript Object Notation (JSON)** files, and so on. Given the wide range of alternatives, we will just briefly touch upon this aspect by offering the basic tools to get your data (even if it is too big) into your computer memory by using either a textual file that's present on your hard disk or the web, or tables in a **relational database management system** (**RDBMS**).

After successfully uploading your data comes the data munging phase. Although now available in-memory, inevitably, your data will surely be in a form that's unsuitable for any analysis and experimentation. Data in the real world is complex, messy, and sometimes even erroneous or missing. Yet, thanks to a bunch of basic Python data structures and commands, you'll address all the problematic data and feed it into the next phases of the project, appropriately transformed into a typical dataset that has observations in rows and variables in columns. A dataset is a basic requirement for any statistical and machine learning analysis, and you may hear it being mentioned as the flat file (when it is the result of joining together multiple relational tables from a database) or data matrix (when columns and rows are unlabeled and the values it contains are just numeric).

Though less rewarding than other intellectually stimulating phases (such as the application of algorithms or machine learning), data munging creates the foundations for every complex and sophisticated value-added analysis that you may have in mind to obtain. The success of your project heavily relies on it.

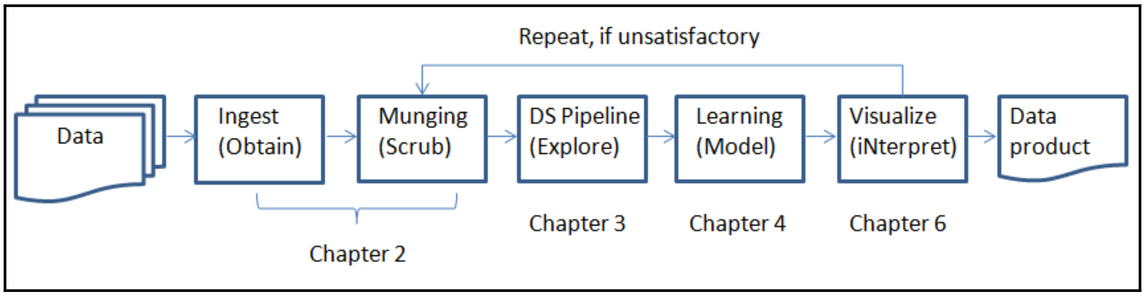
Having completely defined the dataset that you'll be working on, a new phase opens up. At this time, you'll start observing your data; then, you will proceed to develop and test your hypothesis in a recurring loop. For instance, you'll explore your variables graphically. With the help of descriptive stats, you'll figure out how to create new variables by putting your domain knowledge into action. You'll address redundant and unexpected information (outliers, first of all) and select the most meaningful variables and effective parameters to be tested by a selection of machine learning algorithms.

This phase is structured as a pipeline, where your data is processed according to a series of steps. After that, a model is finally created, but you may realize that you have to reiterate and start again from data munging or somewhere in the data pipeline, supplying corrections or trying different experiments, until you have reached a meaningful result.

From our experience on the field, we can assure you that no matter how promising your plans were when starting to analyze the data, in the end, your solution will be much different from any first envisioned idea. The confrontation with the experimental results you will obtain rules the kind of data munging, optimizations, models, and the overall number of iterations you have to go through before reaching a satisfactory end to your project. That is why if you want to be a successful data scientist, it won't suffice at all just to provide theoretically sound solutions. It is necessary to be able to quickly prototype a large number of possible solutions in the fastest time in order to ascertain which is the best path to take. It is our purpose to help you accelerate to the maximum by using the code snippets provided by this book in your data science process.

A result from your project is represented by an error or optimization measure (that you have chosen carefully in order to represent your business targets). Besides an error measurement, your achievement can also be communicated by an interpretable insight that has to be verbally or visually described to your data science project's sponsors or other data scientists. At this point, being able to visualize results and insights appropriately using tables, charts, and plots is indeed essential.

This process can also be described using the acronym **OSEMN** (**Obtain**, **Scrub**, **Explore**, **Model**, **iNterpret**), as introduced by Hilary Mason and Chris Wiggins in a famous post on the blog *dataists* (`http://www.dataists.com/2010/09/a-taxonomy-of-data-science/`), describing a data science taxonomy. OSEMN is also quite memorable since it rhymes with the words *possum* and *awesome*:



We won't ever get tired of remarking how everything starts with munging your data and that munging can easily require up to 80% of your efforts in a data project. Since even the longest journey starts with a single step, let's immediately step into this chapter and learn the building blocks of a successful munging phase!

Data loading and preprocessing with pandas

In the previous chapter, we discussed where to find useful datasets and examined the basic import commands of Python packages. In this section, having kept your toolbox ready, you are about to learn how to structurally load, manipulate, process, and polish data using pandas and NumPy.

Fast and easy data loading

Let's start with a CSV file and pandas. The pandas library offers the most accessible and complete functionality to load tabular data from a file (or a URL). By default, it will store data in a specialized pandas data structure, index each row, separate variables by custom delimiters, infer the right data type for each column, convert data (if necessary), as well as parse dates, missing values, and erroneous values.

We will start by importing the pandas package and reading our `Iris` dataset:

```
In: import pandas as pd
    iris_filename = 'datasets-uci-iris.csv'
    iris = pd.read_csv(iris_filename, sep=',', decimal='.', header=None,
                       names= ['sepal_length', 'sepal_width',
                               'petal_length', 'petal_width',
                               'target'])
```

You can specify the name of the file, the character used as a separator (`sep`), the character used for the decimal placeholder (`decimal`), whether there is a header (`header`), and the variable names (using `names` and a list). The settings of the `sep=','` and `decimal='.'` parameters have default values, and they are redundant in function. For European-style CSV, it is important to point out both since, in many European countries, the separator character and the decimal placeholder are different from the default ones.

If the dataset is not available online, you can follow these steps to download it from the internet:

```
In: import urllib
    url = "http://aima.cs.berkeley.edu/data/iris.csv"
    set1 = urllib.request.Request(url)
    iris_p = urllib.request.urlopen(set1)
    iris_other = pd.read_csv(iris_p, sep=',', decimal='.',
    header=None, names= ['sepal_length', 'sepal_width',
                         'petal_length', 'petal_width',
                         'target'])
    iris_other.head()
```

The resulting object, named `iris`, is a pandas DataFrame. It's more than a simple Python list or dictionary, and in the sections that follow, we will explore some of its features. To get an idea of its content, you can print the first (or the last) row(s) by using the following commands:

```
In: iris.head()
```

The head of the DataFrame will be printed in the output:

	sepal_length	sepal_width	petal_length	petal_width	target
0	5.1	3.5	1.4	0.2	Iris-setosa
1	4.9	3.0	1.4	0.2	Iris-setosa
2	4.7	3.2	1.3	0.2	Iris-setosa
3	4.6	3.1	1.5	0.2	Iris-setosa
4	5.0	3.6	1.4	0.2	Iris-setosa

```
In: iris.tail()
```

The function, if called without arguments, will print five lines. If you want to get back a different number of rows, just call the function using the number of rows you want to see as an argument, as follows:

```
In: iris.head(2)
```

The preceding command will print only the first two lines. Now, to get the names of the columns, you can simply use the following method:

```
In: iris.columns
Out: Index(['sepal_length', 'sepal_width',
            'petal_length', 'petal_width',
            'target'], dtype='object')
```

The resulting object is a very interesting one. It looks like a list, but it is actually a pandas index. As suggested by the object's name, it indexes the columns' names. To extract the target column, for example, you can simply do the following:

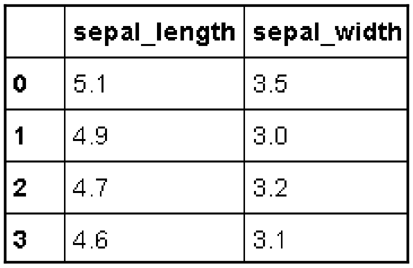
```
In: y = iris['target']
    y

Out: 0     Iris-setosa
     1     Iris-setosa
```

```
2      Iris-setosa
3      Iris-setosa
...
149     Iris-virginica
Name: target, dtype: object
```

The type of the object `y` is a pandas series. Right now, think of it as a one-dimensional array with axis labels, as we will investigate it in depth later on. Now, we just understood that a pandas `Index` class acts like a dictionary index of the table's columns. Note that you can also get a list of columns referring to them by their indexes, as follows:

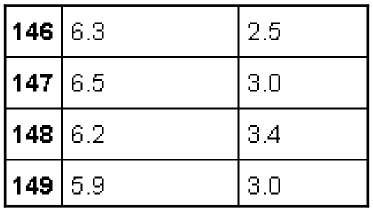
```
In: X = iris[['sepal_length', 'sepal_width']]
    X

Out: [150 rows x 2 columns]
```

Here are the four head rows of the `X` dataset:



	sepal_length	sepal_width
0	5.1	3.5
1	4.9	3.0
2	4.7	3.2
3	4.6	3.1

And here are the four tail ones:



146	6.3	2.5
147	6.5	3.0
148	6.2	3.4
149	5.9	3.0

In this case, the result is a pandas DataFrame. Why such a difference in results when using the same function? In the first case, we asked for a column. Therefore, the output was a 1D vector (that is, a pandas series). In the second example, we asked for multiple columns and we obtained a matrix-like result (and we know that matrices are mapped as pandas DataFrames). A novice reader can simply spot the difference by looking at the heading of the output; if the columns are labeled, then you are dealing with a pandas DataFrame. On the other hand, if the result is a vector and it presents no heading, then that is a pandas series.

So far, we have learned some common steps from the data science process; after you load the dataset, you usually separate the features and target labels.

In a classification problem, target labels are the ordinal numbers or textual strings that indicate the class associated with every set of features.

Then, the following steps require you to get an idea of how large the problem is, and therefore, you need to know the size of the dataset. Typically, for each observation, we count a line, and for each feature, a column.

To obtain the dimensions of the dataset, just use the attribute shape on either a pandas DataFrame or series, as shown in the following example:

```
In: print (X.shape)

Out: (150, 2)

In:  print (y.shape)

Out: (150,)
```

The resulting object is a tuple that contains the size of the matrix/array in each dimension. Also, note that a pandas series follow the same format (that is, a tuple with only one element).

Dealing with problematic data

Now, you should be more confident with the basics of the process and be ready to face datasets that are more problematic, since it is very common to have messy data in reality. Consequently, let's see what happens if the CSV file contains a header and some missing values and dates. For example, to make our example realistic, let's imagine the situation of a travel agency:

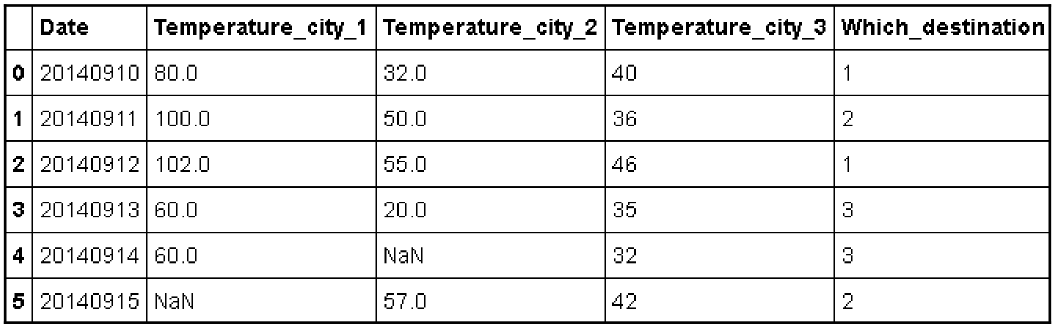
1. According to the temperature of three popular destinations, they record whether the user picks the first, second, or third destination:

   ```
   Date,Temperature_city_1,Temperature_city_2,Temperature_city_3,Which
   _destination
   20140910,80,32,40,1
   20140911,100,50,36,2
   20140912,102,55,46,1
   20140912,60,20,35,3
   20140914,60,,32,3
   20140914,,57,42,2
   ```

2. In this case, all the numbers are integers and the header is in the file. In our first attempt to load this dataset, we can provide the following command:

   ```
   In: import pandas as pd

   In: fake_dataset = pd.read_csv('a_loading_example_1.csv', sep=',')
       fake_dataset
   ```

The top rows of the `fake_dataset` are printed:



	Date	Temperature_city_1	Temperature_city_2	Temperature_city_3	Which_destination
0	20140910	80.0	32.0	40	1
1	20140911	100.0	50.0	36	2
2	20140912	102.0	55.0	46	1
3	20140913	60.0	20.0	35	3
4	20140914	60.0	NaN	32	3
5	20140915	NaN	57.0	42	2

Pandas automatically gave the columns their actual name after picking them from the first data row. We first detect a problem: all of the data, even the dates, have been parsed as integers (or, in other cases, as strings). If the format of the dates is not very strange, you can try the auto-detection routines that specify the column that contains the date data. In the following example, it works well when using the following arguments:

```
In: fake_dataset = pd.read_csv('a_loading_example_1.csv',
                               parse_dates=[0])
    fake_dataset
```

Here is the `fake_dataset` whose date column is now correctly interpreted by the `read_csv`:

	Date	Temperature_city_1	Temperature_city_2	Temperature_city_3	Which_destination
0	2014-09-10	80.0	32.0	40	1
1	2014-09-11	100.0	50.0	36	2
2	2014-09-12	102.0	55.0	46	1
3	2014-09-13	60.0	20.0	35	3
4	2014-09-14	60.0	NaN	32	3
5	2014-09-15	NaN	57.0	42	2

Now, in order to get rid of the missing values that are indicated by `NaN`, replace them with a more meaningful number (let's say, 50 Fahrenheit). We can execute our command in the following way:

```
In: fake_dataset.fillna(50)
```

At this point you will notice that there no more missing variables:

	Date	Temperature_city_1	Temperature_city_2	Temperature_city_3	Which_destination
0	2014-09-10	80.0	32.0	40	1
1	2014-09-11	100.0	50.0	36	2
2	2014-09-12	102.0	55.0	46	1
3	2014-09-13	60.0	20.0	35	3
4	2014-09-14	60.0	50.0	32	3
5	2014-09-15	50.0	57.0	42	2

After that, all of the missing data has disappeared and it has been replaced by the constant **50.0**. Treating missing data can also require different approaches. As an alternative to the previous command, values can be replaced by a negative constant value to mark the fact that they are different from others (and leave the guess for the learning algorithm):

```
In: fake_dataset.fillna(-1)
```

Note that this method only fills missing values in the view of the data (that is, it doesn't modify the original DataFrame). In order to actually change them, use the `inplace=True argument` command.

`NaN` values can also be replaced by the column's mean or median value as a way to minimize the guessing error:

```
In: fake_dataset.fillna(fake_dataset.mean(axis=0))
```

The `.mean` method calculates the mean of the specified axis.

Please note that `axis= 0` implies a calculation of means that spans the rows; the consequently obtained means are derived from column-wise computations. Instead, `axis=1` spans columns and, therefore, row-wise results are obtained. This works in the same way for all other methods that require the axis parameter, both in pandas and NumPy.

The `.median` method is analogous to `.mean`, but it computes the median value, which is useful if the mean is not a very good representation of the central value in the data, given a too skewed distribution (for instance, when there are many extreme values in your feature).

Another possible problem when handling real-world datasets is when loading a dataset containing errors or bad lines. In this case, the default behavior of the `read_csv` method is to stop and raise an exception. A possible workaround, which is feasible when erroneous examples are not the majority, is to ignore the lines causing exceptions. In many cases, such a choice has the sole implication of training the machine learning algorithm without the erroneous observations. As an example, let's say that you have a badly formatted dataset and you want to load just all the good lines and ignore the badly formatted ones.

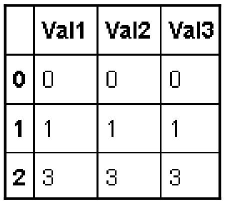
This is now your `a_loading_example_2.csv` file:

```
Val1,Val2,Val3
0,0,0
1,1,1
2,2,2,2
3,3,3
```

And here is what you can do with the error_bad_lines option:

```
In: bad_dataset = pd.read_csv('a_loading_example_2.csv',
                              error_bad_lines=False)
    bad_dataset

Out: Skipping line 4: expected 3 fields, saw 4
```

The resulting output has the fourth line skipped because it has four values instead of three:



	Val1	Val2	Val3
0	0	0	0
1	1	1	1
2	3	3	3

Dealing with big datasets

If the dataset you want to load is too big to fit in the memory, you can deal with it by using a batch machine learning algorithm, which works with only a part of the data at once. Using a batch approach also makes sense if you just need a sample of the data (let's say that you want to take a peek at the data). Thanks to Python, you can actually load the data in chunks. This operation is also called data streaming since the dataset flows into a DataFrame or some other data structure as a continuous flow. As opposed to all the previous cases, the dataset has been fully loaded into the memory in a standalone step.

With pandas, there are two ways to chunk and load a file. The first way is by loading the dataset in chunks of the same size; each chunk is a piece of the dataset that contains all the columns and a limited number of lines, no more than the number you actually have set in the function call (the chunksize parameter). Note that the output of the read_csv function, in this case, is not a pandas DataFrame, but an iterator-like object. In fact, to get the results in memory, you need to iterate that object:

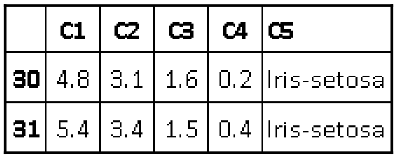
```
In: import pandas as pd
    iris_chunks = pd.read_csv(iris_filename, header=None,
                              names=['C1', 'C2', 'C3', 'C4', 'C5'],
                              chunksize=10)
    for chunk in iris_chunks:
        print ('Shape:', chunk.shape)
        print (chunk,'n')

Out: Shape: (10, 5)
```

```
    C1   C2   C3   C4            C5
0   5.1  3.5  1.4  0.2  Iris-setosa
1   4.9  3.0  1.4  0.2  Iris-setosa
2   4.7  3.2  1.3  0.2  Iris-setosa
3   4.6  3.1  1.5  0.2  Iris-setosa
4   5.0  3.6  1.4  0.2  Iris-setosa
5   5.4  3.9  1.7  0.4  Iris-setosa
6   4.6  3.4  1.4  0.3  Iris-setosa
7   5.0  3.4  1.5  0.2  Iris-setosa
8   4.4  2.9  1.4  0.2  Iris-setosa
9   4.9  3.1  1.5  0.1  Iris-setosa
...
```

There will be 14 other pieces like these, each of them of `Shape: 10, 5`. The other method to load a big dataset is by specifically asking for an iterator of it. In this case, you can dynamically decide the length (that is, how many lines to get) you want for each piece of the pandas DataFrame:

```
In:  iris_iterator = pd.read_csv(iris_filename, header=None,
                                 names=['C1', 'C2', 'C3', 'C4', 'C5'],
                                 iterator=True)

In:  print (iris_iterator.get_chunk(10).shape)

Out: (10, 5)

In:  print (iris_iterator.get_chunk(20).shape)

Out: (20, 5)

In:  piece = iris_iterator.get_chunk(2)
     piece
```

The output represents just a chunk of the original dataset:



	C1	C2	C3	C4	C5
30	4.8	3.1	1.6	0.2	Iris-setosa
31	5.4	3.4	1.5	0.4	Iris-setosa

In this example, we first defined the iterator. Next, we retrieved a piece of data containing 10 lines. We then obtained 20 further rows, and finally the two rows that are printed at the end.

Besides pandas, you can also use the CSV package, which offers two functions to iterate small chunks of data from files: the `reader` and `DictReader` functions. Let's illustrate such functions by importing the CSV package:

```
In:import csv
```

The `reader` inputs the data from disks to the Python lists. `DictReader` instead transforms the data into a dictionary. Both functions work by iterating over the rows of the file being read. The `reader` returns exactly what it reads, stripped of the return carriage, and splits into a list by the separator (which is a comma by default, but this can be modified). `DictReader` will map the list's data into a dictionary, whose keys will be defined by the first row (if a header is present) or the `fieldnames` parameter (using a list of strings that reports the column names).

The reading of lists in a native manner is not a limitation. For instance, it will be easier to speed up the code using a fast Python implementation, such as PyPy. Moreover, we can always convert lists into NumPy `ndarrays` (a data structure that we are going to introduce soon). By reading the data into JSON-style dictionaries, it will be quite easy to get a DataFrame.

Here is a simple example that uses such functionalities from the CSV package.

Let's pretend that our `datasets-uci-iris.csv` file, that was downloaded from `http://mldata.org/`, is a huge file that we cannot fully load in the memory (actually, we just pretend that this is the case because we remember that we saw the file at the beginning of this chapter; it is made up of just 150 examples, and the CSV lacks a header row).

Therefore, our only choice is to load it into chunks. First, let's conduct an experiment:

```
In: with open(iris_filename, 'rt') as data_stream:
      # 'rt' mode
      for n, row in enumerate(csv.DictReader(data_stream,
           fieldnames = ['sepal_length', 'sepal_width',
                         'petal_length', 'petal_width',
                         'target'],
           dialect='excel')):
              if n== 0:
                  print (n, row)
              else:
                  break

Out: 0 OrderedDict([('sepal_length', '5.1'), ('sepal_width', '3.5'),
     ('petal_length', '1.4'), ('petal_width', '0.2'), ('target', 'Iris-
     setosa')])
```

What does the preceding code accomplish? First, it opens a read-binary connection to the file that aliases it as `data_stream`. Using the `with` command assures that the file is closed after the commands placed in the preceding indentation are completely executed.

Then, it iterates (`for...in`) and it enumerates a `csv.DictReader` call, which wraps the flow of the data from `data_stream`. Since we don't have a header row in the file, `fieldnames` provides information about the fields' names. `dialect` just specifies that we are calling the standard comma-separated CSV (we'll provide some hints on how to modify this parameter later).

Inside the iteration, if the row being read is the first one, then it is printed. Otherwise, the loop is stopped by a `break` command. The `print` command presents us with the row number `0` and a dictionary. Therefore, you can recall every piece of data of the row by just calling the keys bearing the variables' names.

Similarly, we can make the same code work for the `csv.reader` command, as follows:

```
In: with open(iris_filename, 'rt') as data_stream:
        for n, row in enumerate(csv.reader(data_stream,
            dialect='excel')):
                if n==0:
                    print (row)
                else:
                    break

Out: ['5.1', '3.5', '1.4', '0.2', 'Iris-setosa']
```

Here, the code is even more straightforward and the output is simpler, providing a list that contains the row values in a sequence.

At this point, based on this second piece of code, we can create a generator callable from a for-loop iteration. This retrieves the data on the fly from the file in the blocks of the size defined by the batch parameter of the function:

```
In: def batch_read(filename, batch=5):
          # open the data stream
          with open(filename, 'rt') as data_stream:
            # reset the batch
            batch_output = list()
            # iterate over the file
            for n, row in enumerate(csv.reader(data_stream, dialect='excel')):
                # if the batch is of the right size
                if n > 0 and n % batch == 0:
                    # yield back the batch as an ndarray
                    yield(np.array(batch_output))
                    # reset the batch and restart
                    batch_output = list()
                # otherwise add the row to the batch
                batch_output.append(row)
            # when the loop is over, yield what's left
            yield(np.array(batch_output))
```

Similar to the previous example, the data is drawn out, thanks to the `csv.reader` function wrapped by the `enumerate` function that accompanies the extracted list of data along with the example number (which starts from zero). Based on the example number, a batch list is either appended with the data list or returned to the main program using the generative `yield` function. This process is repeated until the entire file is read and returned in batches:

```
In: import numpy as np
    for batch_input in batch_read(iris_filename, batch=3):
        print (batch_input)
        break

Out: [['5.1' '3.5' '1.4' '0.2' 'Iris-setosa']
      ['4.9' '3.0' '1.4' '0.2' 'Iris-setosa']
      ['4.7' '3.2' '1.3' '0.2' 'Iris-setosa']]
```

Such a function can provide the basic functionality for learning with stochastic gradient descent, as will be presented in `Chapter 4`, *Machine Learning*, where we will come back to this piece of code and expand this example by introducing some more advanced examples.

Accessing other data formats

So far, we have worked on CSV files only. The pandas package offers similar functionality (and functions) in order to load MS Excel, HDFS, SQL, JSON, HTML, and Stata datasets. Since most of these formats are not used routinely in data science, the understanding of how one can load and handle each of them is mostly left to you, who can refer to the documentation available on the pandas website (`http://pandas.pydata.org/pandas-docs/version/0.16/io.html`). Here, we will only demonstrate the essentials on how to effectively use your disk space to store and retrieve information for machine learning algorithms in a fast and efficient way. In such a case, you can leverage an SQLite database (`https://www.sqlite.org/index.html`) in order to access specific subsets of information and convert them into a pandas DataFrame. If you don't need to make particular selections or filterings on the data, but your only problem is that reading data from a CSV file is time-consuming and requires a lot of effort every time (for instance, setting the right variables types and names), you can speed up saving and loading your data by using the HDF5 data structure (`https://support.hdfgroup.org/HDF5/whatishdf5.html`).

In our first example, we are going to use SQLite and the SQL language to store away some data and retrieve a filtered version of it. SQLite has quite a few advantages over other databases: it is self-contained (all your data will be stored into a single file), serverless (Python will provide the interface to store, manipulate, and access the data), and fast. After importing the `sqlite3` package (which is part of the Python stack, so there's no need to install it anyway), you define two queries: one to drop any previous data table of the same name, and one to create a new table that's capable of keeping the date, city, temperature, and destination data (and you use integer, float, and varchar types, which correspond to `int`, `float`, and `str`).

After opening the database (which at this point is created, if not present on disk), you execute the two queries and then commit the changes (by committing, you actually start the execution of all the previous database commands in a single batch: `https://www.sqlite.org/atomiccommit.html`):

```
In: import sqlite3
    drop_query = "DROP TABLE IF EXISTS temp_data;"
    create_query = "CREATE TABLE temp_data \
                    (date INTEGER, city VARCHAR(80), \
                   temperature REAL, destination INTEGER);"
    connection = sqlite3.connect("example.db")
    connection.execute(drop_query)
    connection.execute(create_query)
    connection.commit()
```

At this point, the database has been created on disk with all of its data tables.

In the previous example, you created a database on disk. You can also create it in-memory by changing the connection output to `':memory:'`, as shown in this snippet of code: `connection = sqlite3.connect(':memory:') you can use ':memory:' to create an in-memory database`.

In order to insert the data into the database table, the best approach is to create a list of tuples of values containing the rows of data you need to store. Then, an insert query will take care of recording each data row. Please note that this time we are using the `executemany` method for multiple commands (each row is inserted separately into the table) instead of the previous command, `execute`:

```
In: data = [(20140910, "Rome",   80.0, 0),
            (20140910, "Berlin", 50.0, 0),
            (20140910, "Wien",   32.0, 1),
            (20140911, "Paris",  65.0, 0)]
    insert_query = "INSERT INTO temp_data VALUES(?, ?, ?, ?)"
```

```
        connection.executemany(insert_query, data)
        connection.commit()
```

At this point, we simply decide, by a selection query, what data, based on specific criteria, we need to get in-memory, and we retrieve it by using the `read_sql_query` command:

```
In: selection_query = "SELECT date, city, temperature, destination \
                       FROM temp_data WHERE Date=20140910"
    retrieved = pd.read_sql_query(selection_query, connection)
```

Now, all the data you need, in pandas DataFrame format, is contained in the `retrieved` variable. All you need to do is to close the connection with the database:

```
In: connection.close()
```

In the following example, we will instead face the situation of a large CSV file that requires a long amount of time for both loading and parsing its column variables. In such a case, we will use a data format, HDF5, which is suitable for storing and retrieving DataFrames in a fast fashion.

HDF5 is a file format that was originally developed by the **National Center for Supercomputing Applications** (**NCSA**) to store and access large amounts of scientific data, based on the requirements of NASA in the 1990s in order to have a portable file format for the data produced by the Earth Observing System and other space observation systems. HDF5 is arranged as a hierarchical data storage that allows saving multidimensional arrays of a homogeneous type or group which are containers of arrays and other groups. As a filesystem, it perfectly fits the DataFrame structure, and by means of automatic data compressions, such a filesystem can make data loading much faster than simply reading a CSV file, in case of large files.

The pandas package allows you to use the HDF5 format to store series and DataFrame data structures. You may find it invaluable for storing binary data as well, such a preprocessed images or video files. When you need to access a large number of files from disk, you may experience some latency in getting the data in-memory because the files are scattered in the filesystem. Storing all the files into a single HDF5 file will simply solve the problem. You can read how to use the `h5py` package, a Python package providing an interface for storing and retrieving data in NumPy array form, at `https://www.h5py.org/` and especially at `http://docs.h5py.org/en/stable/`, its main documentation website. You also can install `h5py` by issuing the `conda install h5py` or `pip install h5py` commands.

We will start by initializing the HDF5 file, `example.h5`, using the `HDFStore` command, which allows for a low-level manipulation of the data file. After instantiating the file, you can start using it as if it were a Python dictionary. In the following code snippet, you store the `Iris` dataset under the dictionary key `iris`. After that, you simply close the HDF5 file:

```
In: storage = pd.HDFStore('example.h5')
    storage['iris'] = iris
    storage.close()
```

When you need to retrieve the data stored in the HDF5 file, you can reopen the file using the `HDFStore` command. First, you check the available keys (as you would do in a dictionary):

```
In: storage = pd.HDFStore('example.h5')
    storage.keys()

Out: ['/iris']
```

Then, you allocate the desired values by recalling them through the corresponding key:

```
In: fast_iris_upload = storage['iris']
    type(fast_iris_upload)

Out: pandas.core.frame.DataFrame
```

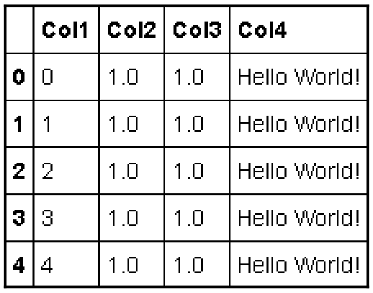
The data is promptly loaded, and the previous DataFrame is now available for further processing under the variable `fast_iris_upload`.

Putting data together

Finally, pandas DataFrames can be created by merging series or other list-like data. Note that scalars are transformed into lists, as follows:

```
In: import pandas as pd
    my_own_dataset = pd.DataFrame({'Col1': range(5),
                                   'Col2': [1.0]*5,
                                   'Col3': 1.0,
                                   'Col4': 'Hello World!'})
    my_own_dataset
```

Here is the output for `my_own_dataset`:



	Col1	Col2	Col3	Col4
0	0	1.0	1.0	Hello World!
1	1	1.0	1.0	Hello World!
2	2	1.0	1.0	Hello World!
3	3	1.0	1.0	Hello World!
4	4	1.0	1.0	Hello World!

It can be easily said that for each of the columns you want to be stacked together, you provide their names (as the dictionary key) and values (as the dictionary value for that key). As seen in the preceding example, `Col2` and `Col3` are created in two different ways, but they provide the same resulting column of values. In this way, you can create a pandas DataFrame that contains multiple types of data with a very simple function.

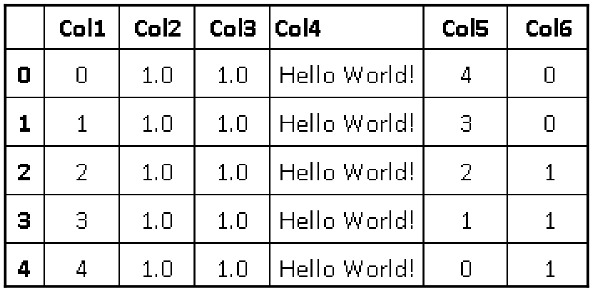
In this process, please ensure that you don't mix lists of different sizes; otherwise, an exception will be raised, as shown here:

```
In: my_wrong_own_dataset = pd.DataFrame({'Col1': range(5),
                           'Col2': 'string', 'Col3': range(2)})

Out: ...
     ValueError: arrays must all be same length
```

In order to assemble entire already existing DataFrames, you have to use a different approach based on concatenation. The pandas package offers the `concat` command, which operates on pandas data structures (`Series` and DataFrames) by stacking rows when working on axis `0` (the default option) or stacking columns when concatenating on axis `1`:

```
In: col5 = pd.Series([4, 3, 2, 1, 0])
    col6 = pd.Series([0, 0, 1, 1, 1])
    a_new_dataset = pd.concat([col5, col6], axis=1,
                              ignore_index = True,
                              keys=['Col5', 'Col6'])

    my_new_dataset = pd.concat([my_own_dataset, a_new_dataset], axis=1)
    my_new_dataset
```

The resulting dataset is a concatenation of the col5 and col6 series:



	Col1	Col2	Col3	Col4	Col5	Col6
0	0	1.0	1.0	Hello World!	4	0
1	1	1.0	1.0	Hello World!	3	0
2	2	1.0	1.0	Hello World!	2	1
3	3	1.0	1.0	Hello World!	1	1
4	4	1.0	1.0	Hello World!	0	1

In the preceding example, we created a new DataFrame, `a_new_dataset`, based on two `Series`. We just stacked the two series together, regardless of their indexes, because we used the `ignore_index` parameter, which is set to `True`. If matching accordingly to the indexes is important for your project, just don't use the `ignore_index` parameter (its default value is `False`) and you'll have a new DataFrame based on the union of the two indexes or on only the index elements that match as a result.

Joining two distinct datasets on the basis of a common column is achieved in `pd.concat` by adding the parameter `join='inner'`, which is equivalent to a SQL inner join, (more on the topic about joins will be dealt with after the following example).

Matching based on indexes could sometimes not be enough for your needs. Sometimes, you may need to match different `Series` or DataFrames on specific columns or series of columns. In that case, you need the `merge` method, which can be run from every DataFrame.

In order to see the `merge` method in action, we will create a reference table containing some values to be matched based on `Col5`:

```
In: key = pd.Series([1, 2, 4])
    value = pd.Series(['alpha', 'beta', 'gamma'])
    reference_table = pd.concat([key, value], axis=1,
                                ignore_index = True,
                                keys=['Col5', 'Col7'])
    reference_table
```

Here is the concatenation between `key` and `value` into a DataFrame:

	Col5	Col7
0	1	alpha
1	2	beta
2	4	gamma

The merge is operated by setting the `how` parameter to `left`, thus achieving a SQL left outer join. Apart from `left`, other possible settings of this parameter are as follows:

- `right`: Equivalent to a SQL right outer join
- `outer`: Equivalent to a SQL full outer join
- `inner`: Equivalent to a SQL inner join (as previously mentioned)

```
In: my_new_dataset.merge(reference_table,
                         on='Col5', how='left')
```

The resulting DataFrame is a left outer join:

	Col1	Col2	Col3	Col4	Col5	Col6	Col7
0	0	1.0	1.0	Hello World!	4	0	gamma
1	1	1.0	1.0	Hello World!	3	0	NaN
2	2	1.0	1.0	Hello World!	2	1	beta
3	3	1.0	1.0	Hello World!	1	1	alpha
4	4	1.0	1.0	Hello World!	0	1	NaN

Getting back to our initial `my_own_dataset`, in order to check the type of data present in each column, you can check the output of the `dtypes` attribute:

```
In: my_own_dataset.dtypes

Out:  Col1      int64
      Col2    float64
      Col3    float64
      Col4     object
      dtype: object
```

The last method seen in this example is very handy if you wish to check whether a datum is categorical, integer numerical, or floating point, and its precision. In fact, sometimes, it is possible to increase the processing speed by rounding up floats to integers and casting double-precision floats to single-precision floats, or by using only a single type of data. Let's see how you can cast the type in the following example. This example can also be seen as a broad example on how to reassign column data:

```
In:  my_own_dataset['Col1'] = my_own_dataset['Col1'].astype(float)
     my_own_dataset.dtypes

Out: Col1    float64
     Col2    float64
     Col3    float64
     Col4     object
     dtype: object
```

You can also obtain information about your DataFrame structure and data types using the `info()` as shown in this example: `my_own_dataset.info()`.

Data preprocessing

We are now able to import datasets, even a big, problematic ones. Now, we need to learn the basic preprocessing routines in order to make it feasible for the next data science step.

First, if you need to apply a function to a limited section of rows, you can create a **mask**. A mask is a series of Boolean values (that is, `True` or `False`) that tells you whether the line is selected or not.

For example, let's say we want to select all the lines of the `Iris` dataset that have a `sepal length` greater than `6`. We can simply do the following:

```
In: mask_feature = iris['sepal_length'] > 6.0
In: mask_feature

Out:   0     False
       1     False
     ...
     146     True
     147     True
     148     True
     149    False
```

In the preceding simple example, we can immediately see which observations are True and which are not (False), and which ones fit the selection query.

Now, let's check how you can use a selection mask on another example. We want to substitute the Iris-virginica target label with the New label label. We can do this by using the following two lines of code:

```
In: mask_target = iris['target'] == 'Iris-virginica'
    iris.loc[mask_target, 'target'] = 'New label'
```

You'll see that all occurrences of Iris-virginica are now replaced by New label. The loc() method is explained in the following code. Just think of it as a way to access the data of the matrix with the help of row-column indexes.

To see the new list of the labels in the target column, we can use the unique() method. This method is very handy if you want to first evaluate the dataset:

```
In: iris['target'].unique()

Out: array(['Iris-setosa', 'Iris-versicolor', 'New label'],
            dtype=object)
```

If you want to see some statistics about each feature, you can group each column accordingly; eventually, you can also apply a mask. The pandas method groupby will produce a similar result to the GROUP BY clause in a SQL statement. The next method to apply should be an aggregate method on one or multiple columns. For example, the mean() pandas aggregate method is the counterpart of the AVG() SQL function to compute the mean of the values in the group; the pandas aggregate method var() calculates the variance; sum() the summation; count() the number of rows in the group; and so on. Note that the result is still a pandas DataFrame, and therefore multiple operations can be chained together.

Many common operations on variables, such as `mean` or `sum`, are DataFrame methods that can be directly used on all the data, by columns (using the parameter `axis=0`, that is, `iris.sum(axis=0)` or by rows (using `axis=1`):

- `count`: The count of non-null (NaN) values
- `median`: Returns the median; that is, the 50th percentile
- `min`: The lowest value
- `max`: The highest value
- `mode`: The mode, which is the most frequently occurring value
- `var`: The variance, which measures the dispersion of the values
- `std`: The standard deviation, which is the square root of the variance
- `mad`: The mean absolute deviation, which is a way to measure the dispersion of the values robust to outliers
- `skew`: The measure of skewness, indicative of the distribution symmetry
- `kurt`: The measure of kurtosis, indicative of the distribution shape

As a next step, we can try a couple of examples with `groupby` in action. By grouping observations by the target (that is, the label), we can check the difference between the average value and the variance of the features for each group:

```
In: grouped_targets_mean = iris.groupby(['target']).mean()
    grouped_targets_mean
```

The output is a grouped `Iris` dataset and the grouping function is the mean:

	sepal_length	**sepal_width**	**petal_length**	**petal_width**
target				
Iris-setosa	5.006	3.418	1.464	0.244
Iris-versicolor	5.936	2.770	4.260	1.326
New label	6.588	2.974	5.552	2.026

```
In: grouped_targets_var = iris.groupby(['target']).var()
    grouped_targets_var
```

Now the grouping function is the variance:

	sepal_length	sepal_width	petal_length	petal_width
target				
Iris-setosa	0.124249	0.145180	0.030106	0.011494
Iris-versicolor	0.266433	0.098469	0.220816	0.039106
New label	0.404343	0.104004	0.304588	0.075433

As you may need multiple statistics on each variable, instead of creating multiple aggregated datasets to be put together by concatenation, you can directly use the `agg` method, and for each variable to apply specific functions. You define the variables by a dictionary where keys are the variable labels and values are lists of functions to be applied – to be called by a string (such as `'mean'`, `'std'`, `'min'`, `'max'`, `'sum'`, and `'prod'`) or by a pre-defined function or even a lambda function declared on the spot:

```
In: funcs = {'sepal_length': ['mean','std'],
             'sepal_width' : ['max', 'min'],
             'petal_length': ['mean','std'],
             'petal_width' : ['max', 'min']}
    grouped_targets_f = iris.groupby(['target']).agg(funcs)
    grouped_targets_f
```

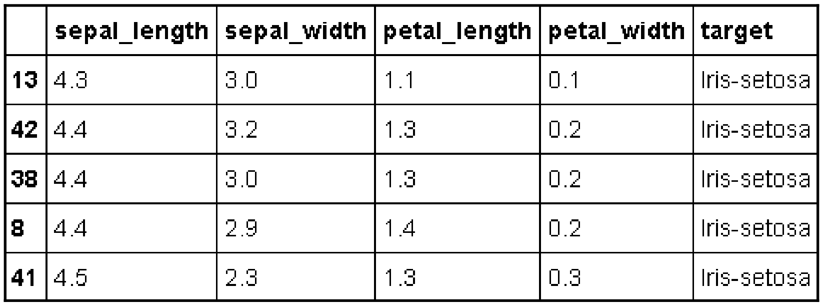
Now each column has different grouping functions:

	sepal_length		sepal_width		petal_length		petal_width	
	mean	**std**	**max**	**min**	**mean**	**std**	**max**	**min**
target								
Iris-setosa	5.006	0.352490	4.4	2.3	1.464	0.173511	0.6	0.1
Iris-versicolor	5.936	0.516171	3.4	2.0	4.260	0.469911	1.8	1.0
New label	6.588	0.635880	3.8	2.2	5.552	0.551895	2.5	1.4

Later, if you need to sort the observations using a function, you can use the `.sort_index()` method, as follows:

```
In: iris.sort_index(by='sepal_length').head()
```

As an output, you get the top rows of the dataset:



	sepal_length	sepal_width	petal_length	petal_width	target
13	4.3	3.0	1.1	0.1	Iris-setosa
42	4.4	3.2	1.3	0.2	Iris-setosa
38	4.4	3.0	1.3	0.2	Iris-setosa
8	4.4	2.9	1.4	0.2	Iris-setosa
41	4.5	2.3	1.3	0.3	Iris-setosa

Finally, if your dataset contains a time series (for example, in the case of a numerical target) and you need to apply a `rolling` operation to it (in the case of noisy data points), you can simply do the following:

```
In: smooth_time_series = pd.rolling_mean(time_series, 5)
```

This can be performed for a rolling average of the values. Alternatively, you can give the following command:

```
In: median_time_series = pd.rolling_median(time_series, 5)
```

Instead, this can be performed in order to obtain a rolling median of the values. In both of these cases, the window had size 5 samples.

More generically, the `apply()` pandas method is able to perform any row-wise or column-wise operation programmatically. `apply()` should be called directly on the DataFrame; the first argument is the function to be applied row-wise or column-wise; the second argument is the axis to apply it on. Note that the function can be a built-in, library-provided, lambda, or any other user-defined function.

As an example of this powerful method, let's try to count how many non-zero elements there are in each line. With the `apply` method, this is simple:

```
In: iris.apply(np.count_nonzero, axis=1).head()

Out:   0    5
       1    5
       2    5
       3    5
       4    5
       dtype: int64
```

Similarly, to compute the non-zero elements feature-wise (that is, per column), you just need to change the second argument and set it to `0`:

```
In: iris.apply(np.count_nonzero, axis=0)

Out:  sepal_length    150
      sepal_width     150
      petal_length    150
      petal_width     150
      target          150
      dtype: int64
```

Finally, to operate element-wise, the `applymap()` method should be used on the DataFrame. In this case, just one argument should be provided: the function to apply.

For example, let's say you're interested in the length of the string representation of each cell. To obtain that value, you should first cast each cell to a string value and then compute the length. With `applymap`, this operation is very easy:

```
In: iris.applymap(lambda x:len(str(x))).head()
```

The top rows of the transformed DataFrame are:

	sepal_length	sepal_width	petal_length	petal_width	target
0	3	3	3	3	11
1	3	3	3	3	11
2	3	3	3	3	11
3	3	3	3	3	11
4	3	3	3	3	11

When applying transformations to your data, you actually don't need to apply the same function to each column. Using pandas `apply` methods, you can actually apply a transformation to a single variable or to multiple ones, by modifying the same variables or creating new ones in addition:

```
In: def square(x):
        return x**2

    original_variables = ['sepal_length', 'sepal_width',
                          'petal_length', 'petal_width']
    squared_iris = iris[original_variables].apply(square)
```

One weak point of such an approach is that transformations can take a long time because the pandas library is not leveraging the multiprocessing capabilities of recent CPU models.

Because of issues with multiprocessing in Windows when using Jupyter, the following example can only run on Linux machines or on Windows machines if transformed into a script, just as this Stack Overflow answer suggests: `https://stackoverflow.com/questions/37103243/multiprocessing-pool-in-jupyter-notebook-works-on-linux-but-not-windows`.

In order to shorten such computation latency, you can leverage the multiprocessing package by creating the `parallel_apply` function. Such a function takes a DataFrame, a function, and the arguments of the function as input, and it creates a pool of workers (many Python duplicates in-memory, where ideally each one is operating on a different CPU of your system) to work in parallel and execute the required transformations:

```
In: import multiprocessing

    def apply_df(args):
        df, func, kwargs = args
        return df.apply(func, **kwargs)

    def parallel_apply(df, func, **kwargs):
         workers = kwargs.pop('workers')
         pool = multiprocessing.Pool(processes=workers)
         df_split = np.array_split(df, workers)
         results = pool.map(apply_df, [(ds, func, kwargs)
                                       for ds in df_split])
         pool.close()
         return pd.concat(list(results))
```

When using this function, it is important to specify the correct number of workers (depending on your system) and the axis the computation will take place on (since you operate by columns, `axis=1` is the usual parameter configuration you'll be using):

```
In: squared_iris = parallel_apply(iris[['sepal_length', 'sepal_width',
                                        'petal_length', 'petal_width']],
                                        func=square,
                                        axis=1,
                                        workers=4)
    squared_iris
```

The `Iris` dataset is a tiny one, and in this case, the execution may take even longer than simply applying a command, but on larger sets of data, the difference could be quite notable, especially if you can count on a large number of workers.

As a tip, on an Intel i5 CPU, you can set `workers=4` for optimal results, while on Intel i7, you can set `workers=8`.

Data selection

The last topic on pandas that we'll focus on is data selection. Let's start with an example. We might come across a situation where the dataset contains an index column. How do we properly import it with pandas? And then, can we actively exploit it to make our job simpler?

We will use a very simple dataset that contains an index column (this is just a counter and not a feature). To make the example very generic, let's start the index from 100. So, the index of row number `0` is `100`:

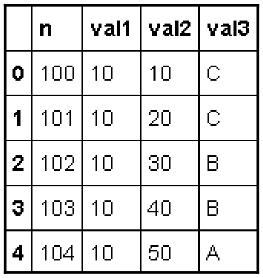
```
n,val1,val2,val3
100,10,10,C
101,10,20,C
102,10,30,B
103,10,40,B
104,10,50,A
```

When trying to load a file the classic way, you'll find yourself in a situation where you have got `n` as a feature (or a column). Nothing is practically incorrect, but an index should not be used by mistake as a feature. Therefore, it is better to keep it separated. If instead, by chance, it is used during the learning phase of your model, you may possibly incur a case of *leakage*, which is one of the major sources of error in machine learning.

In fact, if the index is a random number, no harm will be done to your model's efficacy. However, if the index contains progressive, temporal, or even informative elements (for example, certain numeric ranges may be used for positive outcomes, and others for the negative ones), you might incorporate into the model's leaked information. This will be impossible to replicate when using your model on fresh data:

```
In: import pandas as pd

In: dataset = pd.read_csv('a_selection_example_1.csv')
    dataset
```

Here is the `read` dataset:

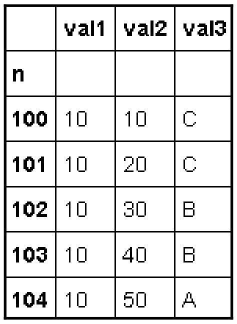


	n	val1	val2	val3
0	100	10	10	C
1	101	10	20	C
2	102	10	30	B
3	103	10	40	B
4	104	10	50	A

Therefore, while loading such a dataset, we might want to specify that `n` is the index column. Since the index `n` is the first column, we can give the following command:

```
In: dataset = pd.read_csv('a_selection_example_1.csv', index_col=0)
    dataset
```

The `read_csv` function now uses the first column as the index:



	val1	val2	val3
n			
100	10	10	C
101	10	20	C
102	10	30	B
103	10	40	B
104	10	50	A

Here, the dataset is loaded and the index is correct. Now, to access the value of a cell, there are a few things we can do. Let's list them one by one:

1. First, you can simply specify the column and the line (by using its index) you are interested in.
2. To extract the `val3` of the fifth line (indexed with *n=104*), you can give the following command:

```
In: dataset['val3'][104]

Out: 'A'
```

3. Apply this operation carefully since it's not a matrix and you might be tempted to first input the row and then the column. Remember that it's actually a pandas DataFrame, and the `[]` operator works first on columns and then on the element of the resulting pandas `Series`.
4. To have something similar to the preceding method of accessing data, you can use the `.loc()` method, which is label-based; that is, it works by the index and column labels:

```
In: dataset.loc[104, 'val3']

Out: 'A'
```

In this case, you should first specify the index and then the columns you're interested in.

Please note that, sometimes, the index in a DataFrame can be expressed in numbers. In such a case, it is easy to confuse it with a positional index, but a numeric index is not necessarily ordered or continuous.

5. Finally, a fully-optimized function that specifies the positions (positional indexing, as in a matrix) is `iloc()`. With it, you must specify the cell by using the row number and column number:

```
In: dataset.iloc[4, 2]

Out: 'A'
```

6. The retrieval of submatrixes is a very intuitive operation; you simply need to specify the lists of indexes instead of scalars:

```
In: dataset[['val3', 'val2']][0:2]
```

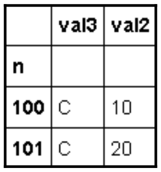
7. This command is equivalent to this:

```
In: dataset.loc[range(100, 102), ['val3', 'val2']]
```

8. And it is also equivalent to the following:

```
In: dataset.iloc[range(2), [2,1]]
```

In all the cases, the resulting DataFrame is as follows:



	val3	val2
n		
100	C	10
101	C	20

There is another method available for indexing in a pandas DataFrame: the `ix` method works by a mix of label-based and positional indexes: `dataset.ix[104, 'val3']`. Note that `ix` has to guess what you are referring to. Therefore, if you don't want to mix labels and positional indexes, `loc` and `iloc` are absolutely preferred in order to create a more safe and effective approach. `ix` is to be deprecated in the upcoming versions of pandas.

Working with categorical and textual data

Typically, you'll find yourself dealing with two main kinds of data: categorical and numerical. Numerical data, such as temperature, amount of money, days of usage, or house number, can be composed of either floating-point numbers (such as 1.0, -2.3, 99.99, and so on) or integers (such as -3, 9, 0, 1, and so on). Each value that the data can assume has a direct relation with others since they're comparable. In other words, you can say that a feature with a value of 2.0 is greater (actually, it is double) than a feature that assumes a value of 1.0. This type of data is very well-defined and comprehensible, with binary operators such as equal to, greater than, and less than.

The other type of data you might see in your career is the categorical type. A categorical datum expresses an attribute that cannot be measured and assumes values in a finite or infinite set of values, often named levels. For example, the weather is a categorical feature, since it takes values in a discrete set [`sunny`, `cloudy`, `snowy`, `rainy`, and `foggy`]. Other examples are features that contain URLs, IPs, device brands, items you put in your e-commerce cart, devices IDs, and so on. On this data, you cannot define the equal to, greater than, and less than binary operators and therefore, you cannot rank them.

A plus point for both categorical and numerical values is Booleans. In fact, they can be seen as categorical (presence/absence of a feature) or, on the other hand, as, the probability of a feature having an exhibit (has displayed, has not displayed). Since many machine learning algorithms do not allow the input to be categorical, Boolean features are often used to encode categorical features as numerical values.

Let's continue with the example of the weather. If we want to map a feature that contains the current weather and which takes values in the set [`sunny`, `cloudy`, `snowy`, `rainy`, and `foggy`] and encodes them to binary features, we should create five `True`/`False` features, with one for each level of the categorical feature. Now, the map is straightforward:

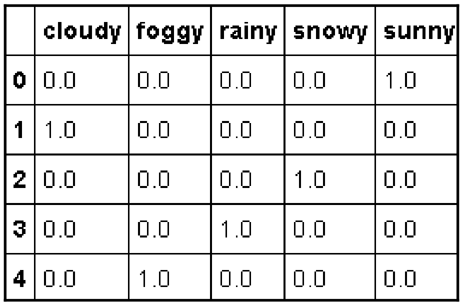
```
Categorical_feature = sunny   binary_features = [1, 0, 0, 0, 0]
Categorical_feature = cloudy  binary_features = [0, 1, 0, 0, 0]
Categorical_feature = snowy   binary_features = [0, 0, 1, 0, 0]
Categorical_feature = rainy   binary_features = [0, 0, 0, 1, 0]
Categorical_feature = foggy   binary_features = [0, 0, 0, 0, 1]
```

Only one binary feature reveals the presence of the categorical feature; the others remain `0`. This is called binary encoding or one hot encoding. By performing this easy step, we moved from the categorical world to a numerical one. The price of this operation is its complexity in terms of memory and computations; instead of a single feature, we now have five features. Generically, instead of a single categorical feature with *N* possible levels, we will create *N* features, each with two numerical values (1/0). This operation is named dummy coding.

The pandas package helps us in this operation, making the mapping easy with one command:

```
In: import pandas as pd
    categorical_feature = pd.Series(['sunny', 'cloudy',
                                     'snowy', 'rainy', 'foggy'])
    mapping = pd.get_dummies(categorical_feature)
    mapping
```

Here is the `mapping` dataset:



	cloudy	foggy	rainy	snowy	sunny
0	0.0	0.0	0.0	0.0	1.0
1	1.0	0.0	0.0	0.0	0.0
2	0.0	0.0	0.0	1.0	0.0
3	0.0	0.0	1.0	0.0	0.0
4	0.0	1.0	0.0	0.0	0.0

The output is a DataFrame that contains the categorical levels as column labels and the respective binary features along the column. To map a categorical value to a list of numerical ones, just use the power of pandas:

```
In: mapping['sunny']

Out: 0    1.0
     1    0.0
     2    0.0
     3    0.0
     4    0.0
     Name: sunny, dtype: float64

In: mapping['cloudy']

Out: 0    0.0
     1    1.0
     2    0.0
     3    0.0
     4    0.0
     Name: cloudy, dtype: float64
```

As seen in this example, `sunny` is mapped into the list of Boolean values `[1, 0, 0, 0, 0]`, `cloudy` to `[0, 1, 0, 0, 0]`, and so on.

The same operation can be done with another toolkit, Scikit-learn. It's somehow more complex since you must first convert text to categorical indices, but the result is the same. Let's take a peek at the previous example again:

```
In: from sklearn.preprocessing import OneHotEncoder
    from sklearn.preprocessing import LabelEncoder
    le = LabelEncoder()
    ohe = OneHotEncoder()
    levels = ['sunny', 'cloudy', 'snowy', 'rainy', 'foggy']
    fit_levs = le.fit_transform(levels)
    ohe.fit([[fit_levs[0]], [fit_levs[1]], [fit_levs[2]],
             [fit_levs[3]], [fit_levs[4]]])
    print (ohe.transform([le.transform(['sunny'])]).toarray())
    print (ohe.transform([le.transform(['cloudy'])]).toarray())

Out: [[ 0.  0.  0.  0.  1.]]
     [[ 1.  0.  0.  0.  0.]]
```

Basically, `LabelEncoder` maps the text to a 0-to-N integer number (note that in this case, it's still a categorical variable since it makes no sense to rank it). Now, these five values are mapped to five binary variables.

A special type of data – text

Let's introduce another type of data. Text data is a frequently used input for machine learning algorithms since it contains a natural representation of data in our language. It's so rich that it also contains the answer to what we're looking for. The most common approach when dealing with text is to use a bag-of-words approach. According to this approach, every word becomes a feature and the text becomes a vector that contains non-zero elements for all the features (that is, the words) in its body. Given a text dataset, what's the number of features? It is simple. Just extract all the unique words in it and enumerate them. For a very rich text that uses all the English words, that number is in the 1 million range. If you're not going to further process it (removal of any third person, abbreviations, contractions, and acronyms), you might find yourself dealing with more than that, but that's a very rare case. In a plain and simple approach, which is the target of this book, we just let Python do its best.

The dataset used in this section is textual; it's the famous *20newsgroup* (for more information about this, visit `http://qwone.com/~jason/20Newsgroups/`). It is a collection of about 20,000 documents that belong to 20 topics of newsgroups. It's one of the most frequently used (if not the topmost used) datasets that's presented while dealing with text classification and clustering. To import it, we're going to use its restricted subset, which contains all the science topics (medicine and space):

```
In: from sklearn.datasets import fetch_20newsgroups
    categories = ['sci.med', 'sci.space']
    twenty_sci_news = fetch_20newsgroups(categories=categories)
```

The first time you run this command, it automatically downloads the dataset and places it in the `$HOME/scikit_learn_data/20news_home/` default directory. You can query the dataset object by asking for the location of the files, their content, and the label (that is, the topic of the discussion where the document was posted). They're located in the `.filenames`, `.data`, and `.target` attributes of the object, respectively:

```
In: print(twenty_sci_news.data[0])

Out: From: flb@flb.optiplan.fi ("F.Baube[tm]")
     Subject: Vandalizing the sky
     X-Added: Forwarded by Space Digest
     Organization: [via International Space University]
     Original-Sender: isu@VACATION.VENARI.CS.CMU.EDU
     Distribution: sci
     Lines: 12
     From: "Phil G. Fraering" <pgf@srl03.cacs.usl.edu>
     [...]
```

```
In: twenty_sci_news.filenames

Out: array([
         '/Users/datascientist/scikit_learn_data/20news_home/20news-bydate-
         train/sci.space/61116',
         '/Users/datascientist/scikit_learn_data/20news_home/20news-
         bydate-train/sci.med/58122',
         '/Users/datascientist/scikit_learn_data/20news_home/20news-
         bydate-train/sci.med/58903',
         ...,
         '/Users/datascientist/scikit_learn_data/20news_home/20news-
         bydate-train/sci.space/60774',
         [...]

In: print (twenty_sci_news.target[0])
    print (twenty_sci_news.target_names[twenty_sci_news.target[0]])

Out: 1
     sci.space
```

The target is categorical, but it's represented as an integer (`0` for `sci.med` and `1` for `sci.space`). If you want to read it, check against the index of the `twenty_sci_news.target` array.

The easiest way to deal with the text is by transforming the body of the dataset into a series of words. This means that, for each document, the number of times a specific word appears in the body will be counted.

For example, let's make a small, easy-to-process dataset:

- `Document_1`: We love data science
- `Document_2`: Data science is hard

In the entire dataset, which contains `Document_1` and `Document_2`, there are only six different words: `we`, `love`, `data`, `science`, `is`, and `hard`. Given this array, we can associate each document with a feature vector:

```
In: Feature_Document_1 = [1 1 1 1 0 0]
    Feature_Document_2 = [0 0 1 1 1 1]
```

Note that we're discarding the positions of the words and retaining only the number of times the word appears in the document. That's all.

In the 20newsletter database, with Python, this can be done in a simple way:

```
In: from sklearn.feature_extraction.text import CountVectorizer
    count_vect = CountVectorizer()
    word_count = count_vect.fit_transform(twenty_sci_news.data)
    word_count.shape

Out: (1187, 25638)
```

First, we instantiate a CountVectorizer object. Then, we call the method to count the terms in each document and produce a feature vector for each of them (fit_transform). We then query the matrix size. Note that the output matrix is sparse because it's very common to have only a limited selection of words for each document (since the number of non-zero elements in each line is very low and it makes no sense to store all the redundant zeros). Anyway, the output shape is (1187, 25638). The first value is the number of observations in the dataset (the number of documents), while the latter is the number of features (the number of unique words in the dataset).

After the CountVectorizer transforms, each document is associated with its feature vector. Let's take a look at the first document:

```
In: print (word_count[0])

Out: (0, 10827)  2
     (0, 10501)  2
     (0, 17170)  1
     (0, 10341)  1
     (0, 4762)  2
     (0, 23381)  2
     (0, 22345)  1
     (0, 24461)  1
     (0, 23137)  7
     [...]
```

You will notice that the output is a sparse vector where only non-zero elements are stored. To check the direct correspondence to words, just try the following code:

```
In: word_list = count_vect.get_feature_names()
    for n in word_count[0].indices:
         print ('Word "%s" appears %i times' % (word_list[n],
                                               word_count[0, n]))

Out: Word: from appears 2 times
     Word: flb appears 2 times
     Word: optiplan appears 1 times
     Word: fi appears 1 times
     Word: baube appears 2 times
```

```
        Word: tm appears 2 times
        Word: subject appears 1 times
        Word: vandalizing appears 1 times
        Word: the appears 7 times
        [...]
```

So far, everything has been pretty simple, hasn't it? Let's move forward to another task of increasing complexity and effectiveness. Counting words is good, but we can manage more; we can compute their frequency. It's a measure that you can compare across differently-sized datasets. It gives an idea of whether a word is a stop word (that is, a very common word such as a, an, the, or is) or a rare, unique one. Typically, these terms are the most important because they're able to characterize an instance and the features based on these words, which are very discriminative in the learning process. To retrieve the frequency of each word in each document, try the following code:

```
In: from sklearn.feature_extraction.text import TfidfVectorizer
    tf_vect = TfidfVectorizer(use_idf=False, norm='l1')
    word_freq = tf_vect.fit_transform(twenty_sci_news.data)
    word_list = tf_vect.get_feature_names()
    for n in word_freq[0].indices:
         print ('Word "%s" has frequency %0.3f' % (word_list[n],
                                                  word_freq[0, n]))

Out: Word "from" has frequency 0.022
     Word "flb" has frequency 0.022
     Word "optiplan" has frequency 0.011
     Word "fi" has frequency 0.011
     Word "baube" has frequency 0.022
     Word "tm" has frequency 0.022
     Word "subject" has frequency 0.011
     Word "vandalizing" has frequency 0.011
     Word "the" has frequency 0.077
     [...]
```

The sum of the frequencies is 1 (or close to 1 due to the approximation). This happens because we chose the `l1` norm. In this specific case, the word `frequency` is a probability distribution function. Sometimes, it's nice to increase the difference between rare and common words. In such cases, you can use the `l2` norm to normalize the feature vector.

An even more effective way to vectorize text data is by using `tf-idf`. In brief, you can multiply the term frequency of the words that compose a document by the inverse document frequency of the word itself (that is, in the number of documents it appears in, or in its logarithmically scaled transformation). This is very handy for highlighting words that effectively describe each document and which are powerful discriminative elements among the dataset:

```
In: from sklearn.feature_extraction.text import TfidfVectorizer
    tfidf_vect = TfidfVectorizer() # Default: use_idf=True
    word_tfidf = tfidf_vect.fit_transform(twenty_sci_news.data)
    word_list = tfidf_vect.get_feature_names()
    for n in word_tfidf[0].indices:
        print ('Word "%s" has tf-idf %0.3f' % (word_list[n],
                                               word_tfidf[0, n]))

Out: Word "fred" has tf-idf 0.089
     Word "twilight" has tf-idf 0.139
     Word "evening" has tf-idf 0.113
     Word "in" has tf-idf 0.024
     Word "presence" has tf-idf 0.119
     Word "its" has tf-idf 0.061
     Word "blare" has tf-idf 0.150
     Word "freely" has tf-idf 0.119
     Word "may" has tf-idf 0.054
     Word "god" has tf-idf 0.119
     Word "blessed" has tf-idf 0.150
     Word "is" has tf-idf 0.026
     Word "profiting" has tf-idf 0.150
     [...]
```

In this example, the four most characterizing words of the first documents are `caste`, `baube`, `flb`, and `tm` (they have the highest `tf-idf` score). This means that their term frequency within the document is high, whereas they're pretty rare in the remaining documents.

So far, for each word, we have generated a feature. What about taking a couple of words together? That's exactly what happens when you consider bigrams instead of unigrams. With bigrams (or generically, n-grams), the presence or absence of a word – as well as its neighbors – matters (that is, the words near it and their disposition). Of course, you can mix unigrams and n-grams and create a rich feature vector for each document. In the following simple example, let's test how n-grams work:

```
In: text_1 = 'we love data science'
    text_2 = 'data science is hard'
    documents = [text_1, text_2]
    documents
```

```
Out: ['we love data science', 'data science is hard']

In: # That is what we say above, the default one
    count_vect_1_grams = CountVectorizer(ngram_range=(1, 1),
    stop_words=[], min_df=1)
    word_count = count_vect_1_grams.fit_transform(documents)
    word_list = count_vect_1_grams.get_feature_names()
    print ("Word list = ", word_list)
    print ("text_1 is described with", [word_list[n] + "(" +
    str(word_count[0, n]) + ")" for n in word_count[0].indices])

Out: Word list =  ['data', 'hard', 'is', 'love', 'science', 'we']
     text_1 is described with ['we(1)', 'love(1)', 'data(1)', 'science(1)']

In: # Now a bi-gram count vectorizer
    count_vect_1_grams = CountVectorizer(ngram_range=(2, 2))
    word_count = count_vect_1_grams.fit_transform(documents)
    word_list = count_vect_1_grams.get_feature_names()
    print ("Word list = ", word_list)
    print ("text_1 is described with", [word_list[n] + "(" +
    str(word_count[0, n]) + ")" for n in word_count[0].indices])

Out: Word list =  ['data science', 'is hard', 'love data',
     'science is', 'we love']
     text_1 is described with ['we love(1)', 'love data(1)',
     'data science(1)']

In: # Now a uni- and bi-gram count vectorizer
    count_vect_1_grams = CountVectorizer(ngram_range=(1, 2))
    word_count = count_vect_1_grams.fit_transform(documents)
    word_list = count_vect_1_grams.get_feature_names()
    print ("Word list = ", word_list)
    print ("text_1 is described with", [word_list[n] + "(" +
    str(word_count[0, n]) + ")" for n in word_count[0].indices])

Out: Word list =  ['data', 'data science', 'hard', 'is', 'is hard', 'love',
     'love data', 'science', 'science is', 'we', 'we love']
     text_1 is described with ['we(1)', 'love(1)', 'data(1)', 'science(1)',
     'we love(1)', 'love data(1)', 'data science(1)']
```

The preceding example very intuitively combines the first and second approach we previously presented. In this case, we used a `CountVectorizer`, but this approach is very common with a `TfidfVectorizer`. Note that the number of features explodes exponentially when you use n-grams.

If you have too many features (the dictionary may be too rich, there may be too many n-grams, or the computer may be just limited), you can use a trick that lowers the complexity of the problem (but you should first evaluate the trade-off performance/trade-off complexity). It's common to use the hashing trick where many words (or n-grams) are hashed and their hashes collide (which makes a bucket of words). Buckets are sets of semantically unrelated words but with colliding hashes. With `HashingVectorizer()`, as shown in the following example, you can decide on the number of buckets of words you want. The resulting matrix, of course, reflects your setting:

```
In: from sklearn.feature_extraction.text import HashingVectorizer
    hash_vect = HashingVectorizer(n_features=1000)
    word_hashed = hash_vect.fit_transform(twenty_sci_news.data)
    word_hashed.shape

Out: (1187, 1000)
```

Note that you can't invert the hashing process (since it's a digest operation). Therefore, after this transformation, you will have to work on the hashed features as they are. Hashing presents quite a few advantages: allowing quick transformation of a bag of words into vectors of features (hash buckets are our features, in this case), easily accommodating never-previously-seen words among the features, and avoiding overfitting by having unrelated words collide together in the same feature.

Scraping the web with Beautiful Soup

In the previous section, we discussed how to operate on textual data, given the fact that we already have the dataset. What if we need to scrape the web and download it manually? This process happens more often than you can expect, and it's a very popular topic of interest in data science. For example:

- Financial institutions scrape the web to extract fresh details and information about the companies in their portfolio. Newspapers, social networks, blogs, forums, and corporate websites are the ideal targets for these analyses.
- Advertisement and media companies analyze sentiment and the popularity of many pieces of the web to understand people's reactions.
- Companies specialized in insight analysis and recommendation scrape the web to understand patterns and model user behaviors.
- Comparison websites use the web to compare prices, products, and services, offering the user an updated synoptic table of the current situation.

Unfortunately, understanding websites is very hard work since each website is built and maintained by different people, with different infrastructures, locations, languages, and structures. The only common aspect among them is represented by the standard exposed language, which, most of the time, is **Hypertext Markup Language** (**HTML**).

That's why the vast majority of web scrapers, available as of today, are only able to understand and navigate HTML pages in a general-purpose way. One of the most used web parsers is named Beautiful Soup. It's written in Python, it's open source, and it's very stable and simple to use. Moreover, it's able to detect errors and pieces of malformed code in the HTML page (always remember that web pages are often human-made products and prone to errors).

A complete description of Beautiful Soup would require an entire book; here, we will see just a few bits. First of all, Beautiful Soup is not a crawler. In order to download a web page, we can (as an example) use the `urllib` library:

1. Let's download the code behind the William Shakespeare page on Wikipedia:

```
In: import urllib.request
    url = 'https://en.wikipedia.org/wiki/William_Shakespeare'
    request = urllib.request.Request(url)
    response = urllib.request.urlopen(request)
```

2. It's time to instruct Beautiful Soup to read the resource and parse it using the HTML parser:

```
In: from bs4 import BeautifulSoup
    soup = BeautifulSoup(response, 'html.parser')
```

3. Now, the `soup` is ready and can be queried. To extract the title, we can simply ask for the title attribute:

```
In: soup.title

Out: <title>William Shakespeare - Wikipedia,
     the free encyclopedia</title>
```

As you can see, the whole title tag is returned, allowing for a deeper investigation of the nested HTML structure. What if we want to know about the categories associated with the Wikipedia page of William Shakespeare? It can be very useful to create a graph of the entry, simply by recurrently downloading and parsing adjacent pages. We should first manually analyze the HTML page itself to figure out what the best HTML tag containing the information we're looking for is. Remember here the *no free lunch* theorem in data science: there are no auto-discovery functions, and furthermore, things can change if Wikipedia modifies its format.

After a manual analysis, we discover that categories are inside a div named `'mw-normal-catlinks'`; excluding the first link, all the others are okay. Now, it's time to program. Let's put what we've observed into some code, printing for each category the title of the linked page and the relative link to it:

```
In: section = soup.find_all(id='mw-normal-catlinks')[0]
    for catlink in section.find_all("a")[1:]:
        print(catlink.get("title"), "->", catlink.get("href"))

Out: Category:William Shakespeare -> /wiki/Category:William_Shakespeare
     Category:1564 births -> /wiki/Category:1564_births
     Category:1616 deaths -> /wiki/Category:1616_deaths
     Category:16th-century English male actors -> /wiki/Category:16th-
     century_English_male_actors
     Category:English male stage actors -> /wiki/Category:
     English_male_stage_actors
     Category:16th-century English writers -> /wiki/Category:16th-
     century_English_writers
```

We've used the `find_all` method twice to find all the HTML tags with the text contained in the argument. In the first case, we were specifically looking for an ID; in the second case, we were looking for all the `"a"` tags.

Given the output, then, and using the same code with the new URLs, it's possible to recursively download the Wikipedia category pages, arriving at this point at the ancestor categories.

A final note about scraping: always remember that this practice is not always allowed, and when so, remember to tune down the rate of the download (at high rates, the website's server may think you're doing a small-scale DoS attack and might eventually blacklist/ban your IP address). For more information, you can read the terms and conditions of the website, or simply contact the administrators.

Data processing with NumPy

Having introduced the essential pandas commands to upload and preprocess your data in memory completely, in smaller batches, or even in single data rows, at this point of the data science pipeline, you'll have to work on it in order to prepare a suitable data matrix for your supervised and unsupervised learning procedures.

As a best practice, we advise that you divide the task between a phase of your work when your data is still heterogeneous (a mix of numerical and symbolic values) and another phase when it is turned into a numeric table of data. A table of data, or matrix, is arranged in rows that represent your examples, and columns that contain the characteristic observed values of your examples, which are your variables.

Following our advice, you have to wrangle between two key Python packages for scientific analysis, pandas and NumPy, and their two pivotal data structures, DataFrame and `ndarray`. This means that your data science pipeline will be more efficient and fast.

Since the target data structure that we want to feed into the following machine learning phase is a matrix represented by the `NumPy ndarray` object, let's start from the result we want to achieve, that is, how to generate a `ndarray` object.

NumPy's n-dimensional array

Python presents native data structures, such as lists and dictionaries, which you should use to the best of your ability. Lists, for example, can store sequentially heterogeneous objects (for instance, you can save numbers, texts, images, and sounds in the same list). On the other hand, because being based on a lookup table (a hash table), dictionaries can recall content. The content can be any Python object, and often it is a list of another dictionary. Thus, dictionaries allow you to access complex, multidimensional data structures.

Anyway, lists and dictionaries have their own limitations, such as the following:

- There's the problem with memory and speed. They are not really optimized for using nearly contiguous chunks of memory, and this may become a problem when trying to apply highly optimized algorithms or multiprocessor computations, because memory handling may turn into a bottleneck.
- They are excellent for storing data but not for operating on it. Therefore, whatever you may want to do with your data, you have to first define custom functions and iterate or map over the list or dictionary elements.
- Iterating may often prove suboptimal when working on a large amount of data.

NumPy offers a `ndarray` object class (n-dimensional array) that has the following attributes:

- It is memory optimal (and, besides other aspects, configured to transmit data to C or Fortran routines in the best-performing layout of memory blocks)

- It allows for fast linear algebra computations (vectorization) and element-wise operations (broadcasting) without any need to use iterations with for loops
- Critical libraries, such as SciPy or Scikit-learn, expect arrays as an input for their functions to operate correctly

All of this comes with some limitations. In fact, `ndarray` objects have the following drawbacks:

- They usually store only elements of a single, specific data type, which you can define beforehand (but there's a way to define complex data and heterogeneous data types, though they could be very difficult to handle for analysis purposes).
- After they are initialized, their size is fixed. If you want to change their shape, you have to create them anew.

The basics of NumPy ndarray objects

In Python, an array is a block of memory-contiguous data of a specific type with a header that contains the indexing scheme and the data type descriptor.

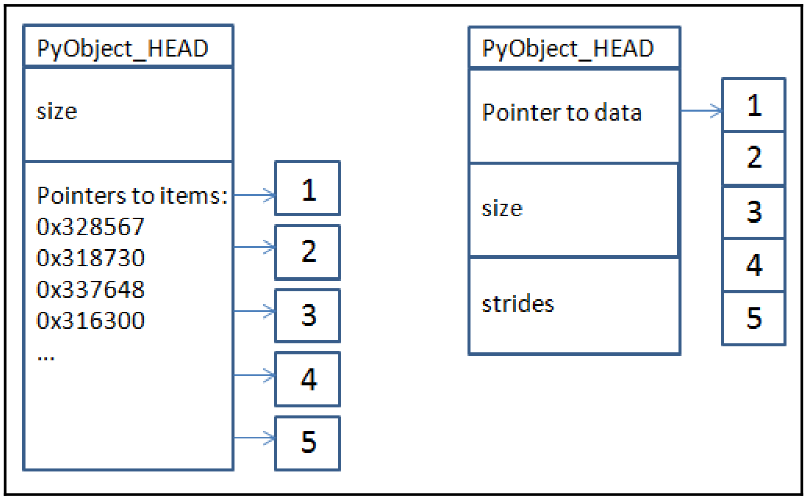
Thanks to the indexing scheme, an array can represent a multidimensional data structure where each element is indexed with a tuple of *n* integers, where *n* is the number of dimensions. Therefore, if your array is unidimensional (that is, a vector of sequential data), the index will start from zero (as in Python lists).

If it is bidimensional, you'll have to use two integers as an index (a tuple of coordinates of type *x*,*y*); if there are three dimensions, the number of integers used will be three (a tuple *x*,*y*,*z*), and so on.

At each indexed location, the array will contain data of the specified data type. An array can store many numerical data types, as well as strings, and other Python objects. It is also possible to create custom data types and therefore handle data sequences of different types, though we advise against it and we suggest that you use the pandas DataFrame in such cases. pandas data structures are indeed much more flexible for any intensive usage of heterogeneous data types as necessary for a data scientist. Consequently, in this book, we will consider only NumPy arrays of a specific, defined type, and leave pandas to deal with heterogeneity.

Since the type (and the memory space it occupies in terms of bytes) of an array should be defined from the beginning, the array creation procedure reserves the exact memory space to contain all the data. The access, modification, and computation of the elements of an array are therefore quite fast, though this also consequently implies that the array is fixed and cannot be changed in its structure.

The Python list data structure is actually much more cumbersome and slow, being a collection of pointers linking the list structure to the scattered memory locations containing the data itself. Instead, as depicted in the following diagram, a NumPy `ndarray` is made of just a pointer addressing a single memory location where data, arranged sequentially, is stored. When you access the data in a `NumPy ndarray`, you'll actually require fewer operations and less access to different memory parts than when using a list, hence the major efficiency and speed when working with large amounts of data. As a drawback, data connected to a NumPy array cannot be changed; it has to be recreated when inserting or removing data:



No matter the dimensions of the NumPy array, data will always be arranged as a continuous sequence of values (a contiguous block of memory). It is the knowledge of the size of the array and of the strides (telling us how many bytes we have to skip in memory to move to the next position along a certain axis) that renders it easy to correctly represent and operate on the array.

Talking of memory optimization for fast performances, in order to store multidimensional arrays, there are strictly two methods called **row-major order** and **column-major order**. Since **RAM** (**random access memory**) is arranged into a linear storage of memory cells (memory cells are contiguous as the points of a line – there is no such thing as an array in RAM), you have to flatten the array to a vector and store it in memory. When flattening, you can just proceed row by row (row-major order), which is typical of C/C++, or column by column (column-major order), which is typical of Fortran or R. Python, in the NumPy package implementation, uses the row-major ordering (also called C-contiguous, whereas the column-major ordering is also called Fortran-contiguous), which means that it is faster in computing operations applied row by row than working column after column. Anyway, when creating your NumPy array, you can decide the ordering of your data structure, based on your expectation of manipulating it more by rows or columns. After importing the package, `import numpy as np`, given an array such as `a = [[1,2,3],[4,5,6],[7,8,9]]`, you can redefine it in row-major order: `c = np.array(a, order='C')` or in column-major order: `f = np.array(a, order='F')`

In contrast, lists of data structures, that represent multiple dimensions, cannot but turn themselves into nested lists, thus increasing both overhead and memory fragmentation when accessing data.

All that you have read so far may sound like a computer scientist blabbering. After all, all data scientists care about is getting Python to do something useful and quick. That's surely true, but doing something quickly from a syntactic point of view sometimes doesn't automatically equate into doing something quick from the point of view of the execution itself. If you can grasp the internals of NumPy and pandas, you could really make your code speed up and achieve more in your projects in less time. We have experience of syntactically correct data munging code using NumPy and pandas that, by the right refactoring, reduced its execution time by half or more.

For our purposes, it is also very important to understand that, when accessing or transforming an array, we may be just viewing it or we may be copying it. When we are *viewing* an array, we actually call a procedure that allows us to convert the data that's present in its structure into something else, but the sourcing array is unaltered. Based on the previous example, when viewing, we are just changing the size attribute of a `ndarray`; the data is left untouched. Consequently, any data transformation experienced as viewing an array is merely ephemeral, unless we fix them into a new array.

Instead, when we are *copying* an array, we are effectively creating a new array with a different structure (thus occupying fresh memory). We do not just change the parameter relative to the size of the array; we are also reserving another sequential chunk of memory and copying our data there.

All pandas DataFrames are actually made of one-dimensional NumPy arrays. For this reason, they inherit the speed and memory efficiency of `ndarrays` when you operate by columns (since each column is a NumPy array). When operating by rows, DataFrames are more inefficient because you are accessing sequentially different columns; that is, different NumPy arrays. For the same reason, it is speedier to address portions of a pandas DataFrame by a positional index, not by a pandas index, because NumPy arrays work using integer numbers as positions. Using pandas indexes (which can also be textual, not just numerical) actually requires a transformation of the index into its corresponding position for the DataFrame to operate correctly on the data.

Creating NumPy arrays

There is more than one way to create NumPy arrays. The following are some of the ways you can create them:

- By transforming an existing data structure into an array
- By creating an array from scratch and populating it with default or calculated values
- By uploading some data from a disk into an array

If you are going to transform an existing data structure, the odds are in favor of you working with a structured list or a pandas DataFrame.

From lists to unidimensional arrays

One of the most common situations you will encounter when working with data is transforming a list into an array.

When operating such a transformation, it is important to consider the objects the lists contain because this will determine the dimensionality and the `dtype` of the resulting array.

Let's start with this first example of a list containing just integers:

```
In: import numpy as np

In: # Transform a list into a uni-dimensional array
    list_of_ints = [1,2,3]
    Array_1 = np.array(list_of_ints)

In: Array_1

Out: array([1, 2, 3])
```

Remember that you can access a one-dimensional array as you would with a standard Python list (the indexing starts from zero):

```
In: Array_1[1] # let's output the second value

Out: 2
```

We can ask for further information about the type of the object and the type of its elements (the effectively resulting type depends on whether your system is 32-bit or 64-bit):

```
In: type(Array_1)

Out: numpy.ndarray

In: Array_1.dtype

Out: dtype('int64')
```

The default `dtype` depends on the system you're operating on.

Our simple list of integers will turn into a one-dimensional array; that is, a vector of 32-bit integers (ranging from -231 to 231-1, the default integer on the platform we used for our examples).

Controlling memory size

You may think that it is a waste of memory to use an `int64` data type if the range of your values is so limited.

In fact, conscious of data-intensive situations, you can calculate how much memory space your `Array_1` object is taking:

```
In: import numpy as np
    Array_1.nbytes

Out: 24
```

Please note that on 32-bit platforms (or when using a 32-bit Python version on a 64-bit platform), the result is 12.

In order to save memory, you can specify the type that best suits your array beforehand:

```
In: Array_1 = np.array(list_of_ints, dtype= 'int8')
```

Now, your simple array occupies just a fourth of the previous memory space. It may seem an obvious and overly simplistic example, but when dealing with millions of rows and columns, defining the best data type for your analysis can really save the day, allowing you to fit everything nicely into memory.

For your reference, here is a table that presents the most common data types for data science applications and their memory usage for a single element:

Type	Size in bytes	Description
`bool`	1	Boolean (`True` or `False`) stored as a byte
`int`	4	Default integer type (normally `int32` or `int64`)
`int8`	1	Byte (-128 to 127)
`int16`	2	Integer (-32768 to 32767)
`int32`	4	Integer (-2**31 to 2**31-1)
`int64`	8	Integer (-2**63 to 2**63-1)

Type	Size in bytes	Description
`uint8`	1	Unsigned integer (0 to 255)
`uint16`	2	Unsigned integer (0 to 65535)
`uint32`	4	Unsigned integer (0 to 2**32-1)
`uint64`	8	Unsigned integer (0 to 2**64-1)
`float_`	8	Shorthand for `float64`
`float16`	2	Half-precision float (exponent 5 bits, mantissa 10 bits)
`float32`	4	Single-precision float (exponent 8 bits, mantissa 23 bits)
`float64`	8	Double-precision float (exponent 11 bits, mantissa 52 bits)

There are some more numerical types, such as complex numbers, that are less usual but which may be required by your application (for example, in a spectrogram). You can get the complete idea from the NumPy user guide at `http://docs.scipy.org/doc/numpy/user/basics.types.html`.

If an array has a type that you want to change, you can easily create a new array by casting a new, specified type:

```
In: Array_1b = Array_1.astype('float32')
    Array_1b

Out: array([ 1.,  2.,  3.], dtype=float32)
```

In case your array is memory consuming, note that the `.astype` method will copy the array, and thus it always creates a new array.

Heterogeneous lists

What if the lists were made of heterogeneous elements, such as integers, floats, and strings? This gets trickier. A quick example can describe the situation to you:

```
In: import numpy as np
    complex_list = [1,2,3] + [1.,2.,3.] + ['a','b','c']
    # at first the input list is just ints
    Array_2 = np.array(complex_list[:3])
    print ('complex_list[:3]', Array_2.dtype)
    # then it is ints and floats
    Array_2 = np.array(complex_list[:6])
    print ('complex_list[:6]', Array_2.dtype)
    # finally we add strings print
    Array_2 = np.array(complex_list)
    ('complex_list[:] ',Array_2.dtype)
```

```
Out: complex_list[:3] int64
     complex_list[:6] float64
     complex_list[:] <U32
```

As explicated by our output, it seems that float types prevail over `int` types, and strings (`<U32` means a Unicode string of size 32 or less) take over everything else.

While creating an array using lists, you can mix different elements, and the most Pythonic way to check the results is by questioning the `dtype` of the resulting array.

Be aware that if you are uncertain about the contents of your array, you really have to check. Otherwise, you may find it impossible to operate on your resulting array and you may incur in an error later (unsupported operand type):

```
In: # Check if a NumPy array is of the desired numeric type
    print (isinstance(Array_2[0],np.number))

Out: False
```

In our data munging process, unintentionally finding out an array of the string type as output would mean that we forgot to transform all variables into numeric ones in the previous steps; for example, when all the data was stored in a pandas DataFrame. In the previous section, *Working with categorical and textual data*, we provided some simple and straightforward ways to deal with such situations.

Before that, let's complete our overview of how to derive an array from a list object. As we mentioned previously, the type of objects in the list influences the dimensionality of the array, too.

From lists to multidimensional arrays

If a list containing numeric or textual objects is rendered into a unidimensional array (that could represent a coefficient vector, for instance), a list of lists translates into a two-dimensional array, and a list of list of lists becomes a three-dimensional one:

```
In: import numpy as np
    # Transform a list into a bidimensional array
    a_list_of_lists = [[1,2,3],[4,5,6],[7,8,9]]
    Array_2D = np.array(a_list_of_lists )
    Array_2D

Out: array([[1, 2, 3],
            [4, 5, 6],
            [7, 8, 9]])
```

As mentioned previously, you can call out single values with indices, as in a list, though here you'll have two indices—one for the row dimension (also called axis 0) and one for the column dimension (axis 1):

```
In: Array_2D[1, 1]

Out: 5
```

Two-dimensional arrays are usually the norm in data science problems, though three-dimensional arrays may be found when a dimension represents time, for instance:

```
In: # Transform a list into a multi-dimensional array
    a_list_of_lists_of_lists = [[[1,2],[3,4],[5,6]],
                                [[7,8],[9,10],[11,12]]]
    Array_3D = np.array(a_list_of_lists_of_lists)
    Array_3D

Out: array([[[ 1,  2],
             [ 3,  4],
             [ 5,  6]],
            [[ 7,  8],
             [ 9, 10],
             [11, 12]]])
```

To access single elements of a three-dimensional array, you just have to point out three indexes:

```
In: Array_3D[0,2,0] # Accessing the 5th element

Out: 5
```

Arrays can be made from tuples in a way that is similar to the method of creating lists. Also, dictionaries can be turned into two-dimensional arrays thanks to the `.items()` method, which returns a copy of the dictionary's list of key-value pairs:

```
In: np.array({1:2,3:4,5:6}.items())

Out: array([[1, 2],
            [3, 4],
            [5, 6]])
```

Resizing arrays

Earlier, we mentioned how you can change the type of the elements of an array. We will now shortly stop for a while to examine the most common instructions to modify the shape of an existing array.

Let's start with an example that uses the `.reshape` method, which accepts an *n*-tuple containing the size of the new dimensions as a parameter:

```
In: import numpy as np
    # Restructuring a NumPy array shape
    original_array = np.array([1, 2, 3, 4, 5, 6, 7, 8])
    Array_a = original_array.reshape(4,2)
    Array_b = original_array.reshape(4,2).copy()
    Array_c = original_array.reshape(2,2,2)
    # Attention because reshape creates just views, not copies
    original_array[0] = -1
```

Our original array is a unidimensional vector of integer numbers from 1 to 8. Here is what we execute in the code:

1. We assign `Array_a` to a reshaped `original_array` of size 4 x 2
2. We do the same with `Array_b`, though we append the `.copy()` method, which will copy the array into a new one
3. Finally, we assign `Array_c` to a reshaped array in three dimensions of size 2 x 2 x 2
4. After having done such an assignment, the first element of `original_array` is changed in value from `1` to `-1`

Now, if we check the content of our arrays, we will notice that `Array_a` and `Array_c`, though they have the desired shape, are characterized by `-1` as the first element. That's because they dynamically mirror the original array they are in view from:

```
In: Array_a

Out: array([[-1, 2],
            [3, 4],
            [5, 6],
            [7, 8]])

In: Array_c

Out: array([[[-1,  2],
             [3,  4]],
                [[5,  6],
                 [7,  8]]])
```

Only the `Array_b` array, having been copied before mutating the original array, has a first element with a value of `1`:

```
In: Array_b

Out: array([[1, 2],
            [3, 4],
            [5, 6],
            [7, 8]])
```

If it is necessary to change the shape of the original array, then the `resize` method is to be favored:

```
In: original_array.resize(4,2)
    original_array

Out: array([[-1,  2],
            [ 3,  4],
            [ 5,  6],
            [ 7,  8]])
```

The same results may be obtained by acting on the `.shape` value by assigning a tuple of values representing the size of the intended dimensions:

```
In: original_array.shape = (4,2)
```

Instead, if your array is two-dimensional and you need to exchange the rows with the columns, that is, to transpose the array, the `.T` or `.transpose()` methods will help you obtain such a kind of transformation (which is a view, like `.reshape`):

```
In: original_array

Out: array([[-1,  2],
            [ 3,  4],
            [ 5,  6],
            [ 7,  8]])
```

Arrays derived from NumPy functions

If you need a vector or a matrix characterized by a particular numeric series (zeros, ones, ordinal numbers, and particular statistical distributions), NumPy functions provide you with quite a large range of choices.

First, creating a NumPy array of ordinal values (integers) is straightforward if you use the `arange` function, which returns integer values in a given interval (usually from zero) and reshapes its results:

```
In: import numpy as np

In: ordinal_values = np.arange(9).reshape(3,3)
    ordinal_values

Out: array([[0, 1, 2],
            [3, 4, 5],
            [6, 7, 8]])
```

If the array has to be reversed in the order of values, use the following command:

```
In: np.arange(9)[::-1]

Out: array([8, 7, 6, 5, 4, 3, 2, 1, 0])
```

If the integers are just random (with no order and possibly repeated), provide the following command:

```
In: np.random.randint(low=1,high=10,size=(3,3)).reshape(3,3)
```

Other useful arrays are either made of just zeros and ones or are identity matrices:

```
In: np.zeros((3,3))

In: np.ones((3,3))

In: np.eye(3)
```

If the array will be used for a grid search to search for optimal parameters, fractional values in an interval or a logarithmic growth should prove most useful:

```
In: fractions = np.linspace(start=0, stop=1, num=10)
    growth = np.logspace(start=0, stop=1, num=10, base=10.0)
```

Instead, statistical distributions, such as normal or uniform, may be handy for the initialization of a vector or matrix of coefficients.

A 3 x 3 matrix of standardized normal values (mean=0, std=1) can be seen here:

```
In: std_gaussian = np.random.normal(size=(3,3))
```

If you need to specify a different mean and standard deviation, just give the following command:

```
In: gaussian = np.random.normal(loc=1.0, scale= 3.0, size=(3,3))
```

The `loc` parameter stands for the mean, and the `scale` is actually the standard deviation.

Another frequent choice for a statistical distribution that is used to initialize a vector is certainly the uniform distribution:

```
In: rand = np.random.uniform(low=0.0, high=1.0, size=(3,3))
```

Getting an array directly from a file

NumPy arrays can also be created directly from the data present in a file.

Let's use an example from the previous chapter:

```
In: import numpy as np
    housing = np.loadtxt('regression-datasets-housing.csv',
                         delimiter=',', dtype=float)
```

NumPy `loadtxt`, given a `filename`, `delimiter`, and `dtype`, will upload the data to an array, unless the `dtype` is wrong; for instance, there's a `string` variable and the required array type is a `float`, as shown in the following example:

```
In: np.loadtxt('datasets-uci-iris.csv',delimiter=',',dtype=float)

Out: ValueError: could not convert string to float: Iris-setosa
```

In this case, a feasible solution could be to be aware of what column is a string (or any other non-numeric format) and prepare a converter function to turn it into numeric thanks to the `converters` parameter of `loadtxt`, which allows you to apply specific transformation functions to specific columns of the array, such as in the following example:

```
In: def from_txt_to_iris_class(x):
         if x==b'Iris-setosa': return 0
         elif x==b'Iris-versicolor': return 1
         elif x== b'Iris-virginica': return 2
         else: return np.nan

    np.loadtxt('datasets-uci-iris.csv', delimiter=',',
               converters= {4: from_txt_to_iris_class})
```

Extracting data from pandas

Interacting with pandas is quite easy. In fact, with pandas being built upon NumPy, arrays can easily be extracted from DataFrame objects, and they can be transformed into DataFrames themselves.

First, let's upload some data into a DataFrame. The `BostonHouse` example we downloaded in the previous chapter from the ML repository is suitable:

```
In: import pandas as pd
    import numpy as np
    housing_filename = 'regression-datasets-housing.csv'
    housing = pd.read_csv(housing_filename, header=None)
```

As demonstrated in the *Heterogeneous lists* section, at this point, the `.values` method will extract an array of a type that accommodates all the different types that are present in the DataFrame:

```
In: housing_array = housing.values
    housing_array.dtype

Out: dtype('float64')
```

In such a case, the selected type is `float64` because the float type prevails over the `int` type:

```
In: housing.dtypes

Out:  0     float64
      1       int64
      2     float64
      3       int64
      4     float64
      5     float64
      6     float64
      7     float64
      8       int64
      9       int64
      10      int64
      11    float64
      12    float64
      13    float64
      dtype: object
```

Asking for the types used by the DataFrame object before extracting your NumPy array by using the `.dtypes` method on the DataFrame allows you to anticipate the `dtype` of the resulting array. Consequently, it allows you to decide whether to transform or change the type of the variables in the DataFrame object before proceeding (please consult the *Working with categorical and textual data* section of this chapter).

NumPy fast operation and computations

When arrays need to be manipulated by mathematical operations, you just need to apply the operation on the array with respect to a numerical constant (a scalar), or an array of the same shape:

```
In: import numpy as np
    a =  np.arange(5).reshape(1,5)
    a += 1
    a*a

Out: array([[ 1,  4,  9, 16, 25]])
```

As a result, the operation is to be performed element-wise; that is, every element of the array is operated by either the scalar value or the corresponding element of the other array.

When operating on arrays of different dimensions, it is still possible to obtain element-wise operations without having to restructure the data if one of the corresponding dimensions is 1. In fact, in such a case, the dimension of size 1 is stretched until it matches the dimension of the corresponding array. This conversion is called broadcasting.

For instance:

```
In: a = np.arange(5).reshape(1,5) + 1
    b = np.arange(5).reshape(5,1) + 1
    a * b

Out: array([[ 1,  2,  3,  4,  5],
            [ 2,  4,  6,  8, 10],
            [ 3,  6,  9, 12, 15],
            [ 4,  8, 12, 16, 20],
            [ 5, 10, 15, 20, 25]])
```

The preceding code is equivalent to the following:

```
In: a2 = np.array([1,2,3,4,5] * 5).reshape(5,5)
    b2 = a2.T
    a2 * b2
```

However, it won't require an expansion of memory of the original arrays in order to obtain pair-wise multiplication.

Furthermore, there exists a wide range of NumPy functions that can operate element-wise on arrays: `abs()`, `sign()`, `round()`, `floor()`, `sqrt()`, `log()`, and `exp()`.

Other usual operations that could be operated by NumPy functions are `sum()` and `prod()`, which provide the summation and product of the array rows or columns on the basis of the specified axis:

```
In: print (a2)

Out: [[1 2 3 4 5]
      [1 2 3 4 5]
      [1 2 3 4 5]
      [1 2 3 4 5]
      [1 2 3 4 5]]

In: np.sum(a2, axis=0)

Out: array([ 5, 10, 15, 20, 25])

In: np.sum(a2, axis=1)

Out: array([15, 15, 15, 15, 15])
```

When operating on your data, remember that operations and NumPy functions on arrays are extremely fast when compared to simple Python lists. Let's try out a couple of experiments. First, let's try to compare a list comprehension to an array when dealing with a sum of a constant:

```
In: %timeit -n 1 -r 3 [i+1.0 for i in range(10**6)]
    %timeit -n 1 -r 3 np.arange(10**6)+1.0

Out: 1 loops, best of 3: 158 ms per loop
     1 loops, best of 3: 6.64 ms per loop
```

On Jupyter, `%time` allows you to easily benchmark operations. Then, the `-n 1` parameter just requires the benchmark to execute the code snippet for only one loop; `-r 3` requires you to retry the execution of the loops (in this case, just one loop) three times and report the best performance recorded from such repetitions.

Results on your computer may vary depending on your configuration and operating system. Anyway, the difference between the standard Python operations and the NumPy ones will remain quite large. Though unnoticeable when working on small datasets, this difference can really impact your analysis when dealing with larger data or when looping over and over the same analysis pipeline for parameter or variable selection.

This also happens when applying sophisticated operations, such as finding a square root:

```
In: import math
    %timeit -n 1 -r 3 [math.sqrt(i) for i in range(10**6)]

Out: 1 loops, best of 3: 222 ms per loop

In: %timeit -n 1 -r 3 np.sqrt(np.arange(10**6))

Out: 1 loops, best of 3: 6.9 ms per loop
```

Sometimes, you may need to apply custom functions to your array instead.
The `apply_along_axis` function lets you use a custom function and apply it on an axis of an array:

```
In: def cube_power_square_root(x):
        return np.sqrt(np.power(x, 3))

    np.apply_along_axis(cube_power_square_root,
                        axis=0, arr=a2)

Out: array([[ 1.,  2.82842712,  5.19615242,  8., 11.18033989],
            [ 1.,  2.82842712,  5.19615242,  8., 11.18033989],
            [ 1.,  2.82842712,  5.19615242,  8., 11.18033989],
            [ 1.,  2.82842712,  5.19615242,  8., 11.18033989],
            [ 1.,  2.82842712,  5.19615242,  8., 11.18033989]])
```

Matrix operations

Apart from element-wise calculations using the `np.dot()` function, you can also apply multiplications to your two-dimensional arrays based on matrix calculations, such as vector-matrix and matrix-matrix multiplications:

```
In: import numpy as np
    M = np.arange(5*5, dtype=float).reshape(5,5)
    M

Out: array([[  0.,   1.,   2.,   3.,   4.],
            [  5.,   6.,   7.,   8.,   9.],
            [ 10.,   11.,   12.,   13.,   14.],
            [ 15.,   16.,   17.,   18.,   19.],
            [ 20.,   21.,   22.,   23.,   24.]])
```

As an example, we will create a 5 x 5 two-dimensional array of ordinal numbers from 0 to 24:

1. We will define a vector of coefficients and an array column stacking the vector and its reverse:

   ```
   In: coefs = np.array([1., 0.5, 0.5, 0.5, 0.5])
       coefs_matrix = np.column_stack((coefs,coefs[::-1]))
       print (coefs_matrix)

   Out: [[ 1.   0.5]
         [ 0.5  0.5]
         [ 0.5  0.5]
         [ 0.5  0.5]
         [ 0.5  1. ]]
   ```

2. We can now multiply the array with the vector by using the `np.dot` function:

   ```
   In: np.dot(M,coefs)

   Out: array([  5.,  20.,  35.,  50.,  65.])
   ```

3. Or the vector by the array:

   ```
   In: np.dot(coefs,M)

   Out: array([ 25.,  28.,  31.,  34.,  37.])
   ```

4. Or the array by the stacked coefficient vectors (which is a 5 x 2 matrix):

   ```
   In: np.dot(M,coefs_matrix)

   Out: array([[  5.,   7.],
               [ 20.,  22.],
               [ 35.,  37.],
               [ 50.,  52.],
               [ 65.,  67.]])
   ```

NumPy also offers an object class, matrix, which is actually a subclass of `ndarray`, inheriting all its attributes and methods. NumPy matrices are exclusively two-dimensional (as arrays are actually multi-dimensional) by default. When multiplied, they apply matrix products, not element-wise ones (the same happens when raising powers), and they have some special matrix methods (`.H` for the conjugate transpose and `.I` for the inverse).

Apart from the convenience of operating in a fashion that is similar to that of MATLAB, they do not offer any other advantage. You may risk confusion in your scripts since you'll have to handle different product notations for matrix objects and arrays.

Since Python 3.5, a new operator, the @ (at) operator, dedicated to matrix multiplication, has been introduced in Python (the change is for all the packages in Python, not just NumPy). The introduction of this new operator brings a couple of advantages.
First, there won't be any more cases where the * operator will be meant to be used for matrix multiplication. The * operator will be used exclusively for element-wise operations (those operations where, having two matrices (or vectors) of the same dimension, you apply the operation between the elements having the same position in the two matrices).
Then, code that is representing formulas will gain in readability, thus becoming much easier to read and interpret. You won't have to evaluate operators (+ - / *) and methods (.dot) together anymore, only operators (+ - / * @).
You can learn more about this introduction (which is just formal – everything you could apply before using the `.dot` method works with the @ operator) and look at some examples of applications by reading the **Python Enhancement Proposal** (**PEP**) **465** at the Python foundation website: `https://www.python.org/dev/peps/pep-0465/`.

Slicing and indexing with NumPy arrays

Indexing allows us to take a view of a `ndarray` by pointing out either what slice of columns and rows to visualize, or an index:

1. Let's define a working array:

```
In: import numpy as np
    M = np.arange(10*10, dtype=int).reshape(10,10)
```

2. Our array is a 10 x 10 two-dimensional array. We can initially start by slicing it into a single dimension. The notation for a single dimension is the same as that in Python lists:

```
[start_index_included:end_index_exclude:steps]
```

3. Let's say that we want to extract even rows from 2 to 8:

```
In: M[2:9:2,:]

Out: array([[20, 21, 22, 23, 24, 25, 26, 27, 28, 29],
            [40, 41, 42, 43, 44, 45, 46, 47, 48, 49],
            [60, 61, 62, 63, 64, 65, 66, 67, 68, 69],
            [80, 81, 82, 83, 84, 85, 86, 87, 88, 89]])
```

4. After slicing the rows, we can slice the columns even further by taking only the columns from index `5`:

```
In: M[2:9:2,5:]

Out: array([[25, 26, 27, 28, 29],
            [45, 46, 47, 48, 49],
            [65, 66, 67, 68, 69],
            [85, 86, 87, 88, 89]])
```

5. As in lists, it is possible to use negative index values in order to start counting from the end. Moreover, a negative number for parameters, such as steps, reverses the order of the output array, like in the following example, where the counting starts from column index `5` but in the reverse order and goes toward index `0`:

```
In: M[2:9:2,5::-1]

Out: array([[25, 24, 23, 22, 21, 20],
            [45, 44, 43, 42, 41, 40],
            [65, 64, 63, 62, 61, 60],
            [85, 84, 83, 82, 81, 80]])
```

6. We can also create Boolean indexes that point out which rows and columns to select. Therefore, we can replicate the previous example by using a `row_index` and a `col_index` variable:

```
In: row_index = (M[:,0]>=20) & (M[:,0]<=80)
    col_index = M[0,:]>=5
    M[row_index,:][:,col_index]
Out: array([[25, 26, 27, 28, 29],
            [35, 36, 37, 38, 39],
            [45, 46, 47, 48, 49],
            [55, 56, 57, 58, 59],
            [65, 66, 67, 68, 69],
            [75, 76, 77, 78, 79],
            [85, 86, 87, 88, 89]])
```

We cannot contextually use Boolean indexes on both columns and rows in the same square brackets, though we can apply the usual indexing to the other dimension using integer indexes. Consequently, we have to first operate a Boolean selection on rows and then reopen the square brackets and operate a second selection on the first, this time focusing on the columns.

7. If we need a global selection of elements in the array, we can also use a mask of Boolean values, as follows:

```
In: mask = (M>=20) & (M<=90) & ((M / 10.) % 1 >= 0.5)
    M[mask]

Out: array([25, 26, 27, 28, 29, 35, 36, 37, 38, 39, 45, 46, 47, 48,
49,
            55, 56, 57, 58, 59, 65, 66, 67, 68, 69, 75, 76, 77, 78,
79,
            85, 86, 87, 88, 89])
```

This approach is particularly useful if you need to operate on the partition of the array selected by the mask (for example, `M[mask]=0`).

Another way to point out which elements need to be selected from your array is by providing a row or column index consisting of integers. Such indexes may be defined either by a `np.where()` function that transforms a Boolean condition on an array into indexes or by simply providing a sequence of integer indexes, where integers may be in a particular order or might even be repeated. Such an approach is called **fancy indexing**:

```
In: row_index = [1,1,2,7]
    col_index = [0,2,4,8]
```

Having defined the indexes of your rows and columns, you have to apply them contextually to select elements whose coordinates are given by the tuple of values of both the indexes:

```
In: M[row_index,col_index]

Out: array([10, 12, 24, 78])
```

In this way, the selection will report the following points: (`1,0`),(`1,2`),(`2,4`), and (`7,8`). Otherwise, as seen previously, you just have to select the rows first and then the columns, which are separated by square brackets:

```
In: M[row_index,:][:,col_index]

Out: array([[10, 12, 14, 18],
            [10, 12, 14, 18],
            [20, 22, 24, 28],
            [70, 72, 74, 78]])
```

Finally, please remember that slicing and indexing are just views of the data. If you need to create new data from such views, you have to use the `.copy` method on the slice and assign it to another variable. Otherwise, any modification to the original array will be reflected on your slice and vice versa. The copy method is shown here:

```
In: N = M[2:9:2,5:].copy()
```

Stacking NumPy arrays

When operating with two-dimensional data arrays, there are some common operations, such as the adding of data and variables, that NumPy functions can render easily and quickly.

The most common such operation is the addition of more cases to your array:

1. Let's start off by creating an array:

   ```
   In: import numpy as np
       dataset = np.arange(10*5).reshape(10,5)
   ```

2. Now, let's add a single row and a bunch of rows that are to be concatenated after each other:

   ```
   In: single_line = np.arange(1*5).reshape(1,5)
       a_few_lines = np.arange(3*5).reshape(3,5)
   ```

3. We can first try to add a single line:

   ```
   In: np.vstack((dataset,single_line))
   ```

4. All you have to do is provide a tuple containing the vertical array preceding it and the one following it. In our example, the same command can work if you have more lines to be added:

   ```
   In: np.vstack((dataset,a_few_lines))
   ```

5. Or, if you want to add the same single line more than once, the tuple can represent the sequential structure of your newly concatenated array:

   ```
   In: np.vstack((dataset,single_line,single_line))
   ```

Another common situation is when you have to add a new variable to an existing array. In this case, you have to use `hstack` (**h** stands for **horizontal**) instead of the just-presented `vstack` command (where **v** is **vertical**).

1. Let's pretend that you have to add a `bias` of unit values to your original array:

   ```
   In: bias = np.ones(10).reshape(10,1)
       np.hstack((dataset,bias))
   ```

2. Without reshaping `bias` (this, therefore, can be any data sequence of the same length as the rows of the array), you can add it as a sequence by using the `column_stack()` function, which obtains the same result but with fewer concerns regarding data reshaping:

   ```
   In: bias = np.ones(10)
       np.column_stack((dataset,bias))
   ```

Adding rows and columns to two-dimensional arrays is basically all that you need to do to effectively wrangle your data in data science projects. Now, let's see a couple of more specific functions for slightly different data problems.

First, although two-dimensional arrays are the norm, you can also operate on a three-dimensional data structure. So, `dstack()`, which is analogous to `hstack()` and `vstack()` but operates on the third axis, will come in quite handy:

```
In: np.dstack((dataset*1,dataset*2,dataset*3))
```

In this example, the third dimension offers the original 2D array with a multiplicand, presenting a progressive rate of change (a time or change dimension).

A further problematic variation could be the insertion of a row or, more frequently, a column to a specific position into your array. As you may recall, arrays are contiguous chunks of memory. Insertion actually requires the recreation of a new array, splitting the original array. The NumPy `insert` command helps you to do so in a fast and hassle-free way:

```
In: np.insert(dataset, 3, bias, axis=1)
```

You just have to define the array where you wish to insert (`dataset`), the position (index `3`), the sequence you want to insert (in this case, the array `bias`), and the axis along which you would like to operate the insertion (axis `1` is the vertical axis).

Naturally, you can insert entire arrays (not just vectors), such as bias, by ensuring that the array to be inserted is aligned with the dimension along which we are operating the insertion. In this example, in order to insert the same array into itself, we have to transpose it as an inserted element:

```
In: np.insert(dataset, 3, dataset.T, axis=1)
```

You can also make insertions on different axes (in the following case, axis `0`, which is the horizontal one, but you can also operate on any dimension of an array that you may have):

```
In: np.insert(dataset, 3, np.ones(5), axis=0)
```

What is being done is that the original array is split at the specified position along the chosen axis. Then, the split data is concatenated with the new data to be inserted.

Working with sparse arrays

Sparse matrices are matrices whose values are mostly zero values. They occur naturally when working with certain kinds of data problems such as **natural language processing** (**NLP**), data counting events (such as customers' purchases), categorical data transformed into binary variables (a technique called one-hot-encoding, which we will be discussing in the next chapter), or even images if they have lots of black pixels.

sparse matrices with the right tools because they represent a memory and computational challenge for most machine learning algorithms.
First of all, sparse matrices are huge (if treated as a normal matrix, they cannot fit into memory) and they mostly contain zero values but for a few cells. Data structures that are optimized for sparse matrices allow us to efficiently store matrices where most of the elements valued as zero do not occupy any memory space. Instead, in any NumPy array (in contrast, we will be calling it a dense array), any zero value occupies some memory space because arrays keep track of all the values.

In addition, sparse matrices, being large, require a lot of computations in order to be processed, yet, most of their values are not used for any prediction. Algorithms that can take advantage of sparse matrix data structures can perform in much less computation time than standard algorithms operating on dense matrices.

In Python, SciPy's sparse module offers different sparse data structures that are able to address sparse problems. More specifically, it offers seven different kinds of sparse matrices:

- `csc_matrix`: Compressed Sparse Column format
- `csr_matrix`: Compressed Sparse Row format
- `bsr_matrix`: Block Sparse Row format
- `lil_matrix`: List of Lists format
- `dok_matrix`: Dictionary of Keys format
- `coo_matrix`: COOrdinate format (also known as IJV, triplet format)
- `dia_matrix`: DIAgonal format

Each kind of matrix features a different way to store sparse information, a particular way that affects how the matrix performs under different circumstances. We are going to illustrate each sparse matrix kind and look at what operations are fast and efficient, and what operations are not performing at all. For instance, the documentation points out `dok_matrix`, `lil_matrix`, or `coo_matrix` as the best ones to construct a sparse matrix from scratch. We will start with this problem and from the `coo_matrix`.

You can find all of SciPy's documentation about sparse matrices at `https://docs.scipy.org/doc/scipy/reference/sparse.html`.

Let's start by creating a sparse matrix:

1. In order to create a sparse matrix, you can either generate it from a NumPy array (just by passing the array to one of SciPy's sparse matrix formats), or by providing three vectors containing row indexes, column indexes, and data values to a COO matrix, respectively:

```
In: row_idx = np.array([0, 1, 3, 3, 4])
    col_idx = np.array([1, 2, 2, 4, 2])
    values  = np.array([1, 1, 2, 1, 2], dtype=float)
    sparse_coo = sparse.coo_matrix((values, (row_idx, col_idx)))
    sparse_coo

Out: <5x5 sparse matrix of type '<class 'numpy.float64'>'
     with 5 stored elements in COOrdinate format>
```

2. Calling the COO matrix will tell you the shape and how many non-zero elements it contains. The number of zero elements against the size of the matrix will provide you with the sparsity measure, which is something that can be otherwise computed as the following:

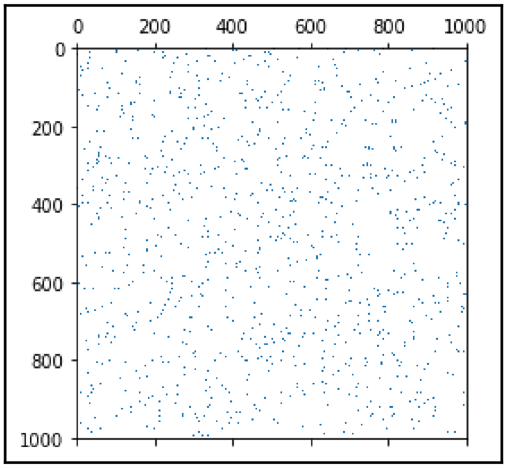
```
In: sparsity = 1.0 - (sparse_coo.count_nonzero() /
    np.prod(sparse_coo.shape))
    print(sparsity)

Out: 0.8
```

The sparsity is `0.8`; that is, 80% of the matrix is actually empty.

You can investigate sparsity graphically as well by using the `spy` command from matplotlib. In the following example, we will create a random sparse matrix and easily represent it in graphic form to provide an idea of how much data is effectively available in the matrix:

```
In: import matplotlib.pyplot as plt

    %matplotlib inline
    large_sparse = sparse.random(10 ** 3, 10 ** 3, density=0.001,
format='coo')
    plt.spy(large_sparse, marker=',')
    plt.show()
```

The resulting graph will provide you with an idea of the empty space in the matrix:



If needed, you can always convert a sparse matrix into a dense one by using the method `to_dense`: `sparse_coo.to_dense()`.

You can try to figure out how a COO matrix is constituted by printing it:

```
In: print(sparse_coo)

Out: (0, 1)    1.0
     (1, 2)    1.0
     (3, 2)    2.0
     (3, 4)    1.0
     (4, 2)    2.0
```

From the output representation, we can figure out that a sparse coordinate format matrix works by storing the printed values in three separated storage arrays: one for x coordinates, one for y coordinates, and one for the values. This means that COO matrices are really fast when inserting the information (each new element is a new row in each storage array) but slowly processing it because it cannot immediately figure out what the values in a row or in a column are in order to scan the arrays.

The same is true for **dictionaries of keys** (**dok**) and **lists in list** (**lil**) matrices. The first operates by using a dictionary of coordinates (so it is fast retrieving single elements), the second uses two lists, both arranged to represent rows, containing the non-zero coordinates in the row, and the other its values (it is easy to expand by adding more rows).
Another advantage of COO matrices is that they can be promptly converted into other kinds of matrices that are specialized in working efficiently at a row or column level: csr and csc matrics.

Compressed sparse row (**csr**) and **compressed sparse column** (**csc**) are the most used formats for operating on sparse matrices after having created them. They use an indexing system that favors computations over the rows for csr and over the columns for csc. However, that makes editing quite computationally costly (for this reason, it is not convenient to change them after having created them).

TIP The performances of csr and csc really depend on the algorithm used and how it optimizes its parameters. You have to actually try them out on your algorithm to find out which performs best.

Finally, diagonal format matrices are sparse data structures that are specialized for diagonal matrices and block sparse row format matrices. These resemble csr matrices in characteristics, apart from the way they store data, which is based on entire blocks of data.

Summary

In this chapter, we discussed how pandas and NumPy can provide you with all the tools to load and effectively mung your data.

We started with pandas and its data structures, DataFrames and series, and went through to the final NumPy two-dimensional arrays with a data structure suitable for subsequent experimentation and machine learning. In doing so, we touched upon subjects such as the manipulation of vectors and matrices, categorical data encoding, textual data processing, fixing missing data and errors, slicing and dicing, merging, and stacking.

pandas and NumPy surely offer many more functions than the essential building blocks we presented here, as well as the commands and procedures illustrated. You can now take any available raw data and apply all the cleaning and shaping transformations necessary for your data science project.

In the next chapter, we will take our data operations to the next step. We have already had a brief overview of all the essential data munging operations necessary for a machine learning process to work. In the next chapter, we will discuss all the operations that can potentially improve or even boost your results.

3
The Data Pipeline

Up until this point, we've explored how to load data into Python and process it to create a bidimensional NumPy array containing numerical values (your dataset). Now, we are ready to be immersed fully in data science, extract meaning from data, and develop potential data products. This chapter on data treatment and transformations and the next one on machine learning are the most challenging sections of this entire book.

In this chapter, you will learn how to do the following:

- Briefly explore data and create new features
- Reduce the dimensionality of data
- Spot and treat outliers
- Decide on the best score or loss metrics for your project
- Apply scientific methodology and effectively test the performance of your machine learning hypothesis
- Reduce the complexity of the data science problem by decreasing the number of features
- Optimize your learning parameters

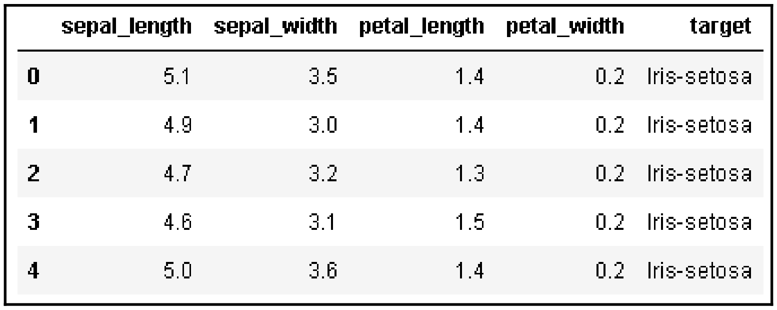
Introducing EDA

Exploratory data analysis (**EDA**), or data exploration, is the first step in the data science process. John Tukey coined this term in 1977 when he first wrote his, book *Exploratory Data Analysis*, emphasizing the importance of EDA. EDA is required to understand the dataset better, check its features and its shape, validate some first hypothesis that you have in mind, and get a preliminary idea about the next step that you want to pursue in subsequent subsequent data science tasks.

In this section, you will work on the Iris dataset, which was already used in the previous chapter. First, let's load the dataset:

```
In: import pandas as pd
    iris_filename = 'datasets-uci-iris.csv'
    iris = pd.read_csv(iris_filename, header=None,
             names= ['sepal_length', 'sepal_width',
             'petal_length', 'petal_width', 'target'])
    iris.head()
```

Calling the `head` method will display the first five rows:

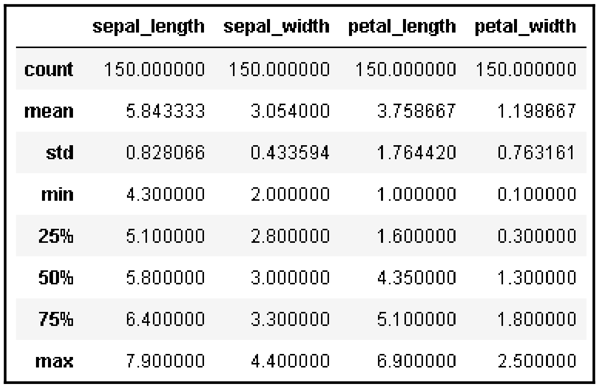


	sepal_length	sepal_width	petal_length	petal_width	target
0	5.1	3.5	1.4	0.2	Iris-setosa
1	4.9	3.0	1.4	0.2	Iris-setosa
2	4.7	3.2	1.3	0.2	Iris-setosa
3	4.6	3.1	1.5	0.2	Iris-setosa
4	5.0	3.6	1.4	0.2	Iris-setosa

Great! Using a few commands, you have already loaded the dataset. Now, the investigation phase starts. Some great insights are provided by the `.describe()` method, which can be used as follows:

```
In: iris.describe()
```

Promptly, a description of the dataset, comprising frequencies, means, and other descriptives appears:

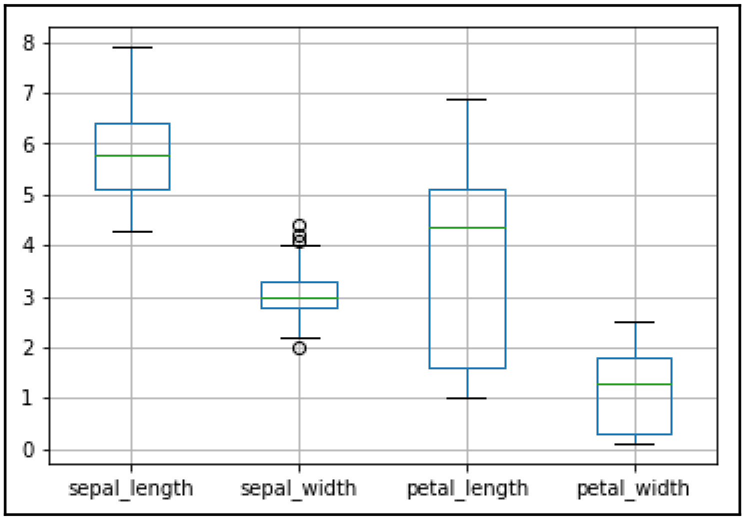


	sepal_length	sepal_width	petal_length	petal_width
count	150.000000	150.000000	150.000000	150.000000
mean	5.843333	3.054000	3.758667	1.198667
std	0.828066	0.433594	1.764420	0.763161
min	4.300000	2.000000	1.000000	0.100000
25%	5.100000	2.800000	1.600000	0.300000
50%	5.800000	3.000000	4.350000	1.300000
75%	6.400000	3.300000	5.100000	1.800000
max	7.900000	4.400000	6.900000	2.500000

For all numerical features, you have the number of observations, their respective average values, standard deviations, minimum and maximum values, and some routinely reported quantiles (at `25` percent, `50` percent, and `75` percent), the so-called quartiles. This provides you with a good idea about the distribution of each feature. If you want to visualize this information, just use the `boxplot()` method, as follows:

```
In: boxes = iris.boxplot(return_type='axes')
```

A boxplot for each variable will appear:

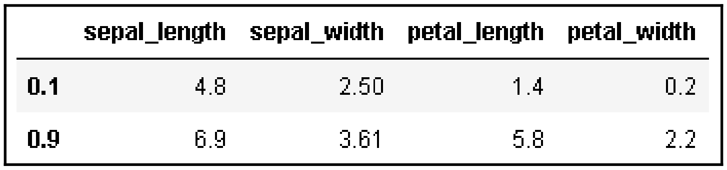


Sometimes, the graphs/diagrams presented in this chapter can be slightly different from the ones obtained on your local computer because graphical layout initialization is made with random parameters.

If you need to learn about other quantile values, you can use the `.quantile()` method. For example, if you need the values at 10 % and 90 % of the distribution of values, you can try out the following code:

```
In: iris.quantile([0.1, 0.9])
```

Here are the values for the required percentiles:



	sepal_length	sepal_width	petal_length	petal_width
0.1	4.8	2.50	1.4	0.2
0.9	6.9	3.61	5.8	2.2

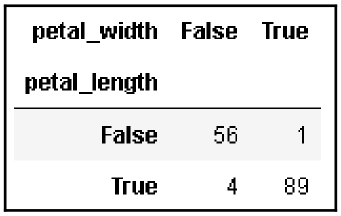
Finally, to calculate the median, you can use the `.median()` method. Similarly, to obtain the mean and standard deviation, the `.mean()` and `.std()` methods are used, respectively. In the case of categorical features, to get information about the levels present in a feature (that is, the different values the feature assumes), you can use the `.unique()` method, as follows:

```
In: iris.target.unique()

Out: array(['Iris-setosa', 'Iris-versicolor', 'Iris-virginica'],
     dtype=object)
```

To examine the relationship between features, you can create a co-occurrence matrix or a similarity matrix.
In the following example, we will count the number of times the `petal_length` feature appears more than the average against the same count for the `petal_width` feature. To do this, you need to use the `crosstab` method, as follows:

```
In: pd.crosstab(iris['petal_length'] > 3.758667,
                iris['petal_width'] > 1.198667)
```

The command produces a two-way table:

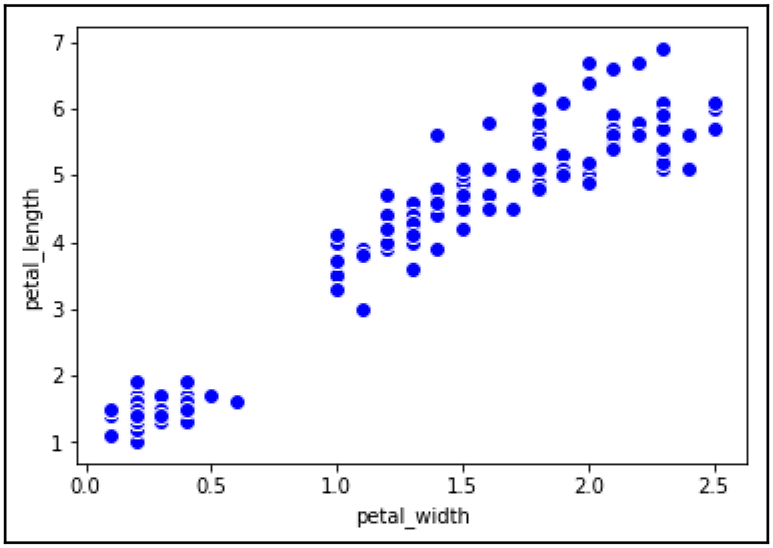


petal_width	False	True
petal_length		
False	56	1
True	4	89

As a result, you will notice that the features will almost always occur conjointly. Consequently, you can suppose that there's a strong relationship between the two events. Graphically, you can check such a hypothesis by using the following code:

```
In: scatterplot = iris.plot(kind='scatter',
                            x='petal_width', y='petal_length',
                            s=64, c='blue', edgecolors='white')
```

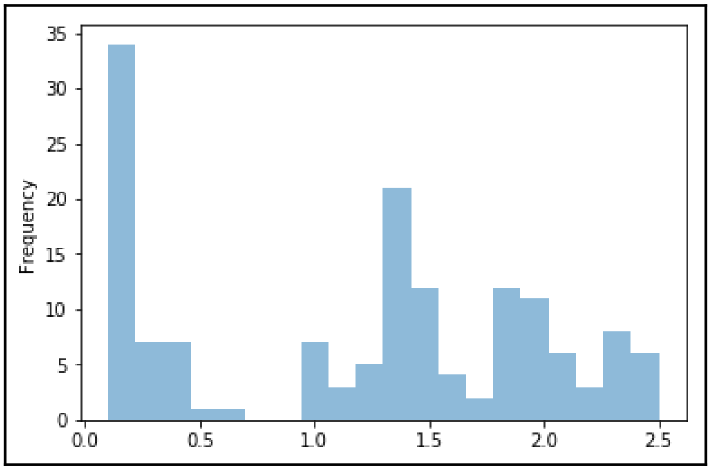
You obtain a scatterplot of the variables you specified as x and y:



The trend is quite marked; we deduce that *x* and *y* are strongly related. The last operation that you usually perform during an EDA is checking the distribution of the feature. To manage this with pandas, you can approximate the distribution using a histogram, which can be done thanks to the following snippet:

```
In: distr = iris.petal_width.plot(kind='hist', alpha=0.5, bins=20)
```

As a result, a histogram is displayed:



We chose 20 bins after a careful search. In other situations, 20 bins might be an extremely low or high value. As a rule of thumb, when drawing a distribution histogram, the starting value is the square root of the number of observations. After the initial visualization, you will then need to modify the number of bins until you recognize a well-known shape in the distribution.

We suggest that you explore all of the features in order to check their relationships and estimate their distribution. In fact, given its distribution, you may decide to treat each feature differently in order subsequently to achieve maximum classification or regression performance.

Building new features

Sometimes, you'll find yourself in a situation where features and `target` variables are not really related. In this case, you can modify the input dataset. You can apply linear or nonlinear transformations that can improve the accuracy of the system, and so on. It's a very important step for the overall process because it completely depends on the skills of the data scientist, who is the one responsible for artificially changing the dataset and shaping the input data for a better fit for the learning model. Although this step intuitively just adds complexity, this approach often boosts the performance of the learner; that's why it is used by bleeding-edge techniques, such as deep learning.

For example, if you're trying to predict the value of a house and you know the height, width, and the length of each room, you can artificially build a feature that represents the volume of the house. This is strictly not an observed feature, but it's a feature that's built on top of the existing ones. Let's start with some code:

```
In: import numpy as np
    from sklearn import datasets
    from sklearn.model_selection import train_test_split
    from sklearn.metrics import mean_squared_error
    cali = datasets.california_housing.fetch_california_housing()
    X = cali['data']
    Y = cali['target']
    X_train, X_test, Y_train, Y_test = train_test_split(X, Y,
                                                        test_size=0.2)
```

We imported the dataset containing house prices in California. This is a regression problem because the `target` variable is the house price (that is, a real number). Applying a simple regressor straight away, called the **KNN regressor** (take it as an example of a simple learner; an in-depth description of regressors will be provided in `Chapter 4`, *Machine Learning*), ends with a **mean absolute error** (**MAE**) of around 1.15 on the test dataset. Don't worry if you cannot fully understand the code; MAE and other regressors are described later on in this book. Right now, assume that the MAE represents the error. Thus, the lower the value of MAE, the better the solution:

```
In: from sklearn.neighbors import KNeighborsRegressor
    regressor = KNeighborsRegressor()
    regressor.fit(X_train, Y_train)
    Y_est = regressor.predict(X_test)
    print ("MAE=", mean_squared_error(Y_test, Y_est))

Out: MAE= 1.07452795578
```

An `MAE` result of `1.07` could seem good, but let's strive to do better. We're going to normalize the input features using Z-scores and compare the regression tasks on this new feature set. Z-normalization is simply the mapping of each feature to a new one with a null mean and unitary variance. With Scikit-learn, this is achieved in the following way:

```
In: from sklearn.preprocessing import StandardScaler
    scaler = StandardScaler()
    X_train_scaled = scaler.fit_transform(X_train)
    X_test_scaled = scaler.transform(X_test)
    regressor = KNeighborsRegressor()
    regressor.fit(X_train_scaled, Y_train)
    Y_est = regressor.predict(X_test_scaled)
    print ("MAE=", mean_squared_error(Y_test, Y_est))

Out: MAE= 0.402334179429
```

With the help of this easy step, we drop the MAE by more than a half, which now has a value of about `0.40`.

Note that we didn't use the original features; we used their linear modification, which is more suitable for learning with a KNN regressor.

Instead of Z-normalization, we can use a scaling function on the features that are more robust to outliers, namely, `RobustScaler`**.** Such a scaler, instead of using mean and standard deviation, uses median and **interquartile range** (**IQR**), that is, the first and the third quartile) to scale each feature independently. It is more robust than outliers since the median and IQR are not influenced as much as mean and variance if a few points (eventually just one) are far away from the center, for example, due to a faulty reading, a transmission error, or a broken sensor:

```
In: from sklearn.preprocessing import RobustScaler
    scaler2 = RobustScaler()
    X_train_scaled = scaler2.fit_transform(X_train)
    X_test_scaled = scaler2.transform(X_test)
    regressor = KNeighborsRegressor()
    regressor.fit(X_train_scaled, Y_train)
    Y_est = regressor.predict(X_test_scaled)
    print ("MAE=", mean_squared_error(Y_test, Y_est))

Out: MAE=0.41749216189
```

Now, let's try to add a nonlinear modification to a specific feature. We can assume that the output is related roughly to the number of occupiers of a house. In fact, there is a big difference between the price of a house occupied by a single person and the price for three people staying in the same house. However, the difference between the price for 10 people living there and the price for 12 people living there is not that great (though there is still a difference of two). So, let's try to add another feature that's built as a nonlinear transformation of another one:

```
In: non_linear_feat = 5 # AveOccup
    X_train_new_feat = np.sqrt(X_train[:,non_linear_feat])
    X_train_new_feat.shape = (X_train_new_feat.shape[0], 1)
    X_train_extended = np.hstack([X_train, X_train_new_feat])
    X_test_new_feat = np.sqrt(X_test[:,non_linear_feat])
    X_test_new_feat.shape = (X_test_new_feat.shape[0], 1)
```

```
        X_test_extended = np.hstack([X_test, X_test_new_feat])
        scaler = StandardScaler()
        X_train_extended_scaled = scaler.fit_transform(X_train_extended)
        X_test_extended_scaled = scaler.transform(X_test_extended)
        regressor = KNeighborsRegressor()
        regressor.fit(X_train_extended_scaled, Y_train)
        Y_est = regressor.predict(X_test_extended_scaled)
        print ("MAE=", mean_squared_error(Y_test, Y_est))

    Out: MAE= 0.325402604306
```

By adding this new feature, we have additionally reduced the `MAE` and finally obtained a more satisfying regressor. Of course, we may try out other transformations in order to improve this, but this straightforward example should hint at how important it is for you to analyze the application of linear and nonlinear transformations found by EDA and obtain features that are conceptually more related to the output variable.

Dimensionality reduction

Oftentimes, you will have to deal with a dataset containing a large number of features, many of which may be unnecessary. This is a typical problem where some features are very informative for the prediction, some are somehow related, and some are completely unrelated (that is, they only contain noise or irrelevant information). Keeping only the interesting features is a way to not only make your dataset more manageable but also have predictive algorithms work better instead of being fooled in their predictions by the noise in the data.

Hence, dimensionality reduction is the operation of eliminating some features of the input dataset and creating a restricted set of features that contains all of the information you need to predict the `target` variable in a more effective and reliable way. As mentioned previously, reducing the number of features usually also reduces the output variability and complexity of the learning process (as well as the time required).

The main hypothesis behind many algorithms used in reduction is the one pertaining to **additive white Gaussian noise** (**AWGN**). We suppose that an independent Gaussian-shaped noise has been added to every feature of the dataset. Consequently, reducing the dimensionality also reduces the energy of the noise since you're decreasing its span set.

The covariance matrix

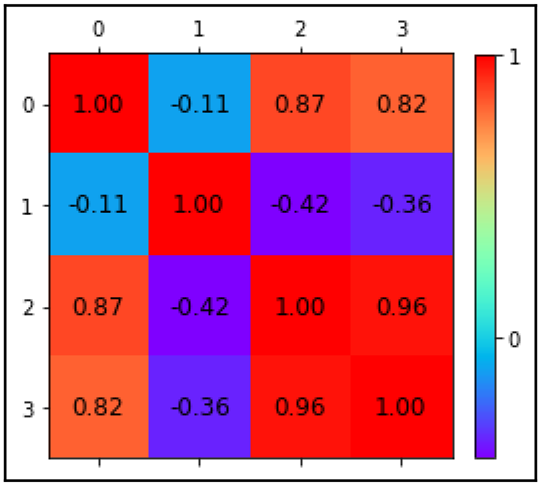
The covariance matrix provides you with an idea of the correlation between all of the different pairs of features. It's usually the first step of dimensionality reduction because it gives you an idea of the number of features that are strongly related (and therefore, the number of features that you can discard) and the ones that are independent. Using the Iris dataset, where each observation has four features, a correlation matrix can be computed easily, and you can understand its results with the help of a simple graphical representation, which can be obtained with the help of the following code:

```
In: from sklearn import datasets
    import numpy as np
    iris = datasets.load_iris()
    cov_data = np.corrcoef(iris.data.T)
    print (iris.feature_names)
    print (cov_data)

Out: ['sepal length (cm)', 'sepal width (cm)', 'petal length (cm)',
      'petal width (cm)']
     [[ 1.         -0.10936925  0.87175416  0.81795363]
      [-0.10936925  1.         -0.4205161  -0.35654409]
      [ 0.87175416 -0.4205161   1.          0.9627571 ]
      [ 0.81795363 -0.35654409  0.9627571   1.        ]]
```

Using a heat map, let's visualize the covariance matrix in a graphical form:

```
In: import matplotlib.pyplot as plt
    img = plt.matshow(cov_data, cmap=plt.cm.rainbow)
    plt.colorbar(img, ticks=[-1, 0, 1], fraction=0.045)
    for x in range(cov_data.shape[0]):
        for y in range(cov_data.shape[1]):
            plt.text(x, y, "%0.2f" % cov_data[x,y],
                     size=12, color='black', ha="center", va="center")
    plt.show()
```

Here is the resulting heat map:



From the previous diagram, you can see that the value of the primary diagonal is 1. This is because we're using the normalized version of the covariance matrix (normalizing each feature covariance to 1.0). We can also notice a high correlation between the first and the third, the first and the fourth, and the third and the fourth features. In addition, we can verify that only the second feature is almost independent of the others; all the other features are somehow correlated to each other.

We now have an idea about the potential number of features in the reduced set, imagining compressing the duplicated information as pointed out by the correlation matrix – we can reduce everything simply to two features.

Principal component analysis

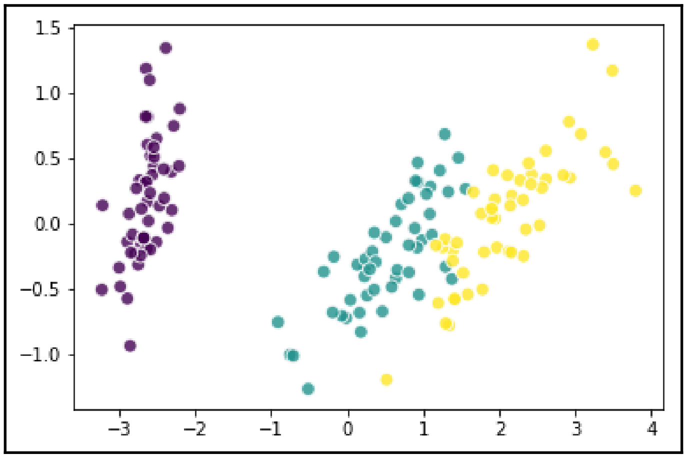
Principal component analysis (**PCA**) is a technique that helps define a smaller and more relevant set of features. The new features obtained from PCA are linear combinations (that is, rotation) of the current features, even if they are binary. After the rotation of the input space, the first vector of the output set contains most of the signal's energy (or, in other words, its variance). The second is orthogonal to the first, and it contains most of the remaining energy; the third is orthogonal to the first two vectors and contains most of the remaining energy, and so on. It's just like restructuring the information in the dataset by aggregating as much as possible of the information onto the initial vectors produced by the PCA.

In the (ideal) case of AWGN, the initial vectors contain all of the information of the input signal; the ones toward the end only contain noise. Moreover, since the output basis is orthogonal, you can decompose and synthesize an approximate version of the input dataset. The key parameter, which is used to decide how many basis vectors one can use, is the energy. Since the algorithm, under the hood, is for singular value decomposition, eigenvectors (the basis vectors) and eigenvalues (the standard deviation associated with that vector) are two terms that are often referred to when reading about PCA. Typically, the cardinality of the output set is the one that guarantees the presence of 95% (in some cases, 90 or 99% are needed) of the input energy (or variance). A rigorous explanation of PCA is beyond the scope of this book, and hence, we will just inform you about the guidelines on how to use this powerful tool in Python.

Here's an example on how to reduce the dataset to two dimensions. In the previous section, we deduced that 2 was a good choice for a dimensionality reduction; let's check if we were right:

```
In: from sklearn.decomposition import PCA
    pca_2c = PCA(n_components=2)
    X_pca_2c = pca_2c.fit_transform(iris.data)
    X_pca_2c.shape

Out: (150, 2)

In: plt.scatter(X_pca_2c[:,0], X_pca_2c[:,1], c=iris.target, alpha=0.8,
                s=60, marker='o', edgecolors='white')
    plt.show()
    pca_2c.explained_variance_ratio_.sum()

Out: 0.97763177502480336
```

When executing the code, you also get a scatterplot of the first two components:



Scatterplot of the first two components

We can immediately see that, after applying the PCA, the output set has only two features. This is because the `PCA()` object was called with the `n_components` parameter set to `2`. An alternative way to obtain the same result would be to run `PCA()` for `1`, `2`, and `3` components and then conclude from the explained variance ratio and the visual inspection that for `n_components = 2`, we got the best result. Then, we will have evidence that when using two basis vectors, the output dataset contains almost 98% of the energy of the input signal, and in the schema, the classes are pretty much neatly separable. Each color is located in a different area of the two dimensional Euclidean space.

Please note that this process is automatic and you don't need to provide labels while training PCA. In fact, PCA is an unsupervised algorithm, and it does not require data related to the independent variable to rotate the projection basis.

For curious readers, the transformation matrix (which turns the initial dataset into the PCA-restructured one) can be seen with the help of the following code:

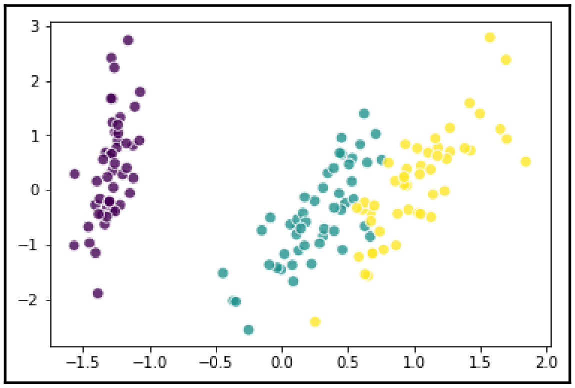
```
In: pca2c.components

Out: array([[ 0.36158968, -0.08226889,  0.85657211,  0.35884393],
           [-0.65653988, -0.72971237,  0.1757674 ,  0.07470647]])
```

The transformation matrix is comprised of four columns (which is the number of input features) and two rows (which is the number of the reduced ones).

Sometimes, you will find yourself in a situation where PCA is not effective enough, especially when dealing with high dimensionality data, since the features may be very correlated and, at the same time, the variance is unbalanced. A possible solution for such a situation is to try to whiten the signal (or make it more spherical). In this occurrence, eigenvectors are forced to unit component-wise variances. Whitening removes information, but sometimes it improves the accuracy of the machine learning algorithms that will be used after the PCA's reduction. Here's what the code looks like when resorting to whitening (in our example, it doesn't change anything except for the scale of the dataset with the reduced output):

```
In: pca_2cw = PCA(n_components=2, whiten=True)
    X_pca_1cw = pca_2cw.fit_transform(iris.data)
    plt.scatter(X_pca_1cw[:,0], X_pca_1cw[:,1], c=iris.target, alpha=0.8,
                s=60, marker='o', edgecolors='white')
    plt.show()
    pca_2cw.explained_variance_ratio_.sum()

Out: 0.9776317750248034
```

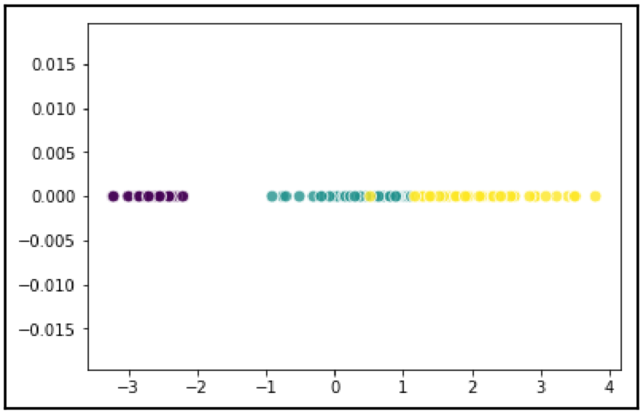
You also get the scatterplot of the first components of the PCA using whitening:



Now, let's see what happens if we project the input dataset on a 1-D space that's generated with PCA, as follows:

```
In: pca_1c = PCA(n_components=1)
    X_pca_1c = pca_1c.fit_transform(iris.data)
    plt.scatter(X_pca_1c[:,0], np.zeros(X_pca_1c.shape),
            c=iris.target, alpha=0.8, s=60, marker='o', edgecolors='white')
    plt.show()
    pca_1c.explained_variance_ratio_.sum()

Out: 0.9246162071742684
```

The projection is distributed along a single horizontal line:



In this case, the output energy is lower (92.4% of the original signal), and the output points are added to the mono-dimensional Euclidean space. This might not be a great feature reduction step since many points with different labels are mixed together.

Finally, here's a trick. To ensure that you generate an output set containing at least 95% of the input energy, you can just specify this value to the PCA object during its first call. A result equal to the one with two vectors can be obtained with the following code:

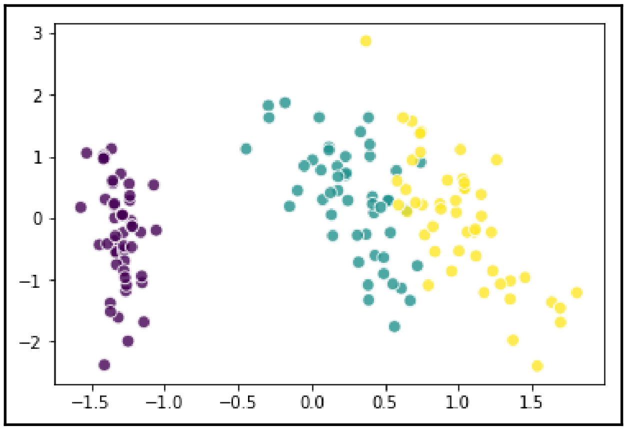
```
In: pca_95pc = PCA(n_components=0.95)
    X_pca_95pc = pca_95pc.fit_transform(iris.data)
    print (pca_95pc.explained_variance_ratio_.sum())
    print (X_pca_95pc.shape)

Out: 0.977631775025
      (150, 2)
```

PCA for big data – RandomizedPCA

The main issue with PCA is the complexity of the underlying **singular value decomposition** (**SVD**) algorithm that does the reduction work, making the whole process very difficult to scale. There is a faster algorithm in Scikit-learn based on randomized SVD. It is a lighter but approximate iterative decomposition method. Using randomized SVD, the full-rank reconstruction is not perfect, and the basis vectors are optimized locally during every iteration. On the other hand, it requires only a few steps to get a good approximation, demonstrating how randomized SVD is much faster than the classical SVD algorithms. Therefore, this reduction algorithm is a great choice if the training dataset is large. In the following code, we will apply it to the Iris dataset. The output is pretty close to the classical PCA since the size of the problem is very small. However, the results vary significantly when the algorithm is applied to large datasets:

```
In: from sklearn.decomposition import PCA
    rpca_2c = PCA(svd_solver='randomized', n_components=2)
    X_rpca_2c = rpca_2c.fit_transform(iris.data)
    plt.scatter(X_rpca_2c[:,0], X_rpca_2c[:,1],
          c=iris.target, alpha=0.8, s=60, marker='o', edgecolors='white')
    plt.show()
    rpca_2c.explained_variance_ratio_.sum()

Out: 0.9776317750248041
```

Here is the scatterplot of the first two components of the PCA using SVD solver:



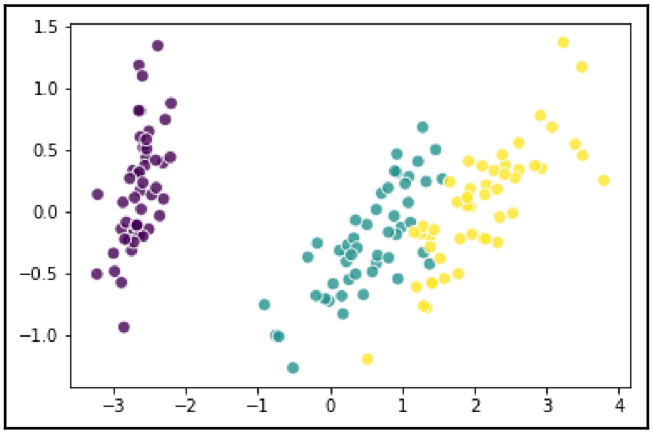
Latent factor analysis

Latent factor analysis (**LFA**) is another technique that helps you reduce the dimensionality of the dataset. The overall idea is similar to PCA. However, in this case, there's no orthogonal decomposition of the input signal, and therefore, no output basis. Some data scientists think that LFA is a generalization of PCA that removes the constraint of orthogonality. Generally, LFA is used when a latent factor or a construct is expected to be present in the system. Under such a hypothesis, all of the features are observations of variables that are derived or influenced by the latent factor that is transformed linearly and which has an **arbitrary waveform generator** (**AWG**) noise. It is generally assumed that the latent factor has a Gaussian distribution and a unitary covariance. Therefore, in this case, instead of collapsing the energy/variance of the signal, the covariance among the variables is explained in the output dataset. The Scikit-learn toolkit implements an iterative algorithm, making it suitable for large datasets.

Here's the code to lower the dimensionality of the Iris dataset by assuming two latent factors in the system:

```
In: from sklearn.decomposition import FactorAnalysis
    fact_2c = FactorAnalysis(n_components=2)
    X_factor = fact_2c.fit_transform(iris.data)
    plt.scatter(X_factor[:,0], X_factor[:,1],
                c=iris.target, alpha=0.8, s=60,
                marker='o', edgecolors='white')
    plt.show()
```

Here are the two latent factors as represented in a scatterplot (a different solution than the previous PCA):



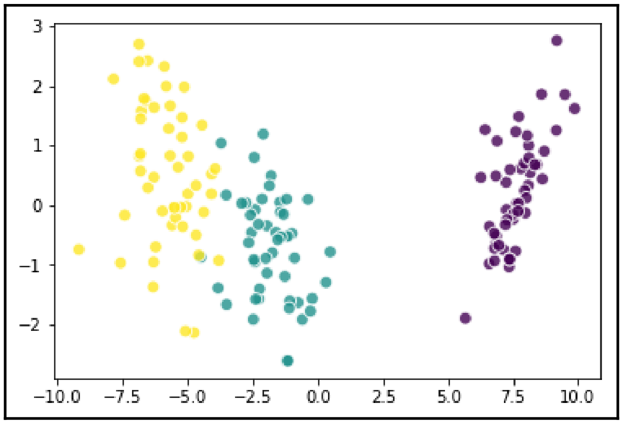
Linear discriminant analysis

Strictly speaking, **linear discriminant analysis** (**LDA**) is a classifier (a classical statistical method developed by Ronald Fisher, the father of modern statistics), but it is often used for dimensionality reduction. It doesn't scale so well to larger datasets (like many statistical methods), but it's something to be tried, which could bring better results than other classification methods such as logistic regression. Since it's a supervised approach, it requires the label set to optimize the reduction step. LDA outputs linear combinations of the input features, trying to model the difference between the classes that best discriminate them (since LDA uses label information). Compared to PCA, the output dataset that is obtained with the help of LDA contains a neat distinction between classes. However, it cannot be used in regression problems, since it is derived from a classification process.

Here's the application of LDA on the Iris dataset:

```
In: from sklearn.lda import LDA
    lda_2c = LDA(n_components=2)
    X_lda_2c = lda_2c.fit_transform(iris.data, iris.target)
    plt.scatter(X_lda_2c[:,0], X_lda_2c[:,1],
                c=iris.target, alpha=0.8, edgecolors='none')
    plt.show()
```

This scatterplot is derived from the first two components generated by the LDA:



Latent semantical analysis

Typically, **latent semantical analysis** (**LSA**) is applied to text after it has been processed by `TfidfVectorizer` or `CountVectorizer`. Compared to PCA, it applies SVD to the input dataset (which is usually a sparse matrix), producing semantic sets of words that are usually associated with the same concept. This is why LSA is used when the features are homogeneous (that is, all the words in the documents) and are present in large numbers.

An example of the same in Python with text and `TfidfVectorizer` is as follows. The output shows part of the content of a latent vector:

```
In: from sklearn.datasets import fetch_20newsgroups
    categories = ['sci.med', 'sci.space']
    twenty_sci_news = fetch_20newsgroups(categories=categories)
    from sklearn.feature_extraction.text import TfidfVectorizer
    tf_vect = TfidfVectorizer()
    word_freq = tf_vect.fit_transform(twenty_sci_news.data)
    from sklearn.decomposition import TruncatedSVD
    tsvd_2c = TruncatedSVD(n_components=50)
    tsvd_2c.fit(word_freq)
    arr_vec = np.array(tf_vect.get_feature_names())
    arr_vec[tsvd_2c.components_[20].argsort()[-10:][::-1]]

Out: array(['jupiter', 'sq', 'comet', 'of', 'gehrels', 'zisfein',
            'jim', 'gene', 'are', 'omen'], dtype='<U79')
```

Independent component analysis

As you can guess from the name, **independent component analysis** (**ICA**) is an approach where you try to derive independent components from the input signal. In fact, ICA is a technique that allows you to create maximally independent additive subcomponents from the initial multivariate input signal. The main hypothesis of this technique focuses on the statistical independence of the subcomponents and their non-Gaussian distribution. ICA has a lot of applications in neurological data and is widely used in the neuroscience domain.

A typical scenario that may require the use of ICA is blind source separation. For example, two or more microphones will record two sounds (for instance, a person speaks and a song plays at the same time). In this case, ICA is able to separate the two sounds into two output features.

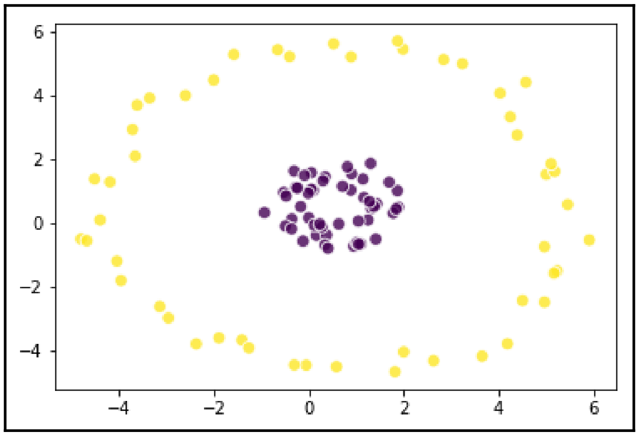
The Scikit-learn package offers a faster version of the algorithm (`sklearn.decomposition.FastICA`), whose use is similar to the other techniques that have been presented thus far.

Kernel PCA

Kernel PCA is a technique that uses a kernel to map the signal on a (typically) nonlinear space and makes it linearly separable (or close to attaining the same). It's an extension of PCA, where the mapping is an actual projection on a linear subspace. There are many well-known kernels (and of course, you can always build your own on the fly), but the most used ones are *linear*, *poly*, *RBF*, *sigmoid*, and *cosine*. They all serve different configurations of input datasets as they are only able to linearize some selected types of data. For example, let's imagine that we have a disk-shaped dataset, like the one we are going to create with the following code:

```
In: def circular_points (radius, N):
        return np.array([[np.cos(2*np.pi*t/N)*radius,
                          np.sin(2*np.pi*t/N)*radius] for t in range(N)])
    N_points = 50
    fake_circular_data = np.vstack([circular_points(1.0, N_points),
                                    circular_points(5.0, N_points)])
    fake_circular_data += np.random.rand(*fake_circular_data.shape)
    fake_circular_target = np.array([0]*N_points + [1]*N_points)
    plt.scatter(fake_circular_data[:,0], fake_circular_data[:,1],
                c=fake_circular_target, alpha=0.8,
                s=60, marker='o', edgecolors='white')
    plt.show()
```

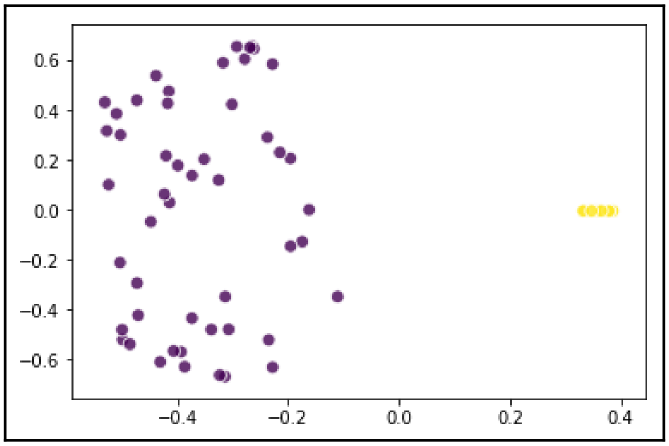
Here is the output of the example:



With this input dataset, all the linear transformations will fail to separate blue and red dots, since the dataset contains circumference-shaped classes. Now, let's try this with the Kernel PCA by using an RBF kernel and see what happens:

```
In: from sklearn.decomposition import KernelPCA
    kpca_2c = KernelPCA(n_components=2, kernel='rbf')
    X_kpca_2c = kpca_2c.fit_transform(fake_circular_data)
    plt.scatter(X_kpca_2c[:,0], X_kpca_2c[:,1], c=fake_circular_target,
                alpha=0.8, s=60, marker='o', edgecolors='white')
    plt.show()
```

The following figure represents the transformation of the example:



Graphs/diagrams in this chapter may be different to the ones obtained on your local computer because graphical layout initialization is made with random parameters.

We achieved our goal – the blue dots are on the left and the red dots are on the right. Thanks to the Kernel PCA's transformation, you can now deal with this dataset by using linear techniques.

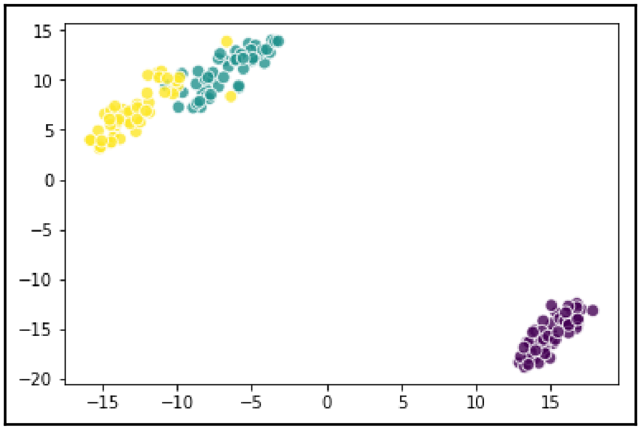
T-SNE

PCA is a widespread technique for dimensionality reduction, yet when we deal with large data, presenting many features, we first need to understand *what's going on* in the feature space. In fact, in the EDA phase, you'll usually make several scatterplots of the data to understand what the relationship between features is. At this point, T-distributed stochastic neighbor embedding, or T-SNE, comes to your aid since it has been designed with the goal of embedding high-dimensional data in a 2-D or 3-D space to make the most of a scatterplot. It is a nonlinear dimensionality reduction technique developed by Laurens van der Maaten and Geoffrey Hinton and the core of the algorithm is based on two rules: the first is that recurrent similar observations must have a greater contribution to the output (and that's achieved with a probability distribution function); second, the distribution in the high-dimensional space must be similar to the one in the small space (and that's achieved by minimizing the **Kullback-Leibler** (**KL**), divergence between the two probability distribution functions). The output is visually nice and allows you to guess nonlinear interactions between features.

Let's see how a simple example works by applying the T-SNE to the Iris dataset and plotting it to a two-dimensional space:

```
In: from sklearn.manifold import TSNE
    from sklearn.datasets import load_iris

    iris = load_iris()
    X, y = iris.data, iris.target
    X_tsne = TSNE(n_components=2).fit_transform(X)
    plt.scatter(X_tsne[:, 0], X_tsne[:, 1], c=y, alpha=0.8,
                s=60, marker='o', edgecolors='white')
    plt.show()
```

Here is the result from the `T_SNE`, completely separating one class from the others:



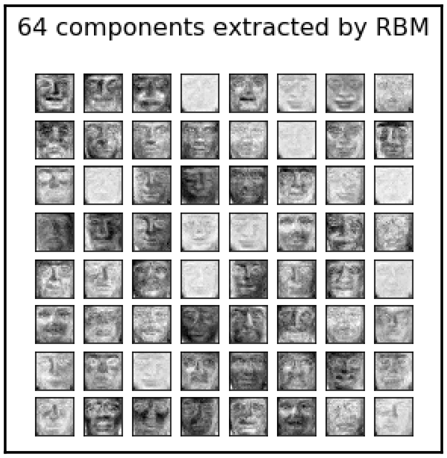
Restricted Boltzmann Machine

The **Restricted Boltzmann Machine** (**RBM**) is another technique that, composed of linear functions (which are usually called hidden units or neurons), creates a nonlinear transformation of the input data. The hidden units represent the status of the system, and the output dataset is actually the status of that layer.

The main hypothesis of this technique is that the input dataset is composed of features that represent probability (binary values or real values in the [0,1] range), since RBM is a probabilistic approach. In the following example, we will feed the RBM using binarized pixels of images as features (1=white, 0=black), and we will print the latent components of the system. These components represent different generic faces that appear in the original images:

```
In: from sklearn import preprocessing
    from sklearn.neural_network
    import BernoulliRBM
    n_components = 64 # Try with 64, 100, 144
    olivetti_faces = datasets.fetch_olivetti_faces()
    X = preprocessing.binarize(
           preprocessing.scale(olivetti_faces.data.astype(float)),
           0.5)
    rbm = BernoulliRBM(n_components=n_components, learning_rate=0.01,
                      n_iter=100)
    rbm.fit(X)
    plt.figure(figsize=(4.2, 4))
    for i, comp in enumerate(rbm.components_):
         plt.subplot(int(np.sqrt(n_components+1)),
                     int(np.sqrt(n_components+1)), i + 1)
         plt.imshow(comp.reshape((64, 64)), cmap=plt.cm.gray_r,
                    interpolation='nearest')
         plt.xticks(()); plt.yticks(())
    plt.suptitle(str(n_components) + ' components extracted by RBM',
                 fontsize=16)
    plt.subplots_adjust(0.08, 0.02, 0.92, 0.85, 0.08, 0.23)
    plt.show()
```

Here are the 64 components extracted by RBM:



Note that Scikit-learn contains just the base layer of RBM processing. If you are working on big datasets, you are better off using GPU-based toolkits (such as the ones built on the top of CUDA or OpenCL) since RBMs are highly parallelizable.

The detection and treatment of outliers

In data science, examples are at the core of learning from data processes. If unusual, inconsistent, or erroneous data is fed into the learning process, the resulting model may be unable to generalize the accommodation of any new data correctly. An unusually high value present in a variable, apart from skewing descriptive measures such as the mean and variance, may also distort how many machine learning algorithms learn from data, causing distorted predictions as a result.

When a data point deviates markedly from the others in a sample, it is called an *outlier*. Any other expected observation is labeled as an *inlier*.

A data point may be an outlier due to the following three general causes (and each one implies different remedies):

- The point represents a rare occurrence, but it is also a possible value, given the fact that the available data is just a sample of the original data distribution. In such an occurrence, the generative underlying process is the same for all the points, but the outlying point may be deemed as unsuitable for a generalization by machine learning due to its rarity. In such a case, the point is commonly removed or underweighted. Another solution is to increase the sample number, thus making the unusual value less relevant in the dataset.
- The point represents the usual occurrence of another distribution. When similar situations occur, it is plausible to imagine an error or a misspecification that has affected the generation of the sample. In any case, your learning algorithm is going to learn from data coming from an extraneous distribution that is not the focus of interest of your data science project (the focus is on the generalization). In such a case, the outlier simply has to be removed.
- The point is clearly some kind of a mistake. For some reason, there has been a data entry error or a problem with data integrity that modified the original value and replaced it with an inconsistent value. The best course of action is to remove the value and treat it as a value that is missing at random. In this case, it is common to replace the outlier with a mean or the most common class depending on whether it is a regression or a classification problem. If it is not convenient or possible to do so, then we suggest that you just remove the example from the dataset.

Univariate outlier detection

To explain the reason behind why a data point is an outlier, you are first required to locate the possible outliers in your data. There are quite a few approaches – some are univariate (you can observe each singular variable at once), while the others are multivariate (they consider more variables at the same time). The univariate methods are usually based on EDA and visualizations such as boxplots (which have been introduced at the beginning of the present chapter; we will talk more about boxplots more specifically in `Chapter 5`, *Visualization, Insights, and Results*).

There are a couple of rules of thumb to keep in mind when chasing outliers by examining single variables. In fact, outliers may be spotted as extreme values:

- If you are observing Z-scores, observations with scores higher than 3 in an absolute value have to be considered as suspect outliers.
- If you are observing a description of data, you can consider the observations that are smaller than the 25th percentile value minus the IQR (that is, the difference between the 75th and 25th percentile values) as suspect outliers – *1.5 and those greater than the 75th percentile value plus the IQR * 1.5. Usually, you can achieve such distinction with the help of a boxplot graph.

In order to present how we can easily detect some outliers using Z-scores, let's load and explore the Boston House Prices dataset. As pointed out by the description of the dataset (which you can get with the help of `boston.DESCR`), the variable CHAS, which is indexed as 3, is a binary. Therefore, it makes little sense to use it while detecting anomalous values. In fact, such a variable can have just a value of either 0 or 1:

```
In: from sklearn.datasets import load_boston
    boston = load_boston()
    continuous_variables = [n for n in range(boston.data.shape[1]) if n!=3]
```

Now, let's quickly standardize all the continuous variables by using the `StandardScaler` function from sklearn. Our target is the fancy indexing of `boston.data` `boston.data[:,continuous_variables]` in order to create another array containing all the variables except the previous one, which was indexed 3.

`StandardScaler` automatically standardizes to zero mean and unit variance. This is a necessary routine operation that should be performed before feeding the data to the learning phase. Otherwise, many algorithms won't work properly (such as linear models powered by gradient descent and support vector machines).

Finally, let's locate the values that are above the absolute value of three standard deviations:

```
In: import numpy as np
    from sklearn import preprocessing
    scaler= preprocessing.StandardScaler()
    normalized_data = scaler.fit_transform(
                                  boston.data[:,continuous_variables])
    outliers_rows, outliers_columns = np.where(np.abs(normalized_data)>3)
```

The `outliers_rows` and `outliers_columns` variables contain the row and column indexes of the suspect outliers. We can print the index of the examples:

```
In: print(outliers_rows)

Out: [ 55  56  57 102 141 199 200 201 202 203 204 225 256 257 262 283 284
       ...
```

Alternatively, we can display the tuple of the row/column coordinates in the array:

```
In: print (list(zip(outliers_rows, outliers_columns)))

Out: [(55, 1), (56, 1), (57, 1), (102, 10), (141, 11), (199, 1), (200, 1),
      ...
```

The univariate approach can reveal quite a lot of potential outliers. It won't disclose an outlier that does not have an extreme value – instead, it is characterized by an unusual combination of values in two or more variables. In such cases, the values of the involved variables may not even be extreme ones, and therefore, the outlier may slip away unnoticed by a univariate inspection. These outliers are called multivariate outliers.

In order to discover multivariate outliers, you can use a dimensionality reduction algorithm, such as the previously illustrated PCA, and then check the absolute values of the components that are beyond three standard deviations, or visually inspect bivariate plots in order to locate isolated clusters of data points.

The Scikit-learn package offers a couple of classes that can automatically work for you straight out of the box and signal all suspect cases:

- The `covariance.EllipticEnvelope` class fits a robust distribution estimation of your data, pointing out the outliers that might be contaminating your dataset because they are the extreme points in the general distribution of the data.
- The `svm.OneClassSVM` class is a support vector machine algorithm that can approximate the shape of your data and find out if any new instances provided should be considered as a novelty (it acts as a novelty detector because, by default, it presumes that there is no outlier in the data). By just modifying its parameters, it can also work on a dataset where outliers are present, providing an even more robust and reliable outlier detection system than `EllipticEnvelope`.

Both classes, based on different statistical and machine learning approaches, need to be known and applied during your modeling phase.

EllipticEnvelope

`EllipticEnvelope` is a function that tries to figure out the key parameters of your data's general distribution by assuming that your entire data is an expression of an underlying multivariate Gaussian distribution. That's an assumption that cannot hold true for all datasets, yet when it does, it proves an effective method indeed for spotting outliers. Simplifying the complex estimations working behind the algorithm as much as possible, we can say that it checks the distance of each observation with respect to a grand mean that takes into account all the variables in your dataset. For this reason, it is able to spot both univariate and multivariate outliers.

The only parameter that you have to take into account when using this function from the covariance module is the contamination parameter, which can take a value of up to 0.5. It provides information to the algorithm about the proportion of the outliers present in your dataset. Situations may vary from dataset to dataset. However, as a starting figure, we suggest a value from 0.01 - 0.02 since it is the percentage of observations that should fall over the absolute value 3 in the Z score distance from the mean in a standardized normal distribution. For this reason, we deem the default value of 0.1 as too high.

Let's see this algorithm in action with the help of a synthetic distribution:

```
In: from sklearn.datasets import make_blobs
    blobs = 1
    blob = make_blobs(n_samples=100, n_features=2, centers=blobs,
                      cluster_std=1.5, shuffle=True, random_state=5)
    # Robust Covariance Estimate
    from sklearn.covariance import EllipticEnvelope
    robust_covariance_est = EllipticEnvelope(contamination=.1).fit(blob[0])
    detection = robust_covariance_est.predict(blob[0])
    outliers = np.where(detection==-1)[0]
    inliers = np.where(detection==1)[0]
    # Draw the distribution and the detected outliers
    from matplotlib import pyplot as plt
    # Just the distribution
    plt.scatter(blob[0][:,0],blob[0][:,1], c='blue', alpha=0.8, s=60,
                marker='o', edgecolors='white')
    plt.show()
    # The distribution and the outliers
    in_points = plt.scatter(blob[0][inliers,0],blob[0][inliers,1],
                            c='blue', alpha=0.8,
                            s=60, marker='o',
                            edgecolors='white')
    out_points = plt.scatter(blob[0][outliers,0],blob[0][outliers,1],
                             c='red', alpha=0.8,
                             s=60, marker='o',
                             edgecolors='white')
```

```
plt.legend((in_points,out_points),('inliers','outliers'),
           scatterpoints=1,
           loc='lower right')
plt.show()
```

Let's examine this code closely.

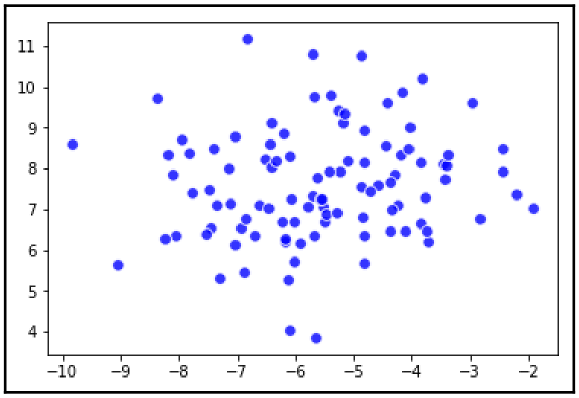
The `make_blobs` function creates a certain number of distributions in a bidimensional space for a total of 100 examples (the `n_samples` parameter). The number of distributions (parameter centers) is related to the user-defined variable blobs, which is initially set to 1.

After creating the artificial example data, running `EllipticEnvelope` with a contamination rate of 10% helps you find out the extreme values in the distribution. The model first deploys the fit by using the `.fit()` method on the `EllipticEnvelope` class. Then, a prediction is obtained by using the `.predict()` method on the data that was used for the fit.

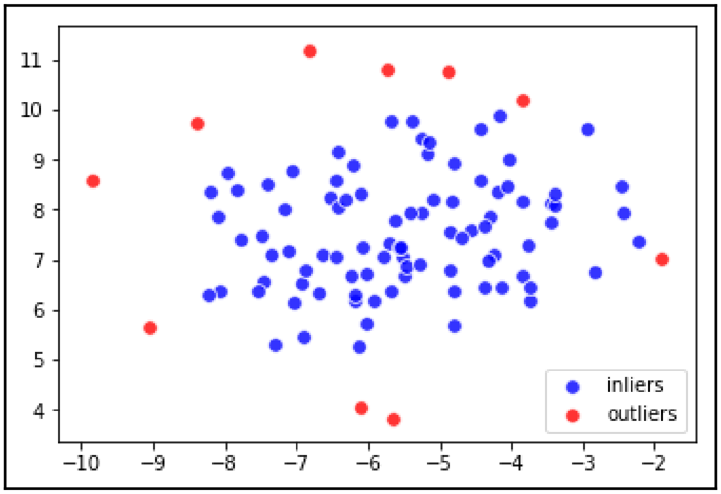
The results, corresponding to a vector of values 1 and -1 (with -1 being the mark for anomalous examples), can be displayed thanks to a couple of scatterplots by using the `plot` function from the `pyplot` module in `matplotlib`.

The distinction between inliers and outliers is recorded in the variable's outliers and inliers, which contain the indexes of the examples.

Now, let's run the code a few more times after changing the number of blobs and examine the results when the blobs have a value of `1` and `4`:



The distributions of data points after changing the number of blobs is as follows:



In the case of a unique, underlying multivariate distribution (when the variable blobs = 1), the `EllipticEnvelope` algorithm has successfully located 10% of the observations on the fringe of the distribution itself and has consequently signaled all the suspect outliers.

Instead, when multiple distributions are present in the data as if there were two or more natural clusters, the algorithm, trying to fit a unique general distribution, tends to locate the potential outliers on just the most remote cluster, thus ignoring other areas of data that might be potentially affected by outlying cases.

This is not an unusual situation with real data, and it represents an important limitation of the `EllipticEnvelope` algorithm.

Now, let's get back to our initial Boston House Prices dataset for the verification of some more data that is more realistic than our synthetic blobs. Here is the first part of the code that we can use for our experiment:

```
In: from sklearn.decomposition import PCA
    # Normalized data relative to continuos variables
    continuous_variables = [n for n in range(boston.data.shape[1]) if n!=3]
    scaler = preprocessing.StandardScaler()
    normalized_data = scaler.fit_transform(
                                   boston.data[:,continuous_variables])
    # Just for visualization purposes pick the first 2 PCA components
    pca = PCA(n_components=2)
    Zscore_components = pca.fit_transform(normalized_data)
    vtot = 'PCA Variance explained ' + str(round(np.sum(
                                         pca.explained_variance_ratio_),3))
    v1 = str(round(pca.explained_variance_ratio_[0],3))
    v2 = str(round(pca.explained_variance_ratio_[1],3))
```

In this script, we will first standardize the data and then, just for subsequent visualization purposes, generate a reduction of two components by using PCA.

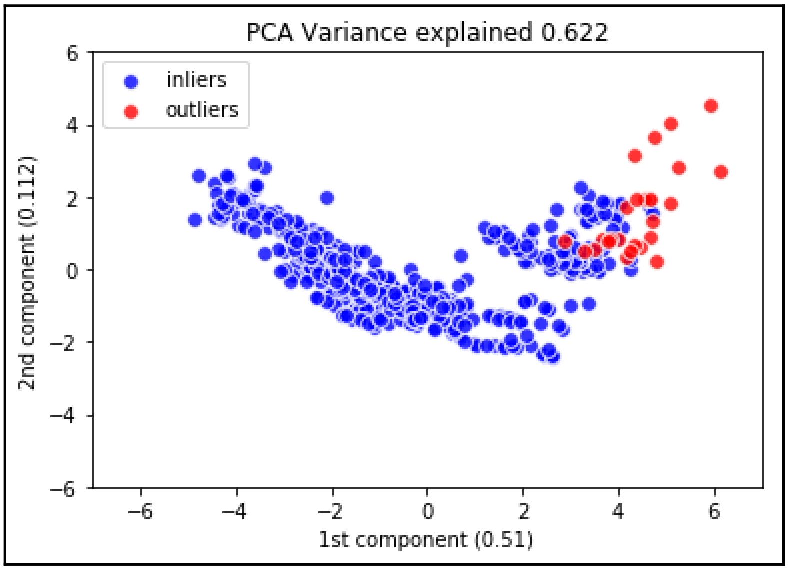
The two PCA components account for about 62% of the initial variance that is expressed by the 12 continuous variables that are available in the dataset (the summed value of the `.explained_variance_ratio_` variable, which is internal to the fitted `PCA` class).

Although only two PCA components are sufficient for visualization purposes, normally, you'd get more than two components for this dataset since the target is to have enough to account for at least 95% of the total variance (as stated previously in this chapter).

We will continue with the script:

```
In: robust_covariance_est = EllipticEnvelope(store_precision=False,
                                         assume_centered = False,
                                         contamination=.05)
    robust_covariance_est.fit(normalized_data)
    detection = robust_covariance_est.predict(normalized_data)
    outliers = np.where(detection==-1)
    regular = np.where(detection==1)

In: # Draw the distribution and the detected outliers
    from matplotlib import pyplot as plt
    in_points = plt.scatter(Zscore_components[regular,0],
                            Zscore_components[regular,1],
                            c='blue', alpha=0.8, s=60, marker='o',
                            edgecolors='white')
    out_points = plt.scatter(Zscore_components[outliers,0],
                             Zscore_components[outliers,1],
                             c='red', alpha=0.8, s=60, marker='o',
                             edgecolors='white')
    plt.legend((in_points,out_points),('inliers','outliers'),
               scatterpoints=1, loc='best')
    plt.xlabel('1st component ('+v1+')')
    plt.ylabel('2nd component ('+v2+')')
    plt.xlim([-7,7])
    plt.ylim([-6,6])
    plt.title(vtot)
    plt.show()
```

The visualization of the first two components accounts for 62.2% of the original variance:



As in the previous example, where we assumed a low contamination that is equivalent to 0.05, the code based on `EllipticEnvelope` predicts the outliers and stores them in an array in the same way as it stores the inliers. Finally, there's the visualization (as mentioned previously, we are going to discuss all of the visualization methods in `Chapter 5`, *Visualization, Insights, and Results*).

Now, let's observe the result offered by the scatterplot we generated to visualize the first two `PCA` components of the data and mark the outlying observations. Concerning the general distribution of the data points in our example, as provided by the two components that account for about 62% of the variance in the data, it appears as if there are two distinct clusters of house prices in Boston, which correspond to the high-end and low-end units present in the market. Generally speaking, the presence of clusters in the data is a no optimal situation for `EllipticEnvelope` estimations. In fact, according to what we've already noticed while experimenting using synthetic blobs, the algorithm has pointed out the outliers on just a cluster – the lesser one. Given such results, there is a strong reason to believe that we just received a biased, partial response, and some further investigation will be required before deeming such points as outliers. The Scikit-learn package actually integrates the robust covariance estimation method, which is fundamentally a statistical approach, with another methodology that is well-rooted in machine learning: the `OneClassSVM` class. Now, we will move on to experimenting with it.

Before leaving this example, please note that to fit both PCA and `EllipticEnvelope`, we used an array named `normalized_data`, which contains just the standardized continuous dataset variables. Please always take into account that using nonstandardized data and mixing binary or categorical data with continuous ones may induce errors and approximated estimations for the `EllipticEnvelope` algorithm.

OneClassSVM

As `EllipticEnvelope` fits a hypothetical Gaussian distribution, leveraging parametric and statistical assumptions, `OneClassSVM` is a machine learning algorithm that learns what the distribution of the features should be from the data itself, and therefore is applicable in a large variety of situations when you want to be able to catch all the outliers but also the unusual data examples.

It is great if you already have a clean dataset and have it fitted by machine learning algorithms. Afterwards, `OneClassSVM` can be summoned to check if any new example fits in the historical distribution, and if it doesn't, it will signal a novel example, which might be both an error or some new, previously unseen situation.

Just think of data science situations as a machine learning classification algorithm trained to recognize posts and news on a website and take online actions. `OneClassSVM` can easily spot a post that is different from the others present on the website (spam, maybe?), whereas other algorithms will just try to fit the new example into the existing topic's categorization.

However, `OneClassSVM` can also be used to spot existing outliers. If this specialized SVM class cannot fit some data, which is pointed out as being at the margins of the data distribution, then there is surely something fishy about those examples.

In order to have `OneClassSVM` work as an outlier detector, you need to work on its core parameters; it requires you to define the kernel, degree, gamma, and nu:

- **Kernel and degree**: These are interconnected. Usually, the values that we suggest based on our experience are the default ones; the type of kernel should be `rbf` and its degree should be 3. Such parameters will inform `OneClassSVM` to create a series of classification bubbles that span through three dimensions, allowing you to model even the most complex multidimensional distribution forms.

- **Gamma**: This is a parameter that's connected to the RBF kernel. We suggest that you keep it as low as possible. A good rule of thumb should be to assign it a minimum value that lies between the inverse of the number of cases and the variables. The role of gamma in SVM will be explained further in `Chapter 4`, *Machine Learning*. It will suffice for now to say that higher values of gamma tend to lead the algorithm to follow the data, but more so define the shape of the classification bubbles.
- **Nu**: This parameter determines whether we have to fit the exact distribution or if we try to obtain a certain degree of generalization by not adapting too much to the present data examples (a necessary choice if outliers are present). It can be easily determined with the help of the following formula:

$$nu\_estimate = 0.95 * outliers\_fraction + 0.05$$

- If the value of the outliers' fraction is very small, nu will be small and the SVM algorithm will try to fit the contour of the data points. On the other hand, if the fraction is high, so will the parameter be, forcing a smoother boundary of the inliers' distributions.

Let's immediately observe the performance of this algorithm on the problem that we faced before on the Boston House Prices dataset:

```
In: from sklearn.decomposition import PCA
    from sklearn import preprocessing
    from sklearn import svm
    # Normalized data relative to continuos variables
    continuous_variables = [n for n in range(boston.data.shape[1]) if n!=3]
    scaler = preprocessing.StandardScaler()
    normalized_data = scaler.fit_transform(
                                   boston.data[:,continuous_variables])
    # Just for visualization purposes pick the first 5 PCA components
    pca = PCA(n_components=5)
    Zscore_components = pca.fit_transform(normalized_data)
    vtot = 'PCA Variance explained ' + str(round(
                                np.sum(pca.explained_variance_ratio_),3))
    # OneClassSVM fitting and estimates
    outliers_fraction = 0.02 #
    nu_estimate = 0.95 * outliers_fraction + 0.05
    machine_learning = svm.OneClassSVM(kernel="rbf",
                                   gamma=1.0/len(normalized_data),
                                   degree=3, nu=nu_estimate)
    machine_learning.fit(normalized_data)
    detection = machine_learning.predict(normalized_data)
    outliers = np.where(detection==-1)
```

```
        regular = np.where(detection==1)
```

We will now proceed to visualize the results:

```
    In: # Draw the distribution and the detected outliers
        from matplotlib import pyplot as plt
        for r in range(1,5):
            in_points = plt.scatter(Zscore_components[regular,0],
                                    Zscore_components[regular,r],
                                    c='blue', alpha=0.8, s=60,
                                    marker='o', edgecolors='white')
            out_points = plt.scatter(Zscore_components[outliers,0],
                                     Zscore_components[outliers,r],
                                     c='red', alpha=0.8, s=60,
                                     marker='o', edgecolors='white')
            plt.legend((in_points,out_points),('inliers','outliers'),
                        scatterpoints=1, loc='best')
            plt.xlabel('Component 1 (' + str(round(
                       pca.explained_variance_ratio_[0],3))+')')
            plt.ylabel('Component '+str(r+1)+'('+str(round(
                       pca.explained_variance_ratio_[r],3))+')')
            plt.xlim([-7,7])
            plt.ylim([-6,6])
            plt.title(vtot)
            plt.show()
```

Compared to the code presented previously, this snippet is different because the resulting PCA decomposition is made up of five components. The larger number is due in order to explore more data dimensions. Another reason for increasing the number of resulting PCA components is because of our intention to use the transformed dataset with `OneClassSVM`.

The core parameters are calculated from the number of observations, as follows:

gamma=1.0/len(normalized_data)

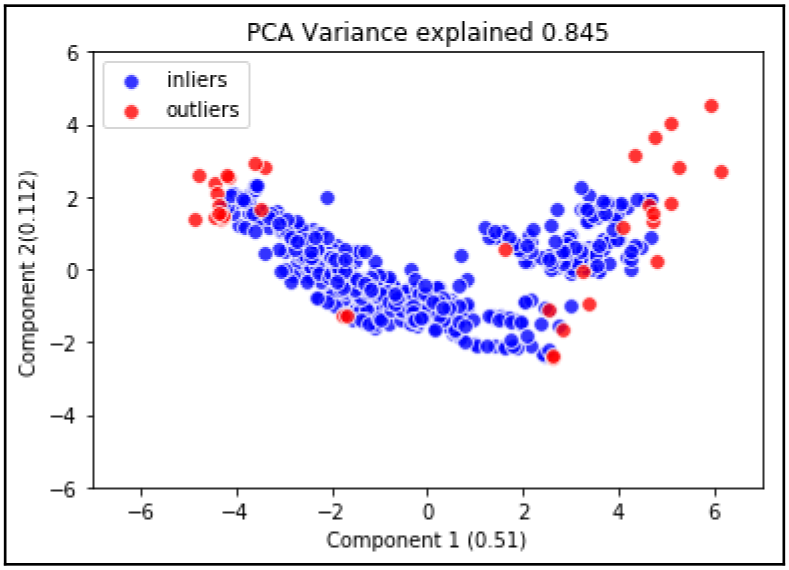
nu=nu_estimate

In particular, nu depends on:

*nu_estimate = 0.95 * outliers_fraction + 0.05*

So, by changing the `outliers_fraction` (from *0.02* to a larger value, such as *0.1*), you require the algorithm to give more attention to possible anomalies when supposing a larger incidence of anomalous cases in your data.

Let's also observe the graphical output of PCA components from 2 to 5 and compare it with the principal component (51% of the explained variance). The first graph of the series (comprised of a total of four scatterplots) is as follows:



From our graphical exploration, it looks as if `OneClassSVM` modeled the distribution of house price data with a good fit and it helped spot a few extreme values on the borders of the distribution.

At this point, you can decide on one of the novelties and outlier detection approaches that we are about to propose. You may even use both:

- To scrutinize the characteristics of the outliers in order to figure out a reason for their presence (a fact that could further make you reflect on the generative processes underlying your data)
- To try to build some machine learning models by using under-weighting for the outlying observations or by just excluding them

In the end, with a pure data science approach, what will help you decide what to do next with any outlying observation is testing the results of your decisions and consequent operations on data. How to test and experiment with a hypothesis about your data is a topic that we are going to discuss with you in the upcoming sections.

Validation metrics

In order to evaluate the performance of the data science system that you have built and check how close you are to the goal that you have in mind, you need to use a function that scores the outcome. Typically, different scoring functions are used to deal with binary classification, multilabel classification, regression, or a clustering problem. Now, let's see the most popular functions for each of these tasks and how they are used by machine learning algorithms.

Learning how to choose the right score/error measure for your data science project is really a matter of experience. We found it very helpful to consult (and participate in) the data science competitions held by Kaggle (`kaggle.com`), a company devoted to organizing data challenges between data scientists from all over the world. By observing the various challenges and what score or error measure they try to optimize, you can surely get useful insights for your own problems. Kaggle's CTO, Ben Hammer, has even created a Python library of commonly used metrics in competitions, which you can consult at `github.com/benhamner/Metrics` and install on your computer by using `pip install ml_metrics`.

Multilabel classification

When your task is to predict more than a single label (for instance: What's the weather like today? Which flower is this? What's your job?), we call the problem a multilabel classification. Multilabel classification is a very popular task, and many performance metrics exist to evaluate classifiers. Of course, you can use all of these measures in the case of a binary classification. Now, let's explain how it works by using a simple, real-world example:

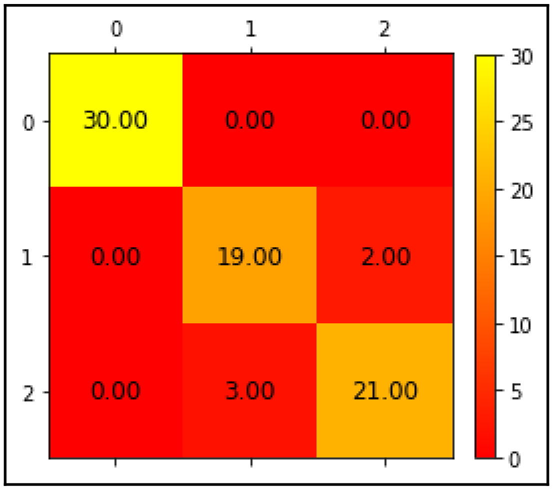
```
In: from sklearn import datasets
    iris = datasets.load_iris()
    # No crossvalidation for this dummy notebook
    from sklearn.model_selection import train_test_split
    X_train, X_test, Y_train, Y_test = train_test_split(iris.data,
                        iris.target, test_size=0.50, random_state=4)
    # Use a very bad multiclass classifier
    from sklearn.tree import DecisionTreeClassifier
    classifier = DecisionTreeClassifier(max_depth=2)
    classifier.fit(X_train, Y_train)
    Y_pred = classifier.predict(X_test)
    iris.target_names

Out: array(['setosa', 'versicolor', 'virginica'], dtype='<U10')
```

Now, let's take a look at the measures that are commonly used in multilabel classification:

- **Confusion matrix**: Before we describe the performance metrics for multilabel classification, let's take a look at the **confusion matrix**, a table that gives us an idea about what the misclassifications are for each class. Ideally, in a perfect classification, all the cells that are not on the diagonal should be 0s. In the following example, you will instead see that class 0 (*Setosa*) is never misclassified, class 1 (*Versicolor*) is misclassified twice as *Virginica*, and class 2 (*Virginica*) is misclassified twice as *Versicolor*:

```
In: from sklearn import metrics
    from sklearn.metrics import confusion_matrix
    cm = confusion_matrix(y_test, y_pred)
    print cm

Out: [[30  0  0]
      [ 0 19  3]
      [ 0  2 21]]

In: import matplotlib.pyplot as plt
    img = plt.matshow(cm, cmap=plt.cm.autumn)
    plt.colorbar(img, fraction=0.045)
    for x in range(cm.shape[0]):
        for y in range(cm.shape[1]):
            plt.text(x, y, "%0.2f" % cm[x,y],
              size=12, color='black', ha="center", va="center")
    plt.show()
```

The confusion matrix is represented graphically in this way:



- **Accuracy**: Accuracy is the portion of the predicted labels that are exactly equal to the real ones. In other words, it's the percentage of overall correctly classified labels:

  ```
  In: print ("Accuracy:", metrics.accuracy_score(Y_test, Y_pred))

  Out: Accuracy: 0.933333333333
  ```

- **Precision**: It is a measure that is taken from the information retrieval world. It counts the number of relevant results in the result set. Equivalently, in a classification task, it counts the number of correct labels in each set of classified labels. Then, results are averaged on all of the labels:

  ```
  In: print ("Precision:", metrics.precision_score(y_test, y_pred))

  Out: Precision: 0.933333333333
  ```

- **Recall**: This is another concept taken from information retrieval. It counts the number of relevant results in the result set, compared to all of the relevant labels in the dataset. In classification tasks, this is the amount of correctly classified labels in the set divided by the total count of labels for that set. Finally, the results are averaged, just like in the following code:

  ```
  In: print ("Recall:", metrics.recall_score(y_test, y_pred))

  Out: Recall: 0.933333333333
  ```

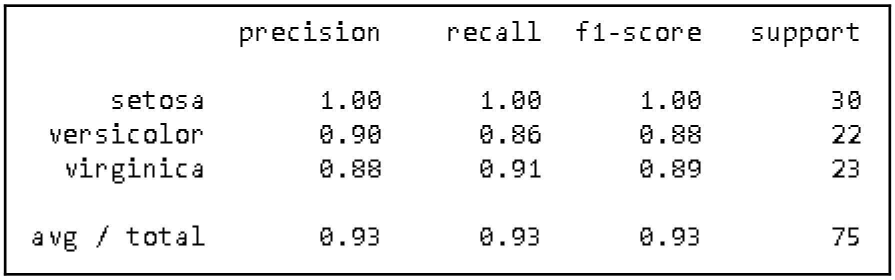
- **F1 Score**: This is the harmonic average of precision and recall, which is mostly used when dealing with unbalanced datasets in order to reveal if the classifier is performing well with all the classes:

  ```
  In: print ("F1 score:", metrics.f1_score(y_test, y_pred))

  Out: F1 score: 0.933267359393
  ```

These are the most used measures in multilabel classification. A convenient function, `classification_report`, shows a report on these measures, which is very handy. Support is simply the number of observations with that label. It's pretty useful to understand whether a dataset is balanced (that is, whether it has the same share of examples for every class) or not:

```
In: from sklearn.metrics import classification_report
    print classification_report(y_test, y_pred,
                                target_names=iris.target_names)
```

Here is the complete report with **precision**, **recall**, **f1-score** and **support** (the number of cases for the class):



```
             precision    recall  f1-score   support

     setosa       1.00      1.00      1.00        30
 versicolor       0.90      0.86      0.88        22
  virginica       0.88      0.91      0.89        23

avg / total       0.93      0.93      0.93        75
```

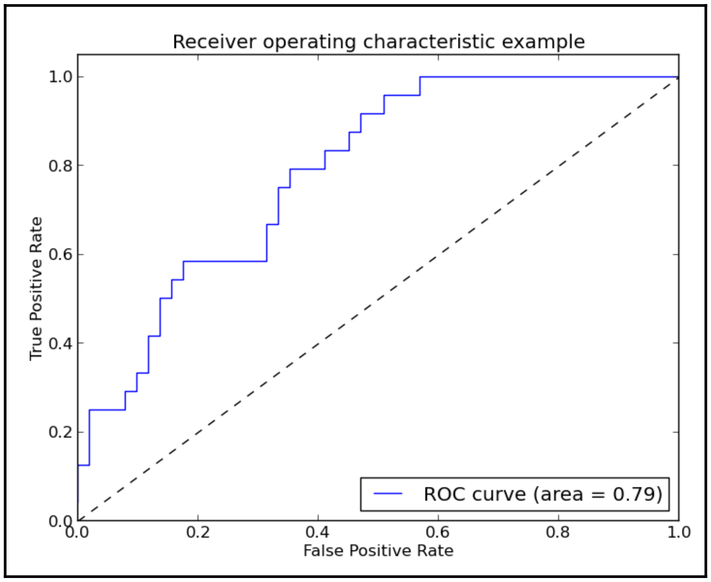
In data science practice, **precision** and **recall** are used more extensively than **accuracy**, as most datasets in data problems tend to be unbalanced. To account for this imbalance, data scientists often present their results in terms of **precision**, **recall**, and **f1-score**. In addition, we have to notice how **accuracy**, **precision**, **recall**, and **f1-score** assume values in the [0.0, 1.0] range. Perfect classifiers achieve the score of **1.0** for all of these measures (but beware of any perfect classification if it's too good to believe, as this usually means that something wrong has happened; real-world data problems never have a perfect solution).

Binary classification

In addition to the error measures shown in the preceding section, in problems where you have only two output classes (for instance, if you have to guess the gender of a user or predict whether the user will click/buy/like the item), there are some additional measures. The most used one, since it's very informative, is the area under the **receiver operating characteristics curve** (**ROC**) or **area under a curve** (**AUC**).

The ROC curve is a graphical way to express how the performances of the classifier change over all the possible classification thresholds (that is, changes in the outcome when its parameters change). Specifically, these performances have a true positive (or hit) rate and a false positive (or miss) rate. The first is the rate of the correct positive results, and the second is the rate of the incorrect ones. The area under that curve represents how well the classifier performs with respect to a random classifier (whose AUC is 0.50).

Here, we have a graphical example of a random classifier (dotted line) and a better one (solid line). You can see that the AUC of a random classifier is 0.5 (it is half of the square), and the other has a higher AUC (with its upper bound at `1.0`):



The function that is used to compute the AUC with Python is `sklearn.metrics.roc_auc_score()`.

Regression

In tasks where you have to predict real numbers or regression, many error measures are derived from Euclidean algebra:

- **Mean absolute error or MAE**: This is the mean L1 norm of the difference vector between the predicted and real values:

```
In: from sklearn.metrics import mean_absolute_error
    mean_absolute_error([1.0, 0.0, 0.0], [0.0, 0.0, -1.0])

Out: 0.666666666666666663
```

- **Mean squared error or MSE**: This is the mean L2 norm of the difference vector between the predicted and real values:

```
In: from sklearn.metrics import mean_squared_error
    mean_squared_error([-10.0, 0.0, 0.0], [0.0, 0.0, 0.0])

Out: 33.333333333333
```

- **R^2 score**: R^2 is also known as the **coefficient of determination**. In a nutshell, R^2 determines how good a linear fit there is that exists between the predictors and the `target` variable. It takes values between 0 and 1 (inclusive); the higher R^2 is, the better the model. It is a good score measure, yet it doesn't tell everything about the story, especially if there are outliers in your data. There are even more intricacies about this metric that you can find in reference books on Statistics. As a suggestion, use it, but accompany it with other score or error measurements. The function to use in this case is `sklearn.metrics.r2_score`.

Testing and validating

After loading our data, preprocessing it, creating new, useful features, checking for outliers and other inconsistent data points, and finally choosing the right metric, we are ready to apply a machine learning algorithm.

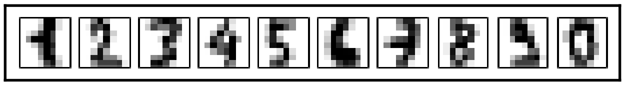
A machine learning algorithm, by observing a series of examples and pairing them with their outcome, is able to extract a series of rules that can be successfully generalized to new examples by correctly guessing their resulting outcome. Such is the supervised learning approach, where it applies a series of highly specialized learning algorithms that we expect can correctly predict (and generalize) on any new data.

But how can we correctly apply the learning process in order to achieve the best model for prediction to be generally used with similar yet new data?

In data science, there are some best practices to be followed that can assure you the best results in the future generalization of your model to any new data. Let's explain this practice by proceeding step by step, first loading the dataset that we will be working on in the following example:

```
In: from sklearn.datasets import load_digits
    digits = load_digits()
    print (digits.DESCR)
    X = digits.data
    y = digits.target
```

The digit dataset contains images of handwritten numbers from 0 to 9. The data format consists of a matrix of 8 x 8 images of this kind:



These digits are actually stored as a vector (resulting from the flattening of each 8 x 8 image) of 64 numeric values from 0 to 16, representing grayscale tonality for each pixel:

```
In: X[0]

Out: array([0., 0., 5., 13., 9., 1., 0., 0., ...])
```

We will also upload three different machine learning hypotheses (a hypothesis, in machine learning language, is an algorithm that's complete with all of its parameters set ready for learning) using three different support vector machines for classification. They will be useful for our practical example:

```
In: from sklearn import svm
    h1 = svm.LinearSVC(C=1.0)
    h2 = svm.SVC(kernel='rbf', degree=3, gamma=0.001, C=1.0)
    h3 = svm.SVC(kernel='poly', degree=3, C=1.0)
```

As a first experiment, let's fit the linear SVM classifier to our data and verify the results:

```
In: h1.fit(X,y)
    print (h1.score(X,y))

Out: 0.984974958264
```

The first method fits a model by using the `X` array in order to correctly predict one of the 10 classes indicated by the `y` vector. After that, by calling the `.score()` method and specifying the same predictors (the `X` array), the method evaluates the performance in terms of mean accuracy with respect to the true values given by the `y` vector. The result is about 98.5% accurate in predicting the correct digit.

This number represents the in-sample performance, which is the performance of the learning algorithm. It is purely indicative, though it represents an upper bound of the performance (providing different examples, the average performance will always be inferior). In fact, every learning algorithm has a certain capability of memorizing the data that it has been trained with. Therefore, the in-sample performance is partly due to the capability of the algorithm to learn some general inference from the data, and partly from its memorization capabilities. In extreme cases, if the model is overtrained or too complex with respect to the available data, the memorized patterns prevail over the derived rules, and the algorithm becomes unfit to predict correctly new observations (though it will be very good on past ones). Such a problem is called overfitting. Since, in machine learning, we cannot separate these two concomitant effects, in order to have a proper estimate of the predictive performances of our hypothesis, we need to test it on some fresh data where there is no memorization effect.

Memorization happens because of the complexity of the algorithm. Complex algorithms own many coefficients, where information about the training data can be stored. Unfortunately, the memorization effect causes high variance in the estimation when predicting unseen examples since its predictive processes become random. Three solutions are possible:

- First, you can increase the number of examples so that it will become infeasible to store information about all the previously seen cases, but it may become more expensive to find all of the necessary data
- Second, you can use a simpler machine learning algorithm which is less prone to memorization, but at the cost of using a machine learning solution that's less capable of fitting the complexity of the rules underlying the data.
- Third, you can use regularization to penalize extremely complex models and force the algorithm to be underweight or even exclude a certain number of variables from the model, thus effectively reducing the number of coefficients in the model and its capacity to memorize data.

In many cases, fresh data is not available, if not at a certain cost. In such a common case, a good approach would be to divide the initial data into a training set (usually 70-80% of the total data) and a test set (the remaining 20-30%). The split between the training and the test set should be completely random, taking into account any possible unbalanced class distribution:

```
In: chosen_random_state = 1
    X_train, X_test, y_train, y_test = model_selection.train_test_split(
                        X, y,
                        test_size=0.30, random_state=chosen_random_state)
    print ("(X train shape %s, X test shape %s, n/y train shape %s, \
           y test shape %s" % (X_train.shape, X_test.shape,
                              y_train.shape, y_test.shape))
    h1.fit(X_train,y_train)
    print (h1.score(X_test,y_test))
    # Returns the mean accuracy on the given test data and labels

Out: (X train shape (1257, 64), X test shape (540, 64),
      y train shape (1257,), y test shape (540,)
      0.953703703704
```

By executing the preceding code, the initial data is randomly split into two mutually exclusive sets by the `model_selection.train_test_split()` function on the basis of the parameter `test_size` (which could be an integer indicating the exact number of examples for the test set or a floating point number, indicating the percentage of the total data to be used for testing purposes). The split is governed by `random_state`, which assures that the operation is reproducible at different times and on different computers (even when you're using completely different operating systems).

The present average accuracy is 0.94. If you try to run the same cell again, using a different integer value for the `chosen_random_state` parameter, you will actually notice that the accuracy will change, hinting that the performance evaluation by a test set is not an absolute measure of performance and that it should be used with care. You have to be aware of its mutability, given different test samples.

Actually, we can even get biased performance estimations from the test set. This could happen if we either choose (after various trials with `random_state`) a test set that can confirm our hypothesis, or start using the test set as a reference in order to take decisions in regard to the learning process (for example, selecting the best hypothesis that fits a certain test sample).

As with evaluating just the fit on the training data, working on a selected test set will make the resulting performance surely look great. Yet, the model you have built would not be replicating the same performances on a different test set (an overfitting problem again).

Therefore, when we have to choose between multiple hypotheses (a common experiment in data science) after fitting each of them onto the training data, we need a data sample that can be used to compare their performances, and it cannot be the test set (because of the reasons that we mentioned previously).

A correct approach is to use a validation set. We suggest that you split the initial data – 60% of the initial data can be reserved for the training set, 20% for the validation set, and 20% for the test set. Our initial code can be changed in order to consider this, and it can be adapted to test all three hypotheses:

```
In: chosen_random_state = 1
    X_train, X_validation_test, y_train, y_validation_test =
    model_selection.train_test_split(X, y,
                                     test_size=.40,
                                     random_state=chosen_random_state)
    X_validation, X_test, y_validation, y_test =
    model_selection.train_test_split(X_validation_test, y_validation_test,
                                    test_size=.50,
                                    random_state=chosen_random_state)
    print ("X train shape, %s, X validation shape %s, X test shape %s,
           /ny train shape %s, y validation shape %s, y test shape %s/n" %
           (X_train.shape, X_validation.shape, X_test.shape,
            y_train.shape, y_validation.shape, y_test.shape))
    for hypothesis in [h1, h2, h3]:
        hypothesis.fit(X_train,y_train)
        print ("%s -> validation mean accuracy = %0.3f" % (hypothesis,
        hypothesis.score(X_validation,y_validation))  )
    h2.fit(X_train,y_train)
    print ("n%s -> test mean accuracy = %0.3f" % (h2,
    h2.score(X_test,y_test)))

Out: X train shape, (1078, 64), X validation shape (359, 64),
     X test shape (360, 64),
     y train shape (1078,), y validation shape (359,), y test shape (360,)

     LinearSVC(C=1.0, class_weight=None, dual=True, fit_intercept=True,
         intercept_scaling=1, loss='squared_hinge', max_iter=1000,
         multi_class='ovr', penalty='l2', random_state=None,  tol=0.0001,
         verbose=0) -> validation mean accuracy = 0.958

     SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
      decision_function_shape=None, degree=3, gamma=0.001, kernel='rbf',
      max_iter=-1, probability=False, random_state=None, shrinking=True,
      tol=0.001, verbose=False) -> validation mean accuracy = 0.992

     SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
      decision_function_shape=None, degree=3, gamma='auto', kernel='poly',
      max_iter=-1, probability=False, random_state=None, shrinking=True,
      tol=0.001, verbose=False) -> validation mean accuracy = 0.989

     SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
      decision_function_shape=None, degree=3, gamma=0.001, kernel='rbf',
      max_iter=-1, probability=False, random_state=None, shrinking=True,
      tol=0.001, verbose=False) -> test mean accuracy = 0.978
```

As reported by the output, now, the training set is made up of 1,078 cases (60% of the total cases). In order to divide the data into three parts – training, validation, and test – the data is at first split between the train set and a test/validation dataset (thus extracting the training sample) using the function `model_selection.train_test_split`. Then, the test/validation dataset is furthermore split into two parts using the same function. Each hypothesis, after being trained, is tested against the validation set. Obtaining an accuracy of 0.992, the SVC using an RBF kernel is the best model according to the validation set. Having decided to use this model, its performance is evaluated on the test set, resulting in an accuracy of 0.978 (which is a measured representative of the real performances of the model).

Since the test's accuracy is different from that of the validation one, is the chosen hypothesis really the best one? We suggest that you try to run the code in the cell multiple times (ideally, running the code at least 30 times should ensure statistical significance), each time changing the `chosen_random_state` value. In such a way, the same learning procedure will be validated with respect to different samples and you can be more confident of your expectations.

Cross-validation

If you have run the previous experiment, you may have realized that:

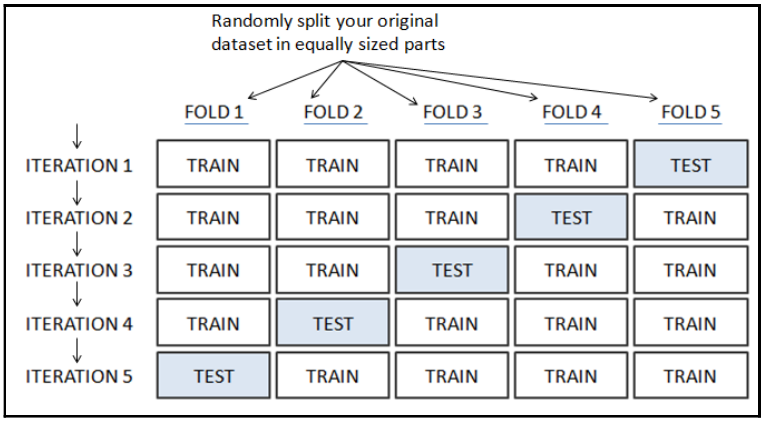
- Both the validation and test results vary, as their samples are different.
- The chosen hypothesis is often the best one, but this is not always the case.

Unfortunately, relying on the validation and testing phases of samples brings uncertainty, along with a reduction of the learning examples dedicated to training (the fewer the examples, the more the variance of the estimates from the model).

A solution would be to use cross-validation, and Scikit-learn offers a complete module for cross-validation and performance evaluation (`sklearn.model_selection`).

By resorting to cross-validation, you'll just need to separate your data into a training and test set, and you will be able to use the training data for both model optimization and model training.

How does cross-validation work? The idea is to divide your training data into a certain number of partitions (called folds) and train your model as many times as the number of partitions there are, keeping out a different partition every time from the training phase. After every model training, you will test the result on the fold that is left out and store it away. In the end, you will have as many results as there are folds, and you can calculate both the average and standard deviation on them:



In the preceding graphical example, the chart depicts a dataset that's been divided into five equally sized folds, which are differently used, depending on the iteration, as part of the train or test set during the machine learning process.

Ten folds is quite a common configuration in the cross-validation that we recommend. Using fewer folds can be fine with biased estimators such as linear regression, but it may penalize machine learning algorithms that are more complex. In some cases, you really need to use more folds to ensure that there is enough training data for the machine learning algorithm to generalize properly. This happens quite commonly in medical datasets where there are not enough data points. On the other hand, if the number of examples at hand is not an issue, using more folds is more computationally intensive and it may take longer for the cross-validation to complete. Sometimes, using five folds is a good compromise between accuracy of estimates and running times.

The standard deviation will provide a hint on how your model is influenced by the data that is provided for training (the variance of the model, actually), and the mean provides a fair estimate of its general performance. Using the mean of the cross-validation results obtained from different models (because of a different model type employed, or because a different selection of the training variables has been used, or because the different hyperparameters of the model), you can confidently choose the best performing hypothesis to be tested for general performance.

We strongly suggest that you use cross-validation just for optimization purposes and not for performance estimation (that is, to figure out what the error of the model might be on fresh data). Cross-validation just points out the best possible algorithm and parameter choice based on the best averaged result. Using it for performance estimation would mean using the best result found, a more optimistic estimation than it should be. In order to report an unbiased estimation of your possible performance, you should prefer using a test set.

Let's execute an example in order to see cross-validation in action. At this point, we can review the previous evaluation of three possible hypotheses for our digits dataset:

```
In: choosen_random_state = 1
    cv_folds = 10 # Try 3, 5 or 20
    eval_scoring='accuracy' # Try also f1
    workers = -1 # this will use all your CPU power
    X_train, X_test, y_train, y_test = model_selection.train_test_split(
                                  X, y,
                                  test_size=0.30,
                                  random_state=choosen_random_state)
    for hypothesis in [h1, h2, h3]:
        scores = model_selection.cross_val_score(hypothesis,
                    X_train, y_train,
                    cv=cv_folds, scoring= eval_scoring, n_jobs=workers)
        print ("%s -> cross validation accuracy: mean = %0.3f \
               std = %0.3f" % (hypothesis, np.mean(scores),
                               np.std(scores)))

Out: LinearSVC(C=1.0, class_weight=None, dual=True, fit_intercept=True,
      intercept_scaling=1, loss='squared_hinge', max_iter=1000,
      multi_class='ovr', penalty='l2', random_state=None, tol=0.0001,
      verbose=0) -> cross validation accuracy: mean = 0.930 std = 0.021

     SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
      decision_function_shape=None, degree=3, gamma=0.001, kernel='rbf',
      max_iter=-1, probability=False, random_state=None, shrinking=True,
      tol=0.001, verbose=False) -> cross validation accuracy:
      mean = 0.990 std = 0.007
```

```
SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
 decision_function_shape=None, degree=3, gamma='auto', kernel='poly',
 max_iter=-1, probability=False, random_state=None, shrinking=True,
 tol=0.001, verbose=False) -> cross validation accuracy:
 mean = 0.987 std = 0.010
```

The core of the script is the `model_selection.cross_val_score` function. The function in our script receives the following parameters:

- A learning algorithm (`estimator`)
- A training set of predictors (`X`)
- A `target` variable (`y`)
- The number of cross-validation folds (`cv`)
- A scoring function (`scoring`)
- The number of CPUs to be used (`n_jobs`)

Given such an input, the function wraps some other complex functions. It creates n-iterations, training a model of the n-cross-validation in-samples, testing the results, and storing scores derived at each iteration from the out-of-sample fold. In the end, the function reports a list of the recorded scores of this kind:

```
In: scores

Out: array([ 0.96899225, 0.96899225, 0.9921875, 0.98412698, 0.99206349,
             1, 1., 0.984, 0.99186992, 0.98347107])
```

The main advantage of using `cross_val_score` resides in its simplicity of usage and in the fact that it automatically incorporates all of the necessary steps for a correct cross-validation. For example, when deciding on how to split the training sample into folds, if a `y` vector is provided, it keeps the same target class label's proportion in each fold as it was in the `y` that was initially provided.

Using cross-validation iterators

Though the `cross_val_score` function from the `model_selection` module acts as a complete helper function for most of the cross-validation purposes, you may have the need to build up your own cross-validation process. In this case, the same `model_selection` module guarantees a formidable selection of iterators.

Before examining the most useful ones, let's provide a clear overview of how they function by studying how one of the iterators, `model_selection.KFold`, works.

`KFold` is quite simple in its functionality. If n-number of folds is given, it returns n iterations to the indexes of the training and validation sets for the testing of each fold.

Let's say that we have a training set made up of 100 examples and we would like to create a 10-fold cross-validation. First, let's set up our iterator:

```
In: kfolding = model_selection.KFold(n_splits=10, shuffle=True,
                                     random_state=1)
    for train_idx, validation_idx in kfolding.split(range(100)):
        print (train_idx, validation_idx)

Out: [ 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 18 19 20 21 22 23 24 25 26
27
       28 29 30 31 32 34 35 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52
53
       54 55 56 57 58 59 60 61 62 63 64 66 67 68 70 71 72 73 74 75 76 77 78
79
       83 85 86 87 88 89 90 91 92 94 95 96 97 98 99] [17 33 36 65 69 80 81
82
       84 93] ...
```

By using the n parameter, we can instruct the iterator to perform the folding on 100 indexes. `n_splits` specifies the number of folds. While shuffle is set to `True`, it will randomly choose the fold components. Instead, if it is set to `False`, the folds will be created with respect to the order of the indexes (so, the first fold will be `[0 1 2 3 4 5 6 7 8 9]`).

As usual, the `random_state` parameter allows for the reproducibility of the fold's generation.

During the iterator loop, the indexes for training and validation are provided with respect to your hypothesis for evaluation. (Let's figure out how it works by using h1, the linear SVC.) You just have to select both `X` and `y` accordingly with the help of fancy indexing:

```
In: h1.fit(X[train_idx],y[train_idx])
    h1.score(X[validation_idx],y[validation_idx])

Out:0.90000000000000002
```

As you can see, a cross-validation iterator provides you with just the index functionality, and it is up to you when it comes to using indexes for your scoring evaluation on your hypothesis. This opens up opportunities for sophisticated operations of validation.

Among the other most useful iterators, the following are worth mentioning:

- `StratifiedKFold` works like `Kfold`, but it always returns folds with approximately the same class percentage as the training set. This leaves each fold balanced; therefore, the learner is fitted on the correct proportion of classes. Instead of the number of cases, as an input parameter, it needs the target variable y. It is the iterator that is wrapped, by default, in the `cross_val_score` function, as we saw in the preceding section.
- `LeaveOneOut` works like `Kfold`, but it returns as a validation set of only one observation. Therefore, in the end, the number of folds will be equivalent to the number of examples in the training set. We recommend that you use this cross-validation approach only when the training set is heavily unbalanced (such as in fraud detection problems) or very small, especially if there are less than 100 observations – a k-fold validation would reduce the training set a lot.
- `LeavePOut` is similar in regards to the advantages and limitations of `LeaveOneOut`, but its validation set is made up of P cases. Therefore, the number of total folds will be the combination of P cases from all the available cases (which actually could be quite a large number as the size of your dataset grows).
- `LeaveOneLabelOut` provides a convenient way to cross-validate according to a scheme that you have prepared or computed in advance. In fact, it will act like `Kfolds`, but for the fact that the folds will already be labeled and provided to the labels parameter.
- `LeavePLabelOut` is a variant of `LeaveOneLabelOut`. In this instance, the test folds are made of a number of labels according to the scheme that you prepare in advance.

To learn more about the specific parameters required by each iterator, we suggest that you check out the Scikit-learn website: `http://Scikit-learn.org/stable/modules/classes.html#module-sklearn.model_selection`.

As a matter of fact, cross-validation can also be used for prediction purposes. In fact, for specific data science projects, you may be required to build a model from your available data and then produce predictions on the very same data. As seen previously, using training predictions will lead to high variance estimates, given that the model has been fitted on that very data and thus it has memorized much of its characteristics.

The cross-validation process applied to prediction can come to the rescue:

- Create a cross-validation iterator (preferably with a large number of k folds).
- Iterate through the cross-validation and each time train your model with the k-1 training folds.
- At each iteration, on the validation fold (which is an out-of-sample fold, actually), produce predictions and store them away, keeping track of their index. The best way of doing so is to have a prediction matrix which will be populated with predictions by using fancy indexing.

Such an approach is commonly referred to as out-of-cross-validation fold prediction.

Sampling and bootstrapping

After illustrating iterators based on folds, p-out, and custom schemes, we'll continue our overview on cross-validation iterators and quote all of the sampling-based ones.

The sampling schemes are different because they do not split the training set, but they sample it using different approaches: subsampling or bootstrapping.

Subsampling is performed when you randomly select a part of the available data, obtaining a smaller dataset than the initial one.

Subsampling is very useful, especially when you need to test your hypothesis extensively, but you prefer not to obtain your validation from extremely small test samples (so, you can opt out of a leave-one-out approach or a `KFold` using a large number of folds). The following is an example of the same:

```
In: subsampling = model_selection.ShuffleSplit(n_splits=10,
    test_size=0.1, random_state=1)
    for train_idx, validation_idx in subsampling.split(range(100)):
        print (train_idx, validation_idx)

Out:[92 39 56 52 51 32 31 44 78 10  2 73 97 62 19 35 94 27 46 38 67 99 54
     95 88 40 48 59 23 34 86 53 77 15 83 41 45 91 26 98 43 55 24  4 58 49
     21 87  3 74 30 66 70 42 47 89  8 60  0 90 57 22 61 63  7 96 13 68 85
     14 29 28 11 18 20 50 25  6 71 76  1 16 64 79  5 75  9 72 12 37] [80
     84 33 81 93 17 36 82 69 65]
     ...
```

Similar to the other iterators, `n_splits` will set the number of subsamples and `test_size` the percentage (if a float is given) or the number of observations to be used as a test.

Bootstrapping, as a resampling method, has been used for a long time to estimate the sampling distribution of statistics. Therefore, it is a proper method according to the evaluation of the out-of-sample performance of a machine learning hypothesis.

Bootstrapping works by randomly choosing observations and allowing repetitions, until a new dataset, which is of the same size as the original one, is built.

Unfortunately, since bootstrapping works by sampling with replacement (that is, by allowing the repetition of the same observation), there are issues that arise due to the following:

- Cases that may appear both on the training and the test set (you just have to use out-of-bootstrap sample observations for test purposes)
- There is less variance and more bias than for the cross-validation estimations due to nondistinct observations resulting from sampling with replacement.

Although the function is useful (at least from our point of view as data science practitioners), we propose to you a simple replacement for `Bootstrap` that is suitable for cross-validating and which can be called by an iteration. It generates a sample bootstrap of the same size as the input data (the length of the indexes) and a list of the excluded indexes (out of the sample) that could be used for testing purposes:

```
In: import random
    def Bootstrap(n, n_iter=3, random_state=None):
        """
        Random sampling with replacement cross-validation generator.
        For each iter a sample bootstrap of the indexes [0, n) is
        generated and the function returns the obtained sample
        and a list of all the excluded indexes.
        """
        if random_state:
            random.seed(random_state)
        for j in range(n_iter):
            bs = [random.randint(0, n-1) for i in range(n)]
            out_bs = list({i for i in range(n)} - set(bs))
            yield bs, out_bs

    boot = Bootstrap(n=100, n_iter=10, random_state=1)
    for train_idx, validation_idx in boot:
        print (train_idx, validation_idx)

Out:[37, 12, 72, 9, 75, 5, 79, 64, 16, 1, 76, 71, 6, 25, 50, 20, 18, 84,
11, 28, 29, 14, 50, 68, 87, 87, 94, 96, 86, 13, 9, 7, 63, 61, 22, 57,
1, 0, 60, 81, 8, 88, 13, 47, 72, 30, 71, 3, 70, 21, 49, 57, 3, 68,
24, 43, 76, 26, 52, 80, 41, 82, 15, 64, 68, 25, 98, 87, 7, 26, 25,
22, 9, 67, 23, 27, 37, 57, 83, 38, 8, 32, 34, 10, 23, 15, 87, 25, 71,
92, 74, 62, 46, 32, 88, 23, 55, 65, 77, 3] [2, 4, 17, 19, 31, 33, 35,
36, 39, 40, 42, 44, 45, 48, 51, 53, 54, 56, 58, 59, 66, 69, 73, 78,
85, 89, 90, 91, 93, 95, 97, 99]
...
```

The function performs subsampling and accepts the parameter `n` for the `n_iter` index to draw the bootstrap samples and the `random_state` index for reproducibility.

Hyperparameter optimization

A machine learning hypothesis is not simply determined by the learning algorithm but also by its hyperparameters (the parameters of the algorithm that have to be fixed prior, and which cannot be learned during the training process) and the selection of variables to be used to achieve the best learned parameters.

In this section, we will explore how to extend the cross-validation approach to find the best hyperparameters that are able to generalize to our test set. We will keep on using the handwritten digits dataset offered by the Scikit-learn package. Here's a useful reminder about how to load the dataset:

```
In: from sklearn.datasets import load_digits
    digits = load_digits()
    X, y = digits.data, digits.target
```

In addition, we will keep on using support vector machines as our learning algorithm:

```
In: from sklearn import svm
    h = svm.SVC()
    hp = svm.SVC(probability=True, random_state=1)
```

This time, we will work with two hypotheses. The first hypothesis is just the plain SVC that outputs a label as a prediction. The second hypothesis is SVC enhanced by the computation of label probabilities (the `probability=True` parameter) with the `random_state` fixed to the value `1` in order to guarantee the reproducibility of the results. SVC outputting probabilities can be evaluated by all of the loss metrics that require a probability and not a label prediction as a result, such as AUC.

After running the preceding code snippet, we are ready to import the `model_selection` module and set the list of hyperparameters that we want to test by cross-validation.

We are going to use the `GridSearchCV` function, which will automatically search for the best parameters according to a search schedule and score the results with respect to a predefined or custom scoring function:

```
In: from sklearn import model_selection
    search_grid = [
          {'C': [1, 10, 100, 1000], 'kernel': ['linear']},
          {'C': [1, 10, 100, 1000], 'gamma': [0.001, 0.0001],
           'kernel': ['rbf']},
          ]
    scorer = 'accuracy'
```

Now, we have imported the module, set the scorer variable using a string parameter (`'accuracy'`), and created a list made of two dictionaries.

The scorer is a string that we chose from a range of possible ones that you can find in the predefined values section of the Scikit-learn documentation, which can be viewed at `Scikit-learn.org/stable/modules/model_evaluation.html`.

Using predefined values just requires you to pick an evaluation metric from the list (there are some for classification and regression, and there are some for clustering) and use the string by plugging it directly, or by using a string variable, into the `GridSearchCV` function.

`GridSearchCV` also accepts a parameter called `param_grid`, which can be a dictionary containing, as keys, an indication of all the hyperparameters to be changed and, as values referring to the dictionary keys, lists of parameters to be tested. Therefore, if you want to test the performances of your hypothesis with respect to the hyperparameter *C*, you can create a dictionary like this:

```
{'C' : [1, 10, 100, 1000]}
```

Alternatively, according to your preference, you can use a specialized NumPy function to generate numbers that are evenly spaced on a log scale (like we saw in the previous chapter):

```
{'C' :np.logspace(start=-2, stop=3, num=6, base=10.0)}
```

You can, therefore, enumerate all of the possible parameters' values and test all of their combinations. However, you can also stack different dictionaries, having each dictionary containing only a portion of the parameters that should be tested together. For example, when working with SVC, the kernel set to *linear* automatically excludes the gamma parameter. Combining it with the linear kernel would be, in fact, a waste of computational power since it would not have any effect on the learning process.

Now, let's proceed with the grid search, timing it (thanks to the `%timeit` command magic command) to know how much time it will take to complete the entire procedure:

```
In: search_func = model_selection.GridSearchCV(estimator=h,
                                   param_grid=search_grid, scoring=scorer,
                                   n_jobs=-1, iid=False, refit=True, cv=10)
    %timeit search_func.fit(X,y)
    print (search_func.best_estimator_)
    print (search_func.best_params_)
    print (search_func.best_score_)

Out: 4.52 s ± 75.6 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
     SVC(C=10, cache_size=200, class_weight=None, coef0=0.0, degree=3,
     gamma=0.001,
       kernel='rbf', max_iter=-1, probability=False, random_state=None,
       shrinking=True, tol=0.001, verbose=False)
     {'kernel': 'rbf', 'C': 10, 'gamma': 0.001}
     0.981081122784
```

It took about `10` seconds to complete the search on our computer. The search pointed out that the best solution is an support vector machine classifier with `rbf` kernel, `C=10`, and `gamma=0.001` with a cross-validated mean accuracy of `0.981`.

As for the `GridSearchCV` command, apart from our hypothesis (the estimator parameter), `param_grid`, and the scoring we just talked about, we decided to set other optional but useful parameters:

1. First, we will set `n_jobs=-1`. This forces the function to use all the processors available on the computer, and so we run the Jupyter cell.
2. We will then set `refit=True` so that the function fits the whole training set, using the best estimator's parameters. Now, we just need to apply the `search_funct.predict()` method to fresh data in order to obtain new predictions.
3. The `cv` parameter is set to 10 folds (however, you can go for a smaller number, trading off speed with the accuracy of testing).

4. The iid parameter is set to False. This parameter decides how to compute the error measure with respect to the classes. If the classes are balanced (as in this case), setting iid won't have much effect. However, if they are unbalanced, by default, iid=True will make the classes with more examples weigh more on the computation of the global error. Instead, iid=False means that all the classes should be considered the same. Since we wanted SVC to recognize every handwritten number from 0 to 9, no matter how many examples were given for each of them, setting the iid parameter to False is the right choice. According to your data science project, you may decide that you actually prefer the default being set to True.

Building custom scoring functions

For our experiment, we picked a predefined scorer function. For classification, there are five measures available (accuracy, AUC, precision, recall, and f1-score), and for regression, there are three (R^2, MAE, and MSE). Though they are some of the most common measures, you may have to use a different measure. In our example, we find it useful to use a loss function in order to figure out if the right answer is still ranked high in probability, even when the classifier is wrong (thus considering if the right answer is the second or the third option of the algorithm). How do we manage that?

In the sklearn.metrics module, there's actually a log_loss function. All we have to do is wrap it in a way that GridSearchCV might use it:

```
In: from sklearn.metrics import log_loss, make_scorer
    Log_Loss = make_scorer(log_loss,
                           greater_is_better=False,
                           needs_proba=True)
```

Here it is. Basically, it's a one-liner. We created another function (Log_Loss) by calling make_scorer to the log_loss error function from sklearn.metrics. We also want to point out that we want to minimize this measure (it is a loss, not a score) by setting greater_is_better=False. We will also specify that it works with probabilities, not predictions (so, set needs_proba=True). Since it works with probabilities, we will use the hp hypothesis, which was just defined in the preceding section, since SVC won't emit any probability for its predictions otherwise:

```
In: search_func = model_selection.GridSearchCV(estimator=hp,
                         param_grid=search_grid, scoring=Log_Loss,
                           n_jobs=-1, iid=False, refit=True, cv=3)
    search_func.fit(X,y)
    print (search_func.best_score_)
```

```
        print (search_func.best_params_)

    Out: -0.16138394082
          {'kernel': 'rbf', 'C': 1, 'gamma': 0.001}
```

Now, our hyperparameters are optimized for log loss, not for accuracy.

A nice thing to remember is that optimizing for the right function can bring much better results to your project. So, time spent working on the score function is always time well spent in data science.

At this point, let's imagine that you have a challenging task. Since it is easy to mistake the handwritten numbers 1 and 7, you have to optimize your algorithm to minimize its mistakes on these two numbers. You can achieve this target by defining a new loss function:

```
In: import numpy as np
    from sklearn.preprocessing import LabelBinarizer
    def my_custom_log_loss_func(ground_truth,
                                p_predictions,
                                penalty = list(),
                                eps=1e-15):
        adj_p = np.clip(p_predictions, eps, 1 - eps)
        lb = LabelBinarizer()
        g = lb.fit_transform(ground_truth)
        if g.shape[1] == 1:
            g = np.append(1 - g, g, axis=1)
        if penalty:
            g[:,penalty] = g[:,penalty] * 2
        summation = np.sum(g * np.log(adj_p))
        return summation * (-1.0/len(ground_truth))
```

As a rule, the first parameter of your function should be the actual answer, and the second should be the predictions or the predicted probabilities. You can also add parameters that have a default value or allow you to have their values fixed later on when you call the `make_scorer` function:

```
In: my_custom_scorer = make_scorer(my_custom_log_loss_func,
                                   greater_is_better=False,
                                   needs_proba=True, penalty = [4,9])
```

In this case, we set the penalty for the highly confusable numbers 4 and 9 (however, you can change it or even leave it empty to check whether the resulting loss will be the same as that of the previous experiment with the sklearn.metrics.log_loss function).

Now, the new loss function computes the log_loss error as double when evaluating the results of the classes of numbers 4 and 9:

```
In: from sklearn import model_selection
    search_grid = [{'C': [1, 10, 100, 1000], 'kernel': ['linear']},
    {'C': [1, 10, 100, 1000], 'gamma': [0.001, 0.0001], 'kernel': ['rbf']}]
    search_func = model_selection.GridSearchCV(estimator=hp,
                param_grid=search_grid, scoring=my_custom_scorer, n_jobs=1,
                iid=False, cv=3)
    search_func.fit(X,y)
    print (search_func.best_score_)
    print (search_func.best_params_)

Out: -0.199610271298
     {'kernel': 'rbf', 'C': 1, 'gamma': 0.001}
```

Please note that, for the last example, we set n_jobs=1. There's a technical reason behind this choice. If you are running this code on Windows (in any Unix or macOS system, it is actually fine), you may incur an error that may block your Jupyter notebook. All cross-validation functions (and many others) on the Scikit-learn package work by using multiprocessors, thanks to the joblib package. Such a package requires all the functions to be run on multiple processors so that they are imported, and it cannot accept them if they are defined on the fly (they should be pickable). A possible workaround is saving the function into a file on the disk, such as custom_measure.py, and importing it by using the from custom_measure import Log_Loss command.

Reducing the grid search runtime

The GridSearchCV function can really manage an extensive amount of work for you by checking all combinations of parameters, as required by your grid specification. Anyway, when the data or grid search space is big, the procedure may take a long time to compute.

A potential remedy to this issue would be the following approach from the `model_selection` module. `RandomizedSearchCV` offers a procedure that randomly draws a sample of combinations and reports the best combination found.

This has some clear advantages:

- You can limit the number of computations.
- You can obtain a good result or, at worst, understand where to focus your efforts on in the grid search.
- `RandomizedSearchCV` has the same options as `GridSearchCV` but:
    1. Has a `n_iter` parameter, which is the number of random samples.
    2. Includes `param_distributions`, which has the same function as that of `param_grid`. However, it only accepts dictionaries and it works even better if you assign distributions as values and not lists of discrete values. For instance, instead of `C: [1, 10, 100, 1000]`, you can assign a distribution such as `C:scipy.stats.expon(scale=100)`.

Let's test this function with our previous settings:

```
In: search_dict = {'kernel': ['linear','rbf'],'C': [1, 10, 100, 1000],
                   'gamma': [0.001, 0.0001]}
    scorer = 'accuracy'
    search_func = model_selection.RandomizedSearchCV(estimator=h,
                                      param_distributions=search_dict,
                                      n_iter=7,
                                      scoring=scorer,
                                      n_jobs=-1,
                                      iid=False,
                                      refit=True,
                                      cv=10,
                                      return_train_score=False)
    %timeit search_func.fit(X,y)
    print (search_func.best_estimator_)
    print (search_func.best_params_)
    print (search_func.best_score_)

Out: 1.53 s ± 265 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
     SVC(C=10, cache_size=200, class_weight=None, coef0=0.0, degree=3,
       gamma=0.001, kernel='rbf', max_iter=-1, probability=False,
       random_state=None, shrinking=True, tol=0.001, verbose=False)
     {'kernel': 'rbf', 'C': 1000, 'gamma': 0.001}
     0.981081122784
```

Using just half of the computations (7 draws against 14 trials with the exhaustive grid search), it found an equivalent solution. Let's also have a look at the combinations that have been tested:

```
In: res = search_func.cvresults
    for el in zip(res['mean_test_score'],
                  res['std_test_score'],
                  res['params']):
       print(el)

Out: (0.9610800248897716, 0.021913085707003094, {'kernel': 'linear',
     'gamma': 0.001, 'C': 1000})
     (0.9610800248897716, 0.021913085707003094, {'kernel': 'linear',
     'gamma': 0.001, 'C': 1})
     (0.9716408520553866, 0.02044204452092589, {'kernel': 'rbf',
     'gamma': 0.0001, 'C': 1000})
     (0.981081122784369, 0.015506818968315338, {'kernel': 'rbf',
     'gamma': 0.001, 'C': 10})
     (0.9610800248897716, 0.021913085707003094, {'kernel': 'linear',
     'gamma': 0.001, 'C': 10})
     (0.9610800248897716, 0.021913085707003094, {'kernel': 'linear',
     'gamma': 0.0001, 'C': 1000})
     (0.9694212166750269, 0.02517929728858225, {'kernel': 'rbf',
     'gamma': 0.0001, 'C': 10})
```

Even without a complete overview of all combinations, a good sample can prompt you to look for just the RBF kernel and for certain `C` and gamma ranges, limiting the following grid search to a limited portion of the potential search space.

Resorting to optimization based on random processes may appear to rely on blind luck, but actually, it is a very efficient way to explore the hyperparameters' space, especially when it is a high-dimensional space. If properly arranged, random search does not sacrifice the completeness of exploration for its extent. In high-dimensional hyperparameter spaces, grid search exploration tends to repeat the testing of similar parameter combinations, proving to be computationally highly inefficient in those case where there are irrelevant parameters or parameters whose effects are very correlated.

Random Search has been devised by James Bergstra and Yoshua Bengio in order to make the search of optimal combinations of hyperparameters in deep learning more efficient. The original paper is a great source for further insight into this method: `http://www.jmlr.org/papers/volume13/bergstra12a/bergstra12a.pdf`.

Statistical tests have demonstrated that for a randomized search to perform well, you should try from a minimum of 30 trials to a maximum of 60 (this rule of thumb is based on the assumption that the optimum covers from 5% to 10% of the hyperparameters' space, and a 95% success rate is an acceptable one). Consequently, it generally makes sense to resort to random search if your grid searching requires a comparable (so you can take advantage of random searching's properties) or a larger number of experiments (allowing you to save on computations).

Feature selection

With respect to the machine learning algorithm that you are going to use, irrelevant and redundant features may play a role in the lack of interpretability of the resulting model, long training times and, most importantly, overfitting and poor generalization.

Overfitting is related to the ratio of the number of observations and the variables available in your dataset. When the variables are many compared to the observations, your learning algorithm will have more chance of ending up with some local optimization or the fitting of some spurious noise due to the correlation between variables.

Apart from dimensionality reduction, which requires you to transform data, feature selection can be the solution to the aforementioned problems. It simplifies high-dimensional structures by choosing the most predictive set of variables; that is, it picks the features that work well together, even if some of them are not such good predictors on an independent level.

The Scikit-learn package offers a wide range of feature selection methods:

- Selection based on the variance
- Univariate selection
- Recursive elimination
- Randomized logistic regression/stability selection
- L1-based feature selection
- Tree-based feature selection

Variance, univariate, and recursive elimination can be found in the `feature_selection` module. The others are a byproduct of specific machine learning algorithms. Apart from tree-based selection (which will be mentioned in `Chapter 4`, *Machine Learning*), we are going to present all the preceding methods and point out how they can help you improve your learning from the data.

Selection based on feature variance

This method is the simplest approach to feature selection, and it's often used as the baseline. It simply removes all the features which have small variance; typically, lower than the one set. By default, the `VarianceThresholder` object removes all the zero-variance features, but you can control it with the threshold parameter.

Let's create a small dataset composed of `10` observations and `5` features, `3` of them informative:

```
In: from sklearn.datasets import make_classification
    X, y = make_classification(n_samples=10, n_features=5,
    n_informative=3, n_redundant=0, random_state=101)
```

Now, let's measure their `Variance`:

```
In: print ("Variance:", np.var(X, axis=0))

Out: Variance: [ 2.50852168  1.47239461  0.80912826  1.51763426
                1.37205498]
```

The lower variance is associated with the third feature; therefore if we want to select the four best features, we should set the threshold of minimum variance to `1.0`. Let's do that, and see what happens with the first observation of the dataset:

```
In: from sklearn.feature_selection import VarianceThreshold
    X_selected = VarianceThreshold(threshold=1.0).fit_transform(X)
    print ("Before:", X[0, :])
    print ("After: ", X_selected[0, :])

Out: Before: [ 1.26873317 -1.38447407  0.99257345  1.19224064 -2.07706183]
     After:  [ 1.26873317 -1.38447407  1.19224064 -2.07706183]
```

As expected, the third column is removed in the feature selection process, and none of the output observations have it. Only the ones with variance greater than 1.0 have remained. Remember not to Z-normalize your dataset (with the `StandardScaler`, for example) before applying `VarianceThresholder`; otherwise, all the features will have unitary variance.

Univariate selection

With the help of univariate selection, we intend to select single variables that are associated the most with your `target` variable according to a statistical test.

There are three available tests to base our selection on:

- The `f_regression` object uses an F-test and a p-value according to the ratio of explained variance against the unexplained one in a linear regression of the variable with the target. This is only useful for regression problems.
- The `f_classif` object is an ANOVA F test that can be used when dealing with classification problems.
- The `Chi2` object is a chi-squared test, which is suitable when the target is a classification and the variables are count or binary data (they should be positive).

All of the tests have a score and a p-value. Higher scores and p-values indicate that the variable is associated and is consequently useful to the target. The tests do not take into account instances where the variable is a duplicate or is highly correlated to another variable. It is, therefore, most suited to rule out the not-so-useful variables than to highlight the most useful ones.

In order to automate the procedure, there are also some selection routines that are available:

- `SelectKBest`, based on the score of the test, takes the k best variables.
- `SelectPercentile`, based on the score of the test, takes the top percentile of performing variables.
- Based on the p-values of the tests, `SelectFpr` (false positive rate test), `SelectFdr` (false discovery rate test), and `SelectFwe` (family-wise error rate procedure).

You can also create your own selection procedure with the `GenericUnivariateSelect` function by using the `score_func` parameter, which takes predictors and the target and returns a score and a p-value based on your favorite statistical test.

The great advantage offered by these functions is that they present a series of methods to select the variables (fit) and later on automatically reduce (transform) all the sets to the best variables. In our example, we use the `.get_support()` method in order to get a Boolean indexing from both the `Chi2` and `f_classif` tests on the top 25 percent predictive variables. We then decide on the variables that have been selected by both tests:

```
In: X, y = make_classification(n_samples=800, n_features=100,
                               n_informative=25,
                               n_redundant=0, random_state=101)
```

`make_classification` creates a dataset of `800` cases and `100` features. The important variables are a quarter of the total:

```
In: from sklearn.feature_selection import SelectPercentile
    from sklearn.feature_selection import chi2, f_classif
    from sklearn.preprocessing import Binarizer, scale
    Xbin = Binarizer().fit_transform(scale(X))
    Selector_chi2 = SelectPercentile(chi2, percentile=25).fit(Xbin, y)
    Selector_f_classif = SelectPercentile(f_classif,
                                          percentile=25).fit(X, y)
    chi_scores = Selector_chi2.get_support()
    f_classif_scores = Selector_f_classif.get_support()
    selected = chi_scores & f_classif_scores # use the bitwise and operator
```

If you use the chi-squared association measure, as in the above example, the input `X` must be non-negative: `X` must contain Booleans or frequencies, hence the choice to binarize after the normalization if the variable is above the average.

The final selected variable contains a Boolean vector, pointing out 21 predictive variables that have been made evident by both of the tests.

As a suggestion based on experience, by operating with different statistical tests and retaining a high percentage of your variables, you can usefully exploit univariate selection by ruling out less informative variables and thus simplify your set of predictors.

Recursive elimination

The problem with univariate selection is the likelihood of selecting a subset containing redundant information, whereas our interest is to get a minimum set that works with our predictor algorithm. In this case, recursive elimination could help provide the answer.

By running the following script, you'll find the reproduction of a problem that is quite challenging and which you may also often come across in datasets of different cases and variable sizes:

```
In: from sklearn.model_selection import train_test_split
    X, y = make_classification(n_samples=100, n_features=100,
                               n_informative=5,
                               n_redundant=2, random_state=101)
    X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                         test_size=0.30,
                                                         random_state=101)
```

```
In: from sklearn.linear_model import LogisticRegression
    classifier = LogisticRegression(random_state=101)
    classifier.fit(X_train, y_train)
    print ('In-sample accuracy: %0.3f' %
                             classifier.score(X_train, y_train))
    print ('Out-of-sample accuracy: %0.3f' %
                             classifier.score(X_test, y_test))

Out: In-sample accuracy: 1.000
     Out-of-sample accuracy: 0.667
```

We have a small dataset with quite a large number of variables. It is a problem of the $p>n$ type, where p is the number of variables and n is the number of observations.

In such cases, there are surely some informative variables in the dataset, but the noise provided by the others may fool the learning algorithm while assigning the correct coefficients to the correct features. Keep in mind that this situation is not the best operative environment to do data science; therefore, expect mediocre results at best.

This reflects in high (in our case, perfect) in-sample accuracy, which drops sharply when tested on an out-of-sample, or when using cross-validation.

In such a case, provided with a learning algorithm, instructions about the scoring/loss function and the cross-validation procedure, the `RFECV` class, starts fitting an initial model on all variables and calculates a score based on cross-validation. At this point, `RFECV` starts pruning the variables until it reaches a set of variables where the cross-validated score starts decreasing (whereas, by pruning, the score should have stayed stable or increased):

```
In: from sklearn.feature_selection import RFECV
    selector = RFECV(estimator=classifier, step=1, cv=10,
                     scoring='accuracy')
    selector.fit(X_train, y_train)
    print('Optimal number of features : %d' % selector.n_features_)

Out: Optimal number of features : 4
```

In our example, from `100` variables, the `RFECV` ended up selecting just four of them. We can check the result on the test set after transforming both the training and test set in order to reflect the variable pruning:

```
In: X_train_s = selector.transform(X_train)
    X_test_s = selector.transform(X_test)
    classifier.fit(X_train_s, y_train)
    print ('Out-of-sample accuracy: %0.3f' %
            classifier.score(X_test_s, y_test))

Out: Out-of-sample accuracy: 0.900
```

As a rule, when you notice a large discrepancy between the training results (based on cross-validation, not the in-sample score) and the out-of-sample results, recursive selection can help you achieve better performance from your learning algorithms by pointing out some of the most important variables.

Stability and L1-based selection

Though effective, recursive elimination is actually a step-by-step algorithm that bases its choices on sequences of single evaluations. While pruning, it opts for certain selections, potentially excluding many others. That's a good way to reduce a particularly challenging and time-consuming problem, such as an exhaustive search among possible sets, into a more manageable one. Anyway, there's another way to solve the problem, which is by using all the variables at hand conjointly. Some algorithms use regularization to limit the weight of the coefficients, thus preventing overfitting and the selection of the most relevant variables without losing predictive power. In particular, the regularization L1 (the lasso) is well-known for the creation of sparse selections of variables' coefficients since it pushes many variables to the 0 value according to the set strength of regularization.

An example will clarify the usage of the logistic regression classifier and the synthetic dataset that we used for recursive elimination.

By the way, `linear_model.Lasso` will work out the L1 regularization for regression, whereas `linear_model.LogisticRegression` and `svm.LinearSVC` will do so for the classification:

```
In: from sklearn.svm import LinearSVC
    classifier = LogisticRegression(C=0.1, penalty='l1', random_state=101)
    classifier.fit(X_train, y_train)
    print ('Out-of-sample accuracy: %0.3f' %
                                    classifier.score(X_test, y_test))

Out: Out-of-sample accuracy: 0.933
```

The out-of-sample accuracy is better than the previous one that was obtained by using the greedy approach. The secret is the `penalty='l1'` and the `C` value that was assigned when initializing the `LogisticRegression` class. Since `C` is the main ingredient of the L1-based selection, it is important to choose it correctly. This can be done by using grid search and cross-validation, but there's an easier and an even more effective way to obtain variable selection through regularization: stability selection.

Stability selection successfully uses L1 regularization, even under the default values (though you may need to change them in order to improve the results) because it verifies its results by subsampling, that is, by recalculating the regularization process a large number of times by using a randomly chosen part of the training dataset.

The result excludes all of the variables that often had their coefficient estimated to be zero. Only if a variable has a nonzero coefficient will the variable be considered stable to the dataset and feature set variations, which is something important to be included in the model (hence the name, "stability selection").

Let's test this by implementing the selection approach (by using the dataset that we used before):

```
In: from sklearn.linear_model import RandomizedLogisticRegression
    selector = RandomizedLogisticRegression(n_resampling=300,
                                            random_state=101)
    selector.fit(X_train, y_train)
    print ('Variables selected: %i' % sum(selector.get_support()!=0))
    X_train_s = selector.transform(X_train)
    X_test_s = selector.transform(X_test)
    classifier.fit(X_train_s, y_train)
    print ('Out-of-sample accuracy: %0.3f' %
           classifier.score(X_test_s, y_test))

Out: Variables selected: 3
     Out-of-sample accuracy: 0.933
```

Actually, we obtained results that were similar to that of the L1-based selection by just using the default parameters of the `RandomizedLogisticRegression` class.

The algorithm works fine. It is reliable and it works out of the box (there are no parameters to tweak unless you want to try lowering the *C* values in order to speed it up). We just suggest that you set the `n_resampling` parameter to a large number so that your computer can handle stability selection in a reasonable amount of time.

If you want to resort to the same algorithm for a regression problem, you should use the `RandomizedLasso` class instead. Let's see how to use it. First, we create a dataset that's adequate for a regression problem. For simplicity, we will use a 100-sample, 10-feature observation matrix; the number of informative features is `4`.

Then, we can leave `RandomizezLasso` to figure out which are the most important features (the informative ones) by printing their score. Note that a resulting score is a floating-point number:

```
In: from sklearn.linear_model import RandomizedLasso
    from sklearn.datasets import make_regression
    X, y = make_regression(n_samples=100, n_features=10,
                           n_informative=4,
                           random_state=101)
    rlasso = RandomizedLasso()
    rlasso.fit(X, y)
    list(enumerate(rlasso.scores_))

Out: [(0, 1.0),
      (1, 0.0),
      (3, 0.0),
      (4, 0.0),
      (5, 1.0),
      (6, 0.0),
      (7, 0.0),
      (8, 1.0),
      (9, 0.0)]
```

As expected, the number of features with nonzero weights is `4`. Select them, since they're the most informative to conduct any further analysis. That is, demonstrate the effectiveness of the method and that you can apply it safely in most feature selection situations in order to quickly have a working selection of useful features to be used in logistic or linear regression models as well as in other linear models.

Wrapping everything in a pipeline

As a concluding topic, we will discuss how to wrap the operations of transformation and selection we have seen so far together, into a single command, a pipeline that will take your data from source to your machine learning algorithm.

Wrapping all of your data operations into a single command offers some advantages:

- Your code becomes clear and more logically constructed because pipelines force you to rely on functions for your operations (each step is a function).
- You treat the test data in the exact same way as your train data without code repetitions or the possibility of any mistakes being made in the process.
- You can easily grid search the best parameters on all the data pipelines you have devised, not just on the machine learning hyperparameters.

We distinguish between two kinds of wrappers, depending on the data flow you need to build: serial or parallel.

Serial processing means that your transformation steps are dependent one on the other, and consequently, they have to be executed in a certain sequence. For serial processing, Scikit-learn offers the `Pipeline` class, which can be found in the `pipeline` module.

On the other hand, parallel processing implies that all of your transformations just take origin from the same data and that they can be easily executed by separate processes, whose results are to be gathered together at the end. Scikit-learn also has a class for parallel processing, `FeatureUnion`, which again is in the `pipeline` module. The interesting aspect of `FeatureUnion` is that it can parallelize any serial pipeline, too.

Combining features together and chaining transformations

What's the best way to figure out how `FeatureUnion` and `Pipeline` operate? Just recall how the Scikit-learn API works: first, a class is instantiated, then it is fitted to some data, and then the same data (or some different data) is transformed based on the previous fitting. Instead of doing so along with your script, you just instruct a pipeline by providing tuples containing the name of the step and the command to be executed. According to the sequence, the operations will be executed by your Python's thread or distributed to different threads on multiple processors.

In our example, we are trying to replicate our previous example, building a logistic regression classifier by stability selection. First, we add some unsupervised learning and feature creation on top of it. We start by setting up the problem by creating train and test datasets:

```
In: import numpy as np
    from sklearn.model_selection import train_test_split
    from sklearn.datasets import make_classification
    from sklearn.linear_model import LogisticRegression
    from sklearn.pipeline import Pipeline
    from sklearn.pipeline import FeatureUnion
    X, y = make_classification(n_samples=100, n_features=100,
                               n_informative=5,
                               n_redundant=2, random_state=101)
    X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                       test_size=0.30,
                                                       random_state=101)
    classifier = LogisticRegression(C=0.1, penalty='l1', random_state=101)
```

After doing so, we instruct the parallel execution of a PCA, a `KernelPCA`, and two custom transformers—one just passing the features as they are and the other one computing the inverse. You can expect each element in `transformer_list` to be fitted, the transformation applied, and all the results stacked together by column, but only when a `transform` method is executed (it is a lazy execution; defining `FeatureUnion` won't trigger any execution).

You will also find it useful to use the `make_pipeline` and `make_union` commands with the same results. In fact, these commands can produce the `FeatureUnion` and `Pipeline` classes, which are ready to set as an output. It is worth mentioning that they do not require you to name the steps since the naming will be done automatically by the function:

```
In: from sklearn.decomposition import PCA
    from sklearn.decomposition import KernelPCA
    from sklearn.preprocessing import FunctionTransformer

    def identity(x):
        return x

    def inverse(x):
        return 1.0 / x

    parallel = FeatureUnion(transformer_list=[
                ('pca', PCA()),
                ('kernelpca', KernelPCA()),
                ('inverse', FunctionTransformer(inverse)),
                ('original',FunctionTransformer(identity))], n_jobs=1)
```

Please note that we have set `n_jobs` to `1`, thus avoiding multiprocessing completely. That's because the `joblib` package, which is responsible for multicore parallelism on Scikit-learn, is not working properly with custom-made functions on a Jupyter Notebook running on Windows. If you are working on macOS or Linux, you can safely set `n_jobs` to multiple workers or set all the multicore resources on the problem (setting it to -1). However, when running on Windows, unless you are not using the custom function but picking them from a package, or you are running your code in a script having set the `__name__` variable to `__main__`, you will surely experience some problems. We already discussed this very same problem in more technical detail at the end of the *Building custom scoring functions* section in this chapter. Please also refer to our advice in the tip in that section for more insights into the problem.

After having defined the parallel operations, we can proceed to get the complete pipeline ready:

```
In: from sklearn.preprocessing import RobustScaler
    from sklearn.linear_model import RandomizedLogisticRegression
    from sklearn.feature_selection import RFECV
    selector = RandomizedLogisticRegression(n_resampling=300,
                                            random_state=101,
                                            n_jobs=1)
    pipeline = Pipeline(steps=[('parallel_transformations', parallel),
                               ('random_selection', selector),
                               ('logistic_reg', classifier)])
```

One great advantage of having a complete pipeline of transformation and learning put together is the possibility to control all of its parameters. We can test a grid search on the pipeline in order to find the best configuration of the hyperparameters:

```
In: from sklearn import model_selection
    search_dict = {'logistic_reg__C':[10,1,0.1], 'logistic_reg__penalty':
                  ['l1','l2']}
    search_func = model_selection.GridSearchCV(estimator=pipeline,
    param_grid =search_dict, scoring='accuracy', n_jobs=1,
    iid=False, refit=True, cv=10)
    search_func.fit(X_train,y_train)
    print (search_func.best_estimator_)
    print (search_func.best_params_)
    print (search_func.best_score_)
```

When defining your parameter grid search, you can refer to the different parts of the pipeline by writing its name, adding a couple of underscores, and then the name of the parameters to tweak. For instance, acting on the `C` hyperparameter of the logistic regression requires you to address it as `'logistic_reg__C'`. If a parameter is nested in multiple pipelines, you just have to name them all, separated by a double underscore, as if you were navigating into a disk directory.

Since a double underscore is used to structure the hierarchy of a pipeline's steps and hyperparameters, you cannot use it when naming the steps of your pipeline.

As a concluding step, we just use the resulting search for predictions on the test set. When this is done, Python will execute the complete pipeline, with the hyperparameters set by the grid search, and provide you with the result. You do not have to worry about replicating to the test set what you've done on the train set; a set of instructions in a pipeline will always assure consistency and reproducibility to your data munging operations:

```
In: from sklearn.metrics import classification_report
    print (classification_report(y_test, search_func.predict(X_test)))

Out:             precision    recall  f1-score   support

              0       0.94      0.94      0.94        17
              1       0.92      0.92      0.92        13

    avg / total       0.93      0.93      0.93        30
```

Building custom transformation functions

As you will have noticed, in our example, we used a couple of custom transformation functions, an identity, and an inverse, in order to have the original features along the transformed one and to make features inverse. Custom transformations can help you deal with the specific munging you have in mind for your problem, and you will also find them useful because they can act as a filter by filtering unwanted or erroneous values.

You can create a custom transformation just by applying the `FunctionTransformer` function from `sklearn.preprocessing`, which turns any function into a Scikit-learn class with the fit and transform method. Creating a transformation from scratch may help to make things clear for you regarding how it works.

First, you have to create a class. Let's see an example for filtering certain columns, which you previously defined from your dataset:

```
In: from sklearn.base import BaseEstimator, TransformerMixin

    class filtering(BaseEstimator, TransformerMixin):
        def __init__(self, columns):
            self.columns = columns

        def fit(self, X, y=None):
            return self

        def transform(self, X):
            if len(self.columns) == 0:
                return X
            else:
                return X[:,self.columns]
```

Using the `__init__` method, you can define the parameters to instantiate the class. In this case, you just record a list with the position of the columns you want to filter. Then, you have to prepare both a `fit` and `transform` method for the class.

In the case of our example, the `fit` method just returns itself. In different situations, it may be useful to use the `fit` method in order to keep track of characteristics of the training set that you will later have to apply on the test set (for instance, the mean and the variance of the features, the maximum and minimum, and so on).

The real operation that you want to achieve on data is executed in the `transform` method.

As you may recall, since Scikit-learn operates internally using NumPy arrays, it is important to treat the data that you transform as a NumPy array.

After defining the class, you can wrap it in a `Pipeline` or a `FeatureUnion` according to your needs. In our example, we just created a pipeline by selecting the first five features of the training set and operating a PCA transformation on them:

```
In: ff = filtering([1,2,3])
    ff.fit_transform(X_train)

Out: array([[ 0.78503915,  0.84999568, -0.63974955],
            [-2.4481912 , -0.38522917, -0.14586868],
            [-0.6506899 ,  1.71846072, -1.14010846],
            ...
```

Summary

In this chapter, we extracted significant meanings from data by applying a number of advanced data operations, from EDA and feature creation to dimensionality reduction and outlier detection.

More importantly, we started developing, with the help of many examples, our data pipeline. This was achieved by encapsulating a train/cross-validation/test setting into our hypothesis, which was expressed in terms of various activities – from data selection and transformation to the choice of learning algorithm and its best hyperparameters.

In the next chapter, we will delve into the principal machine learning algorithms offered by the Scikit-learn package, such as linear models, support vectors machines, ensembles of trees, and unsupervised techniques for clustering, among others.

4
Machine Learning

Having illustrated all the data preparation steps in a data science project, we have finally arrived at the learning phase, where learning algorithms are applied. To introduce you to the most effective machine learning tools that are readily available in scikit-learn and in other Python packages, we have prepared a brief introduction to all the major families of algorithms. We completed it with examples and tips on the hyper-parameters that guarantee the best possible results.

In this chapter, we will present the following topics:

- Linear and logistic regression
- Naive Bayes
- K-Nearest Neighbors (k-NN)
- Support Vector Machines (SVM)
- Ensemble solutions
- Bagged and boosted classifiers
- Stochastic gradient-based classification and regression for big data
- Unsupervised clustering with K-means and DBSCAN

Neural networks and deep learning, instead, will be dealt with in the following chapter.

Preparing tools and datasets

As introduced in the previous chapters, the Python package for machine learning with the lion's share is scikit-learn. In this chapter, we also will use XGboost, LightGBM, and Catboost: you'll find the instructions in the relevant sections.

The motivations for using scikit-learn developed at Inria, the French Institute for Research in Computer Science and Automation (`inria.fr/en/`), are multiple. It is worthwhile at this point to mention the most important reasons for using scikit-learn for the success of your data science project:

- A consistent API (`fit`, `predict`, `transform`, and `partial_fit`) across models that naturally helps to correctly implement data science procedures working on data organized in NumPy arrays
- A complete selection of well-tested and scalable classical models for machine learning, offering many out-of-core implementations for learning from data that won't fit in your RAM memory
- A steady development with many new additions in the pipeline thanks to a group of top contributors (Andreas Mueller, Olivier Grisel, Fabian Pedregosa, Gael Varoquaux, Gilles Loupe, Peter Prettenhofer, and many others)
- Extensive documentation with many examples, to be consulted online or inline using the `help` command

In this chapter, we will apply scikit-learn's machine learning algorithms to some example datasets. We will put apart the very instructive but too commonly used Iris and Boston datasets to demonstrate machine learning as applied to more real-life datasets. We have selected interesting examples from the following:

- The machine learning dataset repository (`mldata.org`) hosted by Technische Universität at Berlin
- The UCI machine learning repository (`archive.ics.uci.edu/ml/datasets.html`)
- LIBSVM datasets (offered by Chih-Jen Lin from National Taiwan University)

To let you have such datasets, and not having to rely on an internet connection every time you want to test the examples, we advise you to download them and store them on your hard disk. Consequently, we have prepared some scripts for automatic downloading of the datasets that will be placed exactly in the directory in which you are working with Python, thus rendering easier data access:

```
In: import pickle
    import urllib
    import ssl
    ssl._create_default_https_context = ssl._create_unverified_context
    from sklearn.datasets import fetch_mldata
    from sklearn.datasets import load_svmlight_file
    from sklearn.datasets import fetch_covtype
    from sklearn.datasets import fetch_20newsgroups
    mnist = fetch_mldata("MNIST original")
    pickle.dump(mnist, open("mnist.pickle", "wb"))
    target_page =
'http://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/binary/ijcnn1.bz2'
    with urllib.request.urlopen(target_page) as response:
         with open('ijcnn1.bz2','wb') as W:
             W.write(response.read())
    target_page =
'http://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/regression/cadata'
    cadata = load_svmlight_file(urllib.request.urlopen(target_page))
    pickle.dump(cadata, open("cadata.pickle", "wb"))

    covertype_dataset = fetch_covtype(random_state=101, shuffle=True)
    pickle.dump(covertype_dataset, open(
                                "covertype_dataset.pickle", "wb"))

    newsgroups_dataset = fetch_20newsgroups(shuffle=True,
              remove=('headers', 'footers', 'quotes'), random_state=6)

    pickle.dump(newsgroups_dataset, open(
                                 "newsgroups_dataset.pickle", "wb"))
```

If any part of the download procedure doesn't work for you, we will provide you a direct download for the datasets. After getting our compressed zip package, all you will have to do is unpack its data into the current working Python directory, which you can discover by running on your Python interface (a Jupyter notebook or any Python IDE) using this command:

```
In: import os
    print ("Current directory is: "%s"" % (os.getcwd()))
```

You can test all the algorithms in the book with other open source and free to use datasets if you feel like. Google provides a search engine for looking for the right data for your experiments at `https://toolbox.google.com/datasetsearch`: you just ask the search engine what you are looking for.

Linear and logistic regression

Linear and logistic regressions are the two methods that can be used to linearly predict a target value or a target class, respectively. Let's start with an example of linear regression predicting a target value.

In this section, we will again use the Boston dataset, which contains 506 samples, 13 features (all real numbers), and a (real) numerical target (which renders it ideal for regression problems). We will divide our dataset into two sections by using a train/test split cross-validation to test our methodology (in the example, 80 percent of our dataset goes in training and 20 percent in the test set):

```
In: from sklearn.datasets import load_boston
    boston = load_boston()
    from sklearn.model_selection import train_test_split
    X_train, X_test, Y_train, Y_test = train_test_split(boston.data,
                                  boston.target, test_size=0.2,
random_state=0)
```

The dataset is now loaded and the train/test pairs have been created. In the next few steps, we're going to train and fit the regressor in the training set and predict the target variable in the test dataset. We are then going to measure the accuracy of the regression task by using the MAE score (as explained in `Chapter 3`, *The Data Pipeline*). As for the scoring function, we decided for the mean absolute error, to penalize errors just proportionally to the size of the error itself (using the more common mean squared error would have emphasized larger errors more, since errors are squared):

```
In: from sklearn.linear_model import LinearRegression
    regr = LinearRegression()
    regr.fit(X_train, Y_train)
    Y_pred = regr.predict(X_test)

    from sklearn.metrics import mean_absolute_error
    print ("MAE", mean_absolute_error(Y_test, Y_pred))

Out: MAE 3.84281058945
```

Great! We achieved our goal in the simplest possible way. Now let's take a look at the time needed to train the system:

```
In: %timeit regr.fit(X_train, y_train)

Out: 544 µs ± 37.4 µs per loop
      (mean ± std. dev. of 7 runs, 1000 loops each)
```

That was really quick! The results, of course, are not all that great (if you see the comparison with another regressor based on Random Forest in the Jupyter notebook presented earlier in the book, in `Chapter 1`, *First Steps*). However, linear regression offers a very good trade-off between performance against the speed of training and simplicity. Now, let's take a look under the hood of the algorithm. Why is it so fast but not that accurate? The answer is somewhat expected—this is because it's a very simple linear method.

Let's briefly dig into a mathematical explanation of this technique. Let's name *X(i)* the *ith* sample (it is actually a row vector of numerical features) and *Y(i)* its target. The goal of linear regression is to find a good weight (column) vector *W*, which is best suited at approximating the target value when multiplied by the observation vector, that is, *X(i) * W* ≈ *Y(i)* (note that this is a dot product). *W* should be the same, and the best for every observation. Thus, solving the following equation becomes easy:

$$\begin{bmatrix} X(0) \\ X(1) \\ . \\ . \\ . \\ X(n) \end{bmatrix} * W = \begin{bmatrix} Y(0) \\ Y(1) \\ . \\ . \\ . \\ Y(n) \end{bmatrix}$$

W can be found easily with the help of a matrix inversion (or, more likely, a pseudo-inversion, which is a computationally efficient way) and a dot product. Here's the reason linear regression is so fast. Note that this is a simplistic explanation—the real method adds another virtual feature to compensate for the bias of the process. Yet, this does not change the complexity of the regression algorithm much.

We progress now to logistic regression. In spite of what the name suggests, it is a classifier and not a regressor. It must be used in classification problems where you are dealing with only two classes (binary classification). Typically, target labels are Boolean; that is, they have values as either True/False or 0/1 (indicating the presence or absence of the expected outcome). In our example, we keep on using the same dataset. The target is to guess whether a house value is over or under the average of a threshold value we are interested in. In essence, we moved from a regression problem to a binary classification one because now our target is to guess how likely an example is to be a part of a group. We start preparing the dataset by using the following commands:

```
In: import numpy as np
    avg_price_house = np.average(boston.target)
    high_priced_idx = (Y_train >= avg_price_house)
    Y_train[high_priced_idx] = 1
```

```
        Y_train[np.logical_not(high_priced_idx)] = 0
        Y_train = Y_train.astype(np.int8)
        high_priced_idx = (Y_test >= avg_price_house)
        Y_test[high_priced_idx] = 1
        Y_test[np.logical_not(high_priced_idx)] = 0
        Y_test = Y_test.astype(np.int8)
```

Now we will train and apply the classifier. To measure its performance, we will simply print the classification report:

```
In: from sklearn.linear_model import LogisticRegression
    clf = LogisticRegression()
    clf.fit(X_train, Y_train)
    Y_pred = clf.predict(X_test)
    from sklearn.metrics import classification_report
    print (classification_report(Y_test, Y_pred))

 Out:
             precision    recall  f1-score   support

          0       0.81      0.92      0.86        61
          1       0.85      0.68      0.76        41

avg / total       0.83      0.82      0.82       102
```

The output of this command can change on your machine depending on the optimization process of the `LogisticRegression` classifier (no seed has been set for replicability of the results).

The `precision` and `recall` values are over `80` percent. This is already a good result for a very simple method. The training speed is impressive, too. Thanks to Jupyter Notebook, we can have a comparison of the algorithm with a more advanced classifier in terms of performance and speed:

```
In: %timeit clf.fit(X_train, y_train)

Out: 2.75 ms ± 120 µs per loop (mean ± std. dev. of 7 runs, 100 loops each)
```

What's under the hood of a logistic regression? The simplest classifier a person could imagine (apart from a mean) is a linear regressor followed by a hard threshold:

$$y\_pred_i = sign\ (X_i * W)$$

Here, *sign(a)* = *+1* if *a* is greater or equal than zero, and 0 otherwise.

To smooth down the hardness of the threshold and predict the probability of belonging to a class, logistic regression resorts to the `logit` function. Its output is a (0 to 1) real number (0.0 and 1.0 are attainable only via rounding; otherwise, the *logit* function just tends toward them), which indicates the probability that the observation belongs to class 1. Using a formula, that becomes as follows:

$$Prob(y_i = +1 \mid X_i) = logistic(X_i . W)$$

In the above formula, you have: logistic(α) = $e^{\alpha}/(1+e^{\alpha})$.

Why the *logistic* function instead of some other function? Well, because it just works pretty well in most real cases. In the remaining cases, if you're not completely satisfied with its results, you may want to try some other nonlinear functions instead (there is a limited variety of suitable ones, though).

Naive Bayes

Naive Bayes is a very common classifier used for probabilistic binary and multiclass classification. Given the feature vector, it leverages the Bayes rule to predict the probability of each class. It's often applied to text classification since it's very effective with large and fat data (that is a data set with many features), characterized by a consistent a priori probability, handling effectively the curse of dimensionality issue.

There are three kinds of Naive Bayes classifiers; each of them has strong assumptions (hypotheses) about the features. If you're dealing with real/continuous data, the Gaussian Naive Bayes classifier assumes that features are generated from a Gaussian process (that is, they are normally distributed). Alternatively, if you're dealing with an event model where events can be modeled with a multinomial distribution (in such a case, features are counters or frequencies), you need to use the Multinomial Naive Bayes classifier. Finally, if all your features are independent and Boolean, and it is safe to assume that they're the outcome of a Bernoulli process, you can use the Bernoulli Naive Bayes classifier.

Let's now try an example of the application of the Gaussian Naive Bayes classifier. Moreover, an example of text classification is given at the end of this chapter. You can test it working with a Naive Bayes by simply substituting the SGDClassifier of the example with a MultinomialNB.

In the following example, we're going to use the Iris dataset, assuming that the features are Gaussian ones:

```
In: from sklearn import datasets
    iris = datasets.load_iris()
    from sklearn.model_selection import train_test_split
    X_train, X_test, Y_train, Y_test = train_test_split(iris.data,
              iris.target, test_size=0.2, random_state=0)

In: from sklearn.naive_bayes import GaussianNB
    clf = GaussianNB()
    clf.fit(X_train, Y_train)
    Y_pred = clf.predict(X_test)

In: from sklearn.metrics import classification_report
    print (classification_report(Y_test, Y_pred))

Out:
             precision    recall  f1-score   support

          0       1.00      1.00      1.00        11
          1       0.93      1.00      0.96        13
          2       1.00      0.83      0.91         6

avg / total       0.97      0.97      0.97        30

In: %timeit clf.fit(X_train, y_train)

Out: 685 µs ± 9.86 µs per loop (mean ± std. dev. of 7 runs, 1000 loops
each)
```

The resulting model seems to have a good performance and a high training speed, although we shouldn't forget that our dataset is also very small. Now, let's see how it works on another multiclass problem.

The aim of the classifier is to predict the probability that a feature vector belongs to the *Ck* class. In the example, there are three classes (`setosa`, `versicolor`, and `virginica`). So, we need to compute the membership probability for all classes; to make the explanation simple, let's name them *1*, *2*, and *3*. Therefore, the goal of the Naive Bayes classifier for the *i*th observation is to compute the following:

$$Prob(Ck \mid X(i))$$

Here, *X(i)* is the vector of the features (in the example, it is composed of four real numbers), whose components are [*X(i, 0)*, *X(i, 1)*, *X(i, 2)*, *X(i, 3)*].

Using the Bayes rule, it becomes the following:

$$Prob(Ck \mid X(i)) = \frac{Prob(Ck)Prob(X(i) \mid Ck)}{Prob(X(i))}$$

We can describe the same formula, as follows:

The a-posteriori probability is the a-priori probability of the class multiplied by the likelihood and then divided by the evidence.

From this probability theory, we know that joint probability can be expressed as follows (simplifying the problem):

$$Prob(Ck, X(i,0), \ldots, X(i,n)) = Prob(X(i,0), \ldots, X(i,n) \mid Ck)$$

Then, the second factor of the multiplication can be rewritten as follows (conditional probability):

$$Prob(X(i,0) \mid Ck)Prob(X(x,1), \ldots, X(i,n) \mid Ck, X(i,0))$$

You can then use the conditional probability definition to express the second member of the multiplication. In the end, you'll have a very long multiplication:

$$Prob(Ck, X(i,0), \ldots, X(i,n)) = Prob(Ck)Prob(X(i,0 \mid Ck)Prob(X(i,1) \mid Ck, X(i,0))\ldots$$

The naive assumption is that each feature is considered conditionally independent of the other features when related to each class. Thus, the probabilities can be simply multiplied. The formula for the same is as follows:

$$Prob(X(i,0) \mid Ck, X(:)) = Prob(X(i,0) \mid Ck)$$

Therefore, wrapping up the math, to select the best class, the following formula is used:

$$Y_{pred}(i) = \underset{k=0,1,2,3}{argmax} \quad Prob(Ck)\prod_{k=0}^{n-1} Prob(X(i,k) \mid Ck)$$

That's a simplification because the evidence probability (the denominator of the Bayes rule) has been removed, since all the classes would have the same probability of the event.

From the previous formula, you can understand why the learning phase is so fast, as it's just a counting of occurrences.

Note that for this classifier, a corresponding regressor doesn't exist, but you can achieve modeling a continuous target variable by binning it, that is, by transforming it into classes (for instance, low, average, and high values for our housing price problem).

K-Nearest Neighbors

K-Nearest Neighbors, or simply k-NN, belongs to the class of instance-based learning, also known as **lazy classifiers**. It's one of the simplest classification methods because the classification is done by just looking at the K-closest examples in the training set (in terms of Euclidean distance or some other kind of distance) in the case that we want to classify. Then, given the K-similar examples, the most popular target (majority voting) is chosen as the classification label. Two parameters are mandatory for this algorithm: the neighborhood cardinality (K), and the measure to evaluate the similarity (although the Euclidean distance, or L2, is the most used and is the default parameter for most implementations).

Let's take a look at an example. We are going to use a large dataset, the `MNIST` handwritten digits. We will later explain why we decided using this dataset for our example. We intend to use only a small portion of it (1,000 samples) to keep the computational time reasonable, and we shuffle the observations to obtain better results (though as a consequence, your final output may be slightly different than ours):

```
In: from sklearn.utils import shuffle
    from sklearn.datasets import fetch_mldata
    from sklearn.model_selection import train_test_split

    import pickle
    mnist = pickle.load(open( "mnist.pickle", "rb" ))
    mnist.data, mnist.target = shuffle(mnist.data, mnist.target)
    # We reduce the dataset size, otherwise it'll take too much time to run
    mnist.data = mnist.data[:1000]
    mnist.target = mnist.target[:1000]
    X_train, X_test, y_train, y_test = train_test_split(mnist.data,
                               mnist.target, test_size=0.8, random_state=0)

In: from sklearn.neighbors import KNeighborsClassifier
    # KNN: K=10, default measure of distance (euclidean)
    clf = KNeighborsClassifier(3)
    clf.fit(X_train, y_train)
    y_pred = clf.predict(X_test)
```

```
In: from sklearn.metrics import classification_report
    print (classification_report(y_test, y_pred))

Out:
                precision    recall  f1-score   support

        0.0       0.79      0.91      0.85        82
        1.0       0.62      0.98      0.76        86
        2.0       0.88      0.68      0.76        77
        3.0       0.71      0.83      0.77        69
        4.0       0.68      0.88      0.77        91
        5.0       0.69      0.66      0.67        56
        6.0       0.93      0.86      0.89        90
        7.0       0.91      0.85      0.88       102
        8.0       0.91      0.41      0.57        73
        9.0       0.79      0.50      0.61        74

avg / total       0.80      0.77      0.76       800
```

The performance is not so high on this dataset. However, please keep under consideration that the classifier has to work on ten different classes. Now let's check the time the classifier needs for the training and predicting:

```
In: %timeit clf.fit(X_train, y_train)
Out: 1.18 ms ± 119 µs per loop (mean ± std. dev. of 7 runs,
     1000 loops each)

In: %timeit clf.predict(X_test)
Out: 179 ms ± 1.68 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

The training speed is exceptional. Now consider the algorithm. The training phase is just copying the data into some data structure the algorithm will later use and nothing else (that's the reason it is called a lazy learner). On the contrary, the prediction speed is connected to the number of samples you have in your training step and to the number of features composing it (that's actually the feature matrix number of elements). In all the other algorithms that we've seen, the prediction speed is independent of the number of training cases that we have in our dataset. In conclusion, we can say that k-NN is great for small datasets, but it's definitely not the algorithm you would use when dealing with big data.

Just one last remark about this classification algorithm—you can also try the analogous regressor, `KNeighborsRegressor`, which works in the same way. Its algorithm is pretty much the same, except that the predicted value is the average of the K-target values of the neighborhood.

Nonlinear algorithms

Support Vector Machine (**SVM**) is a powerful and advanced supervised learning technique for classification and regression that can automatically fit linear and nonlinear models.

SVM algorithms have quite a few advantages against other machine learning algorithms:

- They can handle the majority of supervised problems such as regression, classification, and anomaly detection (anyway, they are actually best at binary classification).
- They provide a good handling of noisy data and outliers. They tend to overfit less, since they only work with some particular examples, the support vectors.
- They work fine with datasets presenting more features than examples, though, as with other machine learning algorithms, SVM would gain both from dimensionality reduction and feature selection.
- As for drawbacks, we have to mention these:
- They provide only estimates, but no probabilities unless you run some time-consuming and computationally intensive probability calibration by means of Platt scaling
- They scale super-linearly with the number of examples (so they cannot work with very large datasets)

Scikit-learn offers an implementation based on LIBSVM, a complete library of SVM classification and regression implementations, and LIBLINEAR, a scalable library for linear classification ideal of large datasets, especially any sparse text-based one. Both libraries have been developed at the National Taiwan University, and both have been written in C++ with a C API to interface with other languages. Both libraries have been extensively tested (being free, they have been used in other open source machine learning toolkits) and have long since been proven to be both fast and reliable. The C API explains well two tricky needs for them to operate optimally under the Python scikit-learn:

- LIBSVM, when operating, needs to reserve some memory for kernel operations. The `cache_size` parameter is used to set the size of the kernel cache, which is specified in megabytes. Though the default value is 200, it is advisable to raise it to 500 or 1000, depending on your available resources.
- They both expect C-ordered NumPy `ndarray` or SciPy `sparse.csr_matrix` (a row-optimized sparse matrix kind), preferably with float64 type. If the Python wrapper receives them under a different data structure, it will have to copy the data in a suitable format, slowing down the training process and consuming more RAM memory.

Neither LIBSVM or LIBLINEAR offer an implementation capable of handling large datasets. SGDClassifier and SGDRegressor are the scikit-learn classes that can produce a solution in a reasonable computational time, even when data is too big to fit into memory. They will be discussed in the following paragraph about handling big data.

SVM for classification

The implementations for SVM classification offered by scikit-learn are shown here:

Class	**Purpose**	**Hyperparameters**
`sklearn.svm.SVC`	The LIBSVM implementation for binary and multiclass linear and kernel classification	C, kernel, degree, and gamma
`sklearn.svm.NuSVC`	Same as for the .SVC version	nu, kernel, degree, and gamma
`sklearn.svm.OneClassSVM`	Unsupervised detection of outliers	nu, kernel, degree, and gamma
`sklearn.svm.LinearSVC`	Based on LIBLINEAR; it is a binary and multiclass linear classifier	Penalty, loss, and C

As an example for classification using SVM, we will use SVC with both a linear and an RBF kernel (**RBF** stands for **Radial Basis Function**, which is an effective nonlinear function). LinearSVC will instead be employed for a complex problem presenting a large number of observations (standard SVC won't perform well when working on more than 10,000 observations, due to the growing cubic complexity; LinearSVC can instead scale linearly).

For our first classification example, a binary one, we'll take on a dataset from the IJCNN'01 neural network competition. It is a time series of 50,000 samples produced by a physical system of a 10-cylinder internal combustion engine. Our target is binary: normal engine firing or misfiring. We will use the dataset as retrieved from the LIBSVM website using the scripts at the beginning of the chapter. The data file is in the LIBSVM format and it is compressed by Bzip2. We operate on it using the `load_svmlight_file` function from scikit-learn:

```
In: from sklearn.datasets import load_svmlight_file
    X_train, y_train = load_svmlight_file('ijcnn1.bz2')
    first_rows = 2500
    X_train, y_train = X_train[:first_rows,:], y_train[:first_rows]
```

For exemplification purposes, we will limit the number of observations from 25,000 to 2,500. The number of available features is 22. Furthermore, we won't preprocess the data, since it is already compatible with the SVM requirements, having already rescaled features in the range between 0 and 1:

```
In: import numpy as np
    from sklearn.model_selection import cross_val_score
    from sklearn.svm import SVC
    hypothesis = SVC(kernel='rbf', random_state=101)
    scores = cross_val_score(hypothesis, X_train, y_train,
                             cv=5, scoring='accuracy')
    print ("SVC with rbf kernel -> cross validation accuracy: \
            mean = %0.3f std = %0.3f" % (np.mean(scores), np.std(scores)))

Out: SVC with rbf kernel -> cross validation accuracy:
     mean = 0.910 std = 0.001
```

In our example, we tested an SVC with an RBF kernel. All the other parameters were kept at the default values. You can try to modify `first_rows` to larger values (up to 25,000) and verify how well the algorithm scales up to an increase in the number of observations. Keeping track of the computation time, you will notice that the scaling is not linear; that is, the computation time will increase more than proportionally with the size of the data. Concerning the SVM scalability, it is interesting to see how such an algorithm behaves when faced with a multiclass problem and a large number of cases. The Covertype dataset, which we are going to use, features as examples a large number of 30x30 meter patches of forest in the US. The data pertaining to them is collected for the task of predicting the dominant species of tree of each patch (cover type). It is a multiclass classification problem (seven `covertypes` to predict). Each sample has 54 features, and there are over 580,000 examples (but for performance reasons, we will work with just 25,000 of such cases). Moreover, the classes are unbalanced, having two kinds of trees with most examples.

Here is the script that you can use to load the previously prepared dataset:

```
In: import pickle
    covertype_dataset = pickle.load(open("covertype_dataset.pickle", "rb"))
    covertype_X = covertype_dataset.data[:25000,:]
    covertype_y = covertype_dataset.target[:25000] -1
```

Using this script, you can have an idea of the examples, features, and targets to be predicted:

```
In: import numpy as np
    covertypes = ['Spruce/Fir', 'Lodgepole Pine', 'Ponderosa Pine',
                  'Cottonwood/Willow', 'Aspen', 'Douglas-fir', 'Krummholz']
    print ('original dataset:', covertype_dataset.data.shape)
    print ('sub-sample:', covertype_X.shape)
```

```
        print('target freq:', list(zip(covertypes,np.bincount(covertype_y))))

    Out: original dataset: (581012, 54)
         sub-sample: (25000, 54)
         target freq: [('Spruce/Fir', 9107), ('Lodgepole Pine', 12122),
         ('Ponderosa Pine', 1583), ('Cottonwood/Willow', 120), ('Aspen', 412),
         ('Douglas-fir', 779), ('Krummholz', 877)]
```

Suppose we consider that since we have seven classes, we will need to train seven different classifiers focused on predicting a single class against the others (one-versus-rest is the default behavior for `LinearSVC` in multiclass problems). We will then have 175,000 data points for each cross-validation test (so it has to be repeated three times if cv=3). This is quite a challenge for many algorithms, considering that there are 54 variables, but `LinearSVC` can demonstrate how to handle it in a reasonable amount of time:

```
    In: from sklearn.cross_validation import cross_val_score, StratifiedKFold
        from sklearn.svm import LinearSVC
        hypothesis = LinearSVC(dual=False, class_weight='balanced')
        cv_strata = StratifiedKFold(covertype_y, n_folds=3,
                                    shuffle=True, random_state=101)
        scores = cross_val_score(hypothesis, covertype_X, covertype_y,
                                 cv=cv_strata, scoring='accuracy')
        print ("LinearSVC -> cross validation accuracy: \
               mean = %0.3f std = %0.3f" % (np.mean(scores), np.std(scores)))

    Out: LinearSVC -> cross validation accuracy: mean = 0.645 std = 0.007
```

The resulting accuracy is `0.65`, which is a good result. Yet, it surely leaves room for some further improvement. On the other hand, the problem seems to be a nonlinear one, though applying SVC with a nonlinear kernel would result in a very long training process as the number of observations is large. We will reprise this problem in the following examples by using other nonlinear algorithms in order to check whether we can improve the score obtained by `LinearSVC`.

SVM for regression

As for regression, the SVM algorithms presented by scikit-learn are shown here:

Class	Purpose	Hyperparameters
`sklearn.svm.SVR`	The LIBSVM implementation for regression	C, kernel, degree, gamma, and epsilon
`sklearn.svm.NuSVR`	Same as for .SVR	nu, C, kernel, degree, and gamma

To provide an example of regression, we decided on a dataset of real estate prices of houses in California (a slightly different problem than the previously seen Boston housing prices dataset):

```
In: import pickle
    X_train, y_train = pickle.load(open( "cadata.pickle", "rb" ))
    from sklearn.preprocessing import scale
    first_rows = 2000
    X_train = scale(X_train[:first_rows,:].toarray())
    y_train = y_train[:first_rows]/10**4.0
```

The cases from the dataset are reduced to `2,000` for performance reasons. The features have been scaled to avoid the influence of the different scale of the original variables. Also, the target variable is divided by `1,000` to render it more readable in thousand-dollar values:

```
In: import numpy as np
    from sklearn.cross_validation import cross_val_score
    from sklearn.svm import SVR
    hypothesis = SVR()
    scores = cross_val_score(hypothesis, X_train, y_train, cv=3,
                             scoring='neg_mean_absolute_error')
    print ("SVR -> cross validation accuracy: mean = %0.3f \
    std = %0.3f" % (np.mean(scores), np.std(scores)))

Out: SVR -> cross validation accuracy: mean = -4.618 std = 0.347
```

The chosen error is the mean absolute error, which is reported by the `sklearn` class as a negative number (but it is actually to be interpreted without a sign; the negative sign is just a computational trick used by scikit-learn's internal functions).

Tuning SVM

Before we start working on the hyperparameters (which are typically a different set of parameters depending on the implementation), there are two aspects that are left to be clarified when working with an SVM algorithm.

The first is about the sensitivity of the SVM to variables of different scale and large numbers. Similar to other learning algorithms based on linear combinations, having variables at different scales leads the algorithm to be dominated by features with the larger range or variance. Moreover, extremely high or low numbers may cause problems in the optimization process of the learning algorithms. It is advisable to scale all the data at limited intervals, such as [0,+1], which is a necessary choice if you are working with sparse arrays. In fact, it is desirable to preserve zero entries. Otherwise, data will become dense, consuming more memory. You can also scale the data into the [-1,+1] interval. Alternatively, you can standardize them to zero mean and unit variance. You can use, from the preprocessing module, the `MinMaxScaler` and `StandardScaler` utility classes by first fitting them on the training data and then transforming both the train and test sets.

The second aspect is regarding unbalanced classes. The algorithm tends to favor the frequent classes. A solution, apart from resampling or downsampling (reducing the majority class to the same number of the lesser one), is to weigh the C penalty parameter according to the frequency of the class (low values will penalize the class more, high values less). There are two ways to achieve this with respect to the different implementations; first, there is the `class_weight` parameter in SVC (which can be set to the keyword `balanced`, or provided with a dictionary containing specific values for each class). Then, there is also the `sample_weight` parameter in the `.fit()` method of `SVC`, `NuSVC`, `SVR`, `NuSVR`, and `OneClassSVM` (it requires a one-dimensional array as input, where each position refers to the weight of each training example).

Having dealt with scale and class balance, you can exhaustively search for optimal settings of the other parameters using `GridSearchCV` from the `model_selection` module in sklearn. Though SVM works fine with default parameters, they are often not optimal, and you need to test various value combinations using cross-validation in order to find the best ones.

According to their importance, you have to set the following parameters:

- `C`: The penalty value. Decreasing it makes the margin larger, thus ignoring more noise but also making the model more generalizable. A best value can be normally considered in the range of `np.logspace(-3, 3, 7)`.
- `kernel`: The non-linearity workhorse for SVM can be set to linear, poly, rbf, sigmoid, or a custom kernel (for experts!). The most commonly used one is certainly `rbf`.
- `degree`: This works with `kernel='poly'`, signaling the dimensionality of the polynomial expansion. Instead, it is ignored by other kernels. Usually, setting its value from 2 to 5 works the best.

- `gamma`: A coefficient for `'rbf'`, `'poly'`, and `'sigmoid'`. High values tend to fit data in a better way but can lead to some overfitting. Intuitively, we can imagine gamma as the influence that a single example exercises on the model. Low values make the influence of each example felt quite far. Since many points have to be considered, the SVM curve will tend to take a shape less influenced by local points and the result will be a morbid contour curve. High values of gamma, instead, make the curve take into account more of how points are arranged locally. Many small bubbles explicating the influence exerted by local points will usually represent the results. The suggested grid search range for this hyperparameter is `np.logspace(-3, 3, 7)`.
- `nu`: For regression and classification with `nuSVR` and `nuSVC`, this parameter approximates the training points that are not classified with confidence, that is, mis-classified points and correct points inside or on the margin. It should be in the range of [0,1], since it is a proportion relative to your training set. In the end, it acts as C, with high proportions enlarging the margin.
- `epsilon`: This parameter specifies how much error SVR is going to accept by defining an epsilon large range where no penalty is associated with respect to the true value of the point. The suggested search range is `np.insert(np.logspace(-4, 2, 7),0,[0])`.
- `penalty`, `loss`, and `dual`: For LinearSVC, these parameters accept the ('l1','squared_hinge',False), ('l2','hinge',True), ('l2','squared_hinge',True), and ('l2','squared_hinge',False) combinations. The ('l2','hinge',True) combination is analogous to the SVC (kernel='linear') learner.

As an example, we will load the IJCNN'01 dataset again, and we will try to improve the initial accuracy of 0.91 by looking for better degree, `C`, and `gamma` values. To save time, we will use the `RandomizedSearchCV` class to increase the accuracy to `0.989` (cross-validation estimate):

```
In: from sklearn.svm import SVC
    from sklearn.model_selection import RandomizedSearchCV
    X_train, y_train = load_svmlight_file('ijcnn1.bz2')
    first_rows = 2500
    X_train, y_train = X_train[:first_rows,:], y_train[:first_rows]
    hypothesis = SVC(kernel='rbf', random_state=101)
    search_dict = {'C': [0.01, 0.1, 1, 10, 100],
                   'gamma': [0.1, 0.01, 0.001, 0.0001]}
    search_func = RandomizedSearchCV(estimator=hypothesis,
                                     param_distributions=search_dict,
                                     n_iter=10, scoring='accuracy',
                                     n_jobs=-1, iid=True, refit=True,
                                     cv=5, random_state=101)
    search_func.fit(X_train, y_train)
    print ('Best parameters %s' % search_func.best_params_)
    print ('Cross validation accuracy: mean = %0.3f' %
            search_func.best_score_)

Out: Best parameters {'C': 100, 'gamma': 0.1}
     Cross validation accuracy: mean = 0.989
```

Ensemble strategies

Until now, we have seen single learning algorithms of growing complexity. Ensembles represent an effective alternative since they achieve better predictive accuracy by combining or chaining the results from models based on different data samples and algorithm settings. Ensemble strategies divide themselves into two branches. According to the method used, they assemble predictions together by the following:

- **Averaging algorithms**: These make predictions by averaging the results of various parallel estimators. The variations in the estimators provide further division into four families: pasting, bagging, subspaces, and patches.
- **Boosting algorithms**: These make predictions by using a weighted average of sequential aggregated estimators.

Before delving into some examples for both classification and regression, we will provide you with the necessary steps to reload the Covertype dataset, a multiclass classification problem that we started exploring before when dealing with linear SVC:

```
In: import pickle
    covertype_dataset = pickle.load(open("covertype_dataset.pickle", "rb"))
    print (covertype_dataset.DESCR)
    covertype_X = covertype_dataset.data[:15000,:]
    covertype_y = covertype_dataset.target[:15000]
    covertypes = ['Spruce/Fir', 'Lodgepole Pine', 'Ponderosa Pine',
                  'Cottonwood/Willow', 'Aspen', 'Douglas-fir', 'Krummholz']
```

Pasting by random samples

Pasting is the first type of averaging ensembling we will discuss. In pasting, a certain number of estimators are built using small samples taken from the data (using sampling without replacement). Finally, the results are pooled and the estimate is obtained by averaging the results, in the case of regression, or by taking the most voted class when dealing with classification. Pasting is very useful when dealing with very large data (such as the case where it cannot fit into the memory) because it allows dealing with only those portions of data manageable by the available RAM and computational resources of your computer.

As a method, Leo Breiman, the creator of the RandomForest algorithm, first devised this strategy. There are no specific algorithms in the scikit-learn package that leverage pasting, though it is easily achievable by using the available bagging algorithms (`BaggingClassifier` or `BaggingRegressor`, the topic of the following paragraph) and setting their `bootstrap` parameter to `False` and `max_features` to 1.0.

Bagging with weak classifiers

Bagging works with samples in a way that is similar to that of pasting, but it allows replacement. Also, theoretically elaborated by Leo Breiman, bagging is implemented in a specific scikit-learn class for regression and one for classification. You just have to decide the algorithm that you'd like to use for the training. Plug it into `BaggingClassifier`, or `BaggingRegressor` for regression problems, and set a sufficiently high number of estimators (and consequently a high number of samples):

```
In: import numpy as np
    from sklearn.model_selection import cross_val_score
    from sklearn.ensemble import BaggingClassifier
    from sklearn.neighbors import KNeighborsClassifier
    hypothesis = BaggingClassifier(KNeighborsClassifier(n_neighbors=1),
                                   max_samples=0.7, max_features=0.7,
                                   n_estimators=100)
    scores = cross_val_score(hypothesis, covertype_X, covertype_y, cv=3,
                                scoring='accuracy', n_jobs=-1)
    print ("BaggingClassifier -> cross validation accuracy: mean = %0.3f
    std = %0.3f" % (np.mean(scores), np.std(scores)))

Out: BaggingClassifier -> cross validation accuracy:
     mean = 0.795 std = 0.001
```

Weak predictors are good choices for the estimator to be used with bagging. A weak learner in classification or prediction is just an algorithm that performs poorly—just above the chance baseline with your data problem—because of its simplicity or high bias in estimation. Some good examples of this are Naive Bayes and K Nearest Neighbors. The advantage of using weak learners and ensembling them is that they can be trained more quickly than complex algorithms. Though weak in prediction, when combined, they usually achieve comparable or even better predictive performances than more sophisticated single algorithms.

Random Subspaces and Random Patches

With random Subspaces, estimators differentiate because of random subsets of the features. Again, such a solution is achievable by tuning the parameters of `BaggingClassifier` and `BaggingRegressor`, by setting `max_features` to a number less than 1.0, representing the percentage of features to be chosen randomly for each model of the ensemble.

Instead, in Random Patches, estimators are built on subsets of both samples and features.

Let's now examine in a table the different characteristics of pasting, bagging, random subspaces, and random patches as implemented using the `BaggingClassifier` and `BaggingRegressor` in scikit-learn:

Ensembling	**Purpose**	**Hyperparameters**
Pasting	A number of models are built using subsamples (sampling without replacement of samples smaller than the original dataset)	`bootstrap=False` `max_samples <1.0` `max_features=1.0`
Bagging	A number of models is built using random selections of bootstrapped cases (sampling with replacement of the same size of the original sample)	`bootstrap=True` `max_samples = 1.0` `max_features=1.0`
Random Subspaces	This is the same as bagging, but also features are sampled when each model is selected	`bootstrap=True` `max_samples = 1.0` `max_features<1.0`
Random Patches	This is the same as bagging, but also features are sampled when each model is selected	`bootstrap=False` `max_samples <1.0` `max_features<1.0`

When `max_features` or `max_samples` have to be less than 1.0, they can be set at any value in the range (0,1) and you can test the best one by grid search. As per our experience, if you need to limit or speed up your search, the values that work best most frequently are between 0.7 and 0.9.

Random Forests and Extra-Trees

Leo Breiman and Adele Cutler have originally devised the idea at the core of the Random Forests algorithms, and the name of the algorithm remains today a trademark of theirs (though the algorithm is open source). Random Forests are implemented in scikit-learn as `RandomForestClassifier` / `RandomForestRegressor`.

Random Forests works in a similar way as bagging, also devised by Leo Breiman, but it operates only using binary split decision trees, which are left to grow to their extremes. Moreover, it samples the cases to be used in each of its models using bootstrapping. And, as the tree is grown, at each split of a branch, the set of variables to be considered for the split is drawn randomly, too. In the end, that's the secret at the heart of the algorithm, because it ensembles trees that, due to different samples and considered variables at splits, are very different than each other. Being different, they are also uncorrelated. That's beneficial because when the results are ensembled, much variance is ruled out as in a mean the extreme values on both sides of a distribution tend to balance each other. In other words, bagging algorithms guarantee a certain level of diversity in the predictions, allowing for developing rules that a single learner (such as a decision tree) might never come across.

Extra-Trees, represented in scikit-learn by the `ExtraTreesClassifier`/`ExtraTreesRegressor` class, are a more randomized kind of Random Forests that produce a lower variance in the estimates, but at a price of greater bias of estimators. Anyway, when it comes to CPU efficiency, Extra-Trees can deliver a considerable speed-up compared to Random Forests, so they can be ideal when you are working with large datasets in terms of both examples and features. The reason for the resulting higher bias but better speed is the way splits are built in an Extra-Tree. Whereas Random Forests carefully search the best values to assign to each branch from among the sampled features to be considered for splitting a branch of a tree, in Extra-Trees this is decided randomly. So, there's no need for much computation, though the randomly chosen split may not be the most effective one (hence the bias).

Let's see how the two algorithms compare with the Covertype forest problem, both in terms of accuracy of the prediction and execution time. To do so, we will use the magic `%%time` cell in a Jupyter notebook's cell in order to measure computational performance:

```
In: import numpy as np
    from sklearn.model_selection import cross_val_score
    from sklearn.ensemble import RandomForestClassifier
    from sklearn.ensemble import ExtraTreesClassifier

In: %%time
    hypothesis = RandomForestClassifier(n_estimators=100, random_state=101)
    scores = cross_val_score(hypothesis, covertype_X, covertype_y,
                              cv=3, scoring='accuracy', n_jobs=-1)
    print ("RandomForestClassifier -> cross validation accuracy: \
            mean = %0.3f std = %0.3f" % (np.mean(scores), np.std(scores)))

Out: RandomForestClassifier -> cross validation accuracy:
     mean = 0.809 std = 0.009
     Wall time: 7.01 s

In: %%time
    hypothesis = ExtraTreesClassifier(n_estimators=100, random_state=101)
    scores = cross_val_score(hypothesis, covertype_X, covertype_y, cv=3,
                                             scoring='accuracy', n_jobs=-1)
    print ("ExtraTreesClassifier -> cross validation accuracy: mean = %0.3f
    std = %0.3f" % (np.mean(scores), np.std(scores)))

Out: ExtraTreesClassifier -> cross validation accuracy:
     mean = 0.821 std = 0.009
     Wall time: 6.48 s
```

For both algorithms, the key hyperparameters that should be set are as follows:

- `max_features`: This is the number of sampled features that are present at every split that can determine the performance of the algorithm. The lower the number, the speedier, but with higher bias.
- `min_samples_leaf` : This allows you to determine the depth of the trees. Large numbers diminish the variance and increase the bias.
- `bootstrap` : This is a Boolean that allows bootstrapping.
- `n_estimators` : This is the number of trees (remember that the more trees the better, but this comes at a computational cost that you have to take into account).

Both RandomForests and Extra-Trees are indeed parallel algorithms. Don't forget to set the appropriate number of `n_jobs` to speed up their execution. When classifying, they decide for the most voted class (majority voting); when regressing, they simply average the resulting values. As an exemplification, we propose a regression example based on the California house prices dataset:

```
In: import pickle
    from sklearn.preprocessing import scale
    X_train, y_train = pickle.load(open( "cadata.pickle", "rb" ))
    first_rows = 2000

In: import numpy as np
    from sklearn.ensemble import RandomForestRegressor
    X_train = scale(X_train[:first_rows,:].toarray())
    y_train = y_train[:first_rows]/10**4.
    hypothesis = RandomForestRegressor(n_estimators=300, random_state=101)
    scores = cross_val_score(hypothesis, X_train, y_train, cv=3,
                             scoring='neg_mean_absolute_error', n_jobs=-1)
    print ("RandomForestClassifier -> cross validation accuracy: mean =
%0.3f
    std = %0.3f" % (np.mean(scores), np.std(scores)))

Out: RandomForestClassifier -> cross validation accuracy:
     mean = -4.642 std = 0.514
```

Estimating probabilities from an ensemble

Random Forests offer a large range of advantages, and they are deemed the first algorithm you should try on your data to figure out what kind of results can be obtained. This is because the Random Forests do not have too many hyperparameters to be fixed, and they work perfectly fine out of the box. They can naturally work with multiclass problems. Moreover, Random Forests offer a way to estimate the importance of variables for your insight or feature selection, and they help in estimating the similarity between the examples since similar cases should end up in the same terminal leaves of many trees of the ensemble.

However, in classification problems, the algorithm lacks the capability of predicting probabilities of an outcome (unless calibrated using the probability calibration offered in scikit-learn by the `CalibratedClassifierCV`). In classification problems, often it does not suffice to predict a response label; we also need the probability associated to it (how likely it is to be true; that's a confidence of the prediction). This is particularly useful for multiclass problems since the right answer may be the second- or the third-most probable one (therefore, probability provides ranks of answers).

However, when Random Forests is required to estimate the probability of the response classes, the algorithm will just report the number of times an example has been classified into a class in the ensemble with respect to the number of all the trees in the ensemble itself. Such a ratio actually doesn't correspond to the correct probability, but it is a biased one (the predicted probability is just correlated to the true one; it doesn't represent it in a numerically correct way).

To help Random Forests and other algorithms affected by a similar situation, such as Naive Bayes or linear SVM, to emit correct response probabilities, the `CalibratedClassifierCV` wrapper class has been introduced in scikit-learn.

`CalibrateClassifierCV` remaps the response of a machine learning algorithm to probabilities using two methods: Platt's scaling and Isotonic regression (the latter is a better performing non-parameter method with the condition that you have enough examples, that is, at least 1,000). Both approaches are, kind of, a second-level model aimed at just modeling a link between the original response of an algorithm and the expected probabilities. The results can be plotted by comparing the original probability distribution against the calibrated ones.

As an example, here we refit the Covertype problem using `CalibratedClassifierCV`:

```
In: import pandas as pd
    import matplotlib.pyplot as plt
    from sklearn.calibration import CalibratedClassifierCV
    from sklearn.calibration import calibration_curve
    hypothesis = RandomForestClassifier(n_estimators=100, random_state=101)
    calibration = CalibratedClassifierCV(hypothesis, method='sigmoid',
                                         cv=5)
    covertype_X = covertype_dataset.data[:15000,:]
    covertype_y = covertype_dataset.target[:15000]
    covertype_test_X = covertype_dataset.data[15000:25000,:]
    covertype_test_y = covertype_dataset.target[15000:25000]
```

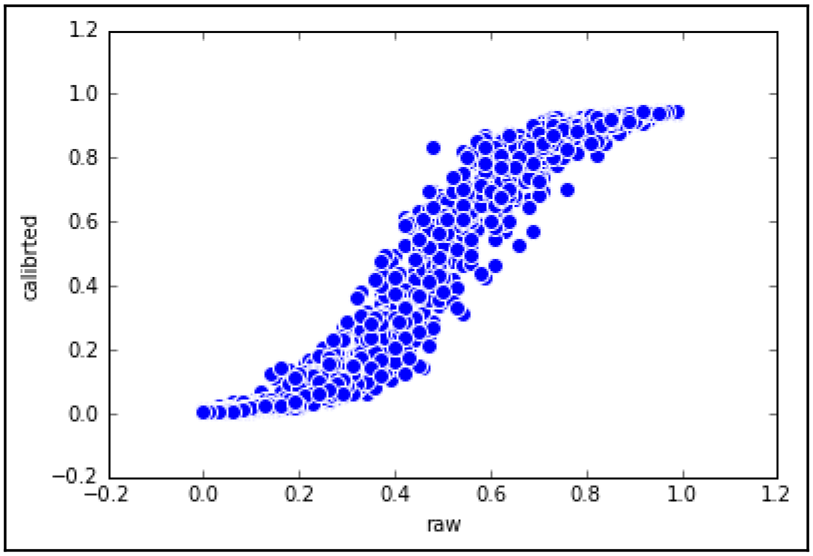
To evaluate the behavior of the calibration, we prepare a test set made of 10,000 examples that we do not use for training. Our calibration model will be based on Platt's model (`method='sigmoid'`) and use five cross-validation folds to tune the calibration:

```
In: hypothesis.fit(covertype_X,covertype_y)
    calibration.fit(covertype_X,covertype_y)
    prob_raw = hypothesis.predict_proba(covertype_test_X)
    prob_cal = calibration.predict_proba(covertype_test_X)
```

After fitting both the raw and the calibrated model, we estimate the probabilities, and we now plot them in a scatterplot to highlight the differences. After projecting the estimated probabilities for the ponderosa pine, it appears that the original Random Forests probabilities (actual percentages of votes) have been rescaled to resemble a logistic curve. We now try to write some code and explore the type of changes that calibration brings about to probability outputs:

```
In: %matplotlib inline
    tree_kind = covertypes.index('Ponderosa Pine')
    probs = pd.DataFrame(list(zip(prob_raw[:,tree_kind],
                                  prob_cal[:,tree_kind])),
                         columns=['raw','calibrted'])
    plot = probs.plot(kind='scatter', x=0, y=1, s=64,
                      c='blue', edgecolors='white')
```

Calibration, though not changing the performance of the model, by reshaping the probability output helps you obtain probabilities that are more correspondent to your training data. In the following plot you can observe how the calibration procedure has modified the original probabilities by adding some non-linearity as a correction:



Sequences of models – AdaBoost

AdaBoost is a boosting algorithm based on the Gradient Descent optimization method. It fits a sequence of weak learners (originally stumps, that is, single-level decision trees) on re-weighted versions of the data. Weights are assigned based on the predictability of the case. Cases that are more difficult are weighted more. The idea is that the trees first learn easy examples and then concentrate more on the difficult ones. In the end, the sequence of weak learners is weighted to maximize the overall performance:

```
In: import numpy as np
    from sklearn.ensemble import AdaBoostClassifier
    hypothesis = AdaBoostClassifier(n_estimators=300, random_state=101)
    scores = cross_val_score(hypothesis, covertype_X, covertype_y, cv=3,
                             scoring='accuracy', n_jobs=-1)
    print ("Adaboost -> cross validation accuracy: mean = %0.3f
    std = %0.3f" % (np.mean(scores), np.std(scores)))
    Out: Adaboost -> cross validation accuracy: mean = 0.610 std = 0.014
```

Gradient tree boosting (GTB)

Gradient boosting is another improved version of boosting. Like AdaBoost, it is based on a gradient descent function. The algorithm has proven to be one of the most proficient ones from the ensemble, though it is characterized by an increased variance of estimates, more sensibility to noise in data (both problems could be attenuated by using sub-sampling), and significant computational costs due to nonparallel operations.

To demonstrate how GTB performs, we will again try checking whether we can improve our predictive performance on the covertype dataset, which was already examined when illustrating linear SVM and ensemble algorithms:

```
In: import pickle
    covertype_dataset = pickle.load(open("covertype_dataset.pickle", "rb"))
    covertype_X = covertype_dataset.data[:15000,:]
    covertype_y = covertype_dataset.target[:15000] -1
    covertype_val_X = covertype_dataset.data[15000:20000,:]
    covertype_val_y = covertype_dataset.target[15000:20000] -1
    covertype_test_X = covertype_dataset.data[20000:25000,:]
    covertype_test_y = covertype_dataset.target[20000:25000] -1
```

After loading the data, the training sample size is limited to 15000 observations to achieve a reasonable training performance. We also extract a validation sample made of 5,000 examples and a test sample made of another 5,000 cases. We now proceed to train our model:

```
In: import numpy as np
    from sklearn.model_selection import cross_val_score, StratifiedKFold
    from sklearn.ensemble import GradientBoostingClassifier
    hypothesis = GradientBoostingClassifier(max_depth=5,
                                            n_estimators=50,
                                            random_state=101)
    hypothesis.fit(covertype_X, covertype_y)

In: from sklearn.metrics import accuracy_score
    print ("GradientBoostingClassifier -> test accuracy:",
             accuracy_score(covertype_test_y,
                            hypothesis.predict(covertype_test_X)))

Out: GradientBoostingClassifier -> test accuracy: 0.8202
```

To obtain the best performance from `GradientBoostingClassifier` and `GradientBoostingRegression`, you have to tweak the following:

- `n_estimators`: Exceeding with estimators, it increases variance. Anyway, if the estimators are not enough, the algorithm will suffer from high bias. The right number cannot be known a-priori and has to be found heuristically, by testing various configurations by cross-validation.
- `max_depth`: It increases the variance and complexity.
- `subsample`: It can effectively reduce variance of the estimates using values from 0.9 to 0.7.
- `learning_rate`: Smaller values can improve optimization in the training process, though that will require more estimators to converge, and thus more computational time.
- `in_samples_leaf`: This can reduce the variance due to noisy data, reserving overfitting to rare cases.

Apart from deep learning, gradient boosting is actually the most developed machine learning algorithm. Since Adaboost and the following Gradient Boosting implementation as developed by Jerome Friedman, there appeared various implementations of the algorithms, the most recent ones being XGBoost, LightGBM, and CatBoost. In the following paragraphs, we will be exploring these new solutions and testing them on the road using the Forest Covertype data.

XGBoost

XGBoost stands for **eXtreme Gradient Boosting**, an open source project that is not part of scikit-learn, though recently it has been expanded by a scikit-Learn wrapper interface that renders using models based on XGBoost more integrated into your data pipeline (`xgboost.readthedocs.io/en/latest/python/python_api.html#module-xgboost.sklearn`).

TIP

The XGBoost source code is available on GitHub, at `github.com/dmlc/XGBoost`; its documentation and some tutorials can be found at `xgboost.readthedocs.io/en/latest`.

The XGBoost algorithm has gained momentum and popularity in data-science competitions such as Kaggle (`www.kaggle.com`) and the KDD-cup 2015. As the authors (Tianqui Chen, Tong He, Carlos Guestrin) report on papers on the algorithm, among 29 challenges were held on Kaggle during 2015, and 17 winning solutions used XGBoost as a standalone solution or as part of an ensemble of multiple different models.

In their paper *XGBoost: A Scalable Tree Boosting System* (which can be found at `learningsys.org/papers/LearningSys_2015_paper_32.pdf`), the authors report that XGBoost was also used by every team that ended in the top 10 of the recent KDD-cup 2015.

Apart from the successful performances in both accuracy and computational efficiency, XGBoost is also a scalable solution from different points of view. XGBoost represents a new generation of GBM algorithms thanks to important tweaks to the initial tree boost GBM algorithm:

- A sparse-aware algorithm; it can leverage sparse matrices, saving both memory (no need for dense matrices) and computation time (zero values are handled in a special way).
- Approximate tree learning (weighted quantile sketch), which bears similar results but in much less time than the classical complete explorations of possible branch cuts.
- Parallel computing on a single machine (using multi-threading in the phase of the search for the best split) and similarly distributed computations on multiple ones.
- Out-of-core computations on a single machine leveraging a data storage solution called Column Block. This arranges data on disk by columns, thus saving time by pulling data from the disk as the optimization algorithm (which works on column vectors) expects it.
- XGBoost can also deal with missing data in an effective way. Other tree ensembles based on standard decision trees require missing data first to be imputed using an off-scale value, such as a negative number, in order to develop an appropriate branching of the tree to deal with missing values.

XGBoost, instead, first fits all the non-missing values. After having created the branching for the variable, it decides which branch is better for the missing values to take in order to minimize the prediction error. Such an approach leads to both trees that are more compact and an effective imputation strategy, leading to more predictive power.

From a practical point of view, XGBoost features mostly the same parameters as Scikit-learn's GBT. The key parameters are as follows:

- `eta`: An equivalent of the learning rate in Scikit-learn's GTB. It impacts how fast the algorithm is learning and thus how many trees are necessary. Higher values help with a better convergence of the learning process, but at the price of more training time and a larger number of trees.
- `gamma`: This acts as a stopping criterion in the tree development since it represents the minimum loss reduction required to make a further partition on a leaf node of the tree. Higher values make the learning more conservative.
- `min_child_weight`: These represent the minimum weight (examples) present on the leaf node of the tree. Higher values prevent overfitting and tree complexity.
- `max_depth`: The number of interactions in the trees.
- `subsample`: The fraction of examples from the training data to be used at each iteration.
- `colsample_bytree`: The fraction of features to be used at each iteration.
- `colsample_bylevel`: The fraction of features to be used at each branch splitting (as in Random Forests).

In our example of how to apply XGBoost, we first recall how to upload the Covertype dataset and divide it into train, validation, and test sets by partially slicing the initial NumPy array containing the complete dataset:

```
In: from sklearn.datasets import fetch_covtype
    from sklearn.model_selection import cross_val_score, StratifiedKFold
    covertype_dataset = fetch_covtype(random_state=101, shuffle=True)
    covertype_dataset.target = covertype_dataset.target.astype(int)
    covertype_X = covertype_dataset.data[:15000,:]
    covertype_y = covertype_dataset.target[:15000] -1
    covertype_val_X = covertype_dataset.data[15000:20000,:]
    covertype_val_y = covertype_dataset.target[15000:20000] -1
    covertype_test_X = covertype_dataset.data[20000:25000,:]
    covertype_test_y = covertype_dataset.target[20000:25000] -1
```

After loading the data, we define the hyperparameters by first setting the objective (as `multi:softprob`, but XGBoost offers other alternatives for regression, classification, multiclass, and ranking) and then set some of the preceding parameters.

When fitting the data, further indications can be given to the algorithm. In our case, we set `eval_metric` to accuracy for multiclass problems (`'merror'`) and provided an `eval_set` that is a validation set that XGBoost has to monitor during training by calculating the evaluation metric on it. If the training does not improve the evaluation metric for 25 rounds (as defined by `early_stopping_rounds`), then the training will stop before reaching the number of estimators (`n_estimators`) previously defined. This approach, called early-stop and derived from neural networks train, effectively helps avoid overfitting during the training phase:

For a complete list of both parameters and evaluation metrics, please see `github.com/dmlc/xgboost/blob/master/doc/parameter.md`. Here we start importing the package, setting its parameters and fitting it to our problem:

```
In: import xgboost as xgb
    hypothesis = xgb.XGBClassifier(objective= "multi:softprob",
                                   max_depth = 24,
                                   gamma=0.1,
                                   subsample = 0.90,
                                   learning_rate=0.01,
                                   n_estimators = 500,
                                   nthread=-1)
    hypothesis.fit(covertype_X, covertype_y,
                   eval_set=[(covertype_val_X, covertype_val_y)],
                   eval_metric='merror', early_stopping_rounds=25,
                   verbose=False)
```

To obtain the predictions, we just use the same methods as Scikit-learn API: `predict` and `predict_proba`. Printing the accuracy reveals how the long fitting of the XGBoost algorithm actually brought about the best test result so far. Examination of the confusion matrix reveals that only the aspen tree type is difficult to predict:

```
In: from sklearn.metrics import accuracy_score, confusion_matrix
    print ('test accuracy:', accuracy_score(covertype_test_y,
           hypothesis.predict(covertype_test_X)))
    print (confusion_matrix(covertype_test_y,
           hypothesis.predict(covertype_test_X)))

Out: test accuracy: 0.848
     [[1512   288     0     0     0     2    18]
      [ 215  2197    18     0     7    11     0]
      [   0    17   261     4     0    19     0]
      [   0     0     4    20     0     3     0]
      [   1    54     3     0    19     0     0]
      [   0    16    42     0     0    86     0]
      [  37     1     0     0     0     0   145]]
```

LightGBM

When your dataset contains a large number of cases or variables, even if XGBoost is compiled from C++, it really takes a long time to train. Therefore, in spite of the success of XGBoost, there was space in January 2017 for another algorithm to appear (XGBoost's first appearance is dated March 2015). It was the high-performance LightGBM, capable of being distributed and fast-handling large amounts of data, and developed by a team at Microsoft as an open source project.

Here is its GitHub page: `https://github.com/Microsoft/LightGBM`. And, here is the academic paper illustrating the idea behind the algorithm: `https://papers.nips.cc/paper/6907-lightgbm-a-highly-efficient-gradient-boosting-decision-tree`.

LightGBM is based on decision trees, as well as XGBoost, yet it follows a different strategy. Whereas XGBoost uses decision trees to split on a variable and exploring different cuts at that variable (the level-wise tree growth strategy), LightGBM concentrates on a split and goes on splitting from there in order to achieve a better fitting (this is the leaf-wise tree growth strategy). This allows LightGBM to reach first and fast a good fit of the data, and to generate alternative solutions compared to XGBoost (which is good, if you expect to blend, i.e. average, the two solutions together in order to reduce the variance of the estimated).

Algorithmically talking, figuring out as a graph the structures of cuts operated by a decision tree, XGBoost peruses a **breadth-first search** (**BFS**), whereas LightGBM a **depth-first search** (**DFS**).

Here are other highlights of the algorithm:

1. It has more complex trees due to the leaf-wise strategy leading to a higher accuracy in prediction but also to a higher risk of overfitting; therefore, it is particularly ineffective with small datasets (uses datasets with more than 10,000 examples).
2. It is faster on larger datasets.
3. It can leverage parallelization and GPU usage; therefore, it can be scaled on even larger problems (actually it is still a GBM, a sequential algorithm; what is parallelized is the *Find Best Split* part of the decision tree).
4. It is memory parsimonious because it doesn’t store and handles continuous variables as they are, but it turns them into discrete bins of values (histogram-based algorithms).

Tuning LightGBM may appear daunting with more than a hundred parameters to fix (you can find them all here: `https://github.com/Microsoft/LightGBM/blob/master/docs/Parameters.rst`), but, actually, you can just tune a few ones and get away with excellent results. Parameters in LightGBM are distinct in terms of the following:

- Core parameters, specifying the task to be done on data
- Control parameters, dictating how the decision trees behave
- Metric parameters, defying your error measures (and there is really a large list to choose from apart from the classical errors for classification and regression)
- IO parameters, mostly ruling about how inputs are dealt with

Here is a quick overview of the principal parameters for each category.

As for as core parameters, you can operate your key choices by the following:

- `task`: The task you want to achieve with your model; it could be `train`, `predict`, `convert_model` (to get it as a series of if-then statements), refit (for updating a model with new data).
- `application`: By default, the expected model is a regression, but it could be `regression`, `binary`, `multiclass` and many others (it is also available as `lambdarank` for ranking tasks such as in search engine optimization).
- `boosting`: LightGBM can use different algorithms for its learning iterations. The default is `gbdt`, the single decision tree, but it could be `rf` (random forest), `darts` (Dropouts meet Multiple Additive Regression Trees) or `goss` (Gradient-based One-Side Sampling).
- `device`: It is `cpu` by default, but you use `gpu` if you have one available on your system.

IO parameters define how data is loaded (and even stored by your model):

- `max_bin`: The maximum number of bins to be used for feature values to be bucketed in (the more, the less approximation when dealing with numeric variables but the more memory and computation time)
- `categorical_feature`: The index of categorical features
- `ignore_column`: The index of features to be ignored
- `save_binary`: If to save the data on disk in binary format to speed up loading and saving memory

Finally, by setting control parameters, you instead decide more specifically how the model has to learn from data:

- `num_boost_round`: The number of boosting iterations to be done.
- `learning_rate`: The rate each boosting iteration weights on the construction of the resulting model.
- `num_leaves`: The maximum number of leaves in a tree, which is 31 by default.
- `max_depth`: The maximum depth that a tree can reach.
- `min_data_in_leaf`: The minimum number of the examples for a leaf to be created.
- `bagging_fraction`: The fraction of data to be randomly used at each iteration.
- `feature_fraction`: When your boosting is rf, this parameter dictates the fraction of total features to be randomly considered for a split.
- `early_stopping_round`: Fixing this parameter, if your model doesn't improve for a certain number of rounds, it will stop training. It helps reducing overfitting and training time.
- `lambda_l1` or `lambda_l2`: Regularization parameters ranging from 0 to 1 (the maximum).
- `min_gain_to_split`: This parameter dictates the minimum gain to create a split on the tree. It limits the complexity of the tree by not developing splits are not contributing much to the model.
- `max_cat_group`: When dealing with categorical variables with high cardinality (a large number of categories), this parameter puts a limit on the number of categories that a variable can have by aggregating the less important. The default value of this parameter is 64.
- `is_unbalance`: For unbalanced datasets in binary classification, is set to True let the algorithm adjust for unbalanced classes.
- `scale_pos_weight`: Also for unbalanced datasets in binary classification, it sets a weight for the positive class.

We actually quoted just a small part of all the possible parameters of a LightGBM model, yet the most essential and important ones. Browsing the documentation, you can find many more parameters that can fit even more specific situations and projects of yours.

How do we tune all these parameters? Actually, you can effectively operate on a few ones. If you want to achieve faster computations, just use `save_binary` and set a small `max_bin`. You can also use `bagging_fraction` and `feature_fraction` with a low number to reduce the size of the training set and speed up the learning process (at the price of increasing the variance of your solution, because it will learn from less data).

If you want to achieve higher accuracy with your error measure, you should instead use a larger max_bin (implying more accuracy when working with numeric variables), use a smaller learning_rate and more num_iterations (necessary because the algorithm will converge in a slower way), and use a larger num_leaves (it may lead to overfitting though).

In the case of overfitting, you can try to set lambda_l1, lambda_l2, and min_gain_to_split and achieve some more regularization. You can also try max_depth to avoid growing too deep trees.

In our example, we take on the same task as before, to classify the Forest Covertype dataset. We start by importing the necessary packages.

Out next steps are then to set the parameters for this boosting algorithm to properly work. We define the objective ('multiclass'), set a low learning rate (0.01), and allow its branches to spread almost completely like a random forest would do: its trees' maximum depth is set to 128 and the number of resulting leaves is 256. In doing so, we also set a random sampling of both cases and features (bagging 90% of them every time):

```
In: import lightgbm as lgb
    import numpy as np
    params = {'task': 'train',
              'boosting_type': 'gbdt',
              'objective': 'multiclass',
              'num_class':len(np.unique(covertype_y)),
              'metric': 'multi_logloss',
              'learning_rate': 0.01,
              'max_depth': 128,
              'num_leaves': 256,
              'feature_fraction': 0.9,
              'bagging_fraction': 0.9,
              'bagging_freq': 10}
```

Then, we set the dataset for train, validation, and test using the Dataset command from the LightGBM package:

```
In: train_data = lgb.Dataset(data=covertype_X, label=covertype_y)
    val_data = lgb.Dataset(data=covertype_val_X, label=covertype_val_y)
```

Finally, we set the training instance, by feeding the previously set parameters, deciding on a maximum number of iterations of 2,500, setting a validation set, and requiring early stopping if the error measure doesn't improve on the validation for over 25 iterations (this will allow us to avoid any overfitting due to too many iterations, that is, boosting trees added):

```
In: bst = lgb.train(params,
                    train_data,
                    num_boost_round=2500,
                    valid_sets=val_data,
                    verbose_eval=500,
                    early_stopping_rounds=25)
```

After a while, the training stops pointing out a log-loss on validation of 0.40 and 851 iterations as the best number to pick. Training until validation scores don't improve for 25 rounds:

```
Out: Early stopping, best iteration is:[851]
     valid_0's multi_logloss: 0.400478
```

Instead of using a validation set, we could also test for the best number of iterations by cross-validation, that is, on the same train set:

```
In: lgb_cv = lgb.cv(params,
                    train_data,
                    num_boost_round=2500,
                    nfold=3,
                    shuffle=True,
                    stratified=True,
                    verbose_eval=500,
                    early_stopping_rounds=25)
    nround = lgb_cv['multi_logloss-mean'].index(np.min(lgb_cv[
                                        'multi_logloss-mean']))
    print("Best number of rounds: %i" % nround)

Out: cv_agg's multi_logloss: 0.468806 + 0.0124661
     Best number of rounds: 782
```

The result is not as brilliant as with the validation set, but the number of rounds is not all that far from what we found before. We will use the initial train by early stop, anyway. First, we get the probability for each class using the predict method, and the best iteration, then we will pick as our prediction the class with the highest probability.

After doing so, we will check for accuracy and plot a confusion matrix. The obtained score is analogous to XGBoost but obtained in a shorter training time:

```
In: y_probs = bst.predict(covertype_test_X,
          num_iteration=bst.best_iteration)
    y_preds = np.argmax(y_probs, axis=1)
    from sklearn.metrics import accuracy_score, confusion_matrix
    print('test accuracy:', accuracy_score(covertype_test_y, y_preds))
    print(confusion_matrix(covertype_test_y, y_preds))

Out: test accuracy: 0.8444
     [[1495 309     0    0    0    2   14]
      [ 221 2196   17    0    5    9    0]
      [   0   20  258    5    0   18    0]
      [   0   0     3   19    0    5    0]
      [   1   51    4    0   21    0    0]
      [   0   14   43    0    0   87    0]
      [  36   1     0    0    0    0  146]]
```

CatBoost

In July 2017, another interesting GBM algorithm was made public by Yandex, the Russian search engine: it is CatBoost (`https://catboost.yandex/`), whose name comes from putting together the two words Category and Boosting. In fact, its strongest point is the capability of handling categorical variables, which actually make the most of information in most relational databases, by adopting a mixed strategy of one-hot-encoding and mean encoding (a way to express categorical levels by assigning them an appropriate numeric value for the problem at hand; more on that later).

As explained in the paper *DOROGUSH, Anna Veronika; ERSHOV, Vasily; GULIN, Andrey. CatBoost: gradient boosting with categorical features support* (`https://pdfs.semanticscholar.org/9a85/26132d3e05814dca7661b96b3f3208d676cc.pdf`), as other GBM solution handle categorical variables by both one-hot-encoding the variables (quite expensive in terms of memory in-print of the data matrix) or by assigning arbitrary numeric codes to categorical levels (an imprecise, at most, approach, requiring large branching in order to turn effective), CatBoost approached the problem differently.

You provide indices of categorical variables to the algorithm, and you set a `one_hot_max_size` parameter, telling CatBoost to handle categorical variables using one-hot-encoding if the variable has less or equal levels. If the variable has more categorical levels, thus exceeding the `one_hot_max_size` parameter, then the algorithm will encode them in a fashion not too different than mean-encoding, as follows:

1. Permuting the order of examples.
2. Turning levels into integer numbers based on the loss function to be minimized.
3. Converting the level number to a float numerical values based on counting level labels based on the shuffle order in respect of your target (more details are given at `https://tech.yandex.com/catboost/doc/dg/concepts/algorithm-main-stages_cat-to-numberic-docpage/` with a simple example).

The idea used by CatBoost to encode the categorical variables is not new, but it has been a kind of feature engineering used various times, mostly in data science competitions like at Kaggle's. Mean encoding, also known as likelihood encoding, impact coding, or target coding, is simply a way to transform your labels into a number based on their association with the target variable. If you have a regression, you could transform labels based on the mean target value typical of that level; if it is a classification, it is simply the probability of classification of your target given that label (probability of your target, conditional on each category value). It may appear as a simple and smart feature engineering trick, but actually, it has side effects, mostly in terms of overfitting because you are taking information from the target into your predictors.

There are a few empirical approaches to limit the overfitting and take advantage of dealing with categorical variables as numeric ones. The best source to know more about is actually a video from Coursera, because there are no formal papers on that: `https://www.coursera.org/lecture/competitive-data-science/concept-of-mean-encoding-b5Gxv`. Our recommendation is to use this trick with care.

CatBoost, apart from having both R and Python APIs and performing in the GBM field at the same degree of the competing XGBoost and LightGBM, also thanks to GPU and multi-GPU support (you can have a look at a performance comparison at `https://s3-ap-south-1.amazonaws.com/av-blog-media/wp-content/uploads/2017/08/13153401/Screen-Shot-2017-08-13-at-3.33.33-PM.png`) is also a completely open source project, and you can read all the code from its GitHub repository here: `https://github.com/catboost/catboost`.

Even in the case of CatBoost, the list of parameters is incredibly large, though well-detailed, at `https://tech.yandex.com/catboost/doc/dg/concepts/python-reference_catboost-docpage/`. For simple applications, you just have to tune the following key parameters:

- `one_hot_max_size` : The threshold over which to target encode any categorical variable
- `iterations` : The number of iterations
- `od_wait`: The number of iterations to wait if the evaluation metric doesn't improve
- `learning_rate`: The learning rate
- `depth`: The depth of trees
- `l2_leaf_reg`: The regularization coefficient
- `random_strength` and `bagging_temperature` to control the randomized bagging

We start by importing all the necessary packages and functions:

1. Since CatBoost excels when dealing with categorical variables, we have to rebuild the Forest Covertype dataset, because all its categorical variables have already been one-hot-encoded. We therefore simply rebuild them and recreate the dataset:

```
In: import numpy as np
    from sklearn.datasets import fetch_covtype
    from catboost import CatBoostClassifier, Pool
    covertype_dataset = fetch_covtype(random_state=101,
                                      shuffle=True)
    label = covertype_dataset.target.astype(int) - 1
    wilderness_area =
    np.argmax(covertype_dataset.data[:,10:(10+4)],
              axis=1)
    soil_type = np.argmax(
                     covertype_dataset.data[:,(10+4):(10+4+40)],
                     axis=1)
    data = (covertype_dataset.data[:,:10],
            wilderness_area.reshape(-1,1),
            soil_type.reshape(-1,1))
    data = np.hstack(data)
```

2. After creating it, we select the train, validation, and test portions as we did before:

```
In: covertype_train = Pool(data[:15000,:],
                           label[:15000], [10, 11])
    covertype_val = Pool(data[15000:20000,:],
                         label[15000:20000], [10, 11])
    covertype_test = Pool(data[20000:25000,:],
                          None, [10, 11])
    covertype_test_y = label[20000:25000]
```

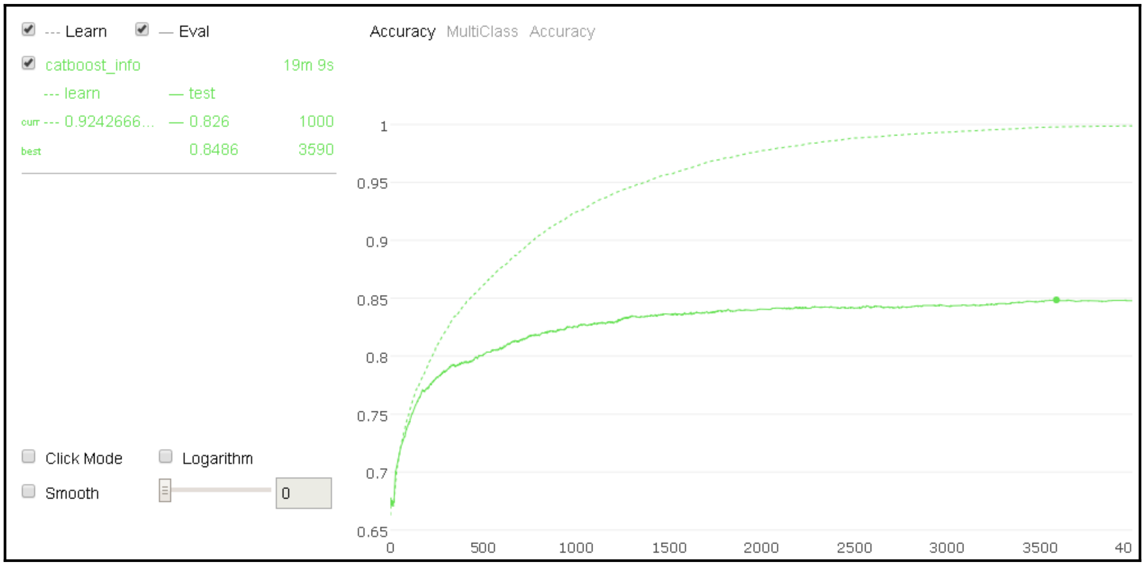
3. It is time now to set the `CatBoostClassifier`. We decide on a low learning rate (0.05) and a high number of iterations, a maximum tree depth of 8 (the actual maximum for CatBoost is 16), optimize for MultiClass (log-loss) but monitor accuracy both on the training and validation set:

```
In: model = CatBoostClassifier(iterations=4000,
                               learning_rate=0.05,
                               depth=8,
                               custom_loss = 'Accuracy',
                               eval_metric = 'Accuracy',
                               use_best_model=True,
                               loss_function='MultiClass')
```

4. We then start training, setting verbosity off but allowing a visual representation of the training and its results, both in-sample and, more importantly, out-of-sample:

```
In: model.fit(covertype_train, eval_set=covertype_val,
              verbose=False, plot=True)
```

Here is an example of what visualization you can get for the model trained on the CoverType dataset:



5. After training, we simply predict the class and its associated probability:

```
In: preds_class = model.predict(covertype_test)
    preds_proba = model.predict_proba(covertype_test)
```

6. An accuracy evaluation points out that the results are equivalent to XGBoost (0.847 against 848) and the confusion matrix looks much cleaner, pointing out a better classification job done by this algorithm:

```
In: from sklearn.metrics import accuracy_score, confusion_matrix
    print('test accuracy:', accuracy_score(covertype_test_y,
                                           preds_class))
    print(confusion_matrix(covertype_test_y, preds_class))

Out: test accuracy:  0.847
     [[1482  320    0    0    0    0   18]
      [ 213 2199   12    0   10   12    2]
      [   0   13  260    5    0   23    0]
      [   0    0    6   18    0    3    0]
      [   2   40    5    0   30    0    0]
      [   0   16   33    1    0   94    0]
      [  31    0    0    0    0    0  152]]
```

Dealing with big data

Big data puts data science projects under four points of view: volume (data quantity), velocity, variety, and veracity (is your data really representing what it should be or is it affected by some bias, distortion, or error?). The Scikit-learn package offers a range of classes and functions that will help you effectively work with data so large that it cannot entirely fit in the memory of a standard computer.

Before providing you with an overview of big data solutions, we have to create or import some datasets in order to give you a better idea of the scalability and performances of different algorithms. This will require about 1.5 gigabytes of your hard disk, which will be let free after the experiment.
(Not big data in itself—nowadays, it is hard to find computers with less than 4 GB of memory—yet, not even a toy dataset, it should provide you some idea).

Creating some big datasets as examples

As a typical example of big data analysis, we will use some textual data from the internet, and we will take advantage of the available `fetch_20newsgroups`, which contains data of 11,314 posts, each one averaging about 206 words, which appeared in 20 different newsgroups:

```
In: import numpy as np
    from sklearn.datasets import fetch_20newsgroups
    newsgroups_dataset = fetch_20newsgroups(shuffle=True,
                         remove=('headers', 'footers', 'quotes'),
                         random_state=6)
    print ('Posts inside the data: %s' % np.shape(newsgroups_dataset.data))
    print ('Average number of words for post: %0.0f' %
           np.mean([len(text.split(' ')) for text in
           newsgroups_dataset.data]))

Out: Posts inside the data: 11314
     Average number of words for post: 206
```

Instead, to work out a generic classification example, we will create three synthetic datasets that contain from 100,000 to 10 million cases. You can create and use any of them according to your computer's resources. We will always refer to the largest one for our experiments:

```
In: from sklearn.datasets import make_classification
    X,y = make_classification(n_samples=10**5, n_features=5,
                              n_informative=3, random_state=101)
    D = np.c_[y,X]
    np.savetxt('large_dataset_10__5.csv', D, delimiter=",")
    # the saved file should be around 14,6 MB
    del(D, X, y)
    X,y = make_classification(n_samples=10**6, n_features=5,
                              n_informative=3, random_state=101)
    D = np.c_[y,X]
    np.savetxt('large_dataset_10__6.csv', D, delimiter=",")
    # the saved file should be around 146 MB
    del(D, X, y)
    X,y = make_classification(n_samples=10**7, n_features=5,
                            n_informative=3, random_state=101)
    D = np.c_[y,X]
    np.savetxt('large_dataset_10__7.csv', D, delimiter=",")
    #the saved file should be around 1,46 GB
    del(D, X, y)
```

After creating and using any of the datasets, you can remove them from disk by the following command:

```
In: import os
    os.remove('large_dataset_10__5.csv')
    os.remove('large_dataset_10__6.csv')
    os.remove('large_dataset_10__7.csv')
```

Scalability with volume

The trick to managing high volumes of data without loading too many megabytes (or gigabytes) of data into your memory is to incrementally update the parameters of your algorithm using only part of the examples at a time, repeating the update on the following data chunks until all the observations have been elaborated at least once by the machine learner.

This is possible in Scikit-learn thanks to the `.partial_fit()` method, which has been made available to a certain number of supervised and unsupervised algorithms. By using the `.partial_fit()` method and providing some basic information (for example, for classification, you should know beforehand the number of classes to be predicted), you can immediately start fitting your model even if you have a single case or a few observations.

This method is called `incremental learning`. The chunks of data that you incrementally fed into the learning algorithm are called batches. The critical points of incremental learning are as follows:

- Batch size
- Data preprocessing
- Number of passes with the same examples
- Validation and parameters fine-tuning

Batch size generally depends on your available memory. The principle is that the larger the data chunks the better, since the data sample will get more representatives of the data distributions as its size grows. In addition, data preprocessing is challenging. Incremental learning algorithms work well with data in the range of [-1,+1] or [0,+1] (for instance, Multinomial Bayes won't accept negative values). However, to scale into such a precise range, you need to know beforehand the range of each variable. Alternatively, you have to do one of these: pass all the data once, record the minimum and maximum values, or derive them from the first batch, trimming the following observations that exceed the initial maximum and minimum values.

A more robust way to cope with this problem is to use a sigmoid normalization that bounds all of the range of possible values between 0 and 1.

The number of passes can become a problem. In fact, as you pass the same examples multiple times, you help the predictive coefficients converge to an optimum solution. If you pass too many of the same observations, the algorithm will tend to overfit; that is, it will adapt too much to the data repeated too many times. Some algorithms, such as the SGD family, are also very sensitive to the order that you propose to the examples to be learned. Therefore, you have to either set their shuffle option (shuffle=True) or shuffle the file rows before the learning starts, keeping in mind that, for efficacy, the order of the rows proposed for the learning should be casual.

Validation is a stream of batches, which can be achieved in two ways:

- Validate in a progressive way; that is, test first how the model predicts newly arrived data chunks before passing them to training.
- Hold out some observations from every chunk. The latter is also the best way to reserve a sample for grid search or some other optimization.

In our example, we entrust the `SGDClassifier` with a log loss (analogous to a logistic regression) to learn how to predict a binary outcome given 10**7 observations:

```
In: from sklearn.linear_model import SGDClassifier
    from sklearn.preprocessing import MinMaxScaler
    import pandas as pd
    streaming = pd.read_csv('large_dataset_10__7.csv',
                            header=None, chunksize=10000)
    learner = SGDClassifier(loss='log', max_iter=100)
    minmax_scaler = MinMaxScaler(feature_range=(0, 1))
    cumulative_accuracy = list()
    for n,chunk in enumerate(streaming):
        if n == 0:
            minmax_scaler.fit(chunk.iloc[:,1:].values)
        X = minmax_scaler.transform(chunk.iloc[:,1:].values)
        X[X>1] = 1
        X[X<0] = 0
        y = chunk.iloc[:,0]
        if n > 8:
            cumulative_accuracy.append(learner.score(X,y))
        learner.partial_fit(X,y,classes=np.unique(y))
    print ('Progressive validation mean accuracy %0.3f' %
           np.mean(cumulative_accuracy))

Out: Progressive validation mean accuracy 0.660
```

First, pandas `read_csv` allows us to iterate over the file by reading batches of 10,000 observations (the number can be increased or decreased according to your computing resources).

We use the `MinMaxScaler` in order to record the range of each variable on the first batch. For the following batches, we will use the rule that if it exceeds one of the limits of [0,+1], they are trimmed to the nearest limit. Otherwise, we can use the `partial_fit` method of the MinMaxScaler and learn the boundaries of the features as we learn with our model. The only caveat to be considered when using the MinMaxScaler though is attention to outliers because they can compress the numeric transformation to a portion of the [0, +1] interval.

Eventually, starting from the tenth batch, we will record the accuracy of the learning algorithm on each newly received batch before using it to update the training. In the end, the accumulated accuracy scores are averaged, offering a global performance estimation.

Keeping up with velocity

Various algorithms work using incremental learning. For classification, we will recall the following:

- `sklearn.naive_bayes.MultinomialNB`
- `sklearn.naive_bayes.BernoulliNB`
- `sklearn.linear_model.Perceptron`
- `sklearn.linear_model.SGDClassifier`
- `sklearn.linear_model.PassiveAggressiveClassifier`

For regression, we will recall the following:

- `sklearn.linear_model.SGDRegressor`
- `sklearn.linear_model.PassiveAggressiveRegressor`

As for velocity, they are all comparable in speed. You can try for yourself with the following script:

```
In: from sklearn.naive_bayes import MultinomialNB
    from sklearn.naive_bayes import BernoulliNB
    from sklearn.linear_model import Perceptron
    from sklearn.linear_model import SGDClassifier
    from sklearn.linear_model import PassiveAggressiveClassifier
    import pandas as pd
    from datetime import datetime
    classifiers = {'SGDClassifier hinge loss' : SGDClassifier(loss='hinge',
                                           random_state=101, max_iter=10),
                   'SGDClassifier log loss' : SGDClassifier(loss='log',
                                           random_state=101, max_iter=10),
                   'Perceptron' : Perceptron(random_state=101,max_iter=10),
                   'BernoulliNB' : BernoulliNB(),
              'PassiveAggressiveClassifier' : PassiveAggressiveClassifier(
                                            random_state=101, max_iter=10)
                   }
    large_dataset = 'large_dataset_10__6.csv'
    for algorithm in classifiers:
        start = datetime.now()
        minmax_scaler = MinMaxScaler(feature_range=(0, 1))
        streaming = pd.read_csv(large_dataset, header=None, chunksize=100)
        learner = classifiers[algorithm]
        cumulative_accuracy = list()
        for n,chunk in enumerate(streaming):
            y = chunk.iloc[:,0]
            X = chunk.iloc[:,1:]
            if n > 50 :
                cumulative_accuracy.append(learner.score(X,y))
            learner.partial_fit(X,y,classes=np.unique(y))
        elapsed_time = datetime.now() - start
        print (algorithm + ' : mean accuracy %0.3f in %s secs'
          % (np.mean(cumulative_accuracy),elapsed_time.total_seconds()))
```

```
Out: BernoulliNB : mean accuracy 0.734 in 41.101 secs
     Perceptron : mean accuracy 0.616 in 37.479 secs
     SGDClassifier hinge loss : mean accuracy 0.712 in 38.43 secs
     SGDClassifier log loss : mean accuracy 0.716 in 39.618 secs
     PassiveAggressiveClassifier : mean accuracy 0.625 in 40.622 secs
```

As a general note, remember that smaller batches are slower, since that implies more disk access from a database or a file, which is always a bottleneck.

Dealing with variety

Variety is another typical characteristic of big data. This is especially true when we are dealing with textual data or very large categorical variables (for example, variables storing website names in programmatic advertising). As you learn from batches of examples and as you unfold categories or words, you will see that each one is an appropriate and exclusive variable. You may find it difficult to handle the challenge of variety and the unpredictability of large streams of data. Scikit-learn provides you with a simple and fast way to implement the hashing trick and completely forget the problem of defining in advance of a rigid variable structure.

The hashing trick uses hash functions and sparse matrices in order to save your time, resources, and hassle. The hash functions are functions that map in a deterministic way any input they receive. It doesn't matter if you feed them with numbers or strings, they will always provide you with an integer number in a certain range. Sparse matrices are, instead, arrays that record only values that are not zero, since their default value is zero for any combination of their row and column. Therefore, the hashing trick bounds every possible input; it doesn't matter if it was previously unseen to a certain range or position on a corresponding input sparse matrix, which is loaded with a value that is not 0.

Apart from the in-built hash function in Python, there are quite a few hashing algorithms available in packages such as `hashlib` (`https://docs.python.org/2/library/hashlib.html`). Interestingly, the hash function is also heavily used by Scikit-learn in many functions and methods, and the MurmurHash 32 (`https://github.com/aappleby/smhasher`) is available for you to use. It can be found among the utilities for developers (`http://Scikit-learn.org/stable/developers/utilities.html`); just import it and use it straight out of the box:

```
In: from sklearn.utils import murmurhash3_32
    print (murmurhash3_32("something", seed=0, positive=True))
```

For instance, if your input is `Python`, a hashing command such as `abs(hash('Python'))` can transform that into the integer number 539294296 and then assign the value of 1 to the cell at the 539294296 column index. The hash function is a very fast and convenient way to invariably locate the same column index given the same input. The use of only absolute values ensures that each index corresponds only to a column in our array (negative indexes just start from the last column, and hence in Python, each column of an array can be expressed by both a positive and negative number).

The example that follows uses the `HashingVectorizer` class, a convenient class that automatically takes documents, separates the words, and transforms them, thanks to the hashing trick, into an input matrix. The script aims at learning why posts are published in 20 distinct newsgroups based on the words used on the existing posts in the newsgroups:

```
In: import pandas as pd
    from sklearn.linear_model import SGDClassifier
    from sklearn.feature_extraction.text import HashingVectorizer
    def streaming():
        for response, item in zip(newsgroups_dataset.target,
                                  newsgroups_dataset.data):
            yield response, item
    hashing_trick = HashingVectorizer(stop_words='english', norm = 'l2')
    learner = SGDClassifier(random_state=101, max_iter=10)
    texts = list()
    targets = list()
    for n, (target, text) in enumerate(streaming()):
        texts.append(text)
        targets.append(target)
        if n % 1000 == 0 and n >0:
            learning_chunk = hashing_trick.transform(texts)
        if n > 1000:
            last_validation_score = learner.score(learning_chunk, targets),
            learner.partial_fit(learning_chunk, targets,
                                classes=[k for k in range(20)])
            texts, targets = list(), list()
    print ('Last validation score: %0.3f' % last_validation_score)

Out: Last validation score: 0.710
```

At this point, no matter what text you may input, the predictive algorithm will always answer by pointing out a class. In our case, it points out a `newsgroup` suitable for the post to appear on it. Let's try out this algorithm with a text taken from a classified ad:

```
    In: New_text = ["A 2014 red Toyota Prius v Five with fewer than 14K" +
                    "miles. Powered by a reliable 1.8L four cylinder " +
                    "hybrid engine that averages 44mpg in the city and " +
                    "40mpg on the highway."]
        text_vector = hashing_trick.transform(New_text)
        print (np.shape(text_vector), type(text_vector))
        print ('Predicted newsgroup: %s' %
               newsgroups_dataset.target_names[learner.predict(text_vector)])

    Out: (1, 1048576) <class 'scipy.sparse.csr.csr_matrix'>
         Predicted newsgroup: rec.autos
```

Naturally, you may change the `New_text` variable and discover where your text most likely will be displayed in a newsgroup. Note that the `HashingVectorizer` class has transformed the text into a `csr_matrix` (which is quite an efficient sparse matrix) to save memory, having a dataset of about one million columns.

An overview of Stochastic Gradient Descent (SGD)

We will complete this part of the chapter devoted to learning from big data with a quick overview of the SGD family, comprising SGDClassifier (for classification) and SGDRegressor (for regression).

Like other classifiers, they can be fit by using the `.fit()` method (passing row by row the in-memory dataset to the learning algorithm) or the previously seen `.partial_fit()` method based on batches. In the latter case, if you are classifying, you have to declare the predicted classes with the class parameter. It can accept a list containing all the class code that it should expect to meet during the training phase.

SGDClassifier can behave as a logistic regression when the loss parameter is set to `loss`. It transforms into a linear SVC if the loss is set to `hinge`. It can also take the form of other loss functions, or even the loss functions working for regression.

SGDRegressor mimics a linear regression using the `squared_loss` loss parameter. Instead, the Huber loss transforms the squared loss into a linear loss over a certain distance epsilon (another parameter to be fixed). It can also act as a linear SVR using the `epsilon_insensitive` loss function or the slightly different `squared_epsilon_insensitive` (which penalizes outliers more).

As in other situations with machine learning, the performance of the different loss functions on your data science problem cannot be estimated a priori. Anyway, please take into account that if you are doing classification and you need an estimation of class probabilities, you will be limited in your choice to `log` or `modified_huber` only.

The key parameters that require tuning for this algorithm to work best with your data are as follows:

- `n_iter`: The number of iterations over the data. As a rule of thumb, the more the passes, the better the optimization of the algorithm. However, there is a higher risk of overfitting if the passes are too many. Empirically, SGD tends to converge to a stable solution after having seen 10**6 examples. Given your examples, set your number of iterations accordingly.
- `penalty`: You have to choose l1, l2, or elasticnet, which are all different regularization strategies, to avoid overfitting because of overparameterization (using too many unnecessary parameters leads to the memorization of observations more than the learning of patterns). Briefly, l1 tends to reduce unhelpful coefficients to zero, l2 just attenuates them, and elasticnet is a mix of l1 and l2 strategies.
- `alpha`: This is a multiplier of the regularization term; the higher the alpha, the more the regularization. We advise you to find the best alpha value by performing a grid search ranging from 10**-7 to 10**-1.
- `l1_ratio`: The l1 ratio is used for elasticnet penalty. The suggested value or 0.15 will usually prove quite effective.
- `learning_rate`: This sets how much the coefficients are affected by every single example. Usually, it is optimal for classifiers and `invscaling` for regression. If you want to use `invscaling` for classification, you'll have to set `eta0` and `power_t (invscaling = eta0 / (t**power_t))`. With `invscaling`, you can start with a lower learning rate, which is less than the optimal rate, though it will decrease slower.
- `epsilon`: This should be used if your loss is `huber`, `epsilon_insensitive`, or `squared_epsilon_insensitive`.
- `shuffle`: If this is `True`, the algorithm will shuffle the order of the training data in order to improve the generalization of the learning.

A peek into natural language processing (NLP)

This section is not strictly related to machine learning, but it contains some machine learning results in the area of natural language processing. Python has many packages to process text data, and one of most powerful and complete toolkit for text processing is **NLTK**, the Natural Language Tool Kit.

Other NLP toolkits available for the Python community are gensim (`https://radimrehurek.com/gensim/`) and spaCy (`https://spacy.io/`)

In the following sections, we'll explore NLTK core functionalities. We will work on the English language; for other languages, you will first need to download the language corpora (note that sometimes languages have no free open source corpora for NLTK).

Please refer to the official website of NLTK data, `http://www.nltk.org/nltk_data/`, to have access to corpora and lexical resources in many languages, ready to work with NLTK.

Word tokenization

Tokenization is the act of splitting the text into words. Chunking whitespace seems very easy, but it's not, because the text contains punctuation and contractions. Let's start with an example:

```
In: my_text = "The coolest job in the next 10 years will be " +\
              "statisticians. People think I'm joking, but " +\
              "who would've guessed that computer engineers " +\
              "would've been the coolest job of the 1990s?"
    simple_tokens = my_text.split(' ')
    print (simple_tokens)

Out: ['The', 'coolest', 'job', 'in', 'the', 'next', '10', 'years', 'will',
      'be', 'statisticians.', 'People', 'think', "I'm", 'joking,', 'but',
      'who', "would've", 'guessed', 'that', 'computer', 'engineers',
      "would've", 'been', 'the', 'coolest', 'job', 'of', 'the', '1990s?']
```

Here, you can immediately see that something is wrong. The following tokens contain more than a word: `statisticians.` (with the final period), `I'm` (two words), `would've`, and `1990s?` (with the final question mark). Let's now see how NLTK performs better in this task (of course, under the hood, the algorithm is more complex than a simple whitespace chunker):

```
In: import nltk
    nltk_tokens = nltk.word_tokenize(my_text)
    print (nltk_tokens)

Out: ['The', 'coolest', 'job', 'in', 'the', 'next', '10', 'years',
      'will', 'be', 'statisticians', '.', 'People', 'think', 'I',
      "'m", 'joking', ',', 'but', 'who', 'would', "'ve", 'guessed',
      'that', 'computer', 'engineers', 'would', "'ve", 'been', 'the',
      'coolest', 'job', 'of', 'the', '1990s', '?']
```

While executing this or some other NLTK package calls, in case of an error saying "`Resource u'tokenizers/punkt/english.pickle' not found.`", just type `nltk.download()` on your console and select to either download everything or browse for the missing resource that triggered the warning.

Here, the quality is better, and each token is associated with a word in the text.

Note that `.`, `,`, and `?` are tokens, too.

There also exists a sentence tokenizer (see the `nltk.tokenize.punkt` module), but it's seldom used in data science.

Also, beyond the general-purpose English tokenizer, NLTK contains many other tokenizers to be used in different contexts. For example, if you're working on tweets, TweetTokenizer can be extremely useful to parse tweet-like documents. The most useful options are to remove handles, shorten consecutive characters, and properly tokenize hashtags. Here's an example:

```
In: from nltk.tokenize import TweetTokenizer
    tt = TweetTokenizer(strip_handles=True, reduce_len=True)
    tweet = '@mate: I looooooove this city!!!!!!! #love #foreverhere'
    tt.tokenize(tweet)

Out: [':', 'I', 'looove', 'this', 'city', '!', '!', '!', '#love',
      '#foreverhere']
```

Stemming

Stemming is the action of reducing inflectional forms of words and taking the words to their core concepts. For example, the concept behind `is`, `be`, `are`, and `am` is the same. Similarly, the concept behind `go` and `goes`, as well as `table` and `tables`, is the same. The operation of deriving the root concept for each word is called stemming. In NLTK, you can choose the stemmer that you'd like to use (there are several ways to get the root part of words). We'll show you one of them, letting the others in Jupyter Notebook associated with this part of the book:

```
In: from nltk.stem import *
    stemmer = LancasterStemmer()
    print ([stemmer.stem(word) for word in nltk_tokens])

Out: ['the', 'coolest', 'job', 'in', 'the', 'next', '10', 'year',
      'wil', 'be', 'stat', '.', 'peopl', 'think', 'i', "'m", 'jok',
      ',', 'but', 'who', 'would', "'ve", 'guess', 'that', 'comput',
      'engin', 'would', "'ve", 'been', 'the', 'coolest', 'job',
      'of', 'the', '1990s', '?']
```

In the example, we used the Lancaster stemmer, which is one of the most powerful and recent algorithms. Checking the result, you will immediately see that it's all lowercase and `statistician` is associated with its root, `stat`. Good job!

Word tagging

Tagging, or **POS-Tagging**, is the association between a word (or a token) and its **part-of-speech tag** (**POS-Tag**). After tagging, you know what (and where) the verbs, adjectives, nouns, and so on, are in the sentence. Even in this case, NLTK makes this complex operation very easy:

```
In: import nltk
    print (nltk.pos_tag(nltk_tokens))

Out: [('The', 'DT'), ('coolest', 'NN'), ('job', 'NN'), ('in', 'IN'),
      ('the', 'DT'), ('next', 'JJ'), ('10', 'CD'), ('years', 'NNS'),
      ('will', 'MD'), ('be', 'VB'), ('statisticians', 'NNS'), ('.', '.'),
      ('People', 'NNS'), ('think', 'VBP'), ('I', 'PRP'), ("'m", 'VBP'),
      ('joking', 'VBG'), (',', ','), ('but', 'CC'), ('who', 'WP'),
      ('would', 'MD'), ("'ve", 'VB'), ('guessed', 'VBN'), ('that', 'IN'),
      ('computer', 'NN'), ('engineers', 'NNS'), ('would', 'MD'),
      ("'ve", 'VB'),  ('been', 'VBN'), ('the', 'DT'), ('coolest', 'NN'),
      ('job', 'NN'), ('of', 'IN'), ('the', 'DT'), ('1990s', 'CD'),
      ('?', '.')]
```

Using the syntax of NLTK, you will realize that the `The` token represents a determiner (DT), `coolest` and `job` represent nouns (NN), `in` represents a conjunction, and so on. The association is really detailed; in the case of a verb, there are six possible tags, as follows:

- Take: `VB` (verb, base form)
- Took: `VBD` (verb, past tense)
- Taking: `VBG` (verb, gerund)
- Taken: `VBN` (verb, past participle)
- Take: `VBP` (verb, singular present tense)
- Takes: `VBZ` (verb, third-person singular present tense)

If you need a more detailed view of the sentence, you may want to use the parse tree tagger to understand its syntactic structure. This operation is rarely used in data science, since it's great for sentence-by-sentence analysis.

Named entity recognition (NER)

The goal of NER is to recognize tokens associated with people, organizations, and locations. Let's use an example to explain it further:

```
In: import nltk
    text = "Elvis Aaron Presley was an American singer and actor. Born in \
            Tupelo, Mississippi, when Presley was 13 years old he and his \
            family relocated to Memphis, Tennessee."
    chunks = nltk.ne_chunk(nltk.pos_tag(nltk.word_tokenize(text)))
    print (chunks)

Out:  (S
      (PERSON Elvis/NNP)
      (PERSON Aaron/NNP Presley/NNP)
      was/VBD
      an/DT
      (GPE American/JJ)
      singer/NN
      and/CC
      actor/NN
      ./.
      Born/NNP
      in/IN
      (GPE Tupelo/NNP)
      ,/,
      (GPE Mississippi/NNP)
      ,/,
      when/WRB
      (PERSON Presley/NNP)
      was/VBD
      13/CD
      years/NNS
      old/JJ
      he/PRP
      and/CC
      his/PRP$
      family/NN
      relocated/VBD
      to/TO
      (GPE Memphis/NNP)
      ,/,
      (GPE Tennessee/NNP)
      ./.)
```

An extract of the Wikipedia page on Elvis is analyzed and NER-processed. A few entities that have been recognized by NER are listed here:

- **Elvis Aaron Presley**: PERSON
- **American**: GPE (Geopolitical entity)
- **Tupelo, Mississippi**: GPE (Geopolitical entity)
- **Memphis, Tennessee**: GPE (Geopolitical entity)

Stopwords

Stopwords are the least informative pieces (or tokens) in text, since they are the most common words (such as the, it, is, as, and not). Stopwords are often removed. And, exactly the way it happens in the feature selection phase if you remove them, the processing takes less time and less memory; also, it is sometimes more accurate. Removing stopwords decreases the overall entropy of the text, thereby making whatever signal is in there more apparent and easier to represent in features.

A list of English stopwords is available in Scikit-learn, too. For the stopwords in other languages, check out NLTK:

```
In: from sklearn.feature_extraction import text
    stop_words = text.ENGLISH_STOP_WORDS
    print (stop_words)

Out: frozenset(['all', 'six', 'less', 'being', 'indeed', 'over', 'move',
                'anyway', 'four', 'not', 'own', 'through', 'yourselves',
                'fify', 'where', 'mill', 'only', 'find', 'before', 'one',
               'whose', 'system', 'how', ...

In: from nltk.corpus import stopwords
    print(stopwords.words('english'))

Out: ['i', 'me', 'my', 'myself', 'we', 'our', 'ours', 'ourselves',
      'you', 'your', 'yours', 'yourself', 'yourselves', 'he', 'him',
      'his', 'himself', 'she', 'her', 'hers', 'herself', 'it', 'its',
      'itself', 'they', 'them', 'their', 'theirs', 'themselves', 'what',
      'which', 'who', 'whom', 'this', 'that', 'these', '...

In: print(stopwords.words('german'))
Out: ['aber', 'alle', 'allem', 'allen', 'aller', 'alles', 'als', 'also',
      'am', 'an', 'ander', 'andere', 'anderem', 'anderen', 'anderer',
      'anderes', 'anderm', 'andern', 'anderr', 'anders', 'auch',
      'auf', 'au', ...
```

A complete data science example – text classification

Now, here's a complete example that allows you to put each text in the right category. We will use the `20newsgroup` dataset, which was already introduced in `Chapter 1`, *First Steps*. To make things more realistic and prevent the classifier from overfitting the data, we'll remove email headers, footers (such as a signature), and quotes. In addition, in this case, the goal is to classify between two similar categories: `sci.med` and `sci.space`. We will use the accuracy measure to evaluate the classification:

```
In: import nltk
    from sklearn.datasets import fetch_20newsgroups
    from sklearn.feature_extraction.text import TfidfVectorizer
    from sklearn.linear_model import SGDClassifier
    from sklearn.metrics import accuracy_score
    from sklearn.datasets import fetch_20newsgroups
    import numpy as np
    categories = ['sci.med', 'sci.space']
    to_remove = ('headers', 'footers', 'quotes')
    twenty_sci_news_train = fetch_20newsgroups(subset='train',
                          remove=to_remove, categories=categories)
    twenty_sci_news_test = fetch_20newsgroups(subset='test',
                         remove=to_remove, categories=categories)
```

Let's start with the easiest approach to preprocess the textual data-using `TfIdf`. Remember that `Tfidf` is the multiplication of the frequency of the word within the document, by the inverse of its frequency across all the documents. High scores indicate that the word is used multiple times in the current document, but it's rare in the others (that is, it's a keyword of the document):

```
In: tf_vect = TfidfVectorizer()
    X_train = tf_vect.fit_transform(twenty_sci_news_train.data)
    X_test = tf_vect.transform(twenty_sci_news_test.data)
    y_train = twenty_sci_news_train.target
    y_test = twenty_sci_news_test.target
```

Now let's use a linear classifier (SGDClassifier) to perform the classification task. One last thing to do is to print out the classification accuracy:

```
In: clf = SGDClassifier()
    clf.fit(X_train, y_train)
    y_pred = clf.predict(X_test)
    print ("Accuracy=", accuracy_score(y_test, y_pred))

Out: Accuracy= 0.878481012658
```

An accuracy of `87.8` percent is a very good result. The entire program consists of less than 20 lines of code. Now, let's see if we can get something better. In this chapter, we've learned stopword removal, tokenization, and stemming. Let's see whether we gain accuracy by using them:

```
In: def clean_and_stem_text(text):
        tokens = nltk.word_tokenize(text.lower())
        clean_tokens = [word for word in tokens if word not in stop_words]
        stem_tokens = [stemmer.stem(token) for token in clean_tokens]
        return " ".join(stem_tokens)
    cleaned_docs_train = [clean_and_stem_text(text) for text in
                          twenty_sci_news_train.data]
    cleaned_docs_test = [clean_and_stem_text(text) for text in
                         twenty_sci_news_test.data]
```

The `clean_and_stem_text` function basically lowercases, tokenizes, stems, and reconstructs every document in the dataset. Finally, we will apply the same preprocessing (`Tfidf`) and classifier (`SGDClassifier`) that we used in the preceding example:

```
In: X1_train = tf_vect.fit_transform(cleaned_docs_train)
    X1_test = tf_vect.transform(cleaned_docs_test)
    clf.fit(X1_train, y_train)
    y1_pred = clf.predict(X1_test)
    print ("Accuracy=", accuracy_score(y_test, y1_pred))

Out: Accuracy= 0.893670886076
```

This processing requires more time, but we gained an accuracy of about 1.5 percent. An accurate tuning of the parameters of `Tfidf` and a cross-validated choice of the parameters of the classifier will eventually boost the accuracy to over 90 percent. So far, we're happy with this performance, but you can try to break that barrier.

An overview of unsupervised learning

In all the methods we've seen so far, every sample or observation has its own target label or value. In some other cases, the dataset is unlabeled and, to extract the structure of the data, you need an unsupervised approach. In this section, we're going to introduce two methods to perform clustering, as they are among the most used methods for unsupervised learning.

It is useful to bear in mind that often the terms *clustering* and *unsupervised learning* are considered synonymous, though, actually, unsupervised learning has a larger meaning.

K-means

The first method that we'll introduce is named K-means, the most commonly used clustering algorithm despite its inevitable shortcomings. In signal processing, K-means is the equivalent of a *vectorial quantization*, that is, the selection of the best *codeword* (from a given *codebook*) that better approximates the input observation (or a word).

You must provide the algorithm with the K parameter, which is the number of clusters. Sometimes, this might be a limitation because you have to investigate first which is the right K for the current dataset.

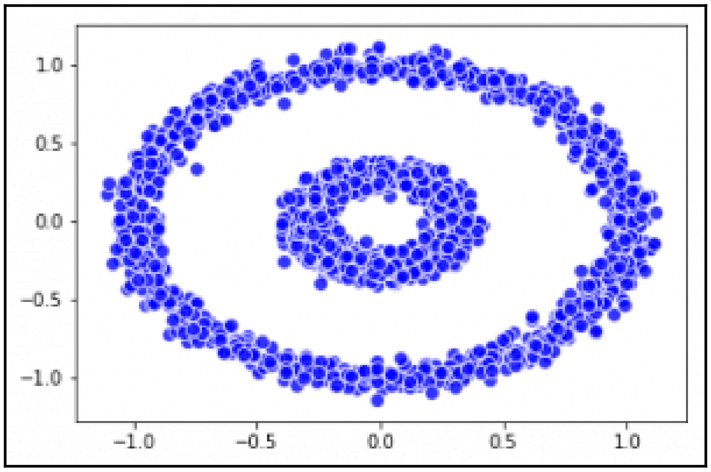
K-means iterates an **EM** (**expectation/maximization**) approach. During the first phase, it assigns each training point to the closest cluster centroid; during the second phase, it moves the cluster centroid to the center of mass of the points assigned to it (to reduce distortion). The initial placement of centroids is random. Consequently, you may need to run the algorithm several times so as not to find a local minimum.

That's all for the theory behind the algorithm; now, let's see it in practice. In this section, we're using two two-dimensional dummy datasets that will explain what's going on better. Both datasets are composed of 2,000 samples so that you can also have an idea about the processing time.

Now, let's create the artificial datasets, and then let's represent them by a plot:

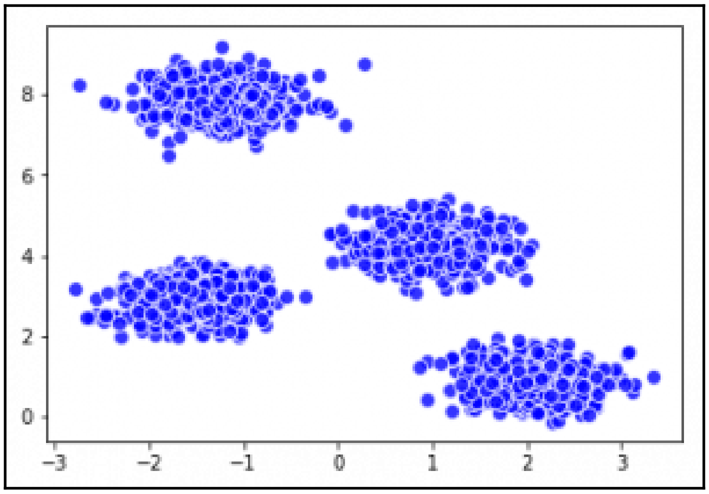
```
In: %matplotlib inline
    import numpy as np
    import matplotlib.pyplot as plt
    from sklearn import datasets
    N_samples = 2000
    dataset_1 = np.array(datasets.make_circles(n_samples=N_samples,
                         noise=0.05, factor=0.3)[0])
    dataset_2 = np.array(datasets.make_blobs(n_samples=N_samples,
                         centers=4, cluster_std=0.4, random_state=0)
    plt.scatter(dataset_1[:,0], dataset_1[:,1], c=labels_1,
                alpha=0.8, s=64, edgecolors='white')
   plt.show()
```

This is the first dataset we created, made of concentric rings of points (a quite tricky problem because the represented clusters are non spherical):



```
In: plt.scatter(dataset_2[:,0], dataset_2[:,1], alpha=0.8, s=64,
                c='blue', edgecolors='white')
    plt.show()
```

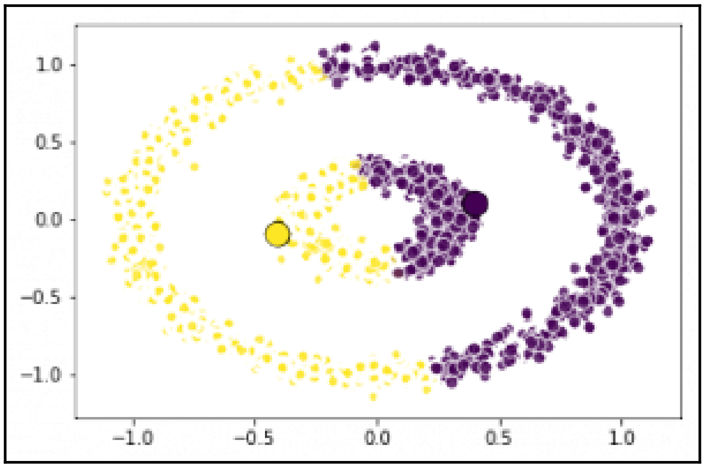
Here is the second one, made of separated bubbles of points:



Now it's time to apply K-means. We will set `K=2` in this case. Let's see the results:

```
In: from sklearn.cluster import KMeans
    K_dataset_1 = 2
    km_1 = KMeans(n_clusters=K_dataset_1)
    labels_1 = km_1.fit(dataset1).labels
    plt.scatter(dataset_1[:,0], dataset_1[:,1], c=labels_1,
                alpha=0.8, s=64, edgecolors='white')
    plt.scatter(km_1.cluster_centers_[:,0], km_1.cluster_centers_[:,1],
                s=200, c=np.unique(labels_1), edgecolors='black')
    plt.show()
```

This is the result with obtain on this problem:

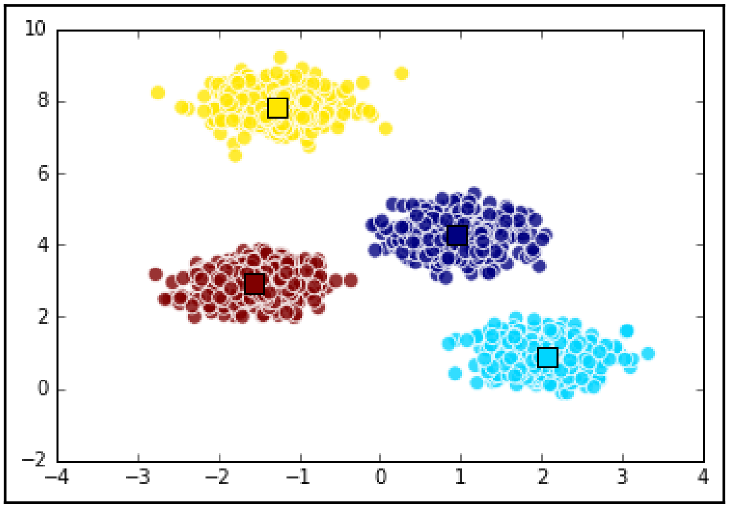


As you can see, K-means is not performing very well on this dataset, because it expects spherical-shaped data clusters. For this dataset, a Kernel-PCA should be applied before using K-means.

Now let's see how it performs on a spherical-clustered data. In this case, based on our knowledge of the problem and the silhouette coefficient, we will set `K=4`:

```
In: K_dataset_2 = 4
    km_2 = KMeans(n_clusters=K_dataset_2)
    labels_2 = km_2.fit(dataset2).labels
    plt.scatter(dataset_2[:,0], dataset_2[:,1], c=labels_2,
                alpha=0.8, s=64, edgecolors='white')
    plt.scatter(km_2.cluster_centers_[:,0], km_2.cluster_centers_[:,1],
          marker='s', s=100, c=np.unique(labels_2), edgecolors='black')
    plt.show()
```

The results we get on this problem are much better:



As expected, the plotted result is great. The centroids and clusters are exactly what we had in mind while looking at the unlabeled dataset. Now we are going to check if there is any other cluster approach that could help us solve the clustering problem when our clusters are non-spherical.

In real-world cases, you may consider using the Silhouette Coefficient to have an idea about how well-defined the clusters are. It is an evaluation metric of consistency within groups, applicable to various clustering results, and even class structures in supervised learning. You can read more about Silhouette Coefficient at `http://Scikit-learn.org/stable/modules/clustering.html#silhouette-coefficient`.

DBSCAN – a density-based clustering technique

Now we will introduce you to **DBSCAN**, a density-based clustering technique. It's a very simple technique. It selects a random point; if the point is in a dense area (if it has more than N neighbors do), it starts growing the cluster, including all the neighbors, and the neighbors of the neighbors, until it reaches a point where there are no more neighbors.

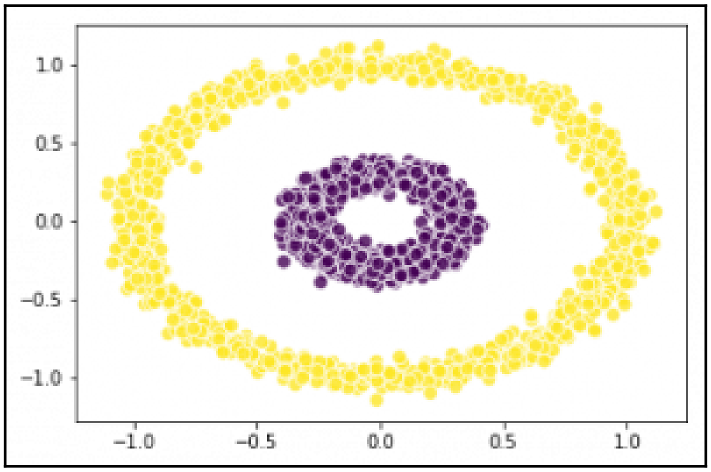
If the point is not in a dense area, it is classified as noise. Then, another unlabeled point is selected randomly and the process starts over. This technique is great for non-spherical clusters, but it works equally well with spherical ones. The input is just the neighborhood radius (the `eps` parameter, that is, the maximum distance between two points that are being considered neighbors), and the output is the cluster membership label for each point.

Note that the points labeled by the value-1 are classified as noise by DBSCAN.

Let's see an example on the dataset we had previously introduced:

```
In: from sklearn.cluster import DBSCAN
    dbs_1 = DBSCAN(eps=0.25)
    labels_1 = dbs_1.fit(dataset1).labels
    plt.scatter(dataset_1[:,0], dataset_1[:,1], c=labels_1,
                alpha=0.8, s=64, edgecolors='white')
    plt.show()
```

Now the clusters are correctly located by the DBSCAN algorithm:



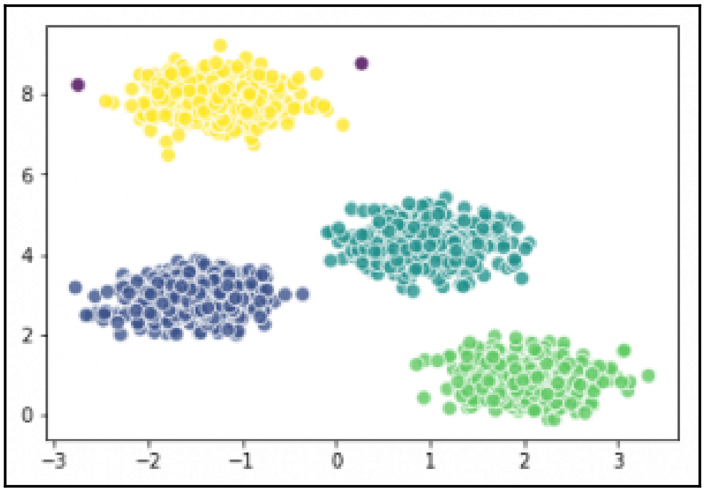
The result is perfect now. No points have been classified as noise (only the `0` and `1` labels appear in the label set):

```
In: np.unique(labels_1)

Out: array([0, 1])
```

Now let's move on to the other dataset:

```
In: dbs_2 = DBSCAN(eps=0.5)
    labels_2 = dbs_2.fit(dataset2).labels
    plt.scatter(dataset_2[:,0], dataset_2[:,1], c=labels_2,
                alpha=0.8, s=64, edgecolors='white')
    plt.show()

In: np.unique(labels_2)

Out: array([-1,  0,  1,  2,  3])
```

It took some time to select the best settings for DBSCAN, and in this case, four clusters have been detected and a few points have been classified as noise (since the label set contains -1):



At the end of this section, a last important note is that in this essential introduction of K-means and DBSCAN, we have always used the Euclidean distance, as it is the default distance metric in these functions (though other distance metrics can also be used if you find them appropriate). When using this distance in real cases, remember that you have to normalize each feature (z-normalization) so that every feature contributes equally to the final distortion. If the dataset is not normalized, the features that have larger support will have more decision power on the output label, and that's something that we don't want.

Latent Dirichlet Allocation (LDA)

For text, instead, a popular unsupervised algorithm that can be used to understand a common set of words in a collection of documents is **Latent Dirichlet Allocation** or **LDA**.

Note that another algorithm, the Linear Discriminant Analysis, also has the same acronym, but the two algorithms are completely unconnected.

LDA aims to extract sets of homogeneous words, or topics, out of a collection of documents. The math behind the algorithm is very advanced; here we will see just a practical notion of it.

Let's start with an example to explain why LDA is popular and why other unsupervised methods aren't good enough when dealing with text. K-means and DBSCAN, for example, provide a hard decision for each sample, putting each point in a disjoint partition. Documents, instead, often describe covering topics together (think about Shakespeare's books; they're a good mix of tragedy, romance, and adventure). On text documents, any hard decision would be almost certainly wrong. LDA, instead, provides as output a mixture of topics composing the document, along with an indication of how much the topic is represented in the document.

Let's use an example to explain how it works. We will train the algorithm on two categories; cars and medicine, from the 20-newsgroup dataset (we have already used the same dataset before in the chapter, in the earlier paragraph, *Preparing tools and datasets*):

```
In: import nltk
    Import gensim
    from sklearn.datasets import fetch_20newsgroups
    def tokenize(text):
        return [token.lower() \
                for token in gensim.utils.simple_preprocess(text) \
                if token not in gensim.parsing.preprocessing.STOPWORDS]

    text_dataset=fetch_20newsgroups(categories=['rec.autos','sci.med'],
                                    random_state=101,
                                    remove=('headers', 'footers', 'quotes'))
    documents = text_dataset.data
    print("Document count:", len(documents))

Out: Document count: 1188
```

Each one of the 1,188 documents composing the dataset is a string. For example, the first document contains the following text:

```
In: documents[0]

Out: 'nI have a new doctor who gave me a prescription today for something
      called nSeptra DS. He said it may cause GI problems and I have a
      sensitive stomach nto begin with. Anybody ever taken this antibiotic.
      Any good?  Suggestions nfor avoiding an upset stomach?  Other tips?n'
```

This document is definitely about medicine; there is nothing really important anyway for the algorithm. Now let's tokenize and create a dictionary of all the words included in the dataset. Mind that the tokenization operation also removes the stopwords and puts each word in lowercase:

```
In: processed_docs = [tokenize(doc) for doc in documents]
    word_dic = gensim.corpora.Dictionary(processed_docs)
    print("Num tokens:", len(word_dic))

Out: Num tokens: 16161
```

In the dataset, there are just over 16,000 distinct words. It's now time to filter too common words and too rare ones. In this step, we will keep the words appearing at least 10 times and no more than in 20% of the documents. At this point, we have the "Bag Of Words" (or BoW) representation of each document; that is, each document is represented as a dictionary containing how many times each word appears in the text. The absolute position of each word in the text is lost, exactly as if you put all the words of the document in a bag. As a result, not all of the signal in the text is captured in the features based on this approach, but most of the time, it suffices to make an effective model:

```
In: word_dic.filter_extremes(no_below=10, no_above=0.2)
    bow = [word_dic.doc2bow(doc) for doc in processed_docs]
```

Finally, here's the core class for LDA. In this example, we instruct LDA that in the dataset there are just two topics. We also provide other parameters to make the algorithm converge (if not, you'll receive a warning from the Python interpreter). Note that this algorithm works on many CPUs on your computer to speed up the process. If it doesn't work, please use the mono-process class, `gensim.models.ldamodel.LdaModel`, with the same parameters:

```
In: lda_model = gensim.models.LdaMulticore(bow, num_topics=2,
                                           id2word=word_dic, passes=10,
                                           iterations=500)
```

Finally, after a couple of minutes, the model is trained. To see the association between words and topics, run the following code:

```
In: lda_model.print_topics(-1)

Out: [(0, '0.011*edu + 0.008*com + 0.007*health + 0.007*medical +
       0.007*new + 0.007*use + 0.006*people + 0.005*time +
       0.005*years + 0.005*patients'), (1, '0.018*car + 0.008*good +
       0.008*think + 0.008*cars + 0.007*msg + 0.006*time +
       0.006*people + 0.006*water + 0.005*food + 0.005*engine')]
```

As you can see, the algorithm went through all the documents and learned that the main topics are cars and medicine. Note that the algorithm doesn't provide a short name for the topics, but their composition (the numbers are the weights of each word inside each topic, ranked from highest to lowest). In addition, note that some words appear in both topics; they are ambiguous words that can be used in both senses.

Finally, let's see how the algorithm works on an unseen document. To make things easier, let's create a sentence that contains both topics, for example *I've shown the doctor my new car. He loved its big wheels!* Then, after having created a Bag-of-Words representation of this new document, LDA will produce two scores, one for each topic:

```
In: new_doc = "I've shown the doctor my new car. He loved its big wheels!"
    bow_doc = word_dic.doc2bow(tokenize(new_doc))
    for index, score in sorted(lda_model[bow_doc], key=lambda tup:
    -1*tup[1]):
    print("Score: {}t Topic: {}".format(score,
         lda_model.print_topic(index, 5)))

Out: Score: 0.5047402389474193   Topic: 0.011*edu + 0.008*com +
            0.007*health + 0.007*medical + 0.007*new
     Score: 0.49525976105258074  Topic: 0.018*car + 0.008*good +
            0.008*think + 0.008*cars + 0.007*msg
```

The scores for both the topics are around 0.5 and 0.5, meaning that the sentence contains a good balance of the subjects `car` and `medicine`. What we've shown here is just an example of two topics; but the same implementation, thanks to the performing library Gensim, can also allocate process the whole English Wikipedia in a matter of few hours.

A different approach than LDA is provided by the Word2Vec algorithm, a very recent model for embedding words in vectors. Compared to LDA, Word2Vec keeps track of the position of the words in a sentence, and this additional context helps to disambiguate some words better. Word2Vec is trained using a deep-learning-like approach, but the implementation provided by the Gensim library makes it very easy to train and use. Note that while LDA aims to understand the topics in a document, Word2Vec works at the word level and tries to understand what the semantic relationship between words in a low-dimensionality space is (that is, creating an n-dimensional vector for each word). Let's see an example, to make things clear.

We will use the movie review dataset to train the Word2Vec model. The training is done simply by passing the sentences composing the corpora to the Word2Vec constructor, and, eventually, the number of workers that can work in parallel on the training task:

```
In: from gensim.models import Word2Vec
    from nltk.corpus import movie_reviews
    w2v = Word2Vec(movie_reviews.sents(), workers=4)
    w2v.init_sims(replace=True)
```

The last line of code simply freezes the model, not allowing any additional updates. This also brings an additional and very welcome benefit: reducing the memory fingerprint of the object.

Visualizing vectors that represent the words may be complicated; therefore, let's see some similarities (that is, similar vectors in the low-dimensional subspace). Here, we will ask the model to provide the top five most similar words (along with the similarity score) to the words `house` and `countryside`. This is just an example; it's possible to retrieve similar words for all words contained in the input corpora:

```
In: w2v.wv.most_similar('house', topn=5)

Out: [('apartment', 0.8799251317977905),
      ('body', 0.8719735145568848),
      ('hotel', 0.8618944883346558),
      ('head', 0.848749041557312),
      ('boat', 0.8469674587249756)]

In: w2v.vw.most_similar('countryside', topn=5)

Out: [('motorcycle', 0.9531803131103516),
      ('marches', 0.9499938488006592),
      ('rural', 0.9467764496803284),
      ('shuttle', 0.9466159343719482),
      ('mining', 0.9461280107498169)]
```

How is Word2Vec able to do so? Simply, with a similarity score in the low-dimensionality vector space. In fact, to see the vector representation of each word, perform the following:

```
In: w2v.wv['countryside']

Out: array([-0.09412272,  0.07695948, -0.14981066,  0.04894404,
           -0.03712097, -0.17099065, -0.0379245 , -0.05336253,
            0.06084964, -0.01273731, -0.03949985, -0.06456301,
           -0.03289359, -0.06889232,   0.02217194, ...
```

The array is composed of 100 dimensions; you can increase or decrease it by setting the `size` parameter while training the model. 100 is the default value.

In the `most_similar` method we've previously used, you can also specify the negative words to use (that is, to subtract similar words). A classic example is finding a similar word to `woman` and `king` without `queen`. The top result is, unsurprisingly, `man`:

```
In: w2v.wv.most_similar(positive=['woman', 'king'], negative=['queen'],
                        topn=3)

Out: [('man', 0.8440324068069458),
      ('girl', 0.7671926021575928),
      ('child', 0.7635241746902466)]
```

The model, thanks to the vector representation, also provides the method to identify the non-matching words in a set of similar words; that is, the word that doesn't match the context (in this case, the context is the bedroom):

```
In: w2v.wv.doesnt_match(['bed', 'pillow', 'cake', 'mattress'])

Out: 'cake'
```

Finally, all the preceding methods are built on similarity scores. The model also provides the raw score of similarity between words; here's an example of the similarity score of `woman` and `girl` and `woman` and `boy`. The first similarity is higher, though the second is not zero, since both words are connected by the fact we're talking about people:

```
In: w2v.wv.similarity('woman', 'girl'), w2v.similarity('woman', 'boy')

Out: (0.90198267746062233, 0.82372486297773828)
```

Summary

In this chapter, we introduced the essentials of machine learning. We started with some easy, but still quite effective, classifiers (linear and logistic regressors, Naive Bayes, and K-Nearest Neighbors). Then, we moved on to the more advanced ones (SVM). We explained how to compose weak classifiers together (ensembles, Random Forests, Gradient Tree Boosting) and touched on three awesome gradient-boosted classifiers: XGboost, LightGBM, and CatBoost. Finally, we had a peek at the algorithms used in big data, clustering, and NLP.

In the next chapter, we are going to introduce you to the basics of visualization with Matplotlib, how to operate EDA with pandas and achieve beautiful visualizations with Seaborn, and how to set up a web server to provide information on demand.

5
Visualization, Insights, and Results

After exploring machine learning, but not because the topic is less relevant than others, we are going to illustrate how to create visualizations with Python to enrich your data science project. Visualization plays an important role in helping you communicate the results and insights derived from data and the learning process.

In this chapter, you will learn how to do the following:

- Use the basic `pyplot` functions from the `matplotlib` package
- Leverage a pandas DataFrame for **Explorative Data Analysis** (**EDA**)
- Create beautiful and interactive charts with Seaborn
- Visualize the machine learning and optimization processes we discussed in `Chapter 3`, *The Data Pipeline*, and `Chapter 4`, *Machine Learning*
- Understand and visually communicate variables' importance and their relationship with the target outcome
- Set up a prediction server that uses HTTP to accept and provide predictions as a service

Introducing the basics of matplotlib

Visualization is a fundamental aspect of data science, allowing data scientists to better and more effectively communicate their findings to the organization they operate in, to both data experts and non-experts. Providing the nuts and bolts of the principles behind communicating information and crafting engaging beautiful visualizations is beyond the scope of our book, but we can recommend suitable resources if you want to improve your skills.

For basic visualization rules, you can visit `https://lifehacker.com/5909501/how-to-choose-the-best-chart-for-your-data`. We also recommend the books of Prof. Edward Tufte on analytic design and visualization.

We can instead provide a fast and to-the-point series of essential recipes that can get you started on visualization using Python, and that you can refer to anytime you need to create a specific graphics chart. Consider all the snippets of code as your visualization building blocks; you can arrange them with different configurations and features just by using the large choice of parameters that we are going to present to you.

`matplotlib` is a Python package for plotting graphics. Created by John Hunter, it has been developed in order to address a lack of integration between Python and external software with graphical capabilities, such as MATLAB or gnuplot. Greatly influenced by MATLAB's way of operating and functions, `matplotlib` presents a quite similar syntax. In particular, the `matplotlib.pyplot` module, perfectly compatible with MATLAB, will be the core of our essential introduction to all the indispensable graphical tools to represent your data and analysis. MATLAB is indeed a standard for visualization in the data analysis and scientific community because of its recognized capabilities when it comes to exploratory analysis, mainly due to its smooth and easy to use plotting functions.

Each `pyplot` command makes a change on an initially instantiated figure. Once you set a figure, all additional commands will operate on it. Thus, it is easy to incrementally improve and enrich your graphic representation. In order for you to take advantage of the code and be able to personalize it to your needs, all the following examples are presented together with commented building blocks so that you can later draft your basic representation, and then look through this chapter for specific parameters among the examples in order to improve your chart as you planned it.

With the `pyplot.figure()` command, you can initialize a new visualization, though it suffices to call a plotting command to automatically start it. Instead, by using `pyplot.show()`, you close the figure that you were operating on, and you can open and operate on new figures.

Before starting with a few visualization examples, let's import the necessary packages in order to run all the examples:

```
In: import numpy as np
    import matplotlib.pyplot as plt
    import matplotlib as mpl
```

In this way, we can always refer to `pyplot`, the MATLAB-like module, as `plt`, and access the complete `matplotlib` functionality set with the help of `mpl`.

If you are using a Jupyter Notebook (or Jupyter Lab), you can use this line magic: `%matplotlib` inline. After writing the command in a cell of the notebook and running it, you can have your plots drawn directly on the notebook itself, instead of having the graphics presented in a separate window (by default, the GUI backend of `matplotlib` is the `TkAgg` backend). If you prefer a different backend such as Qt (`www.qt.io`), which is often distributed with Python scientific distributions, you just have to run this line magic instead: `%matplotlib` Qt.

Trying curve plotting

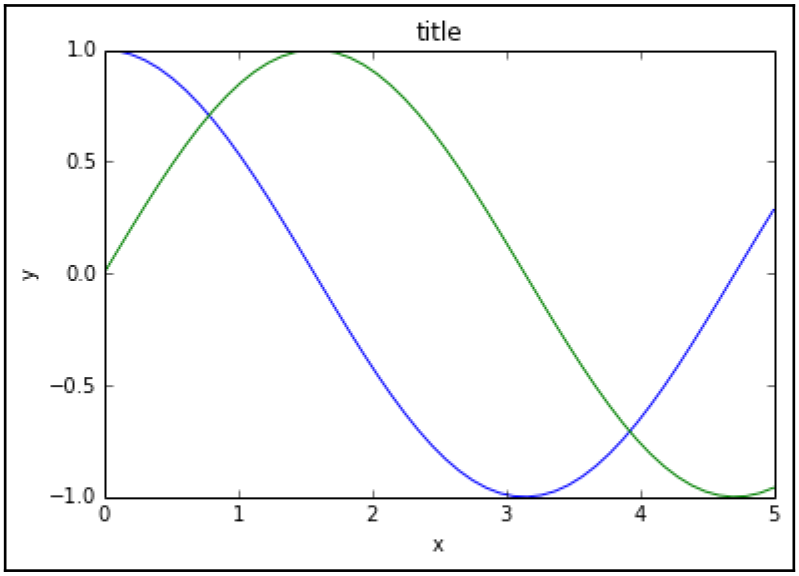
Our first problem will require you to draw a function with `pyplot`. Drawing a function is quite straightforward; you just have to get a series of *x* coordinates and map them to the *y* axis by using the function that you want to plot. Since the mapping results are stored away into two vectors, the `plot` function will deal with the curve representation. The precision of the representation will be greater if the mapped points are enough (50 points is a good sampling number):

```
In: import numpy as np
    import matplotlib.pyplot as plt
    x = np.linspace(0, 5, 50)
    y_cos = np.cos(x)
    y_sin = np.sin(x)
```

Using the NumPy `linspace()` function, we will create a series of 50 equally distanced numbers ranging from 0 to 5. We can use them to map our *y* to the cosine and sine functions:

```
In: plt.figure() # initialize a figure
    plt.plot(x,y_cos) # plot series of coordinates as a line
    plt.plot(x,y_sin)
    plt.xlabel('x') # adds label to x axis
    plt.ylabel('y') # adds label to y axis
    plt.title('title') # adds a title
    plt.show() # close a figure
```

Here is your first plot:



The `pyplot.plot` command can plot more curves in a sequence, with each curve taking a different color according to an internal color schema, which can be customized by explicating the favored color sequence. To do so, you have to manipulate the list containing the sequence of colors that `matplotlib` uses:

```
In: list(mpl.rcParams['axes.prop_cycle'])

Out: [{'color': '#1f77b4'},
      {'color': '#ff7f0e'},
      {'color': '#2ca02c'},
      {'color': '#d62728'},
      {'color': '#9467bd'},
      {'color': '#8c564b'},
      {'color': '#e377c2'},
      {'color': '#7f7f7f'},
      {'color': '#bcbd22'},
      {'color': '#17becf'}]
```

TIP

`#1f77b4`, `#ff7f0e`, `#2ca02c`, and all the others are all colors expressed in hexadecimal form. In order to figure out how they look, you can use the **colorhexa** website, providing you with useful information on each of them: `https://www.colorhexa.com/`.

The hack can be done by using the `cycler` function and feeding it with a list of string names referring to the colors you want to use in sequence:

```
In: mpl.rcParams['axes.prop_cycle'] = mpl.cycler('color',
                                                ['blue', 'red', 'green'])
```

Moreover, the `plot` command, if not given any other information, will assume that you are going to plot a line. Therefore, it will link all the provided points in a curve. If you add a new parameter such as `'.'` – that is, `plt.plot(x,y_cos,'.')` – you signal that you instead want to plot a series of separated points (the string for a line is `'-'`, but we will soon show another example).

In this way, if you've customized `rcParams['axes.prop_cycle']` as proposed previously, the next graphs will first have a blue curve, then the second will be red, and the third green. Then, the color loop will restart. We leave this decision to you. All the examples in this chapter will just follow the standard color sequence, but you are free to experiment with better color settings.

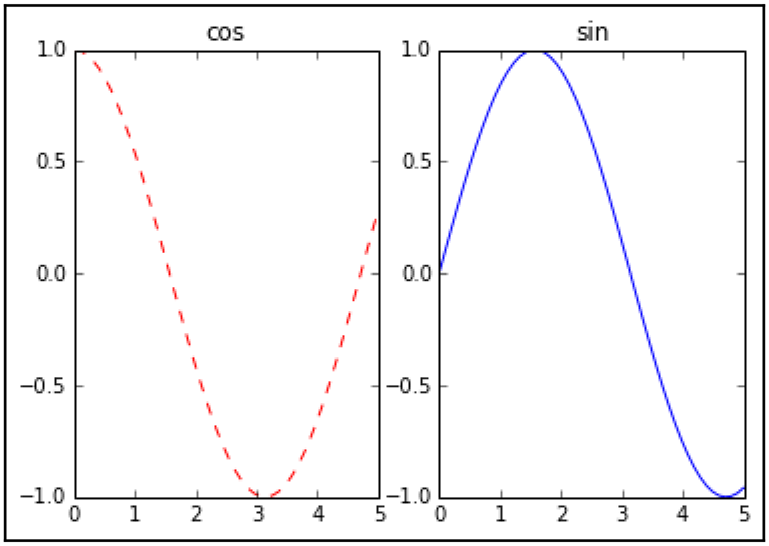
Please note that you can also set the title of the graph and label the axis by the title, `xlabel`, and `ylabel` from `pyplot`.

Using panels for clearer representations

Our second example will demonstrate to you how to create multiple graphics panels and plot a representation on each of them. We will also try to personalize the drawn curves by using different colors, sizes, and styles. Here is the example:

```
In: import matplotlib.pyplot as plt
    # defines 1 row 2 column panel, activates figure 1
    plt.subplot(1,2,1)
    plt.plot(x,y_cos,'r--')
    # adds a title
    plt.title('cos')
    # defines 1 row 2 column panel, activates figure 2
    plt.subplot(1,2,2)
    plt.plot(x,y_sin,'b-')
    plt.title('sin')
    plt.show()
```

The plot displays the cosine and sine curves on two distinct graphic panels:



The `subplot` command accepts the `subplot(nrows, ncols, plot_number)` parameter form. Therefore, when instantiated, it reserves a certain amount of space for the representation based on the `nrows` and `ncols` parameters and number of plots on the `plot_number` area (starting from area `1` on the left).

You can also accompany the `plot` command coordinates with another string parameter, which is useful for the definition of color and the type of the represented curve. The strings work by combining the codes that you can find on the following links:

- `https://matplotlib.org/api/lines_api.html#matplotlib.lines.Line2D.set_linestyle`: Will present the different line styles.
- `http://matplotlib.org/api/colors_api.html`: Offers a complete overview of the basic built-in colors. The page also points out that you can either use the `color` parameter together with the HTML names or hex strings for colors, or define the color you desire by using an RGB tuple, where each value of the tuple lies in the range of *[0,1]*. For instance, a valid parameter is `color = (0.1,0.9,0.9)`, which will create a color made of 10% red, 90% green, and 90% blue.
- `http://matplotlib.org/api/markers_api.html`: Lists all the possible marker styles you can adopt for your points.

Plotting scatterplots for relationships in data

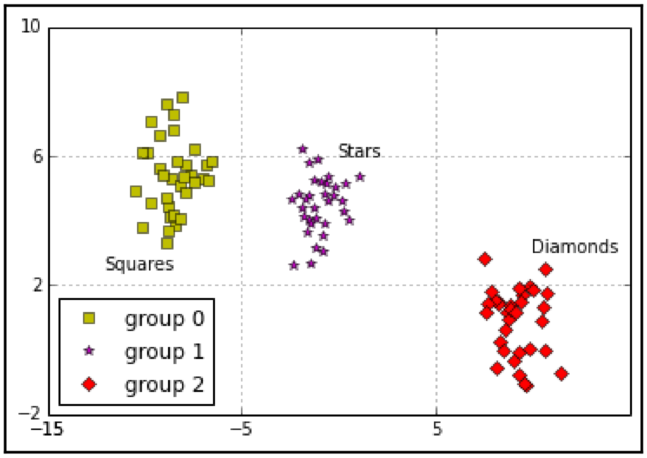
Scatterplots plot two variables as points on a plane, and they can help you figure out the relationship between the two variables. They are also quite effective if you want to represent groups and clusters. In our example, we will create three data clusters and represent them in a scatterplot with different shapes and colors:

```
In: from sklearn.datasets import make_blobs
    import matplotlib.pyplot as plt
    D = make_blobs(n_samples=100, n_features=2,
                   centers=3, random_state=7)
    groups = D[1]
    coordinates = D[0]
```

Since we have to plot three different groups, we will have to use three distinct `plot` commands. Each command specifies a different color and shape (the `'ys'`, `'m*'`, `'rD'` strings, where the first letter is the color and the second is the marker). Please also note that each plot instance is marked by a `label` parameter, which is used to assign a name to the group that has to be reported later in a legend:

```
In: plt.plot(coordinates[groups==0,0],
             coordinates[groups==0,1],
             'ys', label='group 0') # yellow square
    plt.plot(coordinates[groups==1,0],
             coordinates[groups==1,1],
             'm*', label='group 1') # magenta stars
    plt.plot(coordinates[groups==2,0],
             coordinates[groups==2,1],
             'rD', label='group 2') # red diamonds
    plt.ylim(-2,10) # redefines the limits of y axis
    plt.yticks([10,6,2,-2]) # redefines y axis ticks
    plt.xticks([-15,-5,5,-15]) # redefines x axis ticks
    plt.grid() # adds a grid
    plt.annotate('Squares', (-12,2.5)) # prints text at coordinates
    plt.annotate('Stars', (0,6))
    plt.annotate('Diamonds', (10,3))
    plt.legend(loc='lower left', numpoints= 1)
    # places a legend of labelled items
    plt.show()
```

The resulting plot will be a scatterplot of the three groups accompanied by their respective labels:



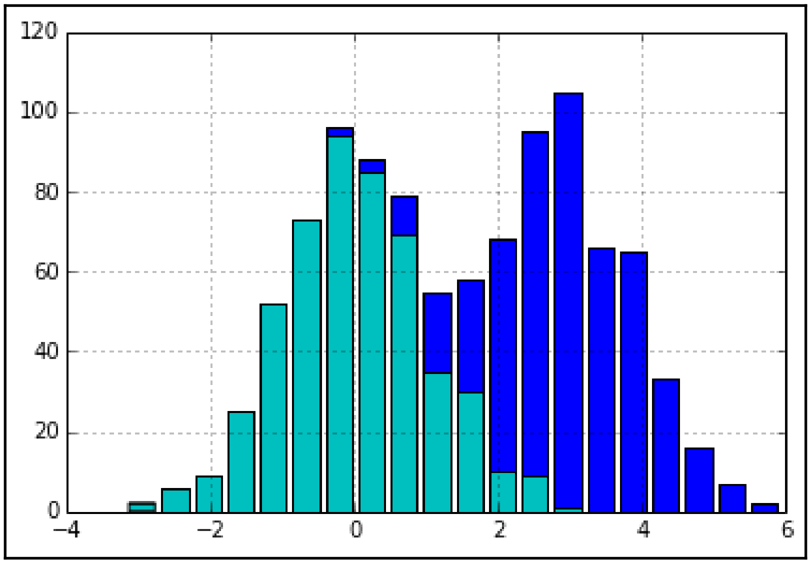
We have also added a legend (`pyplot.legend`), fixed a limit for both the axes (`pyplot.xlim` and `pyplot ylim`), and precisely explicated the ticks (`plt.xticks` and `plt.yticks`) that had to be put on them by specifying a list of values. Therefore, the grid (`pyplot.grid`) divides the plot exactly into nine quadrants and allows you to have a better idea of where the groups are positioned. Finally, we printed some text pointing out the group names (`pyplot.annotate`).

Histograms

Histograms can effectively represent the distribution of a variable. Here, we will visualize two normal distributions, both characterized by unit standard deviation, one having a mean of `0` and the other a mean of `3.0`:

```
In: import numpy as np
    import matplotlib.pyplot as plt
    x = np.random.normal(loc=0.0, scale=1.0, size=500)
    z = np.random.normal(loc=3.0, scale=1.0, size=500)
    plt.hist(np.column_stack((x,z)),
             bins=20,
             histtype='bar',
             color = ['c','b'],
             stacked=True)
    plt.grid()
    plt.show()
```

The conjoint distributions can offer a different insight on the data if there is a classification problem:



There are a few ways to personalize this kind of plot and obtain further insights about the analyzed distributions. First, by changing the number of bins, you will change how the distributions are discretized (discretization is the process that transforms continuous functions or series of values into a reduced, countable set of numbers: `en.wikipedia.org/wiki/Discretization`). Generally, 10 to 20 bins offer a good understanding of the distribution, though it really depends on the size of the dataset as well as the distribution. For instance, the Freedman-Diaconis rule prescribes that the optimal number of bins in a histogram in order to meaningfully visualize your data depends on the bin's width, to be calculated using the **interquartile range** (**IQR**) and the number of observations:

$$h = 2 * IQR * n^{\frac{-1}{3}}$$

Having calculated *h*, which is the bin width, the number of bins is computed by dividing the difference between the maximum and the minimum value by *h*:

bins=(max-min) / h

We can also change the type of visualization from bars to steps by changing the parameters from `histtype='bar'` to `histtype='step'`. By changing the `stacked` Boolean parameter to `False`, the curves won't stack into a unique bar in the parts that overlap, but you will clearly see the separate bars of each one.

Bar graphs

Bar graphs are useful for comparing quantities in different categories. They can be arranged either horizontally or vertically to present the mean estimate and error bands. They can be used to present various statistics of your predictors and how they relate to the target variable.

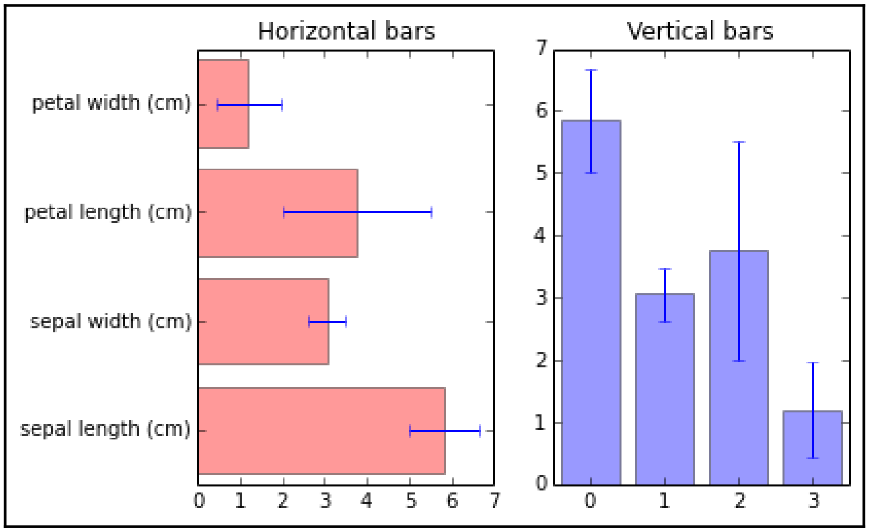
In our example, we will present the mean and standard deviation for the four variables of the Iris dataset:

```
In: from sklearn.datasets import load_iris
    import numpy as np
    import matplotlib.pyplot as plt
    iris = load_iris()
    average = np.mean(iris.data, axis=0)
    std = np.std(iris.data, axis=0)
    range_ = range(np.shape(iris.data)[1])
```

In our representation, we will prepare two subplots: one with horizontal bars (`plt.barh`), and the other with vertical bars (`plt.bar`). The standard error is represented by an error bar, and according to the graph orientation, we can use the `xerr` parameter for horizontal bars and `yerr` for vertical ones:

```
In: plt.subplot(1,2,1) # defines 1 row, 2 columns panel, activates figure 1
    plt.title('Horizontal bars')
    plt.barh(range_,average, color="r",
             xerr=std, alpha=0.4, align="center")
    plt.yticks(range_, iris.feature_names)
    plt.subplot(1,2,2) # defines 1 row 2 column panel, activates figure 2
    plt.title('Vertical bars')
    plt.bar(range_,average, color="b", yerr=std, alpha=0.4, align="center")
    plt.xticks(range_, range_)
    plt.show()
```

Horizontal and verticals bars are now together in the same plot:



It is important to note the use of the `plt.xticks` command (and of `plt.yticks` for the ordinate axis). The first parameter informs the command about the number of ticks that have to be placed on the axis, and the second one explicates the labels that have to be put on the ticks.

Another interesting parameter to notice is `alpha`, which has been used to set the transparency level of the bar. The `alpha` parameter is a float number ranging from 0.0, fully transparent, to 1.0, which causes the color to be shown in different levels of opaqueness.

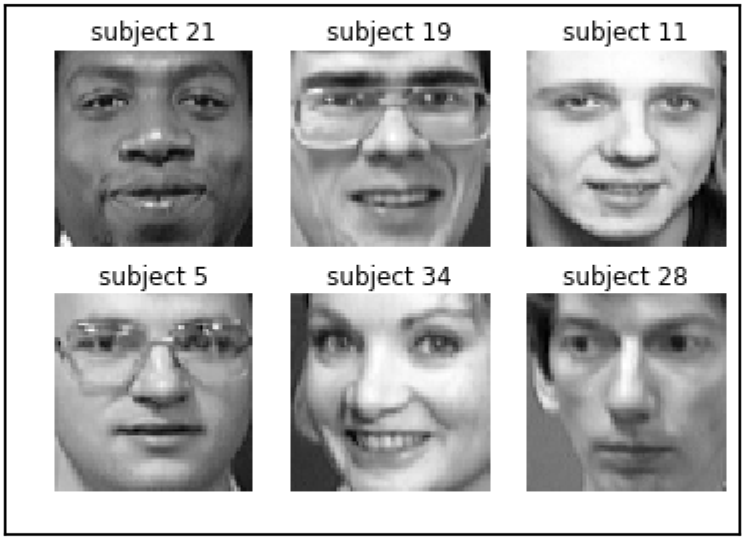
Image visualization

The last possible visualization that we explore using `matplotlib` has to do with images. Resorting to `plt.imgshow` is useful when you are working with image data. Let's take as an example the Olivetti dataset, an open source set of images of 40 people who provided 10 images of themselves at different times (and with different expressions, a fact that makes it more challenging for testing face recognition algorithms). The images from this dataset are provided as feature vectors of pixel intensities. Therefore, it is important to reshape the vectors in order to make them resemble a matrix of pixels. Setting the interpolation to `'nearest'` helps to smooth the picture:

```
In: from sklearn.datasets import fetch_olivetti_faces
    import numpy as np
```

```
        import matplotlib.pyplot as plt
        dataset = fetch_olivetti_faces(shuffle=True, random_state=5)
        photo = 1
        for k in range(6):
            plt.subplot(2, 3, k+1)
            plt.imshow(dataset.data[k].reshape(64, 64),
                       cmap=plt.cm.gray,
                       interpolation='nearest')
            plt.title('subject '+str(dataset.target[k]))
            plt.axis('off')
        plt.show()
```

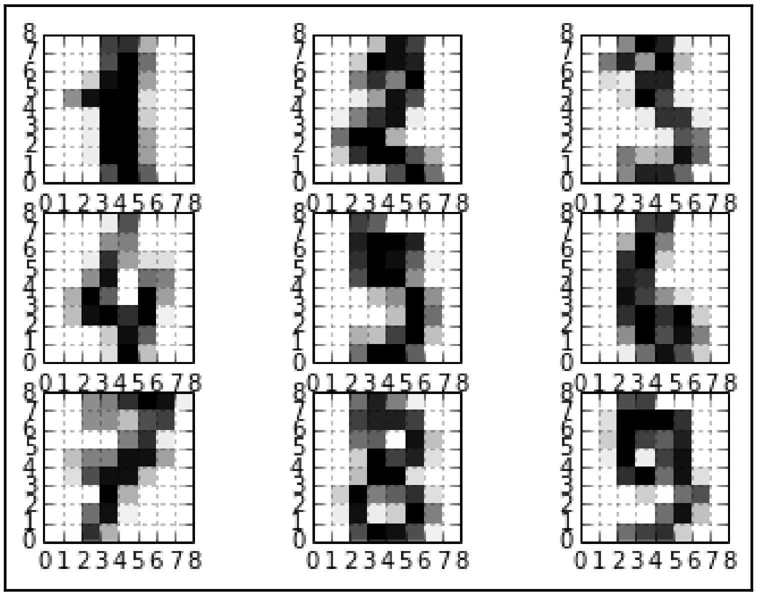
A complete panel of images will be plotted:



We can also visualize handwritten digits or letters. In our example, we will plot the first nine digits from the scikit-learn handwritten digit dataset and set the extent of both the axes (by using the `extent` parameter and providing a list of minimum and maximum values) to align the grid to the pixels:

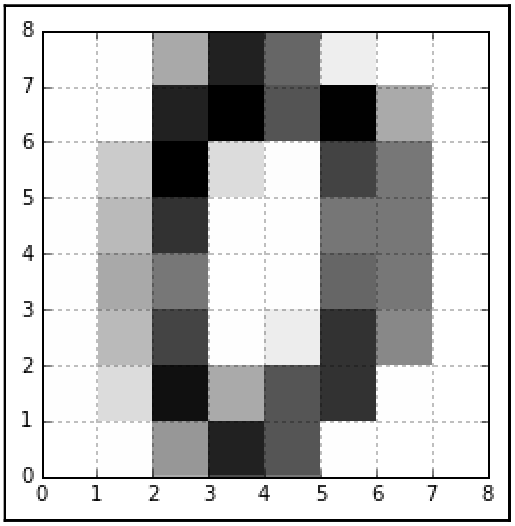
```
    In: from sklearn.datasets import load_digits
        digits = load_digits()
        for number in range(1,10):
            fig = plt.subplot(3, 3, number)
            fig.imshow(digits.images[number],
                       cmap='binary',
                       interpolation='none',
                       extent=[0,8,0,8])
            fig.set_xticks(np.arange(0, 9, 1))
            fig.set_yticks(np.arange(0, 9, 1))
            fig.grid()
        plt.show()
```

A simple close-up on a single number can be obtained by printing only one image:



```
In: plt.imshow(digits.images[0],
               cmap='binary',
               interpolation='none',
               extent=[0,8,0,8])
# Extent defines the images max and min
# of the horizontal and vertical values
plt.grid()
```

The resulting image clearly highlights how pixels constitute the image and their gray levels:



Selected graphical examples with pandas

Using appropriately set hyper-parameters, many machine learning algorithms can optimally learn how to map your data with respect to your target outcome. Yet, their predictive performance can be improved further by fixing hidden and subtle problems in data. It is not simply a matter of detecting any missing or outlying case. Sometimes, it is a matter of whether there are any groups or unusual distributions in the data (for instance, multimodal distributions). Clearly drafted data plots can explicate the relationship between variables, and they can lead to the creation of new and better features in order to predict, with increased accuracy, your target variable.

The just-described practice is called **explorative data analysis** (**EDA**), and it can bring effective results if it is done accordingly with the following:

- It should be fast, allowing you to explore and develop new ideas, and test them, and restart with a new exploration and fresh ideas
- It should be based on graphical representations in order to better describe data as a whole, no matter how high its dimensionality is

The pandas DataFrame offers many EDA tools that can help you in your explorations. However, first you have to transform your data into a DataFrame:

```
In: import pandas as pd
    print ('Your pandas version is: %s' % pd.__version__)
    from sklearn.datasets import load_iris
    iris = load_iris()
    iris_df = pd.DataFrame(iris.data, columns=iris.feature_names)
    groups = list(iris.target)
    iris_df['groups'] = pd.Series([iris.target_names[k] for k in groups])

Out: Your pandas version is: 0.23.1
```

Please check your version of pandas. We tested the code in the book under the version 0.23.1 of pandas, and it should also hold for the later releases.

We will be using the iris_df DataFrame for all the examples presented in the following paragraphs.

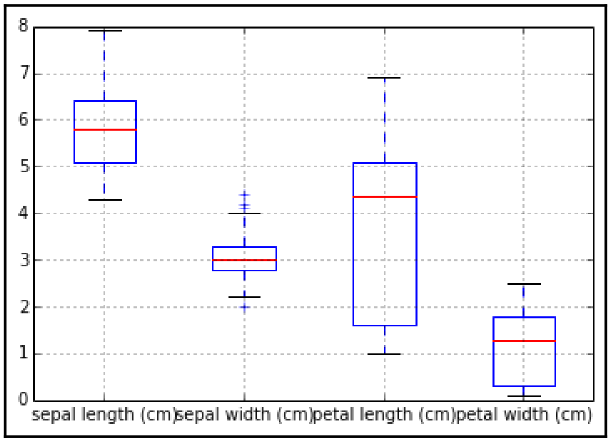
The pandas package actually relies on matplotlib functions for its visualizations. It simply provides a convenient wrapper around the otherwise complex plotting instructions. This offers advantages in terms of speed and simplicity, which are the core values of any EDA process. Instead, if your purpose is to best communicate the findings by using beautiful visualization, you may notice that it is not so easy to customize the pandas graphical outputs. Therefore, when it is paramount to create specific graphics outputs, it is better to start working directly from scratch using matplotlib instructions.

Working with boxplots and histograms

Distributions should always be the first aspect to be inspected in your data. Boxplots draft the key figures in the distribution and help you spot outliers. Just use the boxplot method on your DataFrame for a quick overview:

```
In: boxplots = iris_df.boxplot(return_type='axes')
```

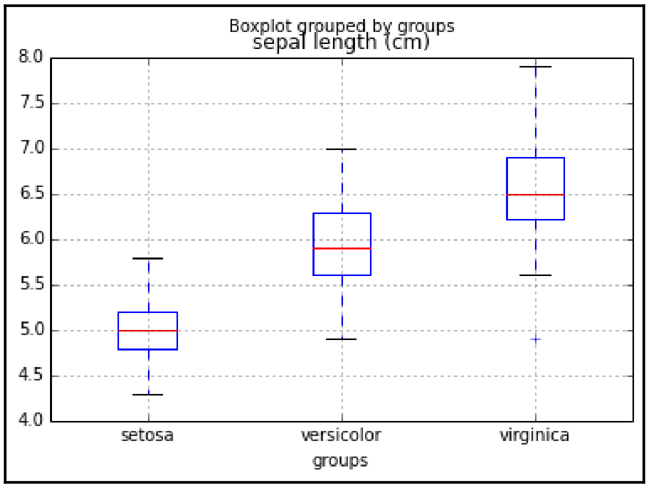
Here are the boxplots of all the numeric variables of the dataset:



If you already have groups in your data (from categorical variables, or derived from unsupervised learning), just point out the variable you need data to be represented in the boxplot and specify that you need to have it separated by the groups (use the `by` parameter followed by the string name of the grouping variable):

```
In: boxplots = iris_df.boxplot(column='sepal length (cm)',
                               by='groups',
                               return_type='axes')
```

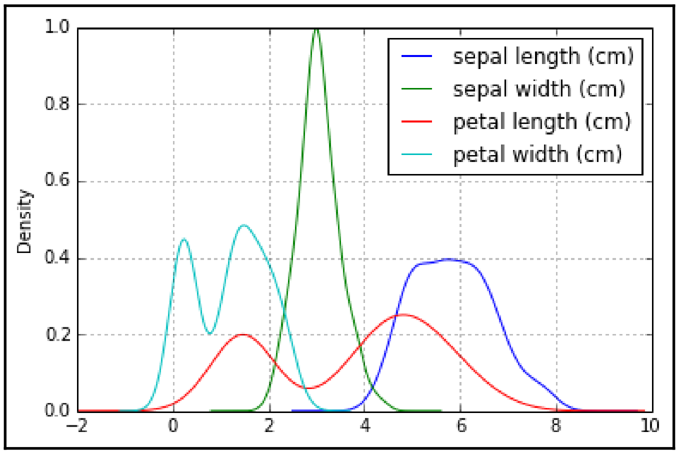
After running the code, you will get the boxplot by groups:



In this way, you can quickly know whether the variable is a good discriminator of the group differences. Anyway, boxplots cannot provide you with a complete view of distributions as histograms and density plots. For instance, by using histograms and density plots, you can figure out whether there are distribution peaks or valleys:

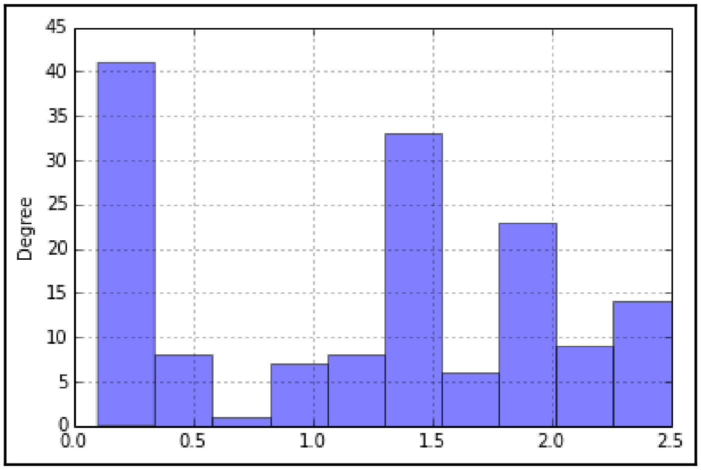
```
In: densityplot = iris_df.plot(kind='density')
```

The code prints the distributions for all the numeric variables of the dataset:



```
In: single_distribution = iris_df['petal width (cm)'].plot(kind='hist',
                                                              alpha=0.5)
```

Here is the resulting distribution represented by a histogram:



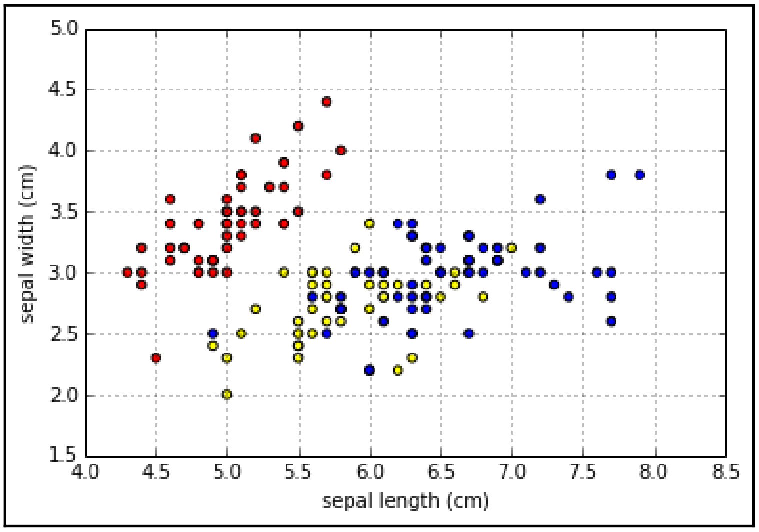
You can obtain both histograms and density plots by using the plot method. This method allows you to represent the whole dataset, specific groups of variables (you just have to provide a list of the string names and do some fancy indexing), or even single variables.

Plotting scatterplots

Scatterplots can be used to effectively understand whether the variables are in a nonlinear relationship, and you can get an idea about their best possible transformations to achieve linearization. If you are using an algorithm based on linear combinations, such as linear or logistic regression, figuring out how to render their relationship more linearly will help you achieve a better predictive power:

```
In: colors_palette = {0: 'red', 1: 'yellow', 2:'blue'}
    colors = [colors_palette[c] for c in groups]
    simple_scatterplot = iris_df.plot(kind='scatter', x=0, y=1, c=colors)
```

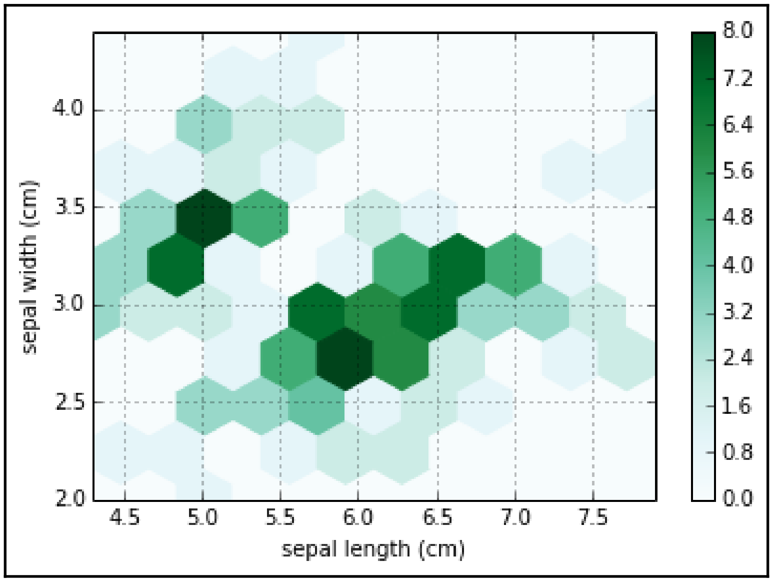
After running the code, a nicely drawn scatterplot will appear:



Scatterplots can be turned into hexagonal binning plots. In addition, they help you effectively visualize the point densities, where the points naturally aggregate together more, thus revealing clusters hidden in your data. For achieving such results, you may use some of the variables originally present in the dataset, or the dimensions obtained by a PCA or by another dimensionality reduction algorithm:

```
In: hexbin = iris_df.plot(kind='hexbin', x=0, y=1, gridsize=10)
```

Here is the resulting `hexbin` plot:

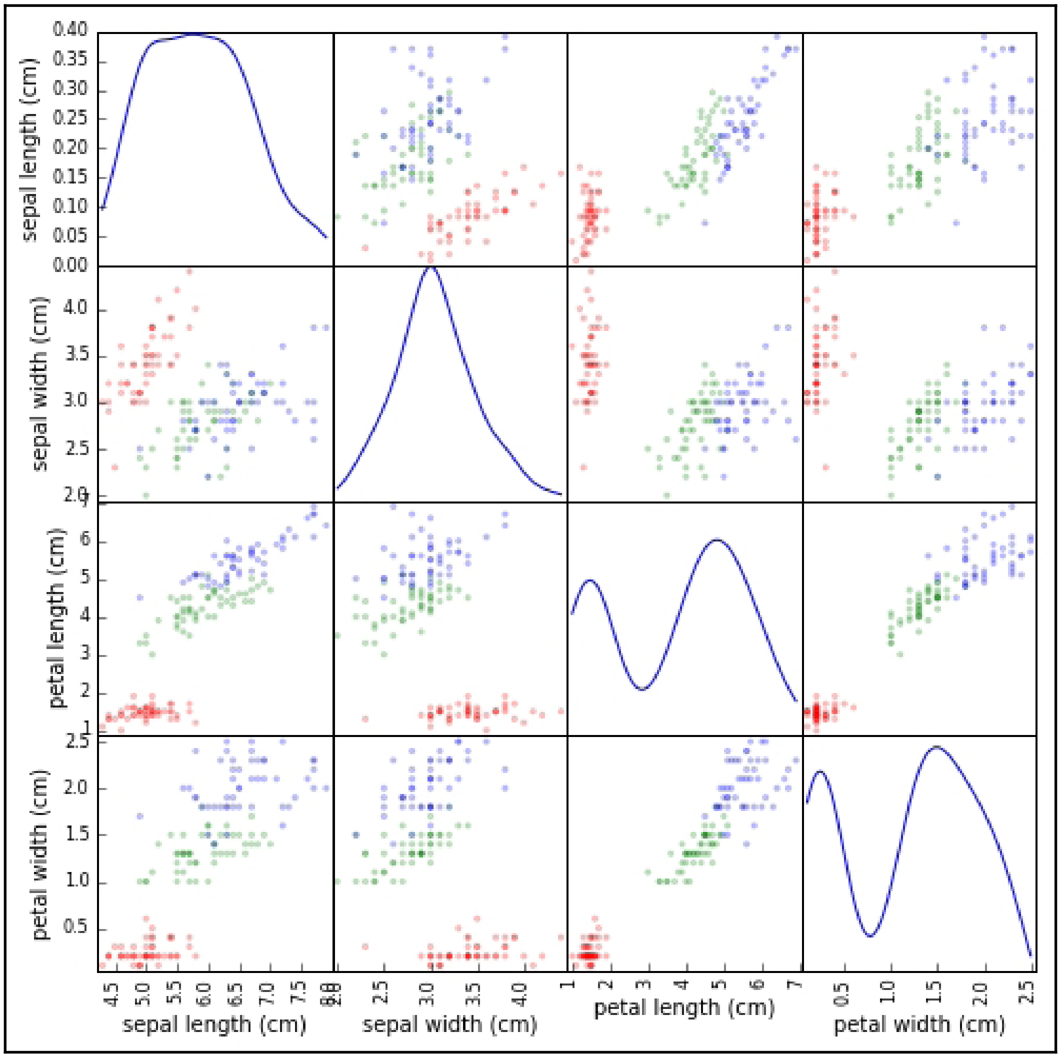


The `gridsize` parameter indicates how many data points the chart will summarize in a single grid. A larger number will create large grid cells, whereas a smaller one will create small cells.

Scatterplots are bivariate. Consequently, you'll require a single plot for every variable combination. If your variables are not so many in number (otherwise, the visualization will be cluttered), a quick solution is to use the `pandas` command to draw a matrix of scatterplots automatically (using the kernel density estimation, `'kde'`, in order to plot the distribution of each feature on the diagonal of the chart):

```
In: from pandas.plotting import scatter_matrix
    colors_palette = {0: "red", 1: "green", 2: "blue"}
    colors = [colors_palette[c] for c in groups]
    matrix_of_scatterplots = scatter_matrix(iris_df,
                                            alpha=0.2,
                                            figsize=(6, 6),
                                            color=colors,
                                            diagonal='kde')
```

After running the previous code, you will get a complete matrix of plots (densities on the diagonal):



A few parameters can control various aspects of the scatterplot matrix. The `alpha` parameter controls the amount of transparency, and `figsize` provides the width and height of the matrix in inches. Finally, `color` accepts a list indicating the color of each point in the plot, thus allowing the depicting of different groups in data. In addition, by selecting `'kde'` or `'hist'` on your `diagonal` parameter, you can opt to represent density curves or histograms of each variable on the diagonal of the scatter matrix.

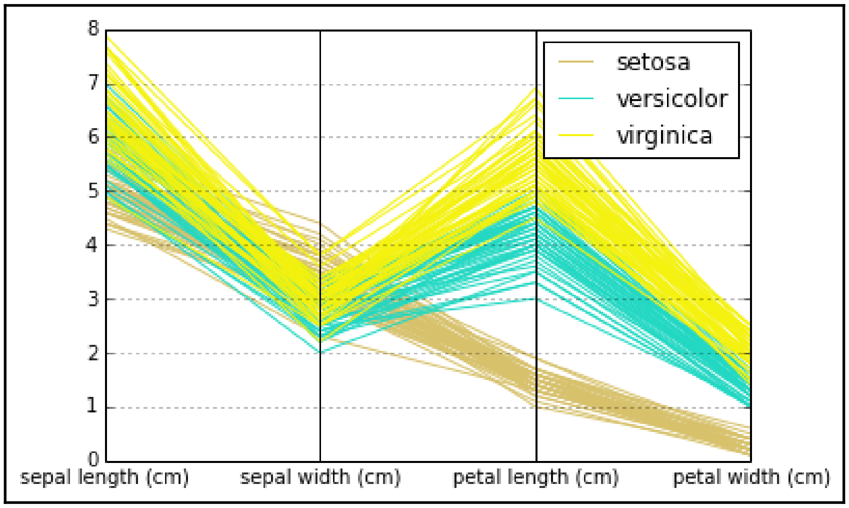
Discovering patterns by parallel coordinates

The scatterplot matrix can inform you about the conjoint distributions of your features. It helps you locate groups in data and verify whether they are distinguishable. Parallel coordinates are another kind of plot that is helpful in providing you with a hint about the most group-discriminating variables present in your data.

By plotting all the observations as parallel lines with respect to all the possible variables (arbitrarily aligned on the abscissa), parallel coordinates will help you spot whether there are streams of observations grouped as your classes, and understand the variables that best separate the streams (the most useful predictor variables). Naturally, in order for the chart to be meaningful, the features in the plot should have the same scale (otherwise, normalize them) as in the Iris dataset:

```
In: from pandas.tools.plotting import parallel_coordinates
    pll = parallel_coordinates(iris_df,'groups')
```

The previous code will output the parallel coordinates:



`parallel_coordinates` is a pandas function that, in order to work properly, just needs as parameters the data DataFrame and the string name of the variable containing the groups whose separability you want to test. For this reason, you should have the group variable available in your dataset. However, don't forget to remove it after you finish exploring by using the `DataFrame.drop('variable name', axis=1, inplace=True)` method.

Wrapping up matplotlib's commands

As we have seen in the previous paragraph, pandas can speed up exploring data visually since it wraps up into single commands what would have required an entire code snippet using matplotlib. The idea behind this is that unless you need to tailor and configure a special visualization, using a wrapper can allow you to create standard graphics faster.

Apart from pandas, other packages assemble low-level instructions from matplotlib into more user-friendly commands for specific representations and usage:

- Seaborn is a package that extends your visualization capabilities by providing you with a set of statistical plots useful for finding out trends and discriminating groups
- `ggplot` is a port of a popular R library, `ggplot2` (`ggplot2.tidyverse.org`), based on the visualization grammar proposed in Leland Wilkinson's book, Grammar of Graphics. The R library is continuously developed and it offers much functionality; the Python porting (`ggplot.yhathq.com`) features the basics (`ggplot.yhathq.com/docs/index.html`) and its complete development is still underway (`github.com/yhat/ggplot`).
- MPLD3 (`mpld3.github.io`) leverages the JavaScript library for graphics manipulation, D3.js, in order to easily transform any matplotlib output into HTML code, which can be rendered using a browser and a tool such as a Jupyter Notebook; or within an internet website.
- Bokeh (`bokeh.pydata.org/en/latest/`) is an interactive visualization package that leverages JavaScript and browser-rendered outputs. It is a great replacement for D3.js since you just need Python in order to leverage the capabilities of JavaScript to quickly represent your data in an interactive way.

In the following pages, we will introduce Seaborn, providing some building blocks for leveraging their visualizations in your data science projects.

Introducing Seaborn

Created by Michael Waskom and hosted on the PyData website (`http://seaborn.pydata.org/`), Seaborn is a library that wraps up the low-level matplotlib with the entire pyData stack, allowing integrating charts with data structures from NumPy and pandas, and with statistical routines from SciPy and StatModels. All that is achieved with a particular care to aesthetics, thanks to built-in themes, and to color palettes especially devised to reveal patterns in data.

If you don't have Seaborn presently installed on your system (the Anaconda distributions provide it by default, for instance), you can easily get it both by `pip` and `conda` (reminding you that the `conda` version may lag behind the `pip` version taken directly from PyPI, the Python Package Index.

```
$> pip install seaborn
$> conda install seaborn
```

In these examples, we have used version 0.9 of the Seaborn package.

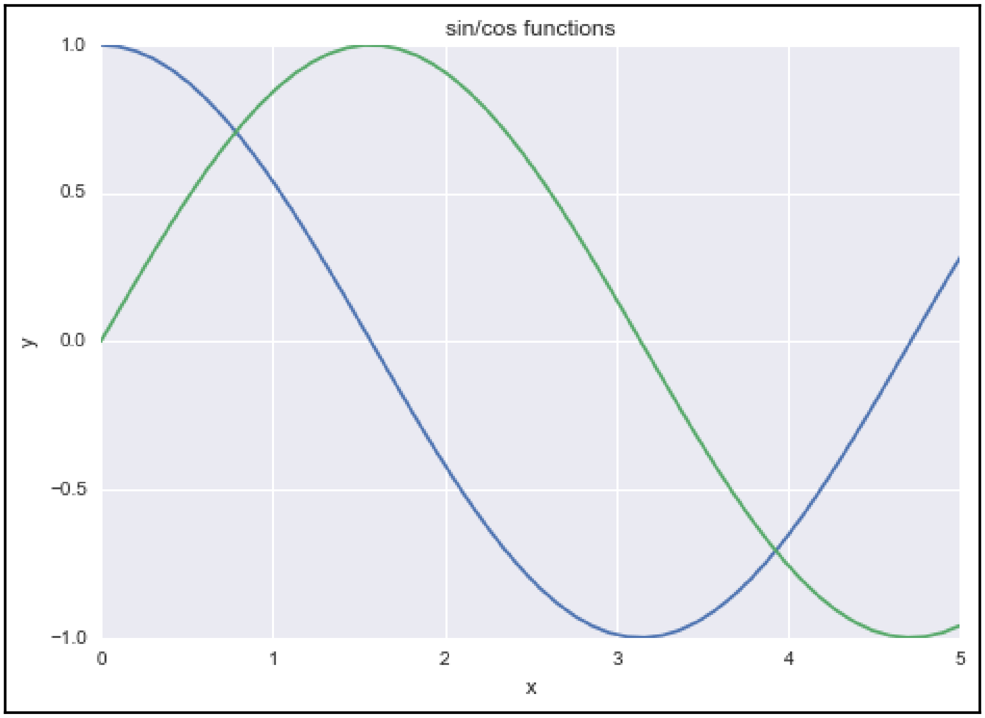
You can upload the package and set the Seaborn style as the default matplotlib style by the following:

```
In: import seaborn as sns
    sns.set()
```

This is enough to turn all your matplotlib-based representations into more visually appealing charts:

```
In: x = np.linspace(0, 5, 50)
    y_cos = np.cos(x)
    y_sin = np.sin(x)
    plt.figure()
    plt.plot(x,y_cos)
    plt.plot(x,y_sin)
    plt.xlabel('x')
    plt.ylabel('y')
    plt.title('sin/cos functions')
    plt.show()
```

Here is the result:



You can obtain interesting results from any of the previously seen charts, even the ones generated using graphical methods in pandas (after all, pandas also relies on matplotlib for creating its explorative plots).

There are five preset themes in Seaborn:

- `darkgrid`
- `whitegrid`
- `dark`
- `white`
- `ticks`

`darkgrid` is the default one. You can easily try each one by using the `set_style` command and the name of your preferred theme, and then running your plot commands:

```
In: sns.set_style('whitegrid')
```

All you have to do is just decide which theme helps you better convey the information on your chart. You can limit a style to a single representation enclosing it:

```
In: with sns.axes_style('whitegrid'):
        # Your plot commands here
        pass
```

Other stylish changes may involve the spines, which are the borders of the chart. Using the `despine` command, you can easily remove the top and right borders:

```
In: sns.despine()
```

Moreover, you can remove the left border using the `left=True` parameter, offset the axis using the `offset` parameter, and trim it (using `trim=True`). All these operations were otherwise not so accessible because of matplotlib commands alone.

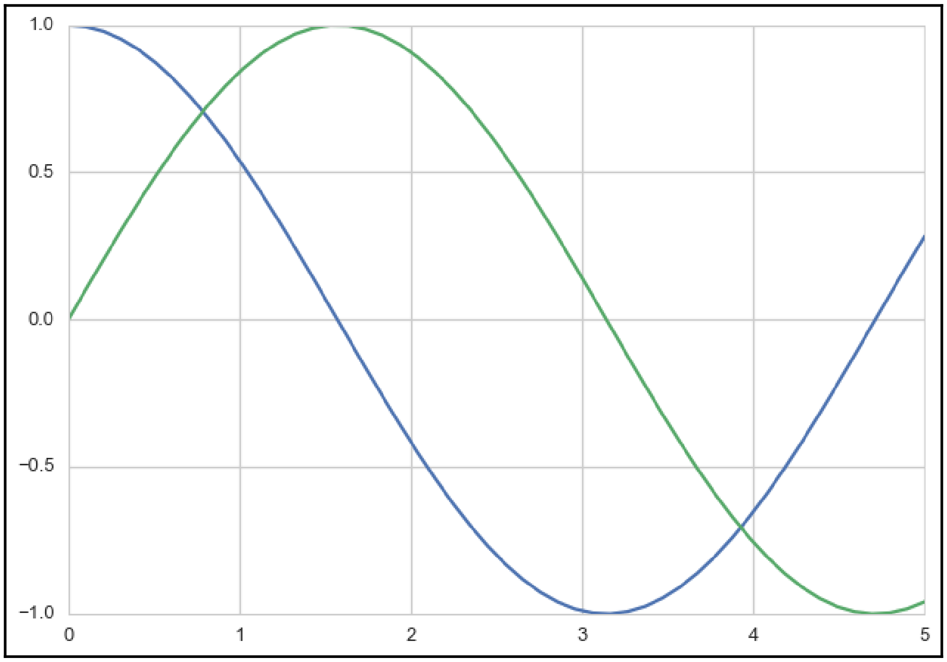
Another useful control that Seaborn permits you regards the scale of the chart. A certain chart scale (involving different thickness of lines, size of fonts, and so on) is called a context, and the available contexts are self-explicative-paper, notebook, talk, and poster as possible options. For instance, if your chart has to be displayed on an MS PowerPoint presentation, just run the following command before creating the graphics:

```
In: sns.set_context("talk")
```

Let's see an example of some of such stylish effects on our initial sin/cos chart:

```
In: sns.set_context("talk")
    with sns.axes_style('whitegrid'):
        plt.figure()
        plt.plot(x,y_cos)
        plt.plot(x,y_sin)
        plt.show()
    sns.set()
```

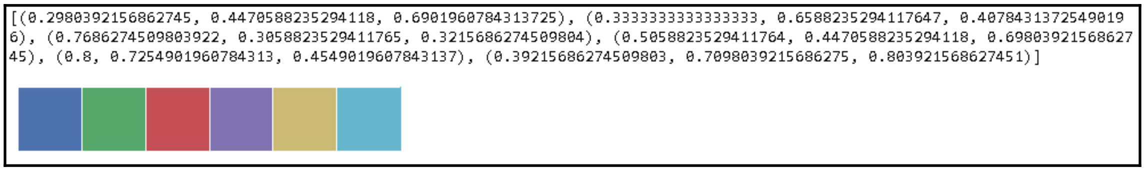
The code will plot the following chart:



Also, choosing the right color cycle or set may help your graphical representation shine. For this, Seaborn offers the `color_palette()` command, which won't just tell the current palette's RBG values (if run with no parameters); it will also accept the name of any palette offered by Seaborn or any matplotlib colormap. It even accepts custom lists of colors provided by you in any matplotlib format (RGB tuples, hex color codes, or HTML color names) in order to create your own palette:

```
In: current_palette = sns.color_palette()
    print (current_palette)
    sns.palplot(current_palette)
```

After running the code, you will visualize the current palette both in values and colors:



```
[(0.2980392156862745, 0.4470588235294118, 0.6901960784313725), (0.3333333333333333, 0.6588235294117647, 0.4078431372549019
6), (0.7686274509803922, 0.3058823529411765, 0.3215686274509804), (0.5058823529411764, 0.4470588235294118, 0.69803921568627
45), (0.8, 0.7254901960784313, 0.4549019607843137), (0.39215686274509803, 0.7098039215686275, 0.803921568627451)]
```

There are a few palettes available, as mentioned. First, all Seaborn palettes are the following:

- `deep`
- `muted`
- `bright`
- `pastel`
- `dark`
- `colorblind`

You also have to add `hls`, `husl`, and all the matplotlib colormaps, which can be reversed by appending *_r* to their name, or made darker by appending *_d*.

Both the names and examples of matplotlib colormaps can be found at this web page: `http://matplotlib.org/examples/color/colormaps_reference.html`.

The `hls` color space is an automatic transformation in the RGB scale of values, which may or may not work for your representations since colors have different intensities (for instance, yellow and green colors are perceived as brighter whereas blue is perceived as darker).

As an alternative to `hsl`, you can use the `husl` palette, which is friendlier for the human eye, as explained by `http://www.hsluv.org/`.

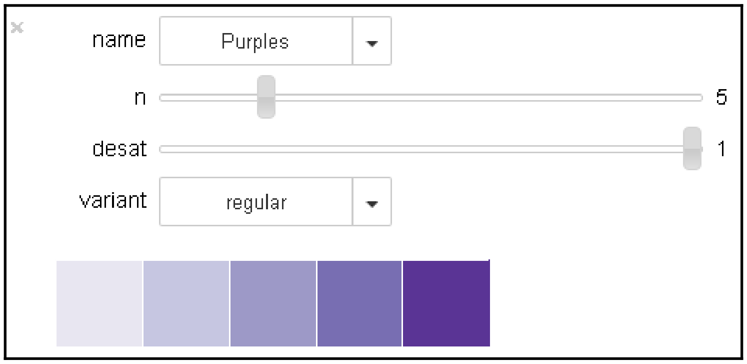
Finally, you can just create a personalized palette using the Color Brewer tool, which can be both found online (`http://www.personal.psu.edu/cab38/ColorBrewer/ColorBrewer_intro.html`) or required in an app from your Jupyter Notebook. In a notebook cell, using the `choose_colorbrewer_palette` command will make an interactive tool appear. For everything to work, it is essential that you specify as a parameter the `data_type`, a string explicating the nature of your palette related to the data you intend to represent:

- **Sequential** if you want to represent continuity
- **Diverging** for representing contrasts
- **Qualitative** when you just want to discriminate between different classes

Let's see how to create a custom sequential palette, and use it:

```
In: your_palette = sns.choose_colorbrewer_palette('sequential')
```

A complete dashboard will appear:



After setting the colors, `your_palette` will turn into a list of the RGB values:

```
In: print(your_palette)

Out:[(0.91109573770971852, 0.90574395025477683, 0.94832756940056306),
    (0.7764706015586853, 0.77908498048782349, 0.88235294818878174),
    (0.61776242186041452, 0.60213766261643054, 0.78345253116944269),
    (0.47320263584454858, 0.43267974257469177, 0.69934642314910889),
    (0.35681661753093497, 0.20525952297098493, 0.58569783322951374)]
```

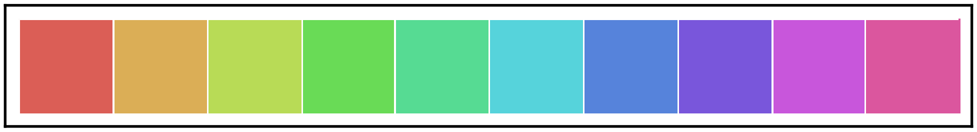
When you are done with your choice, you can just call `sns.set_palette(your_palette)` and have the colors used when drawing all your charts.

If you need just to operate on a chart with some specific colors, using a `with` statement and nesting the chart snippet under it will suffice, as we have seen for the themes before. Instead, if you definitely need to set a certain palette, use `set_palette`.

The color palette is made up of six colors, helping you distinguish at least six trends or classes. If you need to distinguish more, you simply can operate with the `hls` palette and point out the number of colors you need to cycle:

```
In: new_palette=sns.color_palette('hls', 10)
    sns.palplot(new_palette)
```

Here is the resulting palette:



Finally, closing our section about themes and colors, since Seaborn is another, smarter way to use functions offered by matplotlib, we remind you that the resulting charts can be modified further using any basic command coming from matplotlib itself. Or, they can be further transformed by packages such as MPLD3 or Bokeh into JavaScript.

Enhancing your EDA capabilities

Seaborn doesn't just make your charts more beautiful and easily controlled in their aspect; it also provides you with new tools for EDA that helps you discover distributions and relationships between variables.

Before proceeding, let's reload the package and have both the Iris and Boston datasets ready in pandas DataFrame format:

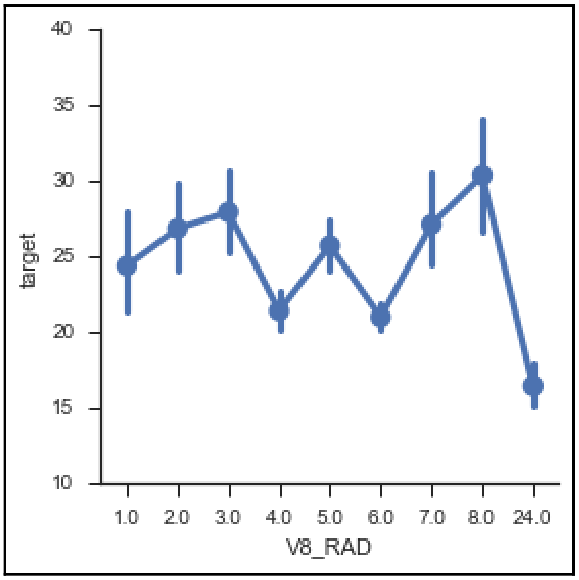
```
In: import seaborn as sns
    sns.set()

    from sklearn.datasets import load_iris
    iris = load_iris()
    X_iris, y_iris = iris.data, iris.target
    features_iris = [a[:-5].replace(' ','_') for a in iris.feature_names]
    target_labels = {j: flower \
                        for j, flower in enumerate(iris.target_names)}
    df_iris = pd.DataFrame(X_iris, columns=features_iris)
    df_iris['target'] = [target_labels[y] for y in y_iris]

    from sklearn.datasets import load_boston
    boston = load_boston()
    X_boston, y_boston = boston.data, boston.target
    features_boston = np.array(['V'+'_'.join([str(b), a])
                                for a,b in zip(boston.feature_names,
                                range(len(boston.feature_names)))])
    df_boston = pd.DataFrame(X_boston, columns=features_boston)
    df_boston['target'] = y_boston
    df_boston['target_level'] = pd.qcut(y_boston,3)
```

As for as the Iris dataset, the target variable has been converted into a descriptive text of the Iris species. For the Boston dataset, the continuous target variable, the median value of owner-occupied homes, has been divided into three equal parts, representing lower, median, and high prices (using the pandas function, `qcut`).

Seaborn can first help your data exploration with figuring out how discretely valued or categorical variables are related to numeric ones. This is achieved using the `catplot` function:

```
In: with sns.axes_style('ticks'):
        sns.catplot(data=df_boston, x='V8_RAD', y='target', kind='point')
```

You will find it insightful exploring similar plots, since they explicit the target level and its variance:

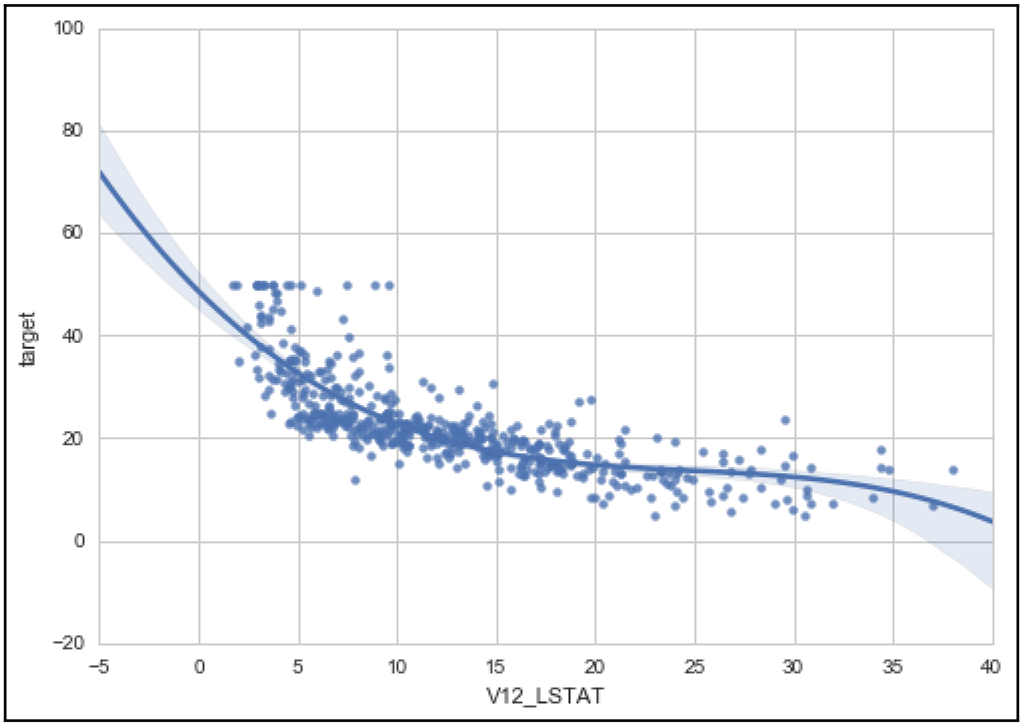


In our example, in the Boston dataset, the index of accessibility to radial highways, which is discretely valued, is compared with the target in order to check both the functional form of its relationships and the associated variance at each level.

In the case, instead, the comparison is between numeric variables; Seaborn offers an enhanced scatterplot with a regression fitted curve trend incorporated, which can clue you in to possible data transformations when the relationship is not linear:

```
In: with sns.axes_style("whitegrid"):
        sns.regplot(data=df_boston, x='V12_LSTAT', y="target", order=3)
```

The fitting line is promptly displayed:

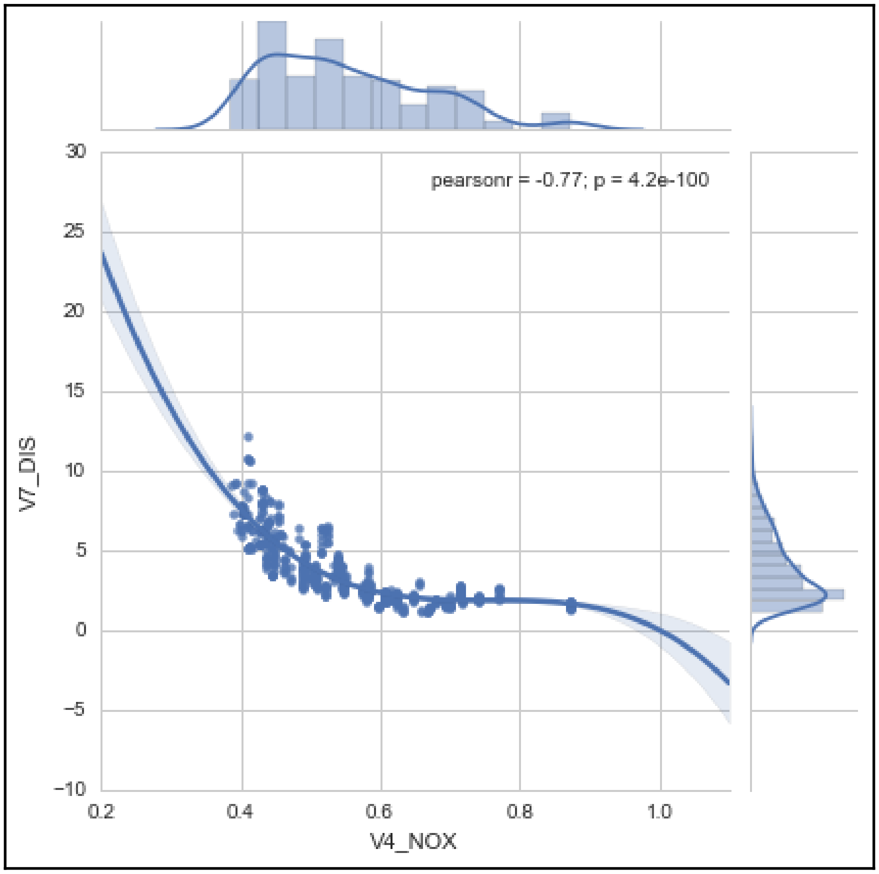


`regplot` in Seaborn can visualize regression plots of any order (we displayed a second-degree polynomial fit). Among the available regression plots, you can use a standard linear regression, a robust regression or even a logistic regression if one of the inspected features is binary.

Where it is necessary to consider distributions too, `jointplot` will provide additional plots on the side of the scatterplot:

```
In: with sns.axes_style("whitegrid"):
        sns.jointplot("V4_NOX", "V7_DIS",
                      data=df_boston, kind='reg',
                      order=3)
```

`jointplot` produces the following chart:

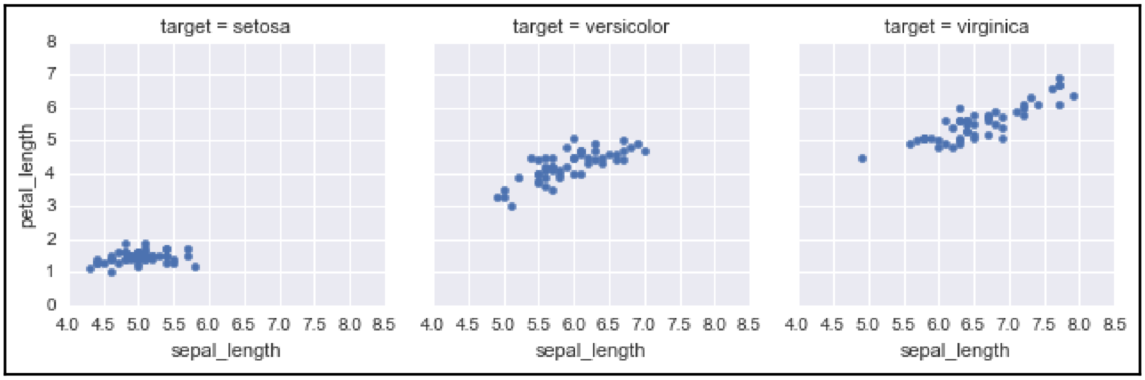


Ideal for representing bivariate relationships by acting on the `kind` parameter, `jointplot` can also represent simple scatterplots or densities (kind=`scatter` or kind=`kde`).

When the purpose is to discover what discriminates classes, `FacetGrid` can arrange different plots in a comparable way and help you understand where there are differences. For instance, we can inspect the scatterplot of Iris species in order to figure out whether they occupy different parts of the feature state:

```
In: with sns.axes_style("darkgrid"):
        chart = sns.FacetGrid(df_iris, col="target_level")
        chart.map(plt.scatter, "sepal_length", "petal_length")
```

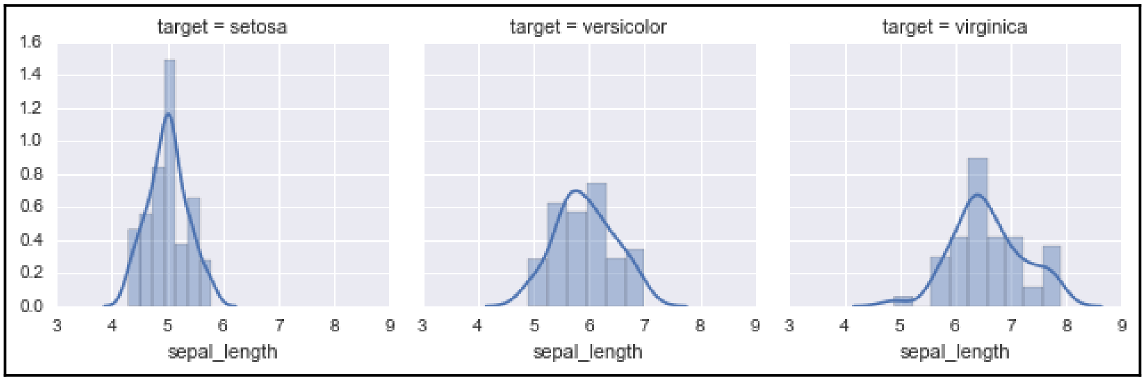
The code will nicely print a panel representing the comparisons based on groups:



Similar comparisons can be made using distributions (`sns.distplot`) or regression slopes (`sns.regplot`):

```
In: with sns.axes_style("darkgrid"):
        chart = sns.FacetGrid(df_iris, col="target")
        chart.map(sns.distplot, "sepal_length")
```

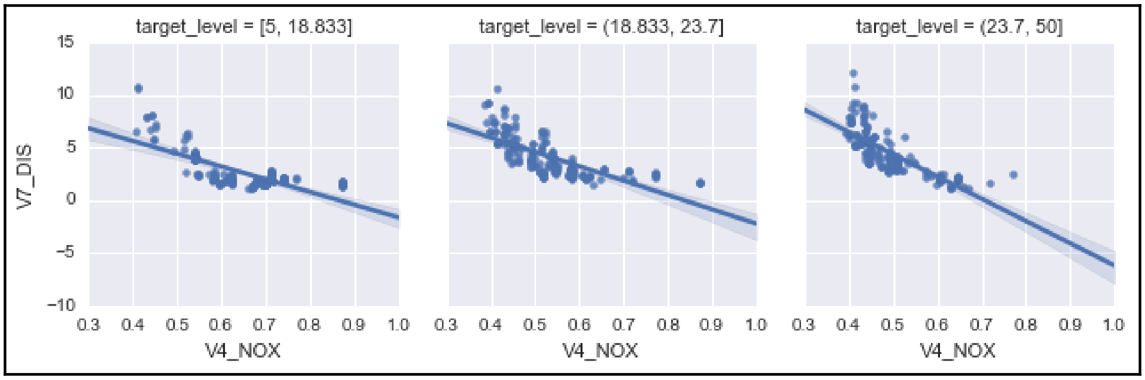
The first comparison is based on distributions:



The subsequent comparison is based on fitting a linear regression line:

```
In: with sns.axes_style("darkgrid"):
        chart = sns.FacetGrid(df_boston, col="target_level")
        chart.map(sns.regplot, "V4_NOX", "V7_DIS")
```

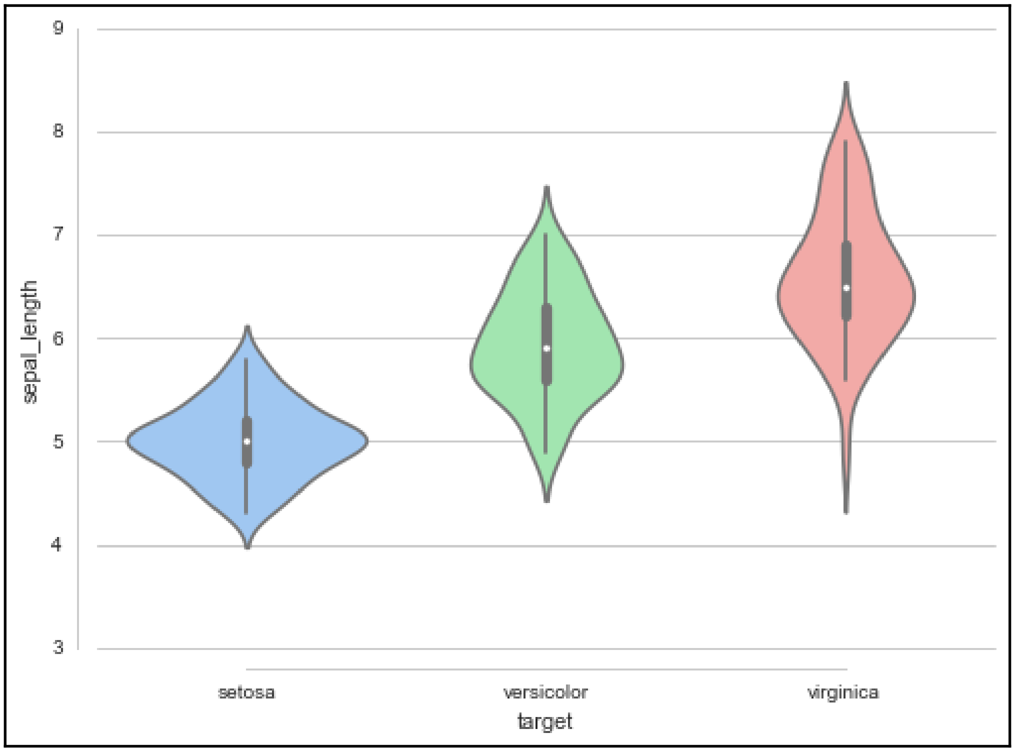
Here is the regression-based comparison:



As for evaluating data distributions across classes, Seaborn offers an alternative tool, which is the violin plot (`https://medium.com/@bioturing/5-reasons-you-should-use-a-violin-graph-31a9cdf2d0c6`). A violin plot is simply a boxplot whose box is shaped based on density estimation, thus visually conveying information that is more intuitive:

```
In: with sns.axes_style("whitegrid"):
        ax = sns.violinplot(x="target", y="sepal_length",
                            data=df_iris, palette="pastel")
        sns.despine(offset=10, trim=True)
```

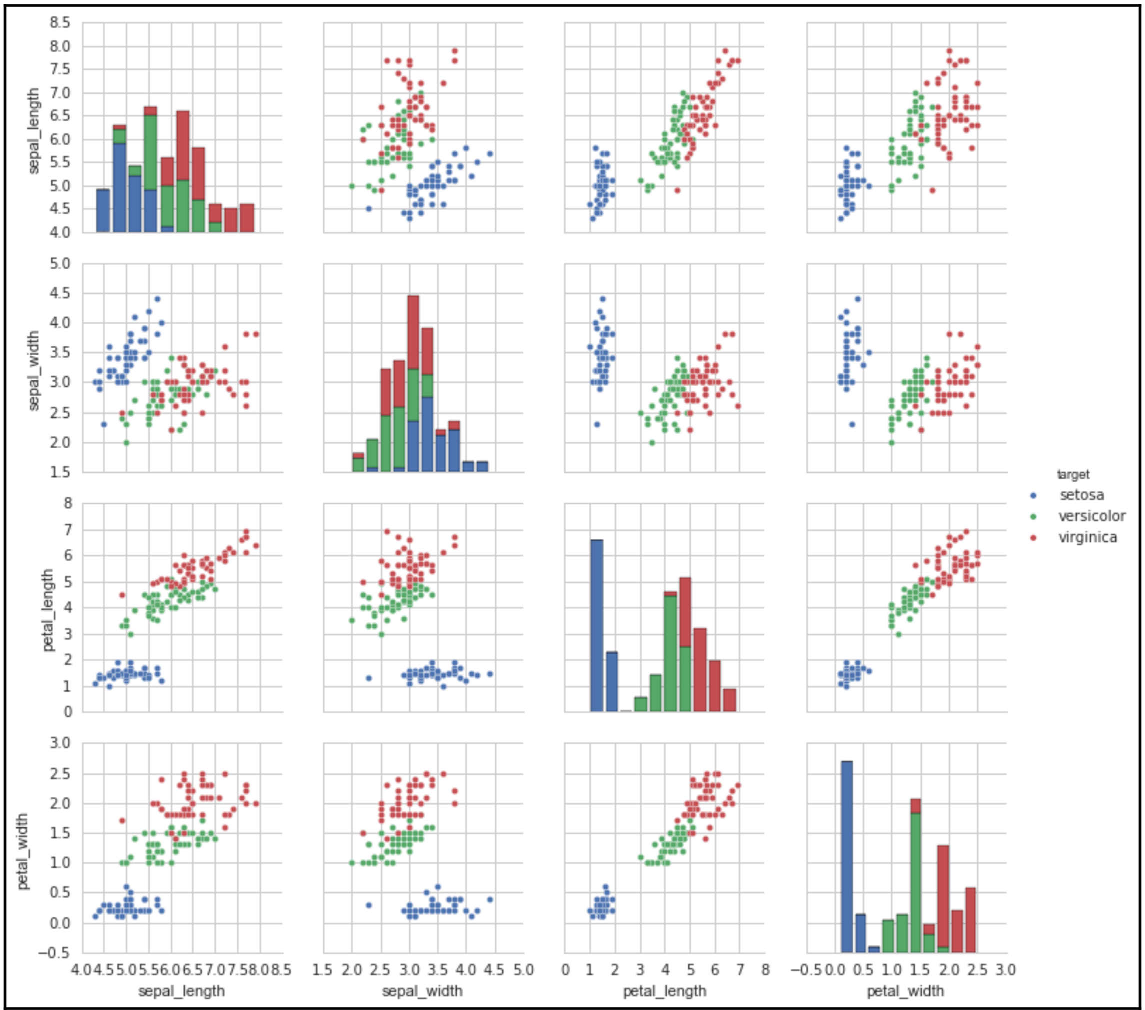
The violin plot produced by the previous code can provide interesting insights into the dataset:



Finally, Seaborn offers a much better way of creating a matrix of scatterplots by using the `pairplot` command and allowing you to define group colors (parameter hue) and how to populate the diagonal row. This is by using the `diag_kind` parameter, which can be a histogram (`'hist'`) or kernel density estimation (`'kde'`):

```
In: with sns.axes_style("whitegrid"):
        chart = sns.pairplot(data=df_iris, hue="target", diag_kind="hist")
```

The previous code will output a complete matrix of scatterplots for the dataset:



Advanced data learning representation

Some useful representations can be derived from the data science process. That is, the representation is not done directly from the data, but is achieved by using machine learning procedures, which inform us about how the algorithms operate and offer us a more precise overview of the role of each predictor in the predictions obtained. In particular, learning curves can provide a quick diagnosis to improve your models. This helps you figure out whether you need more observations, or need to enrich your variables.

Learning curves

A learning curve is a useful diagnostic graphic that depicts the behavior of your machine learning algorithm (your hypothesis) with respect to the available quantity of observations. The idea is to compare how the training performance (the error or accuracy of the in-sample cases) behaves with respect to the cross-validation (usually tenfold) using different in-sample sizes.

As far as the training error is concerned, you should expect it to be high at the start and then decrease. However, depending on the bias and variance level of the hypothesis, you will notice different behaviors:

- A high-bias hypothesis tends to start with average error performances, decreases rapidly on being exposed to more complex data, and then remains at the same level of performance no matter how many cases you further add.
- A low-bias learners tend to generalize better in the presence of many cases, but they are limited in their capability to approximate complex data structures, hence their limited performance.
- A high-variance hypothesis tends to start high in error performance and then slowly decreases as you add more cases. It tends to decrease slowly because it has a high capacity of recording the in-sample characteristics.

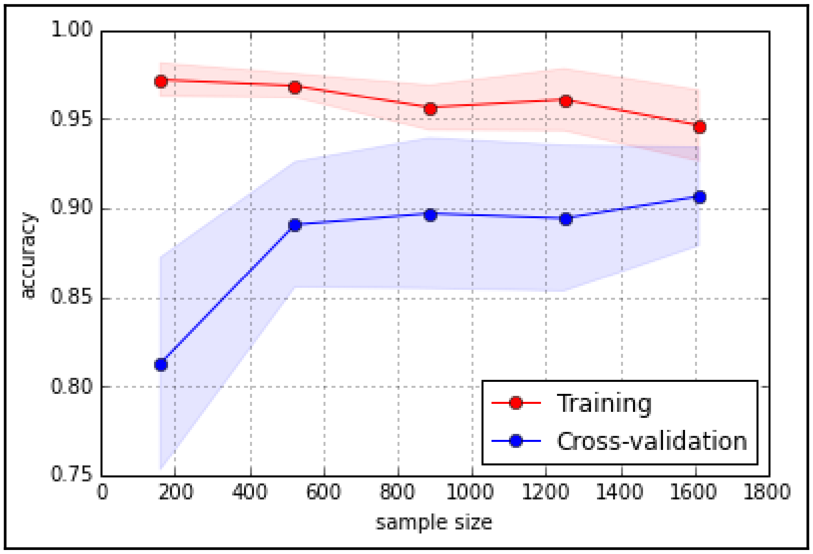
As for cross-validation, we can notice two behaviors:

- High-bias hypothesis tends to start with low performance, but it grows very rapidly until it reaches almost the same performance as that of the training. Then, it stops growing.
- High-variance hypothesis tends to start with very low performance. Then, steadily but slowly, it improves as more cases help generalize. It hardly reads the in-sample performances, and there is always a gap between them.

Being able to estimate whether your machine learning solution is behaving as a high-bias or high-variance hypothesis immediately helps you in deciding how to improve your data science project. Scikit-learn makes it simpler to calculate all the statistics that are necessary for the drawing of the visualization thanks to the `learning_curve` class, although visualizing them properly requires a few further calculations and commands:

```
In: import numpy as np
    from sklearn.learning_curve import learning_curve, validation_curve
    from sklearn.datasets import load_digits
    from sklearn.linear_model import SGDClassifier

    digits = load_digits()
    X, y = digits.data, digits.target
    hypothesis = SGDClassifier(loss='log', shuffle=True,
                               n_iter=5, penalty='l2',
                               alpha=0.0001, random_state=3)
    train_size, train_scores, test_scores = learning_curve(hypothesis, X,
                              y, train_sizes=np.linspace(0.1,1.0,5), cv=10,
                               scoring='accuracy',
                               exploit_incremental_learning=False,
                               n_jobs=-1)
    mean_train  = np.mean(train_scores,axis=1)
    upper_train = np.clip(mean_train + np.std(train_scores,axis=1),0,1)
    lower_train = np.clip(mean_train - np.std(train_scores,axis=1),0,1)
    mean_test = np.mean(test_scores,axis=1)
    upper_test = np.clip(mean_test + np.std(test_scores,axis=1),0,1)
    lower_test = np.clip(mean_test - np.std(test_scores,axis=1),0,1)
    plt.plot(train_size,mean_train,'ro-', label='Training')
    plt.fill_between(train_size, upper_train,
                     lower_train, alpha=0.1, color='r')
    plt.plot(train_size,mean_test,'bo-', label='Cross-validation')
    plt.fill_between(train_size, upper_test, lower_test,
                     alpha=0.1, color='b')
    plt.grid()
    plt.xlabel('sample size') # adds label to x axis
    plt.ylabel('accuracy') # adds label to y axis
    plt.legend(loc='lower right', numpoints= 1)
    plt.show()
```

Based on different sample sizes, you soon get a learning curve plot:



The `learning_curve` class requires the following as an input:

- A series of training sizes stored in a list
- An indication of the number of folds to use, and the error measure
- Your machine learning algorithm to test (parameter estimator)
- The predictors (parameter `X`) and the target outcome (parameter `y`)

As a result, the class will produce three arrays; the first one containing the effective training sizes, the second presenting the training scores obtained at each cross-validation iteration, and the last one carrying the cross-validation scores.

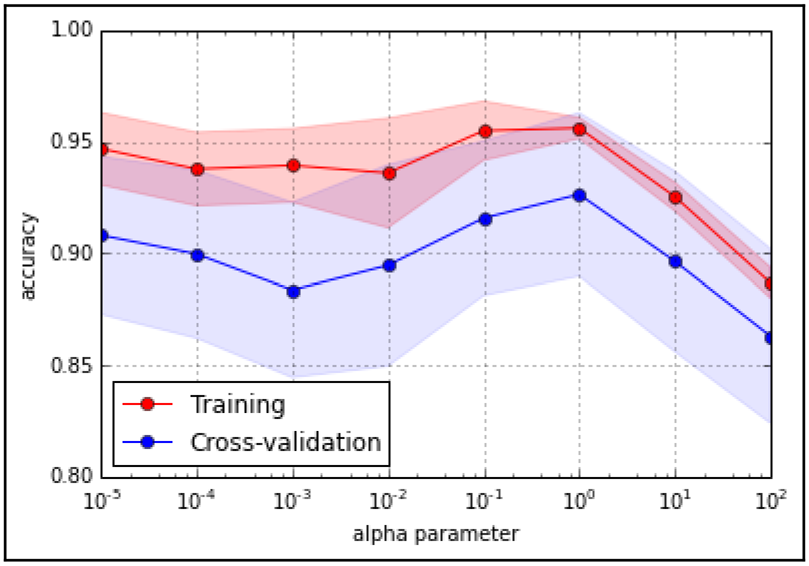
By applying the mean and the standard deviation for both training and cross-validation, it is possible to display in the graph both the curve trends and their variation. You can also provide information about the stability of the recorded performances.

Validation curves

As learning curves operate on different sample sizes, validation curves estimate the training and cross-validation performance with respect to the values that a hyper-parameter can take. As in learning curves, similar considerations can be applied, though this particular visualization will grant you further insight about the optimization behavior of your parameter, visually suggesting to you the part of the hyper-parameter space that you should concentrate your search on:

```
In: from sklearn.learning_curve import validation_curve
    testing_range = np.logspace(-5,2,8)
    hypothesis = SGDClassifier(loss='log', shuffle=True,
                               n_iter=5, penalty='l2',
                               alpha=0.0001, random_state=3)
    train_scores, test_scores = validation_curve(hypothesis, X, y,
                                 param_name='alpha',
                                 param_range=testing_range,
                                 cv=10, scoring='accuracy', n_jobs=-1)
    mean_train  = np.mean(train_scores,axis=1)
    upper_train = np.clip(mean_train + np.std(train_scores,axis=1),0,1)
    lower_train = np.clip(mean_train - np.std(train_scores,axis=1),0,1)
    mean_test = np.mean(test_scores,axis=1)
    upper_test = np.clip(mean_test + np.std(test_scores,axis=1),0,1)
    lower_test = np.clip(mean_test - np.std(test_scores,axis=1),0,1)
    plt.semilogx(testing_range,mean_train,'ro-', label='Training')
    plt.fill_between(testing_range, upper_train, lower_train,
                     alpha=0.1, color='r')
    plt.fill_between(testing_range, upper_train, lower_train,
                     alpha=0.1, color='r')
    plt.semilogx(testing_range,mean_test,'bo-', label='Cross-validation')
    plt.fill_between(testing_range, upper_test, lower_test,
                     alpha=0.1, color='b')
    plt.grid()
    plt.xlabel('alpha parameter') # adds label to x axis
    plt.ylabel('accuracy') # adds label to y axis
    plt.ylim(0.8,1.0)
    plt.legend(loc='lower left', numpoints= 1)
    plt.show()
```

After some computations, you will get a representation of the validation curve for the parameter:



The syntax of the `validation_curve` class is similar to that of the previously seen `learning_curve` but for the `param_name` and `param_range` parameters, which should be provided respectively with the hyper-parameter and the range that has to be tested. As for the results, the training and test results are returned in arrays.

Feature importance for RandomForests

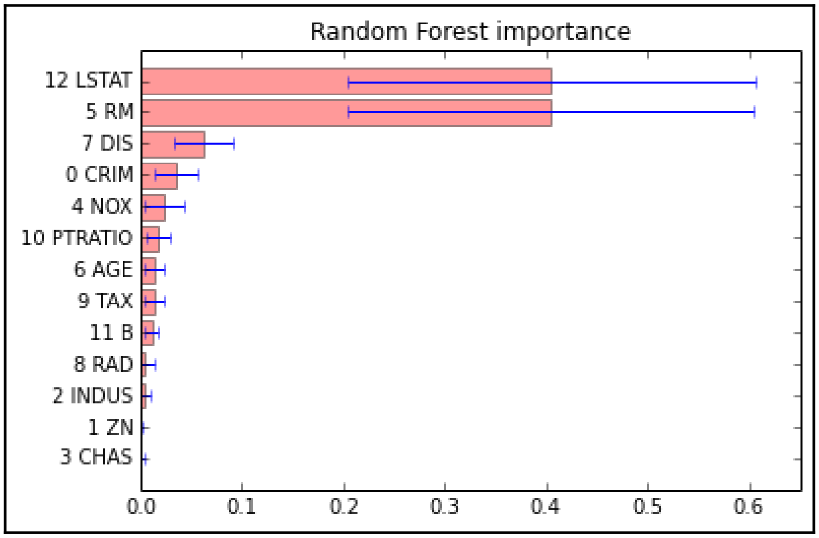
As discussed in the conclusion of `Chapter 3`, *The Data Pipeline*, selecting the right variables can improve your learning process by reducing noise, the variance of estimates, and the burden of too many computations. Ensemble methods, such as RandomForest in particular, can provide you with a different view of the role played by a variable when working together with other ones in your dataset.

Here, we show you how to extract the importance of RandomForest and Extra-Tree models. Importance is calculated in the fashion originally described in the book Classification and Regression Trees by Breiman, Friedman et al. in 1984. It was a true classic that laid solid foundations for classification trees. In the book, importance is described in terms of *gini importance* or *mean decrease impurity*, which is the total decrement in node impurity due to a specific variable averaged over all trees of the ensemble. In other words, mean decrease impurity is the total error reduction of nodes split on that variable multiplied by the number of samples that were routed to each of the nodes. Noticeably, accordingly to this importance calculation method, not only does error reduction depend on the error measure-Gini or Entropy for classification, and MSE for regression, but also splits at the head of the tree are deemed more important because they involve dealing with more examples.

In a few steps, we'll learn how to obtain such information and project it onto a clear visualization:

```
In: from sklearn.datasets import load_boston
    boston = load_boston()
    X, y = boston.data, boston.target
    feature_names = np.array([' '.join([str(b), a]) for a,b in
                              zip(boston.feature_names,range(
                              len(boston.feature_names)))])
    from sklearn.ensemble import RandomForestRegressor
    RF = RandomForestRegressor(n_estimators=100,
                               random_state=101).fit(X, y)
    importance = np.mean([tree.feature_importances_ for tree in
                          RF.estimators_],axis=0)
    std = np.std([tree.feature_importances_ for tree in
                  RF.estimators_],axis=0)
    indices = np.argsort(importance)
    range_ = range(len(importance))
    plt.figure()
    plt.title("Random Forest importance")
    plt.barh(range_,importance[indices],
             color="r", xerr=std[indices], alpha=0.4, align="center")
    plt.yticks(range(len(importance)), feature_names[indices])
    plt.ylim([-1, len(importance)])
    plt.xlim([0.0, 0.65])
    plt.show()
```

The code will produce the following chart highlighting important features of the model:



For each of the estimators (in our case, we have 100 models), the algorithm estimated a score to rank each variable's importance. The RandomForest model is made up of decision trees that can be made up of many branches, since the algorithm tries to obtain very small terminal leaves. One of its variables is deemed important if, after casually permuting its original values, the resulting predictions of the permuted model are very different in terms of accuracy as compared to the predictions of the original model.

The importance vectors are averaged over the number of estimators, and the standard deviation of the estimations is computed by a list comprehension (the assignment of variables importance and `std`). Now, sorted according to the importance score (the vector indices), the results are projected onto a bar graph with an error bar provided by the standard deviation.

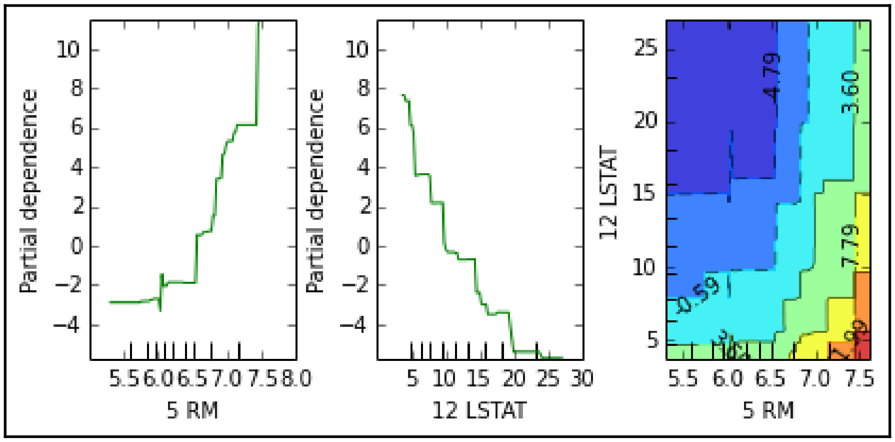
In our LSTAT analysis, the percentage of the lower status population in the area and RM, which is the average number of rooms per dwelling, are pointed out as the most decisive variables in our RandomForest model.

Gradient Boosting Trees partial dependence plotting

The estimate of the importance of a feature is a piece of information that can help you operate on the best choices to determine the features to be used. Sometimes, you may need to understand better why a variable is important in predicting a certain outcome. Gradient Boosting Trees, by controlling the effect of all the other variables involved in the analysis, provide you with a clear point of view of the relationship of a variable with respect to the predicted results. Such information can provide you with more insights into causation dynamics than what you may have obtained by using a very effective EDA:

```
In: from sklearn.ensemble.partial_dependence import
    plot_partial_dependence
    from sklearn.ensemble import GradientBoostingRegressor
    GBM = GradientBoostingRegressor(n_estimators=100,
                                    random_state=101).fit(X, y)
    features = [5,12,(5,12)]
    fig, axis = plot_partial_dependence(GBM, X, features,
                                        feature_names=feature_names)
```

As an output, you get three plots, which constitute the partial plots of RM and LSTAT features:



The `plot_partial_dependence` class will automatically provide you with the visualization after you provide an analysis plan on your part. You need to present a list of indexes of the features to be plotted singularly, and the tuples of the indexes of those that you would like to plot on a heat map (the features are the axis, and the heat value corresponds to the outcome).

In the preceding example, both the average number of rooms and the percentage of the lower status population have been represented, thus displaying an expected behavior. Interestingly, the heat map, which explains how they together contribute to the value of the outcome, reveals that they do not interact in any particular way (it is single hill-climbing). However, it is also revealed that LSTAT is a strong delimiter of the resulting housing values when it is above 5.

Creating a prediction server with machine-learning-as-a-service

Many times, during your working career as a data scientist, you'll find yourself having need of a predictor decoupled from the code you're currently working on; for example, as follows:

- You're developing an app for your phone, and you want to save on memory
- You're coding in a non-Python programming language (Java, Scala, C, C++, and so on) and you need to call the predictor you've developed in Python
- You're operating on big data, and the model is trained in the same remote location where the data is stored

In all these cases, it would be nice to have a service over HTTP that does predictions-as-a-service, or generically, any **machine-learning-as-a-service** (**ML-AAS**).

Bottle, a Python web framework, is the starting point for micro apps over HTTP. It is a very simple library for Python, providing the essential objects and functions to create a web app. Also, it can be paired with all the other libraries available in Python. Before going into the prediction-as-a-service, let's see how a basic `Hello World` program is built with Bottle. Please note that the following listings are meant for Python REPL, as a script, and not for a Jupyter Notebook:

```
# File: bottle1.py

from bottle import route, run, template

port = 9099
```

```
@route('/personal/<name>')
def homepage(name):
    return template('Hi <b>{{name}}</b>!', name=name)

print("Try going to http://localhost:{}/personal/Tom".format(port))
print("Try going to http://localhost:{}/personal/Carl".format(port))

run(host='localhost', port=port)
```

Let's analyze the code line by line before executing it:

1. We started importing the functions and the classes that we need from the Bottle module.
2. Then, we specified the port that the HTTP server would listen to.
3. In the example, we selected port `9099`; feel free to change it to another one, but first check whether any other service is using it (remember that HTTP is on top of TCP).
4. The next step is the definition of the API endpoint. The *route* decorator applies the function defined after it when an HTTP call to the path specified as an argument is performed. Note that in the path, it says `name`, and that is the argument of the coming function. That means `name` is a parameter of the call; you can select whatsoever string you like in the HTTP call, and your selection will be passed to the function as the parameter name.
5. Then, inside the function home page, a template with an HTML code was returned. In a simpler way, think of it as the `template` function creating the page you'll see from your browser.

Template, is this example, is just a plain HTML page, but it can be more complex (it can actually be a template page with some blanks to fill in). A complete description of templates is out of the scope of this section since we will be using the framework just for a simple, plain output. If you need additional information, surf the Bottle help pages.

6. Finally, after the `print` functions, there's the core `run` function. It's a blocking function and will set up the web server on the host and port provided as arguments. When you run the code in the listing, once that function is executed, you can open your browser and point it to `http://localhost:9099/personal/Carl`, and you'll find the following text: `Hi Carl!`

Of course, changing the name in the HTTP call from `Carl` to `Tom` or any other name will result in a different page, containing the name specified in the call.

Please note that in this dummy example, we just defined the `/personal/<name>` route. Any other call will result in `Error 404`, unless defined in the code.

To turn it off, we need to press *Ctrl* + *C* in the command line (remember that the `run` function is blocking).

Let's now create a service that is more data science-oriented; we will create an HTML page with a form asking for the sepal length and width, and the petal length and width, to classify the iris sample. For this example, we will use the iris dataset to train our scikit-learn classifier. Then, for each prediction, we simply call the `predict` function on the classifier, sending back the prediction:

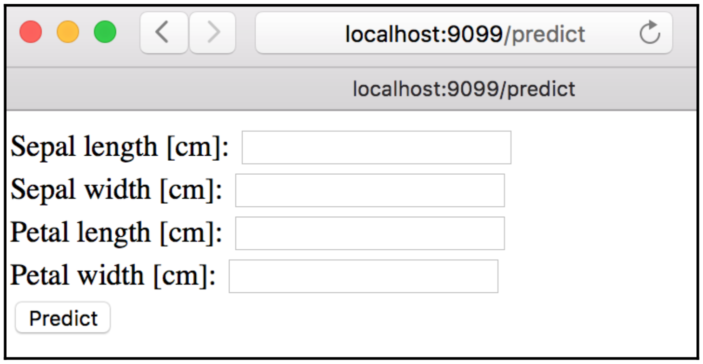
```
# File: bottle2.py

from sklearn.datasets import load_iris
from sklearn.linear_model import LogisticRegression
from bottle import run, request, get, post
import numpy as np

port = 9099

@get('/predict')
def predict():
    return '''
        <form action="/prediction" method="post">
            Sepal length [cm]: <input name="sl" type="text" /><br/>
            Sepal width [cm]: <input name="sw" type="text" /><br/>
            Petal length [cm]: <input name="pl" type="text" /><br/>
            Petal width [cm]: <input name="pw" type="text" /><br/>
            <input value="Predict" type="submit" />
        </form>
    '''

@post('/prediction')
def do_prediction():

    try:
        sample = [float(request.POST.get('sl')),
                  float(request.POST.get('sw')),
                  float(request.POST.get('pl')),
                  float(request.POST.get('pw'))]

        pred = classifier.predict(np.matrix(sample))[0]
        return "<p>The predictor says it's a <b>{}</b></p>"\
              .format(iris['target_names'][pred])
    except:
        return "<p>Error, values should be all numbers</p>"

iris = load_iris()
classifier = LogisticRegression()
classifier.fit(iris.data, iris.target)


print("Try going to http://localhost:{}/predict".format(port))
run(host='localhost', port=port)

# Try insert the following values:
# [ 5.1, 3.5, 1.4, 0.2] -> setosa
# [ 7.0  3.2, 4.7, 1.4] -> versicolor
# [ 6.3, 3.3, 6.0, 2.5] -> virginica
```

After some imports, here we use the get decorator, specifying a route valid only for HTTP GET calls. The decorator, as well as the function following, has no parameters since all the features should be inserted into the HTML form, defined in the `predict` function. The form, when submitted, is passed to the `/prediction` page using an HTTP `POST`.

Now, we need to create a route for this call, and that's what we do in the `do_prediction` function. Its decorator is `post` (that is, opposite to `get`; it defines only `POST` routes) on the /prediction page. Data is parsed and transformed into a double (default parameters are strings), and then the feature vector is fed into the `classifier` global variable to obtain a prediction. This is returned using a simple template. The object request contains all the parameters passed to the service, including the entire variable we *POST-ed* to the route. Finally, it seems we just need to define the global variable classifier – that is, a classifier trained on the iris dataset – and lastly, we can call the `run` function.

For this dummy example, we've used a logistic regressor as a classifier and trained on the full Iris dataset, leaving all the parameters as default. In a real case, here you would tune your classifier as best as possible.

When this code is run, if everything works well, you can point your browser to `http://localhost:9099/predict` and you'll see the form:



Sepal length [cm]:
Sepal width [cm]:
Petal length [cm]:
Petal width [cm]:
Predict

Inserting the values (`5.1`, `3.5`, `1.4`, `0.2`) after clicking on the **Predict** button, you should be redirected to `http://localhost:9099/prediction`, where the `The predictor says it's a setosa` string should be displayed. Also, note that if you insert invalid entries in the form (for example, leaving it empty or inserting a string instead of a number), you'll get an HTML page that says that there's an error.

We're halfway through this section, and we've already seen how easy and quick it is to create an HTTP endpoint with Bottle. Now, let's try to create a prediction-as-a-service that can be called in any program. We will submit the feature vector as a `get` call, and the returned prediction will be in JSON format. Here's the code for this solution:

```
# File: bottle3.py

from sklearn.datasets import load_iris
from sklearn.linear_model import LogisticRegression
from bottle import run, request, get, response
import numpy as np
import json

port = 9099

@get('/prediction')
def do_prediction():

    pred = {}

    try:
        sample = [float(request.GET.get('sl')),
                  float(request.GET.get('sw')),
                  float(request.GET.get('pl')),
                  float(request.GET.get('pw'))]

        pred['predicted_label'] =
             iris['target_names']
[classifier.predict(np.matrix(sample))[0]]
        pred['status'] = "OK"
    except:
        pred['status'] = "ERROR"

    response.content_type = 'application/json'
    return json.dumps(pred)

iris = load_iris()
classifier = LogisticRegression()
classifier.fit(iris.data, iris.target)

print("Try going to http://localhost:{}/prediction\
       sl=5.1&sw=3.5&pl=1.4&pw=0.2".format(port))
print("Try going to http://localhost:{}/prediction\
       sl=A&sw=B&pl=C&pw=D".format(port))
run(host='localhost', port=port)
```

The solution is pretty straightforward and easy; still, let's analyze it step by step. The entry point of the feature is defined by the `get` decorator on the `/prediction` path. In there, we will access the `GET` values to extract the predictions (note that if your classifier needs many features, it may be better to use a `POST` call here). Exactly as in the previous example, the prediction is generated; finally, the value is inserted in a Python dictionary, altogether with the `OK` value for the `status` key. If an exception is raised in this function, there will be no prediction, but an `ERROR` string in the `status` key. Then, we set the output application format to JSON, and we serialize the Python dictionary to a JSON string.

When it runs, we can access the URL, `localhost:9099/prediction`, followed by the feature values, and we will get back the prediction as JSON. Note that we don't need a browser to interpret the returned HTTP response since it's a JSON. Therefore, we can call the endpoint from different applications (`wget`, browser, or `curl`) or any programming language (including Python itself). To see it working, start it and point your browser to (or request the URL in any way) `http://localhost:9099/prediction?sl=5.1&sw=3.5&pl=1.4&pw=0.2`. You'll get back the valid JSON: `{"predicted_label": "setosa", "status": "OK"}`. Also, if something goes wrong in the parsing of the parameters, you'll get this JSON: `{"status": "ERROR"}`. And that's your first ML-AAS!

Although simple and quick, Bottle has many other functions to be explored. It's not as complete as other frameworks, however. If your application needs some extraordinary functionality, check out Flask or Django modules.

Summary

This chapter provided an overview of essential data science by providing examples of both basic and advanced graphical representations of data, machine learning processes, and results. We explored the `pylab` module from matplotlib, which gives the easiest and fastest access to the graphical capabilities of the package. We used pandas for EDA, and tested the graphical utilities provided by scikit-learn. All examples were like building blocks, and they are all easily customizable in order to provide you with a fast template for visualization.

In the next chapter, you'll be introduced to **graphs**, which are an interesting deviation from the predictors/target flat matrices. They are quite a hot topic in data science now. Expect to delve into very complex and intricate networks.

6 Social Network Analysis

Social network analysis, usually referred to as **SNA**, creates a model and studies the relationships of a group of social entities that exist in the form of a network. An entity can be a person, a computer, or a web page, and a relationship can be a like, link, or friendship (that is, a connection between entities).

In this chapter, you'll learn about the following:

- Graphs, since social networks are usually represented in this form
- Important algorithms that are used to gain insights from a graph
- How to load, dump, and sample large graphs

Introduction to graph theory

Basically, a graph is a data structure that's able to represent relations in a collection of objects. Under this paradigm, the objects are the graph's nodes and the relations are the graph's links (or edges). The graph is directed if the links have an orientation (conceptually, they're like the one-way streets of a city); otherwise, the graph is undirected. In the following table, examples of well-known graphs are provided:

Graph example	**Type**	**Nodes**	**Edges**
World Wide Web	Directed	Web pages	Links
Facebook	Undirected	People	Friendship
Twitter	Directed	People	Follower
IP network	Undirected	Hosts	Wires/Connections
Navigation systems	Directed	Places/Addresses	Streets
Wikipedia	Directed	Pages	Anchor links
Scientific literature	Directed	Papers	Citations
Markov chains	Directed	Statuses	Emission probability

All of the preceding examples can be expressed as relations between nodes, as in a traditional **relational database management system** (**RDBMS**), such as MySQL or Postgres. Now, we are going to discover the advantages of a graph data structure, and start to think about how complex the following query in SQL would be for a social network such as Facebook (think about a recommender system that helps you find people you may know):

1. Examine the following query:

   ```
   Find all people who are friends of my friends, but not my friends
   ```

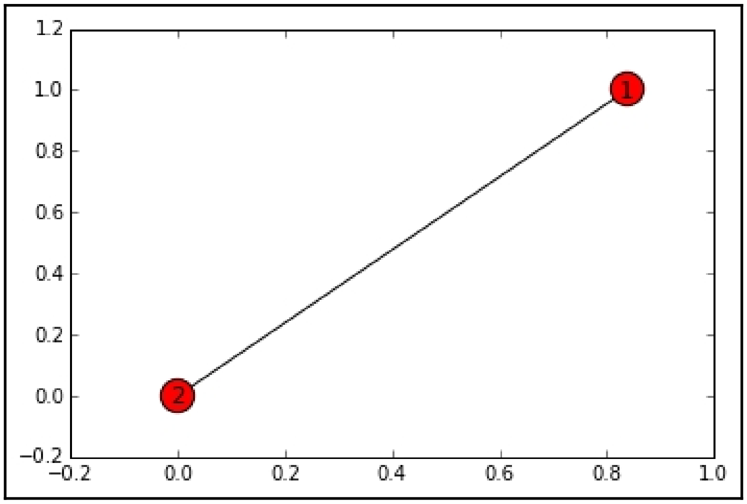
2. Compare the preceding query to the following query on a graph:

   ```
   Get all friends connected to me having distance=2
   ```

3. Now, let's see how to create a graph or a social network with Python. The library that we're going to use extensively throughout this chapter is named `NetworkX`. It is capable of handling small to medium-sized graphs and it is complete and powerful:

   ```
   In: %matplotlib inline
       import networkx as nx
       import matplotlib.pyplot as plt

       G = nx.Graph()
       G.add_edge(1,2)
       nx.draw_networkx(G)
       plt.show()
   ```

The following graph is a visualization of the preceding code, presenting the two nodes and their connecting edge:

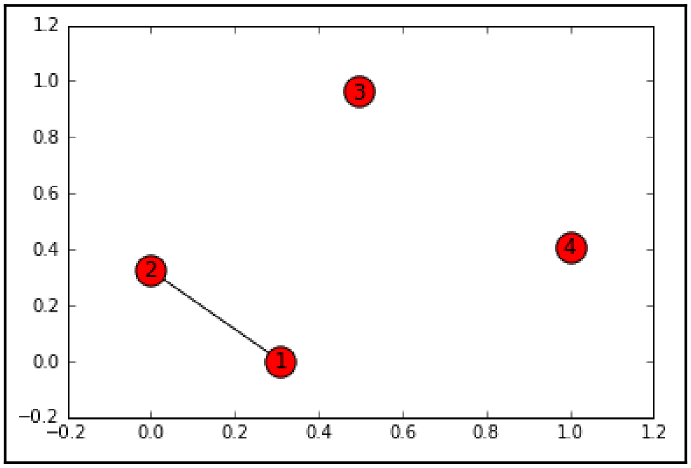


The command is self-explanatory. Examining the previous code, after the package imports, we will first define a (`NetworkX`) graph object (by default, it's an undirected one). Then, we will add an edge (that is, a connection) between two nodes (since the nodes are not already in the graph, they're automatically created). Finally, we will plot the graph. The graph layout (the positions of the nodes) is automatically generated by the library.

With the `.add_note()` method, adding other nodes to the graph is pretty straightforward. For example, if you want to add the nodes `3` and `4`, you can simply use the following code:

```
In: G.add_nodes_from([3, 4])
    nx.draw_networkx(G)
    plt.show()
```

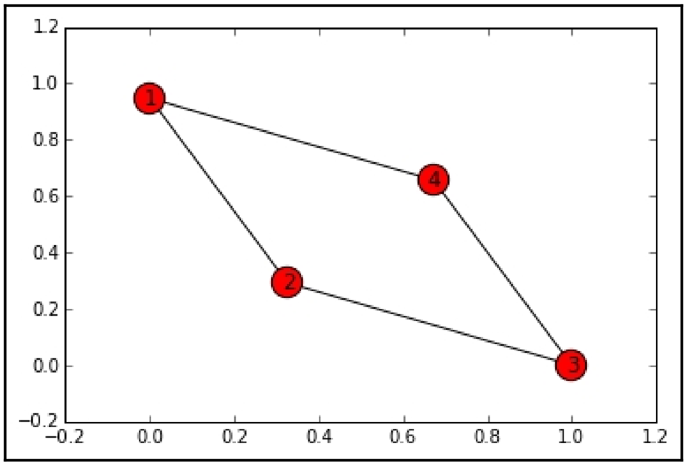
Now, our graph is getting more complex, as you can see from the plot:



The preceding code will add the two nodes. Since they're not linked to the other nodes, they'll be unconnected. Similarly, to add more edges to the graph, you can use the following code:

```
In: G.add_edge(3,4)
    G.add_edges_from([(2, 3), (4, 1)])
    nx.draw_networkx(G)
    plt.show()
```

By using the previous code, we have completed connecting the nodes in our graph:



To obtain a collection of nodes in the graph, just use the `.nodes()` method. Similarly, `.edges()` gives you the list of edges as a list of connected nodes:

```
In: G.nodes()

Out: [1, 2, 3, 4]

In: G.edges()

Out: [(1, 2), (1, 4), (2, 3), (3, 4)]
```

There are several ways to represent and describe a graph. In the following section, we'll illustrate the most popular ones. The first option is to use an adjacency list. It lists the neighbors of every node; that is, `list[0]` contains the adjacency nodes expressed in the adjacency list format:

```
In: list(nx.generate_adjlist(G))

Out: ['1 2 4', '2 3', '3 4', '4']
```

In this format, the first number is always the source and the ones that follow are the targets, as detailed at the following URL: `https://networkx.github.io/documentation/stable/reference/readwrite/adjlist.html`.

To make the description self-contained, you can represent the graph as a dictionary of lists. This is the most popular (and practical) way to describe a graph, due to its succinctness. Here, the nodes' names are the dictionary keys, and their values are the nodes' adjacency lists:

```
In: nx.to_dict_of_lists(G)

Out: {1: [2, 4], 2: [1, 3], 3: [2, 4], 4: [1, 3]}
```

On the other hand, you can describe a graph as a **collection of edges**. In the output, the third element of each tuple is the attribute of the edge. In fact, every edge can have one or more attributes (such as its weight, its cardinality, and so on). Since we created a very simple graph, in the following example, we have no attributes:

```
In: nx.to_edgelist(G)

Out: [(1, 2, {}), (1, 4, {}), (2, 3, {}), (3, 4, {})]
```

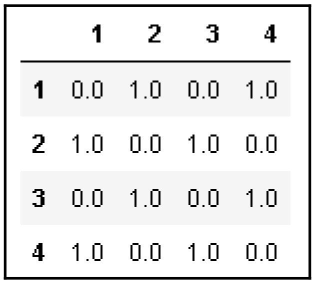
Finally, a graph can be described as a NumPy matrix. If the matrix contains a `1` in the `(i, j)` position, it means that there is a link between the `i` and `j` nodes. Since the matrix usually contains very few ones (compared to the number of zeros), it's usually represented as a sparse (SciPy) matrix, a NumPy matrix, or a `pandas` DataFrame.

Please note that the matrix description is exhaustive. Therefore, undirected graphs are transformed into directed ones, and a link connecting `(i, j)` is transformed into two links, `(i, j)` and `(j, i)`. This representation is often named an adjacency matrix or a connection matrix.

Thus, a symmetric matrix is created, as in the following example:

```
In: nx.to_numpy_matrix(G)

Out: matrix([[ 0., 1., 0., 1.],
             [ 1., 0., 1., 0.],
             [ 0., 1., 0., 1.],
             [ 1., 0., 1., 0.]])

In: print(nx.to_scipy_sparse_matrix(G))

Out:   (0, 1) 1
       (0, 3) 1
       (1, 0) 1
       (1, 2) 1
       (2, 1) 1
       (2, 3) 1
       (3, 0) 1
       (3, 2) 1

In: nx.convert_matrix.to_pandas_adjacency(G)
```

The resulting output is shown in the following table:



	1	2	3	4
1	0.0	1.0	0.0	1.0
2	1.0	0.0	1.0	0.0
3	0.0	1.0	0.0	1.0
4	1.0	0.0	1.0	0.0

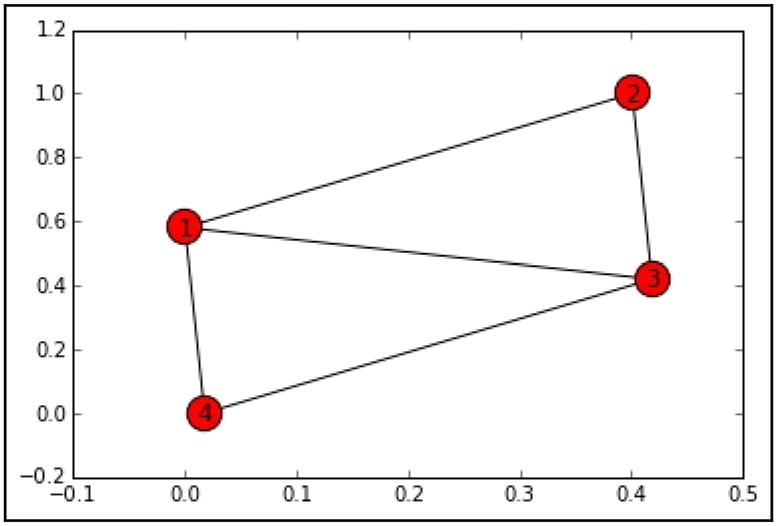
Of course, if you want to load a NetworkX graph, you can use the opposite functions (changing *to* into *from* in the function name), and you'll be able to load NetworkX graphs from a dictionary of lists, edge lists, and NumPy, SciPy, and `pandas` structures.

An important measure of each node in a graph is their degree. In an undirected graph, the degree of a node represents the number of links the node has. For directed graphs, there are two types of degree: an in-degree and an out-degree. These count the inbound and outbound links of the node, respectively.

Let's add a node (to unbalance the graph) and calculate the nodes' degrees, as follows:

```
In: G.add_edge(1, 3)
    nx.draw_networkx(G)
    plt.show()
```

The resulting plot of the graph is as follows:



The graphs in this chapter may be different to the ones obtained on your local computer, because graphical layout initialization is made with random parameters.

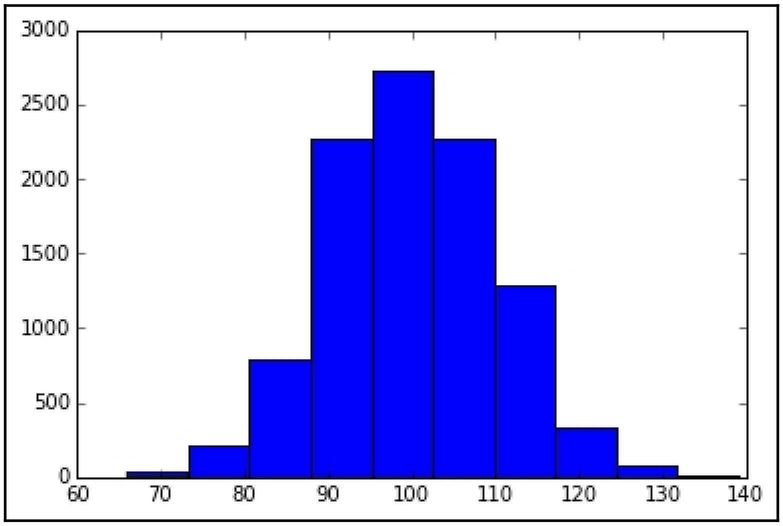
The degree of the nodes is displayed as follows:

```
In: G.degree()

Out: {1: 3, 2: 2, 3: 3, 4: 2}
```

For large graphs, this measure is impractical since the output dictionary has an item for every node. In such cases, a histogram of the nodes' degree is often used to approximate its distribution. In the following example, a random network with 10,000 nodes and a link probability of 1 % is built. Then, the histogram of the node degree is extracted, as follows:

```
In: k = nx.fast_gnp_random_graph(10000, 0.01).degree()
    plt.hist(list(dict(k).values()))
```

The histogram for the preceding code is as follows:

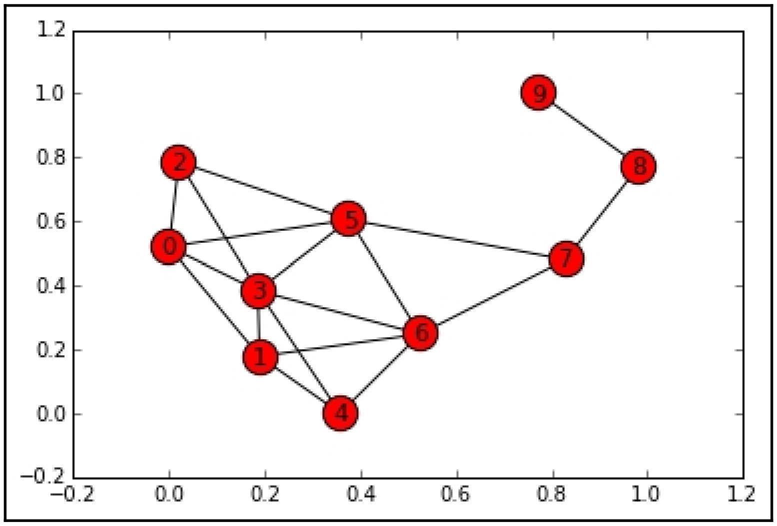


Graph algorithms

To get insights from graphs, many algorithms have been developed. In this chapter, we'll use a well-known graph in `NetworkX`, that is, the `Krackhardt Kite` graph. It is a dummy graph containing 10 nodes, and it is typically used to proof graph algorithms. David Krackhardt is the creator of the structure, which has the shape of a kite. It's composed of two different zones. In the first zone (composed of nodes 0 to 6), the nodes are interlinked; in the other zone (nodes 7 to 9), they are connected as a chain:

```
In: G = nx.krackhardt_kite_graph()
    nx.draw_networkx(G)
    plt.show()
```

In the following plot, you can examine the Krackhardt Kite's graph structure:



Let's start with connectivity. Two nodes of a graph are connected if there is at least a path (that is, a sequence of nodes) between them.

If at least one path exists, the shortest path between the two nodes is the one with the shortest collection of nodes you should pass (or traverse) to go from the source to the destination node.

Note that, in a directed graph, you must follow the link's directions.

In `NetworkX`, checking whether a path exists between two nodes, calculating the shortest route, and getting its length is very easy. For example, to check the connectivity and the path between nodes 1 and 9, you can use the following code:

```
In: print(nx.has_path(G, source=1, target=9))
    print(nx.shortest_path(G, source=1, target=9))
    print(nx.shortest_path_length(G, source=1, target=9))

Out: True
     [1, 6, 7, 8, 9]
     4
```

This function just gives the shortest path from one node to another. What about if we want to see all the paths to reach node 9 from node 1? An algorithm proposed by Jin Yen provides this answer, and it's implemented in the function `shortest_simple_paths` in NetworkX. This function returns a generator of all the paths, from the shortest to the longest, between the node sources and the target in the graph:

```
In: print (list(nx.shortest_simple_paths(G, source=1, target=9)))

Out: [[1, 6, 7, 8, 9], [1, 0, 5, 7, 8, 9], [1, 6, 5, 7, 8, 9],
      [1, 3, 5, 7, 8, 9], [1, 4, 6, 7, 8, 9], [1, 3, 6, 7, 8, 9],
      [1, 0, 2, 5, 7, 8, 9], [...]]
```

Finally, another handy function provided by NetworkX is the `all_pairs_shortest_path` function, which returns a Python dictionary containing the shortest path between all of the pairs of nodes in the network. For example, to see the shortest path from node `5`, you just need to see what's inside key `5`:

```
In: paths = list(nx.all_pairs_shortest_path(G))
    paths[5][1]

Out: {0: [5, 0],
      1: [5, 0, 1],
      2: [5, 2],
      3: [5, 3],
      4: [5, 3, 4],
      5: [5],
      6: [5, 6],
      7: [5, 7],
      8: [5, 7, 8],
      9: [5, 7, 8, 9]}
```

As expected, the paths between `5` and all the other nodes start with `5` itself. Note that this structure is also a dictionary, and therefore, to obtain the shortest path between nodes `a` and `b`, it can just be called **paths[a][b]**. Use this function carefully on large networks. In fact, under the hood, it computes all the pairwise shortest paths with a computational complexity of $O(N^2)$.

Types of node centrality

We will now start talking about node centrality, which roughly represents the importance of the node inside the network. It also gives an idea of how well the node connects the network. There are multiple types of centrality that we will look at here, including betweenness centrality, degree centrality, closeness centrality, harmonic centrality, and eigenvector centrality.

- **Betweenness centrality**: This type of centrality gives you an idea about the number of shortest paths in which the node is present. Nodes with high betweenness centrality are the core components of the network, and many shortest paths route through them. In the following example, `NetworkX` offers a straightforward way to compute the betweenness centrality of all the nodes:

```
In: nx.betweenness_centrality(G)

Out: {0: 0.023148148148148143,
      1: 0.023148148148148143,
      2: 0.0,
      3: 0.10185185185185183,
      4: 0.0,
      5: 0.23148148148148148,
      6: 0.23148148148148148,
      7: 0.38888888888888884,
      8: 0.2222222222222222,
      9: 0.0}
```

  As you can imagine, the highest betweenness centrality is achieved by node `7`. It seems very important since it's the only node that connects elements `8` and `9` (it's their gateway to the network). On the contrary, nodes such as `9`, `2`, and `4` are on the extreme border of the network, and they are not present in any of the shortest paths of the network. Therefore, these nodes can be removed without affecting the connectivity of the network.

- **Degree centrality**: This type of centrality is simply the percentage of the vertexes that are incident upon a node. Note that, in directed graphs, there are two degree centralities for every node: that is in-degree and out-degree centrality. Let's take a look at the following example:

```
In: nx.degree_centrality(G)

Out: {0: 0.4444444444444444,
      1: 0.4444444444444444,
      2: 0.3333333333333333,
      3: 0.6666666666666666,
      4: 0.3333333333333333,
      5: 0.5555555555555556,
      6: 0.5555555555555556,
      7: 0.3333333333333333,
      8: 0.2222222222222222,
      9: 0.1111111111111111}
```

As expected, node `3` has the highest degree centrality since it's the node with the maximum number of links (it's connected to six other nodes). On the contrary, node `9` is the node with the lowest degree since it has only one edge.

- **Closeness centrality**: To compute this for every node, calculate the shortest path distance to all other nodes, average it, divide the average by the maximum distance, and take the inverse of that value. This results in a score between 0 (the greater average distance) and 1 (the lower average distance). In our example, for node `9`, the shortest path distances are [1, 2, 3, 3, 4, 4, 4, 5, 5]. The average (3.44) is then divided by 5 (the maximum distance) and subtracted from 1, resulting in a closeness centrality score of 0.31. You can use the following code to compute the closeness centrality for all the nodes in the example graph:

```
In: nx.closeness_centrality(G)

Out: {0: 0.5294117647058824,
      1: 0.5294117647058824,
      2: 0.5,
      3: 0.6,
      4: 0.5,
      5: 0.6428571428571429,
      6: 0.6428571428571429,
      7: 0.6,
      8: 0.42857142857142855,
      9: 0.3103448275862069}
```

The nodes with high closeness centrality are `5`, `6`, and `3`. In fact, they are the nodes that are present in the middle of the network, and on average, they can reach all the other nodes with a few hops. The lowest score belongs to node `9`. In fact, its average distance to reach all the other nodes is pretty high.

- **Harmonic centrality:** This measure is similar to closeness centrality, but instead of having the inverse of the sum of the reciprocal of the distances, it has the sum of reciprocal of distances. Doing so, it emphasizes the extremes of distances. Let's see what the harmonic distances look like in our network:

```
In: nx.harmonic_centrality(G)

Out: {0: 6.083333333333333,
      1: 6.083333333333333,
      2: 5.583333333333333,
      3: 7.083333333333333,
      4: 5.583333333333333,
      5: 6.833333333333333,
      6: 6.833333333333333,
      7: 6.0,
      8: 4.666666666666666,
      9: 3.4166666666666665}
```

  Node `3` is the one with the highest harmonic centrality, while `5` and `6` have a comparable but lower value. Again, those nodes are in the center of the network, and on average, they can reach all the other nodes with a few hops. Opposite, node `9` has the lowest harmonic centrality; in fact, it's the farthest from all the other nodes on average.

- **Eigenvector centrality**: If the graph is directed, the nodes represent web pages and the edges represent page links. A slightly modified version is named PageRank. This metric, invented by Larry Page, is the core ranking algorithm of Google, as well as Bing, and possibly other search engines. It gives every node a measure of how important the node is from the point of view of a random surfer. Its name derives from the fact that if you think of the graph as a Markov Chain, the graph represents the eigenvector associated with the greatest eigenvalue. Therefore, from this point of view, this probabilistic measure represents the static distribution of the probability of visiting a node. Let's take a look at the following example:

```
In: nx.eigenvector_centrality(G)

Out: {0: 0.35220918419838565,
      1: 0.35220918419838565,
      2: 0.28583482369644964,
      3: 0.481020669200118,
      4: 0.28583482369644964,
      5: 0.3976909028137205,
      6: 0.3976909028137205,
      7: 0.19586101425312444,
      8: 0.04807425308073236,
      9: 0.011163556091491361}
```

In this example, nodes 3 and 9 have the highest and the lowest scores according to the eigenvector centrality measure. Compared to degree centrality, eigenvalue centrality gives an idea about the static distribution of the surfers across the network because it considers, for each node, not only the directly connected neighbors (as in degree centrality), but also the whole structure of the network. If the graph represented web pages and their connections, this makes them the most/least (probable) visited pages.

As a concluding topic, we'll introduce the clustering coefficient. In brief, it is the proportion of the node's neighbors that are also neighbors with each other (that is, the proportion of possible triplets or triangles that exist). Higher values indicate higher cliquishness. It's named this way because it represents the degree to which nodes tend to cluster together. Let's take a look at the following example:

```
In: nx.clustering(G)

Out: {0: 0.6666666666666666,
      1: 0.6666666666666666,
      2: 1.0,
      3: 0.5333333333333333,
      4: 1.0,
      5: 0.5,
      6: 0.5,
      7: 0.3333333333333333,
      8: 0.0,
      9: 0.0}
```

Higher values can be seen in the highly connected sections of the graph and lower values can be seen in the least connected areas.

Partitioning a network

Now, let's look at the way in which you can partition the network into multiple subnetworks of nodes. One of the most used algorithms is the Louvain method, which was specifically created to accurately detect communities in large graphs (with a million nodes). We will first introduce the modularity measure. This is a measure of the structure of the graph (it's not node-oriented), whose formal math definition is very long and complex and which is beyond the scope of this book (readers can find more information at `https://sites.google.com/site/findcommunities/`). It intuitively measures the quality of the division of a graph into communities, comparing the actual community linkage with a random one. The modularity score falls between -0.5 and +1.0; the higher the value, the better the division (there is a dense intragroup connectivity and a sparse intergroup connectivity).

It's a two-step iterative algorithm: first, there's a local optimization, then a global one, then a local again, and so on:

1. In the first step, the algorithm locally maximizes the modularity of small communities.
2. Then, it aggregates the nodes of the same community and hierarchically builds a graph whose nodes are the communities.
3. The method repeats these two steps iteratively until the maximum global modularity score is reached.

To take a peek at this algorithm in a practical example, we first need to create a larger graph. Let's consider a random network with 100 nodes:

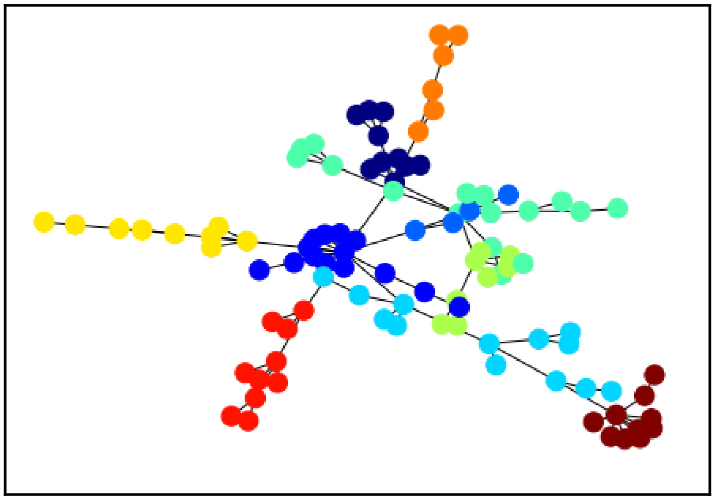
1. In this example, we will build a graph with the `powerlaw` algorithm, which tries to maintain an approximate average clustering.
2. For every new node added to the graph, an `m` number of random edges will also be added to it, with each of them having a probability of `p` to create a triangle.
3. The source code is not included in `NetworkX`, but it's in a separate module named `community`. An implementation of this algorithm is shown in the following example:

```
In: import community
    # Module for community detection and clustering

    G = nx.powerlaw_cluster_graph(100, 1, .4, seed=101)
    partition = community.best_partition(G)

    for i in set(partition.values()):
        print("Community", i)
```

```
            members = [nodes for nodes in partition.keys()
                       if partition[nodes] == i]
            print(members)

        values = [partition.get(node) for node in G.nodes()]
        nx.draw(G, pos=nx.fruchterman_reingold_layout(G),
                cmap = plt.get_cmap('jet'),
                node_color = values,
                node_size=150,
                with_labels=False)
        plt.show()
        print ("Modularity score:", community.modularity(partition, G))

    Out: Community 0
         [0, 46, 50, 61, 73, 74, 75, 82, 86, 96]
         Community 1
         [1, 2, 9, 16, 20, 28, 29, 35, 57, 65, 78, 83, 89, 93]
         [...]
         Modularity score: 0.7941026425874911
```

The first output of the program is the list of communities detected in the graph (each community is a collection of nodes). In this case, the algorithm detected eight groups. We wanted to highlight that we didn't specify the number of output communities that we were looking for, but it was automatically decided by the algorithm. That's a desirable feature shared with not all the clustering algorithms (k-means, for example, needs the number of clusters as a parameter).

Then, we printed the graph, assigning a different color to each community. You can see that the colors are pretty homogeneous on the edge nodes:



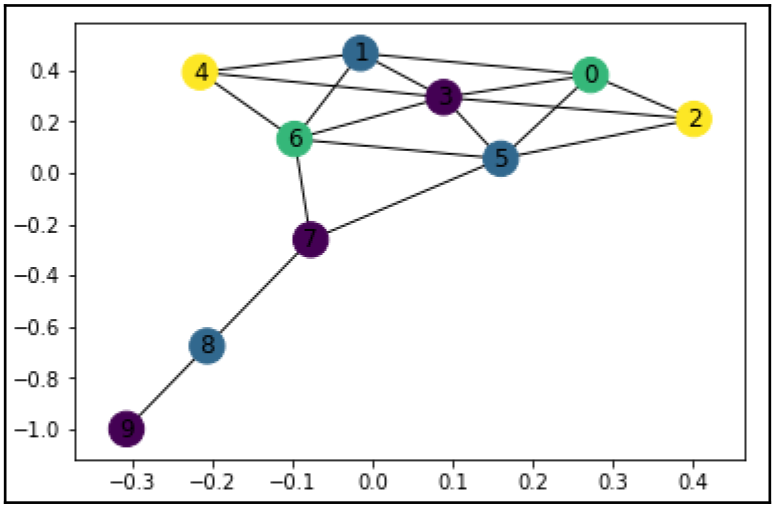
Lastly, the algorithm returns the modularity score of the solution: 0.79 (that's a pretty high score).

The last algorithm that this short introduction about graphs is going to present is `coloring`. It is a graphical way of assigning labels to the nodes, in a way that neighbors (that is, nodes with a link) must have different labels (or colors). To explain why this algorithm is important, we will use a practical example. Telecommunication networks are composed of antennas at different frequencies spread across the Earth. Think about each antenna as a node, and the frequency as a label of the node. If antennas are closer than a defined distance—let's say close enough to cause interference—they're connected with an edge. Can we find the lowest number of different frequencies to allocate (to minimize the bill the company has to pay) and avoid interferences between close antennas (that is, by allocating different frequencies to linked nodes)?

The solution is given by the graph-coloring algorithms. In theory, the solution of such a class of algorithm is NP-hard, and it's almost impossible to find the optimal solution, though there are many approximations to obtain suboptimal solutions quickly. NetworkX implements a greedy approach to solve the coloring problem. What's returned by the function is a dictionary containing, for each node (the key in the dictionary), the color (the value of the key in the dictionary). As an example, let's see the allocation of colors in our example graph, and then let's see it colored:

```
In: G = nx.krackhardt_kite_graph()
    d = nx.coloring.greedy_color(G)
    print(d)
    nx.draw_networkx(G,
       node_color=[d[n] for n in sorted(d.keys())])
    plt.show()

Out:{3: 0, 5: 1, 6: 2, 0: 2, 1: 1, 2: 3, 4: 3, 7: 0, 8: 1, 9: 0}
```

Here is the plot of the graph, using different colors for the linked nodes:



As expected, linked nodes have different colors. It seems that for this configuration of the network, four colors were needed. If this were representing a telecommunications network, it would show us that four frequencies were needed to avoid interference.

Graph loading, dumping, and sampling

Beyond `NetworkX`, graphs and networks can be generated and analyzed with other software. One of the best open source multiplatform software that can be used for their analysis is named Gephi. It's a visual tool and it doesn't require programming skills. It's freely available at `http://gephi.github.io`.

As in machine learning datasets, even graphs have standard formats for storing, loading, and exchanging. This way, you can create a graph with NetworkX, dump it to a file, and then load and analyze it with Gephi.

One of the most frequently used formats is **Graph Modeling Language** (**GML**). Now, let's see how we can dump a graph into a GML file:

```
In: dump_file_base = "dumped_graph"

    # Be sure the dump_file file doesn't exist
    def remove_file(filename):
        import os
        if os.path.exists(filename):
            os.remove(filename)

    G = nx.krackhardt_kite_graph()

    # GML format write and read
    GML_file = dump_file_base + '.gml'
    remove_file(GML_file)

    to_string = lambda x: str(x)
    nx.write_gml(G, GML_file, stringizer=to_string)
    to_int = lambda x: int(x)
    G2 = nx.read_gml(GML_file, destringizer = to_int)
    assert(G.edges() == G2.edges())
```

In the preceding chunk of code, we did the following:

1. We removed the dumped file, if it did exist in the first place.
2. Then, we created a graph (the Kite), and after that, we dumped and loaded it.
3. Finally, we compared the original and the loaded structure, asserting that they're equal.

Beyond GML, there are a variety of formats. Each of these formats has different features. Note that some of them remove information pertaining to the network (like edge/node attributes). Similar to the `write_gml` function and its equivalent, `read_gml`, are the following ones (the names are self-explanatory):

- The adjacency list (`read_adjlist` and `write_adjlist`)
- The multiline adjacency list (`read_multiline_adjlist` and `write_multiline_adjlist`)
- The edge list (`read_edgelist` and `write_edgelist`)
- GEXF (`read_gexf` and `write_gexf`)
- Pickle (`read_gpickle` and `write_gpickle`)
- GraphML (`read_graphml` and `write_graphml`)
- LEDA (`read_leda` and `parse_leda`)
- YAML (`read_yaml` and `write_yaml`)
- Pajek (`read_pajek` and `write_pajek`)
- GIS Shapefile (`read_shp` and `write_shp`)
- JSON (load/loads and dump/dumps, and provides JSON serialization)

The last topic of this chapter is sampling. Why sample a graph? We sample graphs because working with large graphs is sometimes impractical (remember that in the best case, the processing time is proportional to the graph size). Therefore, it's better to sample it, create an algorithm by working on a small-scale scenario, and then test it on the full-scale problem. There are several ways to sample a graph. Here, we're going to introduce the three most frequently used techniques.

In the first technique, which is known as node sampling, a limited subset of nodes, along with their links, forms the sampled set. In the second technique, which is known as link sampling, a subset of links forms the sampled set. Both of these methods are simple and fast, but they may potentially create a different structure for the network. The third method is named snowball sampling. The initial node, all its neighbors, and the neighbors of the neighbors (expanding the selection this way until we reach the maximum traversal depth parameter) form the sampled set. In other words, the selection is like a rolling snowball.

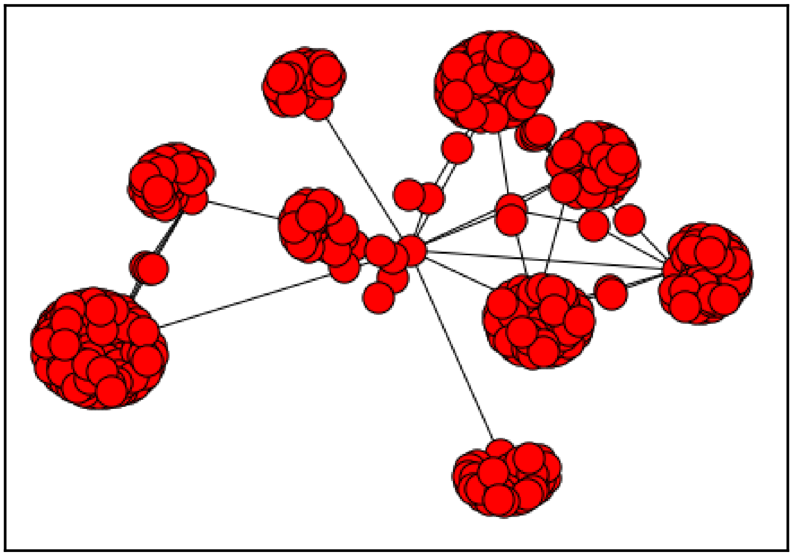
Note that you can also subsample the traversed links. In other words, each link has a probability of `p` that has to be followed and selected in the output set.

The last sampling method is not a part of `NetworkX`, but you can find an implementation for the same in the `snowball_sampling.py` file.

In this example, we will subsample the `LiveJournal` network by starting with the person with an `alberto` ID and then expand recursively twice (in the first example) and three times (in the second example). In the latter instance, every link is followed by a probability of 20%, thus decreasing the retrieval time. Here is an example that demonstrates the same:

```
In: import snowball_sampling
    import matplotlib.pyplot as plot
    my_social_network = nx.Graph()
    snowball_sampling.snowball_sampling(my_social_network, 2, 'alberto')
    nx.draw(my_social_network)
    ax = plot.gca()
    ax.collections[0].set_edgecolor("#000000")
    plt.show()

Out:  Reching depth 0
      new nodes to investigate: ['alberto']
      Reching depth 1
      new nodes to investigate: ['mischa', 'nightraven', 'seraph76',
      'adriannevandal', 'hermes3x3', 'clymore', 'cookita', 'deifiedsoul',
      'msliebling', 'ph8th', 'melisssa', '______eric_', 'its_kerrie_duhh',
      'eldebate']
```

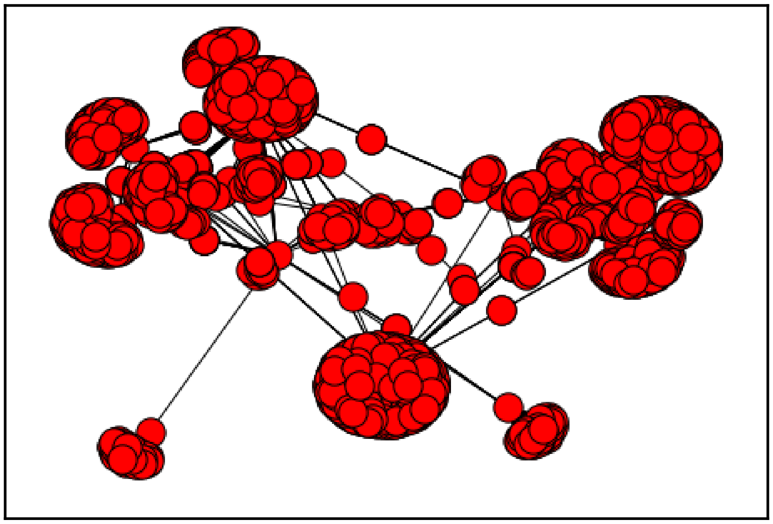
Here is the result of the sampling code:



We will now proceed by using a specific sampling rate of `0.2`:

```
In: my_sampled_social_network = nx.Graph()
    snowball_sampling.snowball_sampling(my_sampled_social_network, 3,
                                         'alberto', sampling_rate=0.2)
    nx.draw(my_sampled_social_network)
    ax = plot.gca()
    ax.collections[0].set_edgecolor("#000000")
    plt.show()

Out:  Reching depth 0
      new nodes to investigate: ['alberto']
      Reching depth 1
      new nodes to investigate: ['mischa', 'nightraven', 'seraph76',
      'adriannevandal', 'hermes3x3', 'clymore', 'cookita', 'deifiedsoul',
      'msliebling', 'ph8th', 'melisssa', '______eric_', 'its_kerrie_duhh',
      'eldebate']
      Reching depth 2
      new nodes to investigate: ['themouse', 'brynna', 'dizzydez', 'lutin',
      'ropo', 'nuyoricanwiz', 'sophia_helix', 'lizlet', 'qowf', 'cazling',
      'copygirl', 'cofax7', 'tarysande', 'pene', 'ptpatricia', 'dapohead',
      'infinitemonkeys', 'noelleleithe', 'paulisper', 'kirasha',
'lenadances',
      'corianderstem', 'loveanddarkness', ...]
```

The resulting graph is more detailed:



Summary

In this chapter, we learned what a social network is, including its creation and modification, representation, and some of the important measures of the social network and its nodes. Finally, we discussed the loading and saving of large graphs and ways to deal with the same.

With this chapter, almost all of the essential data science algorithms have been presented. Machine learning techniques were discussed in `Chapter 4`, *Machine Learning*, and social network analysis methods were discussed here. We will finally discuss the most advanced and cutting-edge techniques of deep learning and neural networks in the next chapter, *Deep Learning Beyond the Basics*.

7
Deep Learning Beyond the Basics

In this chapter, we will introduce deep models, and we will show three examples of how to build deep models. More specifically, in this chapter, you'll learn the following:

- The basics of deep learning
- How to optimize a deep net
- The speed/complexity/accuracy problem
- How to classify images with a CNN
- How to use a pre-trained network for classification and transfer learning
- How to operate on sequences using a LSTM

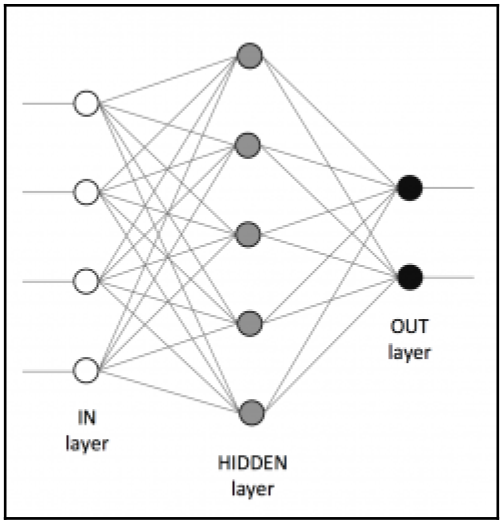
We will be using the Keras package (`https://keras.io/`), which is a high-level API for deep learning that will render approaching neural networks for deep learning much easier and more understandable because it is characterized by a Lego-like approach (here, the bricks are a neural network's composing elements).

Approaching deep learning

Deep learning is an extension of the classical machine-learning approach using neural networks: instead of building networks of a few layers (so-called *shallow networks*), we can stack hundreds of layers to create an elaborate, but more powerful, learner. Deep learning is one of the most popular methods of **artificial intelligence** (**AI**) nowadays since it's very effective and helps to solve many problems in pattern recognition, such as object or sequence identification, which seemed unbreakable using standard machine learning tools.

The idea of neural networks came from the human central nervous system, where multiple nodes (or *neurons)* that are able to process simple information are connected together to create a network capable of processing complex information. In fact, neural networks are so named because they can learn the weights of the model autonomously and adaptively, and, given enough complex network architecture, they're able to approximate any nonlinear function. In deep learning, the nodes are usually called units or neurons.

Let's see how a deep architecture is built and what its components are. We will start with a small deep architecture for a classification problem composed of three layers, as shown in the following figure:



This network has the following characteristics:

- It has three layers. The left-hand one is called the input layer, the right-hand one is called the output layer, and the central one is the hidden layer. Generically, in a neural network, there is always one input and one output layer, and zero or more hidden layers (when there are zero hidden layers, the whole neural architecture will effectively turn into a logistic-regression system).
- The input layer is composed of five units, which means that each observation vector is composed of five numerical features (that is, the observation matrix has five columns). Note that the features must be numeric and in a bounded range of values (for better numeric convergence, the range is ideally 0 to +1, but -1 to +1 is also fine). Therefore, categorical features must be preprocessed in order to become numerical.

- The output layer is composed of three units, which means we want to differentiate among three output classes (that is, perform a three-class classification). In the case of a regression problem, there should be just one unit in this layer.
- The hidden layer is composed of eight units. Note that there's no rule about how many hidden layers should appear in the deep architecture and how many units each should have. These parameters are left to the scientist, and, usually, they require some optimization and fine-tuning in order to work best.
- Each connection has a weight associated with it. This is optimized during the learning algorithm.

Each unit of the input layer is connected to all the units of the next layer. There are neither connections between the units in the same layers nor connections between units in two of the layers at a distance greater than 1 from each other.

In the example, the flow of information is passed forward, from the input to the output (passing eventually through the hidden layers); in literature, this network is referred to as a *feed-forward neural network*.

How does it create the final prediction? Let's see how it works step by step:

1. Starting from the top unit of the hidden layer, it performs a dot product between the output vector of the first layer (that is, the input-observation vector) and the vector of weights of the connections between the first layer and the first unit of the hidden layer.
2. The value is then transformed with the activation function of the unit.
3. This operation is repeated for all the units in the hidden layer.
4. Finally, we can compute the feed-forward propagated values between the hidden layer and the output layer in the same way, which produces the outputs of the network.

The process seems very easy, and it's composed of multiple embarrassingly parallel tasks. The last missing point of the explanation is the activation function: What is it and why is it needed? The activation function helps to make binary decisions more separable (it makes the decision boundary non-linear, thus helping to separate the examples better) and it's a property (or an attribute) of each unit; ideally, each unit should have a different activation function, although they're usually grouped by layer.

Typical activation functions are the sigmoid, the hyperbolic tangent, and the `softmax` (for classification problems) functions, although one of the most popular currently is the **rectified linear unit** (or **ReLU**), whose output is the maximum between 0 and the input (where the input is the dot product between the previous layer output and the weights of the connections).

The activation function, as the number of units and the number of hidden layers, is a parameter of a deep network and should be optimized by the scientist to obtain a better performance.

Training a neural network characterized by many layers is a hard operation since there is a very high number (sometimes millions) of parameters to tune: the weights. The most common way to assign weights to connections uses a similar approach to a gradient descent, and it's called backpropagation, because it propagates back the errors from the output layer toward the input layer, updating each weight proportionally to the gradient of the error at that point in the network. Initially, weights are assigned at random, but, after a few steps, they should converge toward the optimal value.

This was a very short introduction to deep learning and neural networks; if you find the topic interesting and you want to dig more into it, we recommend the following video series from Packt, where you can find a better explanation and some nice tricks to master the learning process:

- Deep Learning with Python [Video] (`https://www.packtpub.com/big-data-and-business-intelligence/deep-learning-python-video`)
- Deep Learning with TensorFlow [Video] (`https://www.packtpub.com/big-data-and-business-intelligence/deep-learning-tensorflow-video`)

Now let's see something practical: how to solve a classification problem with neural networks. We will use Keras in this example. The first is a Python library for low-level primitives, which is typically used in deep learning and is able to take advantage of recent GPUs and numerical speed-up to process multi-dimensional arrays efficiently. Keras is an advanced, fast, and modular Python library for neural networks able to run on top of different numerical computation frameworks, such as TensorFlow, Microsoft Cognitive Tool (previously named CNTK), or Theano.

Classifying images with CNN

Let's now apply a deep neural network to an image-classification problem. Here, we will try to predict a traffic sign from its image. For this task, we will use a **CNN** (**convolutional neural network**), which is able to exploit the spatial correlation between nearby pixels in an image, and is the state of the art in deep learning when working on this kind of problem.

The dataset is available here: `http://benchmark.ini.rub.de/?section=gtsrbsubsection=dataset`. We would like to thank the team for having released the dataset free of charge, and reference the publication dealing with this dataset:
J. Stallkamp, M. Schlipsing, J. Salmen, and C. Igel. The German Traffic Sign Recognition Benchmark: A multi-class classification competition. In Proceedings of the IEEE International Joint Conference on Neural Networks, pages 1453–1460. 2011.

First, download the dataset and then unzip it. The filename of the dataset is `GTSRB_Final_Training_Images.zip`, and, when unzipped, you'll find a new directory named `GTSRB`, which contains all the images located in the same directory as the Jupyter notebook.

The next step is to import Keras and check if the backend is configured properly. In this chapter, we will use the TensorFlow backend, and all the code is tested on that backend.

The backend choice is reversible. If you want to switch from TensorFlow to another backend, follow the guide here: `https://keras.io/backend`. Scripts that are written using Keras can operate successfully no matter what backend they use (the performance in terms of computation time and minimized errors may differ, though).

To check your backend, run the following code, and check if the operation performs successfully and the resulting output matches that reported here.

```
In: import keras

Out: Using TensorFlow backend.
```

It's now time to start the processing, so we have to define some static parameters for the task. There are two of these, primarily: the number of different signals we want to recognize (that is, the number of classes) and the size of the pictures. The number of classes is 43; that is, we have 43 different traffic signs to recognize.

The second parameter, the image size, is important because the input images can be of different sizes and shapes; we need to resize them to a standard size in order to run our deep net on them. We picked 32x32 pixels as the standard: it's small enough to recognize the signal, and, at the same time, it doesn't require too much memory (that is, every grayscale image uses just 1,024 bytes or 1 KB). Increasing the size means increasing the memory needed to keep the dataset, plus the input layer of the deep net and the time necessary for computations. In the literature, 32x32 is a pretty standard choice for images with just one item; so, in our case, we have good reasons to decide on that size.

```
In: N_CLASSES = 43
    RESIZED_IMAGE = (32, 32)
```

At this point, we have to read the images and resize them, creating the observation matrix and the array of labels. To do so, we perform the following steps:

1. Import the modules needed for the processing. The most important is Scikit-learn, or sklearn, which contains loads of functions to process the images.
2. We read the images one after another. The label is contained in the path. For example, the image `GTSRB/Final_Training/Images/00000/00003_00024.ppm` has label `00000`, which is `0`; and the image `GTSRB/Final_Training/Images/00025/00038_00005.ppm` has label `00025`, which is `25`. The label is stored as a labeled-encoded array, which is an array 43-cells long with only one that has a value of `1` (all the others are `0`).
3. The image is stored in the **PPM** (**Portable PixMap**) format, and it's a lossless way to store the pixels in an image. Scikit-image, or just skimage (`https://scikit-image.org/`), is able to read that format by using the function `imread`. If you don't have Scikit-image already installed on your system, just type the following in a shell: `conda install scikit-image` or `pip install -U scikit-image`. The returned object is a 3D NumPy array.
4. The 3D NumPy array, containing the pixel representation of the image (with three channels—red, blue and green) is then converted to grayscale. Here, we first convert to the LAB color space (see `https://hidefcolor.com/blog/color-management/what-is-lab-color-space`—this color space is more perceptually linear than others, which implies that the same amount of change in a color value should produce an impact of the same visual importance), and then the first channel (containing the luminance) is kept. Again, this operation is easily done with skimage. As a result, we have a 1D NumPy array containing the image pixels.
5. The image is finally resized to the 32x32 pixel format, again using a skimage function.

6. Finally, all the images are squeezed into a 4-dimensional matrix: the first dimension is used to index the image within the dataset; the second and the third represent the height and the width of the image, respectively; and the last dimension is the channel. Having 39,208 images, with all 32x32 pixels in grayscale, the observation matrix is therefore in the shape (39,208, 32, 32, 1).
7. Labels are compacted into a two-dimensional matrix. The first dimension is the index of the image and the second dimension is the class. Due to having the same number of images, and 43 possible classes, this matrix will be shaped (39,208, 43).

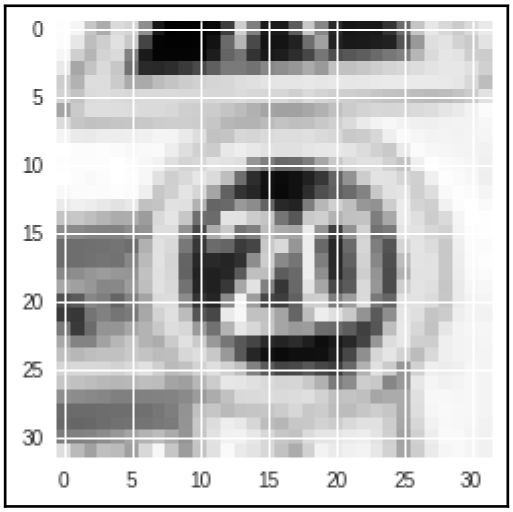
The following shows all seven steps translated into code:

```
In: import matplotlib.pyplot as plt
    import glob
    from skimage.color import rgb2lab
    from skimage.transform import resize
    from collections import namedtuple
    import numpy as np
    np.random.seed(101)
    %matplotlib inline

    Dataset = namedtuple('Dataset', ['X', 'y'])

    def to_tf_format(imgs):
        return np.stack([img[:, :, np.newaxis] for img in imgs],
                        axis=0).astype(np.float32)

    def read_dataset_ppm(rootpath, n_labels, resize_to):
        images = []
        labels = []
        for c in range(n_labels):
            full_path = rootpath + '/' + format(c, '05d') + '/'
            for img_name in glob.glob(full_path + "*.ppm"):
                img = plt.imread(img_name).astype(np.float32)
                img = rgb2lab(img / 255.0)[:,:,0]
                if resize_to:
                    img = resize(img, resize_to, mode='reflect',
                                 anti_aliasing=True)
                label = np.zeros((n_labels, ), dtype=np.float32)
                label[c] = 1.0
                images.append(img.astype(np.float32))
                labels.append(label)
        return Dataset(X = to_tf_format(images).astype(np.float32),
                       y = np.matrix(labels).astype(np.float32))

    dataset = read_dataset_ppm('GTSRB/Final_Training/Images', N_CLASSES,
                                       RESIZED_IMAGE)
    print(dataset.X.shape)
    print(dataset.y.shape)

Out: (39209, 32, 32, 1)
     (39209, 43)
```

The dataset is composed of almost 40,000 images; let's see what the first of them looks like, after the color change and the resize:

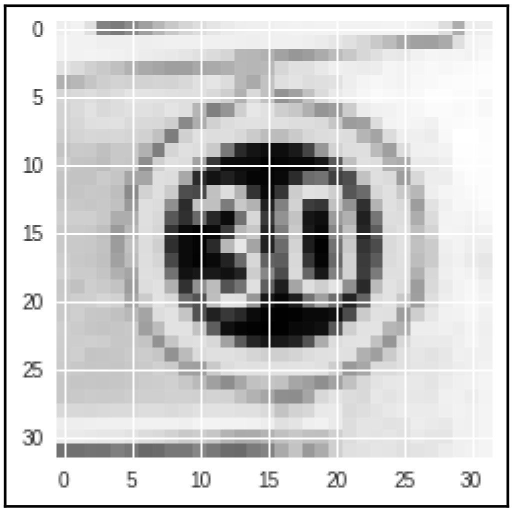
```
In: plt.imshow(dataset.X[0, :, :, :].reshape(RESIZED_IMAGE))
    print("Label:", dataset.y[0, :])

Out: Label: [[1. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.
              0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0.
              0. 0. 0.]]
```

The following is the plotted sample image:



Even though the image has a very low definition, 32x32 pixels, we can immediately recognize which sign is represented. So far, it seems that the reshaping operation is leaving the images intelligible, even to humans. Note again that the label is a 43-dimensional vector; since this image belongs to the first class (that is, class `00000`), just the first element of the label is not null.

Another element, of a different class, is shown as follows. That's image number 1,000 in the dataset, and its class is the 2nd (in fact, it's a different sign):



Let's now split the dataset into training and testing. We use Scikit-learn to randomly separate and shuffle the images. In this cell, we select 25% of the dataset as a test set; that is, almost 10,000 images, leaving the other 29K+ images for training the deep net:

```
In: from sklearn.model_selection import train_test_split
    idx_train, idx_test = train_test_split(range(dataset.X.shape[0]),
                                           test_size=0.25,
                                           random_state=101)
    X_train = dataset.X[idx_train, :, :, :]
    X_test = dataset.X[idx_test, :, :, :]
    y_train = dataset.y[idx_train, :]
    y_test = dataset.y[idx_test, :]

    print(X_train.shape)
    print(y_train.shape)
    print(X_test.shape)
    print(y_test.shape)

Out: (29406, 32, 32, 1)
     (29406, 43)
     (9803, 32, 32, 1)
     (9803, 43)
```

Here's the moment of creating a convolutional deep network. We start with a simple, easy to understand, neural network. Then we'll move to something that is more complex but accurate.

Creating deep nets with Keras is very easy: you have to define all layers in a sequential way, one after another. The Keras object needs to define the layers in a sequence named `Sequential`. Here, we will create a deep net with three layers:

1. The input layer, defined as a convolutional 2D layer (which is actually a convolutional operation between the image and the kernel), contains 32 filters in the shape of 3x3 pixels and with an activation layer of type ReLU.
2. A layer that flattens the output of the previous; that is, square observations will be unrolled to create a 1D array.
3. A dense output layer, with `softmax` activation and which is composed of 43 units, one for each class.

The model is then compiled and, finally, fitted to the training data. During this operation we selected the following:

- **The optimizer**: SGD, the simplest one
- **The batch size**: 32 images/batch
- **The numbers of epochs**: 10

Here is the code that will generate the model we have just described:

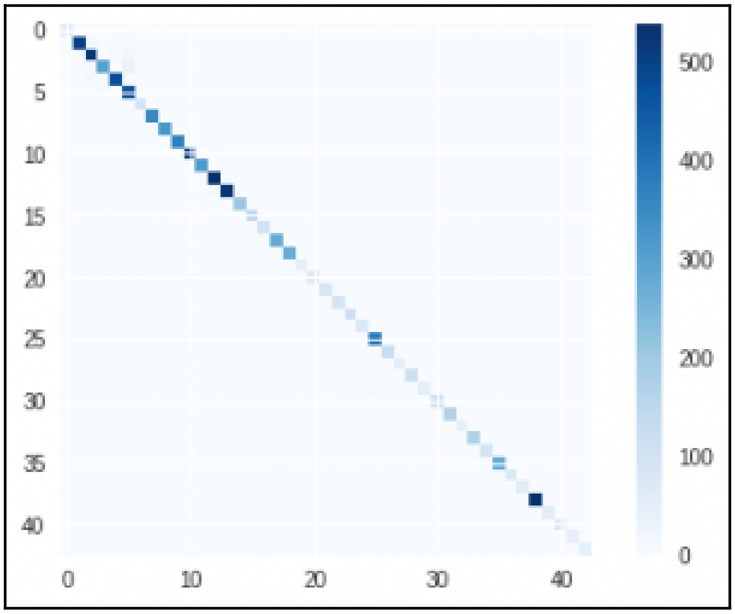
```
In: from keras.models import Sequential
    from keras.layers.core import Dense, Flatten
    from keras.layers.convolutional import Conv2D
    from keras.optimizers import SGD
    from keras import backend as K
    K.set_image_data_format('channels_last')
    def cnn_model_1():
        model = Sequential()
        model.add(Conv2D(32, (3, 3),
                    padding='same',
                    input_shape=(RESIZED_IMAGE[0], RESIZED_IMAGE[1], 1),
                    activation='relu'))
        model.add(Flatten())
        model.add(Dense(N_CLASSES, activation='softmax'))
        return model

    cnn = cnn_model_1()
    cnn.compile(loss='categorical_crossentropy',
                optimizer=SGD(lr=0.001, decay=1e-6),
                metrics=['accuracy'])
    cnn.fit(X_train, y_train,
            batch_size=32,
            epochs=10,
            validation_data=(X_test, y_test))

Out: Train on 29406 samples, validate on 9803 samples
     Epoch 1/10
     29406/29406 [==============================] - 11s 368us/step -
     loss: 2.7496 - acc: 0.5947 - val_loss: 0.6643 - val_acc: 0.8533
     Epoch 2/10
     29406/29406 [==============================] - 10s 343us/step -
     loss: 0.4838 - acc: 0.8937 - val_loss: 0.4456 - val_acc: 0.9001
     [...]
     Epoch 9/10
     29406/29406 [==============================] - 10s 337us/step -
     loss: 0.0739 - acc: 0.9876 - val_loss: 0.2306 - val_acc: 0.9553
     Epoch 10/10
     29406/29406 [==============================] - 10s 343us/step -
     loss: 0.0617 - acc: 0.9897 - val_loss: 0.2208 - val_acc: 0.9574
```

The final accuracy is close to 99% on the training set and almost 96% on the test set. We're overfitting a bit, but let's see the confusion matrix and the classification report of this model on the test set. We'll also print the `log2` of the confusion matrix to better identify misclassifications.

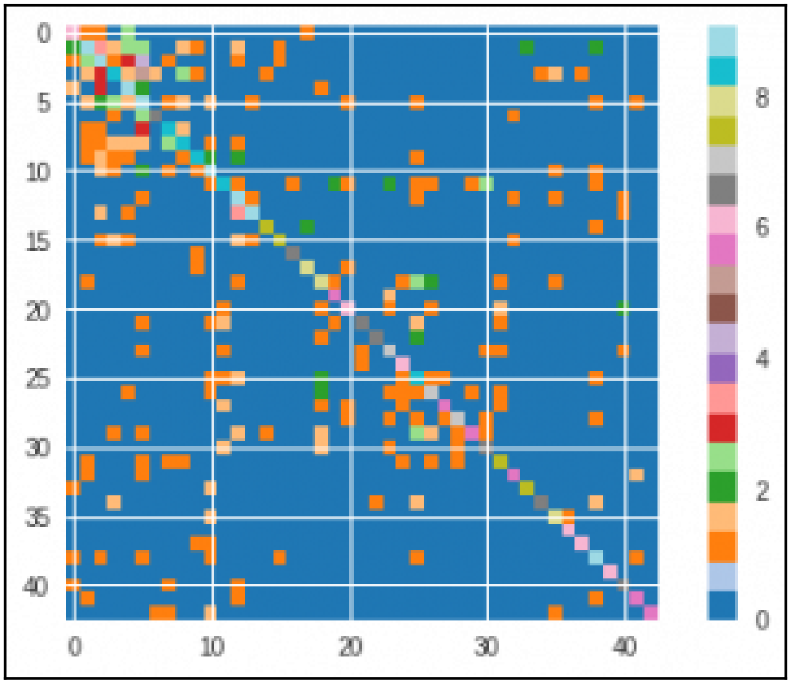
To do so, we first need to predict the labels and then apply the `argmax` operator to select the most likely class:

```
In: from sklearn.metrics import classification_report, confusion_matrix

    def test_and_plot(model, X, y):
        y_pred = cnn.predict(X)
        y_pred_softmax = np.argmax(y_pred, axis=1).astype(np.int32)
        y_test_softmax = np.argmax(y, axis=1).astype(np.int32).A1
        print(classification_report(y_test_softmax, y_pred_softmax))
        cm = confusion_matrix(y_test_softmax, y_pred_softmax)
        plt.imshow(cm, interpolation='nearest', cmap=plt.cm.Blues)
        plt.colorbar()
        plt.tight_layout()
        plt.show()
        # And the log2 version, to emphasize the misclassifications
        plt.imshow(np.log2(cm + 1), interpolation='nearest',
                   cmap=plt.get_cmap("tab20"))
        plt.colorbar()
        plt.tight_layout()
        plt.show()

test_and_plot(cnn, X_test, y_test)

Out:
                 precision    recall  f1-score   support
              0          0.87      0.90      0.88        67
              1          0.97      0.94      0.95       539
              2          0.93      0.94      0.94       558
              [........]
             40          0.93      0.96      0.95        85
             41          0.92      0.94      0.93        47
             42          1.00      0.91      0.95        53
    avg / total          0.96      0.96      0.96      9803
```

The following are the diagnostic plots, which provide you with evidence on the performance of the model:



And here's the `log2` version of the confusion matrix:



The classification already seems to be pretty good. Can we do something better and avoid the overfitting? Yes, here is what we can use:

- **Dropout layers**: This is the equivalent of regularization, and it prevents overfitting. Basically, at each step during the training, a portion of units is deactivated, so the output of the layer doesn't rely too much on just a few of them.
- **BatchNormalization layer**: This z-normalizes the layer, by subtracting the batch mean and dividing it by the standard deviation. It's useful for recentering the data, and it amplifies/attenuates the signal at each step.
- **MaxPooling**: This is a nonlinear transformation, which is used to downsample the input by applying a max filter to each region under the kernel. It's used to select the max feature, which can be in a slightly different position within the same class.

Beyond these, there's always space to change the deep net and training properties; that is, the optimizer (and its parameters), the batch size, and the number of epochs. Here, in the next cell, is an improved deep net with the following layers:

1. Convolutional layer, with 32 3x3 filters and ReLU activation
2. BatchNormalization layer
3. Another convolutional layer followed by a BatchNormalization layer
4. Dropout layer, with a probability of 0.4 of being dropped
5. Flattening layer
6. 512-units dense layer, with ReLU activation
7. BatchNormalization layer
8. Dropout layer, with a probability of 0.5 of being dropped
9. Output layer; as in the previous example, this is a `softmax` dense layer with 43 units

How will that perform on our dataset?

```
In: from keras.layers.core import Dropout
    from keras.layers.pooling import MaxPooling2D
    from keras.optimizers import Adam
    from keras.layers import BatchNormalization

    def cnn_model_2():
        model = Sequential()
        model.add(Conv2D(32, (3, 3), padding='same',
                         input_shape=(RESIZED_IMAGE[0], RESIZED_IMAGE[1], 1),
                         activation='relu'))
        model.add(BatchNormalization())
        model.add(Conv2D(32, (3, 3),
                         padding='same',
                         input_shape=(RESIZED_IMAGE[0], RESIZED_IMAGE[1], 1),
                         activation='relu'))
        model.add(BatchNormalization())
        model.add(MaxPooling2D(pool_size=(2, 2)))
        model.add(Dropout(0.4))
        model.add(Flatten())
        model.add(Dense(512, activation='relu'))
        model.add(BatchNormalization())
        model.add(Dropout(0.5))
        model.add(Dense(N_CLASSES, activation='softmax'))
        return model

    cnn = cnn_model_2()
    cnn.compile(loss='categorical_crossentropy',
        optimizer=Adam(lr=0.001, decay=1e-6), metrics=['accuracy'])
    cnn.fit(X_train, y_train,
            batch_size=32,
            epochs=10,
            validation_data=(X_test, y_test))
```

```
Out: Train on 29406 samples, validate on 9803 samples
     Epoch 1/10
     29406/29406 [==============================] - 24s 832us/step -
     loss: 0.7069 - acc: 0.8145 - val_loss: 0.1611 - val_acc: 0.9584
     Epoch 2/10
     29406/29406 [==============================] - 23s 771us/step -
     loss: 0.1784 - acc: 0.9484 - val_loss: 0.1065 - val_acc: 0.9714
     [...]
     Epoch 10/10
     29406/29406 [==============================] - 23s 770us/step -
     loss: 0.0370 - acc: 0.9878 - val_loss: 0.0332 - val_acc: 0.9920

     <keras.callbacks.History at 0x7fd7ac0f17b8>
```

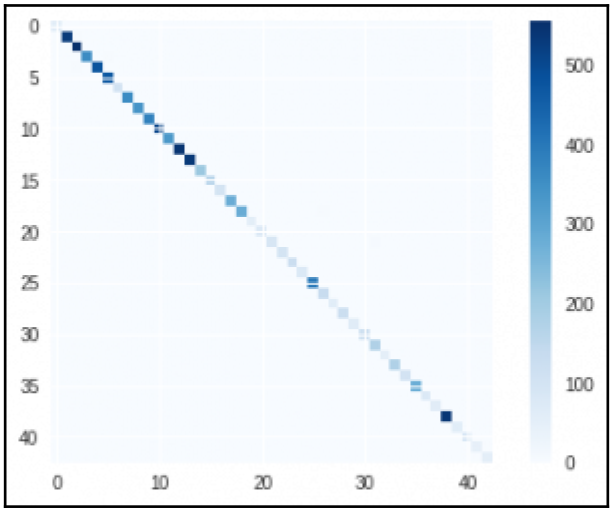
The training set's accuracy is similar to that for the test set, and they're both around 99%; that is, 99 out of 100 images are classified with the correct label! This network is longer and it requires more memory and computational power, but it's less prone to overfitting and it performs better.

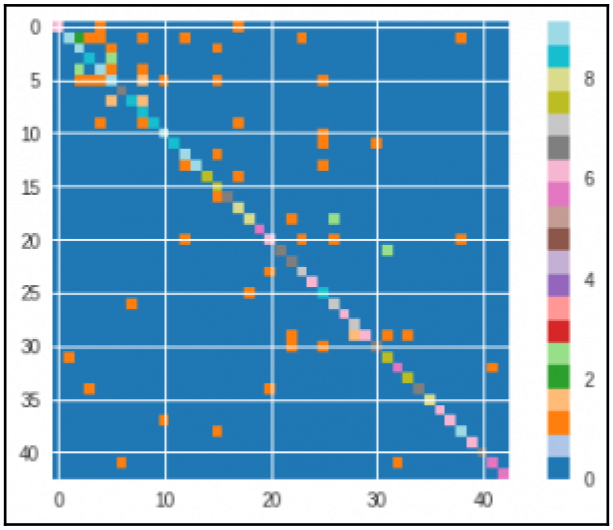
Let's now see the classification report and the confusion matrix (the full one and the `log2` version):

```
In: test_and_plot(cnn, X_test, y_test)
```

```
Out:
                  precision    recall  f1-score   support
               0       1.00      0.97      0.98        67
               1       1.00      0.98      0.99       539
               2       0.99      1.00      0.99       558
              [..........]
              38       1.00      1.00      1.00       540
              39       1.00      1.00      1.00        60
              40       1.00      1.00      1.00        85
              41       0.98      0.96      0.97        47
              42       1.00      1.00      1.00        53
     avg / total       0.99      0.99      0.99      9803
```

Here are the visual representations of the results:





It is clear that the number of misclassifications has decreased quite significantly. Now, let's try to do something better, by changing the parameters.

Using pre-trained models

As you saw in the previous example, increasing the complexity of the network increases the time and the memory needed to train it. Sometimes, we have to accept that we don't have a machine powerful enough to try all the combinations. What can we do in that situation? Basically, we can do two things:

- Simplify the network; that is, by removing parameters and variables
- Use a pre-trained network, which has already been trained by someone with a powerful enough machine

In both situations, we will work in sub-optimal conditions, since the deep network won't be as powerful as the one we could have used. More specifically, in the first case, the network won't be very accurate because we have fewer parameters; in the second case, well, we have to cope with someone else's decisions and training set. Although it's not very easy to do, pre-trained models can also be fine-tuned with your dataset; in this case, the network won't have a random initialization of the parameters. Although this is very interesting, this operation is out of the scope of this book.

In this section, we will quickly show how to use pre-trained models, which is a common way to proceed. Bear in mind that pre-trained models can be used in multiple situations:

- Feature augmentation, to add a feature (in this case, the predicted label), along with observation vectors, into your model
- Transfer learning, to add more features (coefficients coming from one or model layers), along with observation vectors, into your model
- Prediction; that is, to compute the label

Let's now see how to use a pre-trained network to serve our purpose.

In Keras, various pre-trained models are available from here: `https://keras.io/applications`.

Let's first download some images to test. In the following example, we will use the dataset provided by Caltech, which is available here: `http://www.vision.caltech.edu/Image_Datasets/Caltech101/`.

We would like to thank the authors of the dataset, and suggest to read their paper: *L. Fei-Fei, R. Fergus and P. Perona. One-Shot learning of object categories. IEEE Trans. Pattern Recognition and Machine Intelligence*.

It contains several images in 101 categories and comes in the `tar.gz` format.

Now, with a new notebook, import the modules we will use. In this example, we will use the InceptionV3 pre-trained network, which is able to recognize objects in images very well. It has been developed by Google, and its output is comparable to the human eye.

1. First, we import the functions that are needed to set up the network, to preprocess the inputs, and to extract the predictions:

```
In: from keras.applications.inception_v3 import InceptionV3
    from keras.applications.inception_v3 import preprocess_input
    from keras.applications.inception_v3 import decode_predictions
    from keras.preprocessing import image
    import numpy as np
    import matplotlib.pyplot as plt
    %matplotlib inline

Out: Using TensorFlow backend.
```

2. Now, let's load the huge network and its coefficient:

```
In: model = InceptionV3(weights='imagenet')
```

   It's simple, isn't it?

3. The next step (and the final one) is to create a function to make the prediction. In this case, we will predict the top three labels:

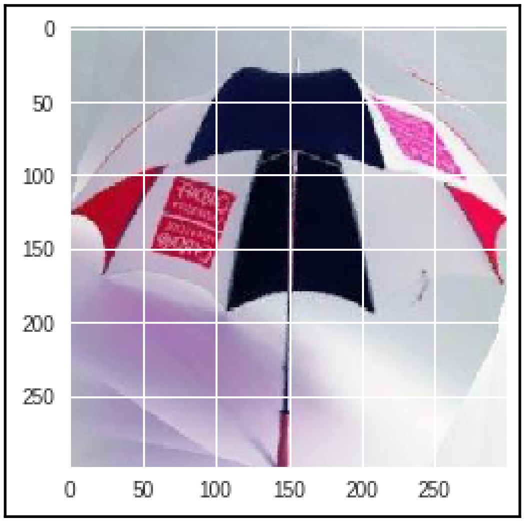
```
In: def predict_top_3(model, img_path):
    img = image.load_img(img_path, target_size=(299, 299))
    plt.imshow(img)
    x = image.img_to_array(img)
    x = np.expand_dims(x, axis=0)
    x = preprocess_input(x)
    preds = model.predict(x)
    print('Predicted:', decode_predictions(preds, top=3)[0])
```

Basically, this function loads and resizes the image to 299x299 pixels (which is the default input size for the pre-trained network InceptionV3), and converts the image to the correct format for the model. After that, it predicts all the labels of the image and selects (and prints) the top three.

Let's see how it performs with an example image by using the pre-trained model and asking for the top three predictions in terms of probability:

```
In: predict_top_3(model, "101_ObjectCategories/umbrella/image_0001.jpg")
```

The image we want to predict and the resulting output from the top three predictions are as follows:

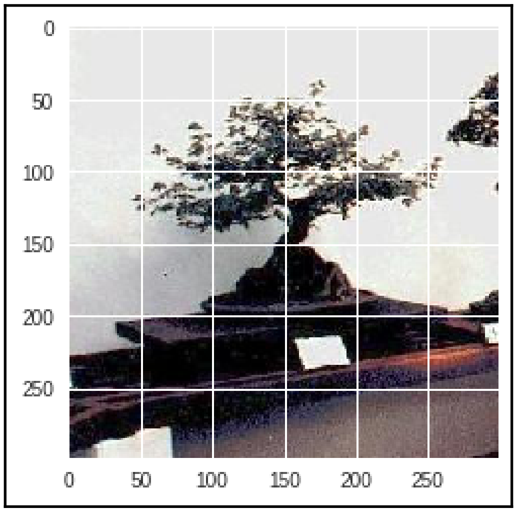


```
Out: Predicted: [('n04507155', 'umbrella', 0.88384396),
                 ('n04254680', 'soccer_ball', 0.07257448),
                 ('n03888257', 'parachute', 0.012849103)]
```

We confirm that this is a great result; the first label (with a score of 88%) is an umbrella, followed by a soccer ball and a parachute. Let's now test a certainly more difficult image, which is one whose label is not included in the InceptionV3 training set:

```
In: predict_top_3(model, "101_ObjectCategories/bonsai/image_0001.jpg")
```

Here is the image and its top three results:



```
Out: Predicted: [('n02704792', 'amphibian', 0.20315942),
                 ('n04389033', 'tank', 0.07383019),
                 ('n04252077', 'snowmobile', 0.055828683)]
```

As expected, as it is not among its pre-defined classes, the network is not able to recognize the bonsai in the first predicted label.

Actually, pre-trained models can be taught to recognize even completely new classes by the so-called **transfer learning technique**. This technique is out of the scope of this book, but you can read about it on this example from Keras's blog: `https://blog.keras.io/building-powerful-image-classification-models-using-very-little-data.html`.

Finally, let's see how to extract features from the intermediate layers, as follows:

1. As the first step, let's verify the label names:

```
In: print([l.name for l in model.layers])

Out: ['input_1', 'conv2d_1', 'batch_normalization_1',
      ..........
      'activation_94', 'mixed10', 'avg_pool', 'predictions']
```

2. We can select any of these layers; we will go for the one before the `softmax` prediction. Let's create an object `Model` whose output is the `avg_pool` layer:

```
In: from keras.models import Model
    feat_model = Model(inputs=model.input,
                       outputs=model.get_layer('avg_pool').output)

    def extract_features(feat_model, img_path):
        img = image.load_img(img_path, target_size=(299, 299))
        x = image.img_to_array(img)
        x = np.expand_dims(x, axis=0)
        x = preprocess_input(x)
        return feat_model.predict(x)
```

3. Finally, to extract the features for a picture, let's call the previous function with an image:

```
In: f = extract_features(feat_model,
                    "101_ObjectCategories/bonsai/image_0001.jpg")
    print(f.shape)
    print(f)

Out: (1, 2048)
     [[0.12340261 0.0833823 0.7935947 ... 0.50869745 0.34015656]]
```

As you can check, the `avg_pool` layer contains `2048` units, and the output of the function is exactly a 2,048D array. You can now concatenate this array to any other feature array of your choice.

Working with temporal sequences

The last example in this chapter is about dealing with temporal sequences; more specifically, we will see how to deal with text, which is a variable-length sequence of words.

Some data-science algorithms deal with text using the bag-of-words approach; that is, they don't care where the words are and how they're placed in the text, they just care about their presence/absence (and maybe their frequency). Instead, a special class of deep networks is specifically designed to operate on sequences, where the order is important.

Some examples are as follows:

- **Predict a future stock price, given its historical data**: In this case, the input is a sequence of numbers, and the output is a number
- **Predict whether the market will go up or down**: In this case, given a sequence of numbers, we want to predict a class (up or down)
- **Translate an English text to French**: In this case, the input sequence is converted into another sequence
- **Chatbot**: In this case, the input and the output are both sequences (in the same language)

For this example, let's do something easy. We will try to detect the sentiment of a movie review. In this specific example, the input data is a sequence of words (and the order counts!), and the output is a binary label (which is the sentiment *positive* or *negative*).

Let's start importing the dataset. Fortunately, Keras already includes this dataset, and it's already pre-indexed; that is, each review is not composed of words but of indexes of a dictionary. Also, it's possible to select just the top words, and, with this code, we select a dictionary containing the top `25000` words:

```
In: from keras.datasets import imdb
    ((data_train, y_train),
     (data_test, y_test)) = imdb.load_data(num_words=25000)
```

Let's see what's inside the `data` and the `shape`:

```
In: print(data_train.shape)
    print(data_train[0])
    print(len(data_train[0]))

Out: (25000,)
     [1, 14, 22, 16, 43, 530, .......... 19, 178, 32]
     218
```

Firstly, there are `25000` reviews; that is, observations. Secondly, each review is composed of a sequence of numbers between 1 and 24,999; 1 indicates the start of the sequence, while the last number signals a word that is not in the dictionary. Note that each review has a different size; for example, the first one is `218` words in length.

It's now time to trim or pad all the sequences to a specific size. With Keras, this is easily done, and, for padding, the integer 0 is added:

```
In: from keras.preprocessing.sequence import pad_sequences
    X_train = pad_sequences(data_train, maxlen=100)
    X_test = pad_sequences(data_test, maxlen=100)
```

Our training matrix now has a rectangular shape. The first element after the trimming/padding operation becomes the following:

```
In: print(X_train[0])
    print(X_train[0].shape)

Out: [1415, .......... 19, 178, 32]
     (100,)
```

For this observation, just the last 100 words are maintained. Overall, now, all the observations have 100 dimensions. Let's now create a temporal deep model to predict the review sentiment.

The model proposed here has three layers:

1. An embedding layer. The original dictionary is set to 25,000 words, and the number of units composing the embedding (that is, the layer's output) is 256.
2. An LSTM layer. **LSTM** stands for **long short-term memory**, and it's one of the most powerful deep models for sequences. Thanks to its deep architecture, it's able to extract information from close and distant words in the sequence (hence the name). In this example, the number of cells is set to 256 (as the previous layer output dimension), with a dropout of 0.4 for regularization.
3. A dense layer with a sigmoid activation. That's what we need for a binary classifier.

Here's the code for doing so:

```
In: from keras.models import Sequential
    from keras.layers import LSTM, Dense
    from keras.layers.embeddings import Embedding
    from keras.optimizers import Adam
    model = Sequential()
    model.add(Embedding(25000, 256, input_length=100))
    model.add(LSTM(256, dropout=0.4, recurrent_dropout=0.4))
    model.add(Dense(1, activation='sigmoid'))
    model.compile(loss='binary_crossentropy',
    optimizer=Adam(),
    metrics=['accuracy'])
```

```
            model.fit(X_train, y_train,
                      batch_size=64,
                      epochs=10,
                      validation_data=(X_test, y_test))

        Out: Train on 25000 samples, validate on 25000 samples
             Epoch 1/10
             25000/25000 [==============================] - 139s 6ms/step -
             loss:0.4923 - acc:0.7632 - val_loss:0.4246 - val_acc:0.8144
             Epoch 2/10
             25000/25000 [==============================] - 139s 6ms/step -
             loss:0.3531 - acc:0.8525 - val_loss:0.4104 - val_acc: 0.8235
             Epoch 3/10
             25000/25000 [==============================] - 138s 6ms/step -
             loss:0.2564 - acc:0.9000 - val_loss:0.3964 - val_acc: 0.8404
             ...
             Epoch 10/10
             25000/25000 [==============================] - 138s 6ms/step -
             loss:0.0377 - acc:0.9878 - val_loss:0.8090 - val_acc:0.8230
```

And that's the accuracy on the 25K-review test dataset. That's an acceptable result since we achieved more than 80% of correct classifications with such a simple model. If you feel like improving it, you could try to make the architecture more sophisticated, but always keep in mind that, by increasing the complexity of the network, there is an increase in the time needed to train it and to predict the outcome, as well as the memory footprint.

Summary

In this chapter, we saw the essentials and some advanced models for deep networks. We were introduced to how neural networks work and the difference between shallow networks and deep learning. Then, we learnt ho to build a CNN deep network capable of classifying images of traffic signs. We also predicted the class of an image using a pre-trained network. Detecting the sentiment of a movie review using text found in reviews was also a part of the learning.

Deep learning models are indeed very powerful, though at the cost of having many degrees of freedom to handle and many coefficients to train, which requires having at hand large amounts of data.

In the next chapter, we'll see how Spark helps when the amount of data becomes too large to be handled and processed by a single computer.

8
Spark for Big Data

The amount of data stored in the world is increasing in a quasi-exponential fashion. Nowadays, for a data scientist, having to process a few terabytes of data a day is not an unusual request anymore and, to make things even more complex, this implies having to deal with data that comes from many different heterogeneous systems. In addition, in spite of the size of the data you have to deal with, the expectation of business is constantly to produce a model within a short time, as you were simply operating on a toy dataset.

In conclusion of our journey around the essentials of data science, we cannot elude such a key necessity in data science. Therefore, we are going to introduce you to a new way of processing large amounts of data, scaling through multiple computers in order to acquire data, processing it, and building effective machine learning algorithms. Dealing with large amounts of data and producing an effective machine learning model won't be an after our essential introduction.

In this chapter, you will:

- Understand distributed frameworks, explaining Hadoop, MapReduce, and Spark technologies
- Start with PySpark, the Python API interface for Spark
- Experiment with Resilient Distributed Datasets, a new way to operate on large data
- Define and share variables in a distributed system in Spark
- Process data using DataFrames in Spark
- Apply machine learning algorithms in Spark

At the end of this chapter, given an appropriate cluster of machines, you will be capable of facing any data science problem, regardless of the scale of the data at hand.

From a standalone machine to a bunch of nodes

Handling big data is not just a matter of size; it's actually a multifaceted phenomenon. In fact, according to the **3V model** (volume, velocity and variety), systems operating on big data can be classified using three (orthogonal) criteria:

- The first criterion to consider is the **velocity** that the system achieves to process the data. Although a few years ago, speed was used to indicate how quickly a system was able to process a batch, nowadays, velocity indicates whether a system can provide real-time outputs on streaming data.
- The second criterion is **volume**; that is, how much information is available to be processed. It can be expressed in the number of rows or features, or just a bare count of the bytes. In streaming data, the volume indicates the throughput of data arriving in the system.
- The last criterion is **variety**; that is, the types of data source. A few years ago, the variety was limited by structured datasets, but, nowadays, data can be structured (tables, images, and so on), semi-structured (JSON, XML, and so on), and unstructured (web pages, social data, and so on). Usually, big-data systems try to process as many relevant sources as possible and mix all kinds of sources.

Beyond these criteria, many other Vs have appeared in the last few years, which are trying to explain other features of big data. Some of these are as follows:

- **Veracity**: Providing an indication of abnormality, bias, and noise contained in the data; ultimately, indicating its accuracy
- **Volatility**: Indicating how long the data can be used to extract meaningful information
- **Validity**: The correctness of the data
- **Value**: Indicating the return on the investment from the data

In recent years, all of the Vs have increased dramatically. Now, many companies have found that the data they retain has a huge value that can be monetized, and they want to extract information out of it. The technical challenge has moved to have enough storage and processing power in order to be able to extract meaningful insights quickly, at scale, and using different input data streams.

Current computers, even the newest and most expensive ones, have a limited amount of disk, memory, and CPU. It seems to be very hard to process terabytes (or petabytes) of information per day, and produce a model in a timely fashion. Moreover, a standalone server containing both data and processing software needs to be replicated; otherwise, it could become the single point of failure of the system.

The world of big data has therefore moved to clusters: they're composed of a variable number of *not-very-expensive* nodes and sit on a high-speed internet connection. Usually, some clusters are dedicated to storing data (a big hard disk, little CPU, and a low amount of memory), and others are devoted to processing the data (a powerful CPU, a medium-to-large amount of memory, and a small hard disk). Moreover, if a cluster is properly set, it can ensure reliability (having no single point of failure) and high availability.

Making sense of why we need a distributed framework

The easiest way to build a cluster is to use some nodes as storage nodes and others as processing ones. This configuration seems very easy to use as we don't need a complex framework to handle this situation. In fact, many small clusters are built exactly in this way: a couple of servers handle the data (plus their replica) and another bunch process the data. Although this may appear as a great solution, it's not often used for many reasons:

- It only works for embarrassingly parallel algorithms. If an algorithm requires a common area of memory shared among the processing servers, this approach cannot be used.
- If one or many storage nodes die, the data is not guaranteed to be consistent. (Think about a situation where a node and its replica die at the same time, or where a node dies just after a write operation that has not yet been replicated.)
- If a processing node dies, we are not able to keep track of the process that it was executing, making it hard to resume the processing on another node.
- If the network experiences a failure, it's very hard to predict the situation after it goes back to normality.

A crash event (or even more than one) is quite likely, which is a fact requiring that such an occurrence must be thought of in advance and handled properly to ensure the continuity of operations on the data. Furthermore, when using cheap hardware or a bigger cluster, it looks almost certain that at least one node will fail. So far, the vast majority of cluster frameworks use the approach named *Divide et Impera* (split and conquer):

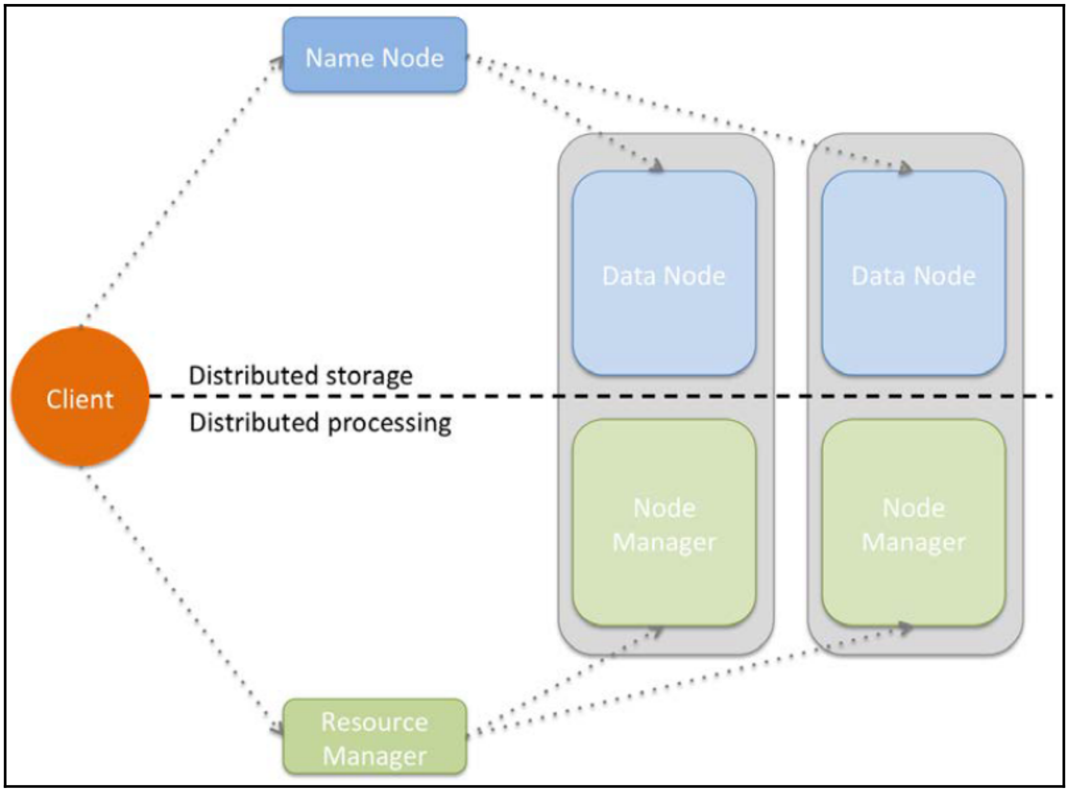
- There are *specialized* modules for the data nodes and some other specialized modules for data processing nodes (also named workers).
- Data is replicated across the data nodes, and one node is the master, ensuring that both the write and read operations succeed.
- The processing steps are split across the worker nodes. They don't share any state (unless stored in the data nodes), and their master ensures that all the tasks are performed positively and in the right order.

The Hadoop ecosystem

Apache Hadoop is a very popular software framework for distributed storage and distributed processing on a cluster. Its strengths are in its price (it's free), flexibility (it's open source, and although it is written in Java, it can be used by other programming languages), scalability (it can handle clusters composed of thousands of nodes), and robustness (it was inspired by a published paper from Google and has been around since 2011), making it the de facto standard to handle and process big data. Moreover, lots of other projects from the Apache foundation have extended its functionalities.

Hadoop architecture

Logically, Hadoop is composed of two pieces: distributed storage (HDFS) and distributed processing (YARN and MapReduce). Although the code is very complex, the overall architecture is fairly easy to understand. A client can access both storage and processing through two dedicated modules; they are then in charge of distributing the job across all the working nodes, as shown in the following diagram:



All the Hadoop modules run as services (or instances); that is, a physical or virtual node can run many of them. Typically, for small clusters, all the nodes run both distributed computing and processing services; for big clusters, it may be better to separate the two functionalities and specialize the nodes.

We will see the functionalities offered by the two layers in detail.

Hadoop Distributed File System

The **Hadoop Distributed File System (HDFS)** is a fault-tolerant distributed filesystem, which is designed to run on low-cost hardware, and able to handle very large datasets (in the order of hundreds of petabytes to exabytes). Although the HDFS requires a fast network connection to transfer data across nodes, the latency can't be as low as in classic filesystems (it may be in the order of seconds); therefore, the HDFS has been designed for batch processing and high throughput. Each HDFS node contains a part of the filesystem's data; the same data is also replicated in other instances, and this ensures a high throughput access and fault-tolerance.

The HDFS's architecture is master-slave. If the master (called **NameNode**) fails, there is a secondary/backup node ready to take control. All the other instances are slaves (**DataNodes**); if one of them fails, it's not a problem as the HDFS has been designed with this in mind, so no data is lost (it is redundantly replicated) and operations are quickly redistributed to surviving nodes. **DataNodes** contain blocks of data: each file saved in the HDFS is broken up into chunks (or blocks), typically 64 MB each, and then distributed and replicated in a set of **DataNodes**. The **NameNode** stores only the metadata of the files in the distributed file system; it doesn't store any actual data, rather it just stores the right indications on how to access the files in the multiple **DataNodes** that it manages.

A client asking to read a file must first contact the **NameNode**, which will give back a table containing an ordered list of blocks and their locations (as in **DataNodes**). At this point, the client should contact the **DataNodes** separately, downloading all the blocks and reconstructing the file (by appending the blocks together).

To write a file, a client should instead first contact the **NameNode**, which will first decide how to handle the request, then update its records and reply to the client with an ordered list of **DataNodes** of where to write each block of the file. The client will now contact and upload the blocks to the **DataNodes**, as reported in the **NameNode** reply. Namespace queries (for example, listing a directory content, creating a folder, and so on) are instead completely handled by the **NameNode** by accessing its metadata information.

Moreover, the **NameNode** is also responsible for properly handling a **DataNode** failure (it's marked as dead if no heartbeat packets are received) and its data re-replication to other nodes.

Although these operations are long and hard to implement with robustness, they're completely transparent to the user, thanks to many libraries and the HDFS shell. The way you operate on the HDFS is pretty similar to what you're currently doing on your filesystem, and this is a great benefit of Hadoop: hiding the complexity and letting the user use it simply.

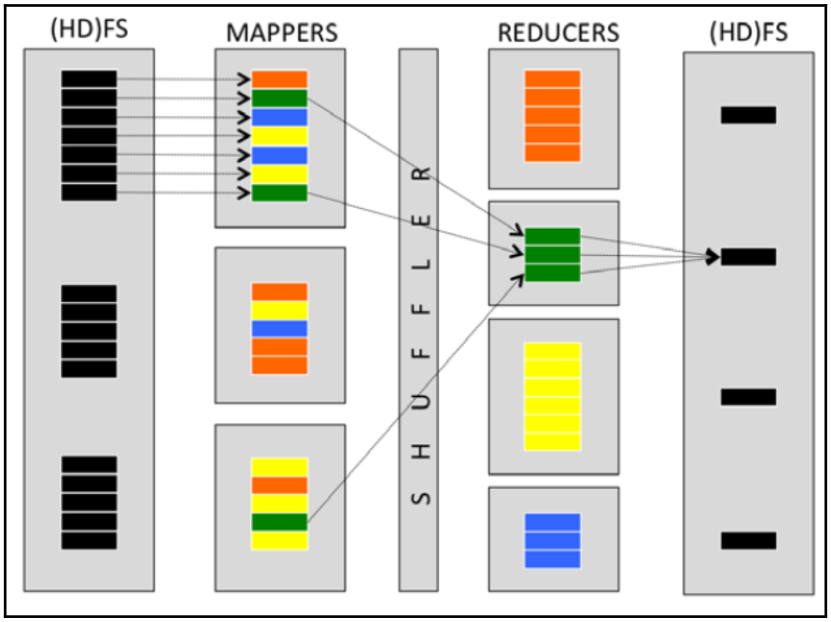
MapReduce

MapReduce is the programming model that was implemented in the earliest versions of Hadoop. It's a very simple model and is designed to process large datasets on a distributed cluster in parallel batches. The core of MapReduce is composed of two programmable functions—a mapper that performs filtering, and a reducer that performs aggregation—and a shuffler that moves the objects from the mappers to the right reducers. Google published a paper in 2004 on MapReduce (`https://ai.google/research/pubs/pub62`), a few months after having been granted a patent on it.

Specifically, here are the steps of MapReduce for the Hadoop implementation:

- **Data chunker**: Data is read from the filesystem and split into chunks. A chunk is a piece of the input dataset, which is typically either a fixed-size block (for example, an HDFS block read from a **DataNode**) or another more appropriate split. For instance, if we want to count the number of characters, words, and lines in a text file, a nice split can be a line of text.
- **Mapper**: From each chunk, a series of key-value pairs is generated. Each mapper instance applies the same mapping function onto different chunks of data. Continuing the preceding example, for each line, three key-value pairs are generated in this step—one containing the number of characters in the line (the key can simply be a *chars* string), one containing the number of words (in this case, the key must be different, so let's say *words*), and one containing the number of lines, which is always one (in this case, the key can be *lines*).
- **Shuffler**: From the key and number of available reducers, the shuffler distributes all the key-value pairs with the same key to the same reducers. Typically, this operation is calculating the hash of the key, dividing it by the number of reducers and using the remainder in order to point out a specific reducer. This should ensure a fair amount of keys for each reducer. This function is not user-programmable, but is provided by the MapReduce framework.
- **Reducer**: Each reducer receives all the key-value pairs for a specific set of keys and can produce zero or more aggregate results. In the example, all the values connected to the *words* key arrive at a reducer; its job is just summing up all the values. The same happens for the other keys, which results in three final values: the number of characters, the number of words, and the number of lines. Note that these results may be on different reducers.
- **Output writer**: The outputs of the reducers are written on the filesystem (or HDFS). In the default Hadoop configuration, each reducer writes a file (`part-r-00000` is the output of the first reducer, `part-r-00001` is the output of the second, and so on). To have a full list of results on a file, you should concatenate all of them.

Visually, this operation can be simply communicated and understood as follows:



There's also an optional step that can be run by each mapper instance after the mapping step—the combiner. It basically anticipates, if possible, the reducing step on the mapper and is often used to decrease the amount of information to shuffle, which speeds up the process. In the preceding example, if a mapper processes more than one line of the input file, during the (optional) combiner step, it can pre-aggregate the results, and output a smaller number of key-value pairs. For example, if the mapper processes 100 lines of text in each chunk, why output 300 key-value pairs (100 for the number of chars, 100 for words, and 100 for lines) when the information can be aggregated in three? That's actually the goal of the combiner.

In the MapReduce implementation provided by Hadoop, the shuffle operation is distributed, which optimizes the communication cost, and it's possible to run more than one mapper and reducer per node, which makes full use of the hardware resources available on the nodes. Also, the Hadoop infrastructure provides redundancy and fault-tolerance, as the same task can be assigned to multiple workers.

Introducing Apache Spark

Apache Spark is an evolution of Hadoop and has become very popular in the last few years. In contrast to Hadoop, and its Java and batch-focused design, Spark is able to produce iterative algorithms in a fast and easy way. Furthermore, it has a very rich suite of APIs for multiple programming languages, and natively supports many different types of data processing (machine learning, streaming, graph analysis, SQL, and so on).

Apache Spark is a cluster framework designed for the quick and general-purpose processing of big data. One of the improvements in speed results from the fact that the data, after every job, is kept in-memory and not stored on the filesystem (unless you want to do so) as would have happened with Hadoop, MapReduce, and the HDFS. This thing makes iterative jobs (such as the clustering K-means algorithm) faster and faster, as the latency and bandwidth provided by the memory are more performant than the physical disk. Clusters running Spark, therefore, need a high amount of RAM memory for each node.

Although Spark has been developed in Scala (which runs on the JVM, like Java), it has APIs for multiple programming languages, including Java, Scala, Python, and R. In this book, we will focus on Python.

Spark can operate in two different ways:

- **Standalone mode**: It runs on your local machine. In this case, the maximum parallelization is the number of cores of the local machine, and the amount of memory available is exactly the same as the local one.
- **Cluster mode**: It runs on a cluster of multiple nodes, using a cluster manager such as YARN. In this case, the maximum parallelization is the number of cores across all the nodes composing the cluster, and the amount of memory is the sum of the amount of memory of each node.

PySpark

In order to use the Spark functionalities (or PySpark, which contains the Python APIs of Spark), we need to instantiate a special object named `SparkContext`. It tells Spark how to access the cluster, and contains some application-specific parameters. In the Jupyter notebook provided in the virtual machine, this variable is already available and is called `sc` (it's the default option when an IPython Notebook is started); let's see what it contains in the next section.

Starting with PySpark

The data model used by Spark is named **Resilient Distributed Dataset** (**RDD**), which is a distributed collection of elements that can be processed in parallel. An RDD can be created from an existing collection (a Python list, for example) or from an external dataset, which is stored as a file on the local machine, HDFS, or other sources.

Setting up your local Spark instance

Making a full installation of Apache Spark is not an easy task to do from scratch. This is usually accomplished on a cluster of computers, often accessible on the cloud, and it is delegated to experts of the technology (namely, data engineers). This could be a limitation, because you may then not have access to an environment in which to test what you will be learning in this chapter.

However, in order to test the contents of this chapter, you actually do not need to make too-complex installations. By using Docker (`https://www.docker.com/`), you can have access to an installation of Spark, together with a Jupyter notebook and PySpark, on a Linux server on your own computer (it does not matter if it is a Linux, macOS, or Windows-based machine).

Actually, that is mainly possible because of Docker. Docker allows operating-system-level virtualization, also known as **containerization**. Containerization means that a computer is allowed to run multiple, isolated filesystem instances, where each instance is simply separated from the other (though sharing the same hardware resources) as if they were single computers themselves. Basically, any piece of software running in Docker is wrapped in a complete, stable, and previously defined filesystem that is totally independent of the filesystem you are running Docker from. Using a Docker container implies that your code will run as perfectly as expected (and as presented in this chapter). Consistency in the execution of commands is the main reason why Docker is the best way to put your solutions into production: you just need to move the container you used into a server and make an API to access your solution (a topic we previously discussed in `Chapter 5`, *Visualization, Insights, and Results*, where we presented the Bottle package).

Here are the steps you need to take:

1. First, you start by installing the Docker software suitable for your system. You can find all you need here, depending on the operating system you operate on:

Windows	`https://docs.docker.com/docker-for-windows/`
Linux	`https://docs.docker.com/engine/getstarted/`
macOS	`https://docs.docker.com/docker-for-mac/`

   The installation is straightforward, yet you can find any further information you may need on the very same pages you are downloading the software from.

2. After having completed the installation, we can use the Docker image that can be found at `https://github.com/jupyter/docker-stacks/tree/master/pyspark-notebook`. It contains a complete installation of Spark, accessible by a Jupyter notebook, plus a Miniconda installation with the most recent versions of Python 2 and 3. You can find out more about the image's contents here: `http://jupyter-docker-stacks.readthedocs.io/en/latest/using/selecting.html#jupyter-pyspark-notebook`.
3. At this point, just open the Docker interface; there, a shell will appear with the ASCII-art of a whale and an IP address. Just take note of the IP address (in our case it was `192.168.99.100`). Now, run the following command in the shell:

```
$> docker run -d -p 8888:8888 --name spark jupyter/pyspark-notebook
start-notebook.sh –NotebookApp.token=''
```

4. If you prefer security over ease of use, just type this:

```
$> docker run -d -p 8888:8888 --name spark jupyter/pyspark-notebook
start-notebook.sh –NotebookApp.token='mypassword'
```

   Replace the `mypassword` placeholder with your chosen password. Please note that the Jupyter notebook will then ask for that password when starting it.

5. After running the preceding command, Docker will then start downloading the `pyspark-notebook image` (it could take a while); assign it the name `spark`, copy the `8888` port on the Docker image to the `8888` port on your machine, then execute the `start-notebook.sh` script, and set the notebook password to empty (that will allow you to immediately access Jupyter just by using the previously noted IP address and the `8888` port).

At this very point, the only other thing you need to do is just type this into your browser:

```
http://192.168.99.100:8888/
```

That is, put into your browser the IP address Docker gave you when you started, a colon, and then `8888`, which is the port number. Jupyter should immediately appear.

6. As a simple test, you could immediately open a new notebook and test this:

```
In: import pyspark
    sc = pyspark.SparkContext('local[*]')

    # do something to prove it works
    rdd = sc.parallelize(range(1000))
    rdd.takeSample(False, 5)
```

7. It is also important to notice that you have commands to stop the Docker machine and commands that will even destroy it. This shell command will stop it:

```
$> docker stop spark
```

In order to destroy the container after it has been stopped, use the following command (you will lose all your work in the container, by the way):

```
$> docker rm spark
```

If your container has not been destroyed, in order to have the container run again after it has been stopped, just use this shell command:

```
$> docker start spark
```

Additionally, you need to know that, on the Docker machine, you operate on the `/home/jovyan` directory, and you can get a list of its contents directly from the Docker shell:

```
$> docker exec -t -i spark ls /home/jovyan
```

You can also execute any other Linux bash command.

Notably, you can also copy data to and from the container (since, otherwise, your work will be just kept inside the machine's operating system). Let's pretend that you have to copy a file (`file.txt`) from a directory on your Windows desktop to the Docker machine:

```
$> docker cp c:/Users/Luca/Desktop/spark_stuff/file.txt
spark:/home/jovyan/file.txt
```

Also, the opposite is possible:

```
$> docker cp spark:/home/jovyan/test.ipynb
c:/Users/Luca/Desktop/spark_stuff/test.ipynb
```

That's really all there is; in just a few steps, you should have a locally operating Spark environment to run all your experiments on (clearly, it will use only one node and it will be limited to the power of a single CPU).

Experimenting with Resilient Distributed Datasets

Now let's create a Resilient Distributed Dataset containing integers from 0 to 9. To do so, we can use the `parallelize` method provided by the `SparkContext` object:

```
In: numbers = range(10)
    numbers_rdd = sc.parallelize(numbers)
    numbers_rdd

Out: PythonRDD[2672] at RDD at PythonRDD.scala:49
```

As you can see, you can't simply print the RDD content, as it is split into multiple partitions (and distributed in the cluster). The default number of partitions is twice the number of CPUs (so, it's four in the provided VM), but it can be set manually using the second argument of the `parallelize` method.

To print out the data contained in the RDD, you should call the `collect` method. Note that this operation, while running on a cluster, collects all the data on the node; therefore, the node needs to have enough memory to contain it all:

```
In: numbers_rdd.collect()

Out: [0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
```

To obtain just a partial peek, use the `take` method, indicating how many elements you'd want to see. Note that, as it's a distributed dataset, it's not guaranteed that elements are in the same order as when we inserted it:

```
In: numbers_rdd.take(3)

Out: [0, 1, 2]
```

To read a text file, we can use the `textFile` method provided by the `SparkContext`. It allows for the reading of both the HDFS files and local files, and it splits the text on the newline characters; therefore, the first element of the RDD is the first line of the text file (using the first method). Note that, if you're using a local path, all the nodes composing the cluster should access the same file through the same path. To do that, we first download the complete plays by William Shakespeare:

```
In: import urllib.request
    url = "http://www.gutenberg.org/files/100/100-0.txt"
    urllib.request.urlretrieve(url, "shakespeare_all.txt")

In: sc.textFile("file:////home//jovyan//shakespeare_all.txt").take(6)

Out: ['',
'Project Gutenberg's The Complete Works of William Shakespeare, by William',
'Shakespeare', '',
'This eBook is for the use of anyone anywhere in the United States and',
'most other parts of the world at no cost and with almost no restrictions']
```

To save the content of an RDD onto the disk, you can use the `saveAsTextFile` method provided by the RDD:

```
In: numbers_rdd.saveAsTextFile("file:////home//jovyan//numbers_1_10.txt")
```

An RDD supports just two types of operation:

- Transformations, which transform the dataset into a different one. The inputs and outputs of transformations are both RDDs; therefore, it's possible to chain together multiple transformations, approaching a functional style of programming. Moreover, transformations are lazy; that is, they don't compute their results straight away.
- Actions return values from RDDs, such as the sum of the elements and the count, or just collect all the elements. Actions are the triggers to execute the chain of (lazy) transformations as an output is required.

Typical Spark programs are a chain of transformations with an action at the end. By default, all the transformations on the RDD are executed each time you run an action (that is, the intermediate state after each transformer is not saved). However, you can override this behavior using the `persist` method (on the RDD) whenever you want to `cache` the value of the transformed elements. The `persist` method allows both memory and disk persistence.

In the following example, we will square all the values contained in an RDD and then sum them up; this algorithm can be executed through a mapper (square elements), followed by a reducer (summing up the array). According to Spark, the `map` method is a transformer, as it just transforms the data element by element; reduce is an action, as it creates a value out of all the elements together.

Let's approach this problem step by step to see the multiple ways in which we can operate. First, we start with the function that we will be used to transform (map) all the data: we first define a function that returns the square of the input argument, then we pass this function to the `map` method in the RDD, and, finally, we collect the elements in the RDD:

```
In: def sq(x):
        return x**2
    numbers_rdd.map(sq).collect()

Out: [0, 1, 4, 9, 16, 25, 36, 49, 64, 81]
```

Although the output is correct, the `sq` function takes a lot of space; we can rewrite the transformation more concisely, thanks to Python's `lambda` expression, in this way:

```
In: numbers_rdd.map(lambda x: x**2).collect()

Out: [0, 1, 4, 9, 16, 25, 36, 49, 64, 81]
```

Do you remember why we needed to call `collect` to print the values in the transformed RDD? This is because the `map` method will not spring to action, but will be just lazily evaluated. The `reduce` method, on the other hand, is an action; therefore, adding the `reduce` step to the previous RDD should output a value. As for `map`, `reduce` takes as an argument a function that should have two arguments (a left value and a right value), and should return a value. In this case, it can be a `verbose` function defined with `def` or a `lambda` function:

```
In: numbers_rdd.map(lambda x: x**2).reduce(lambda a,b: a+b)

Out: 285
```

To make it even simpler, we can use the `sum` action instead of the reducer:

```
In: numbers_rdd.map(lambda x: x**2).sum()

Out: 285
```

Let's now advance one step and introduce the key-value pairs. Although RDDs can contain any kind of object (we've seen integers and lines of text so far), a few operations can be made when the elements are tuples composed by two elements: key and value.

To give an example, let's group the numbers in the RDD into odds and evens, and then compute the sum of the two groups separately. As for the MapReduce model, it would be nice to map each number with a key (odd or even) and then, for each key, reduce using a sum operation.

We can start with the `map` operation: let's first create a function that tags the numbers, outputting `even` if the argument number is even, and `odd` otherwise. Then, we will create a key-value mapping that creates a key-value pair for each number, where the key is the tag and the value is the number itself:

```
In: def tag(x):
        return "even" if x%2==0 else "odd"

    numbers_rdd.map(lambda x: (tag(x), x)).collect()

Out: [('even', 0),
      ('odd', 1),
      ('even', 2),
      ('odd', 3),
      ('even', 4),
      ('odd', 5),
      ('even', 6),
      ('odd', 7),
      ('even', 8),
      ('odd', 9)]
```

To reduce each key separately, we can now use the `reduceByKey` method (which is not a Spark action). As an argument, we should pass the function that we need to apply to all the values of each key; in this case, we will sum up all of them. Finally, we should call the `collect` method to print the results:

```
In: numbers_rdd.map(lambda x: (tag(x), x) ) \
           .reduceByKey(lambda a,b: a+b).collect()

Out: [('even', 20), ('odd', 25)]
```

Now, let's list some of the most important methods available in Spark; it's not an exhaustive guide, but just includes the most used ones.

We start with transformations; they can be applied to an RDD, and they produce an RDD:

- `map(function)`: This returns an RDD formed by passing each element through the function.
- `flatMap(function)`: This returns an RDD formed by flattening the output of the function for each element of the input RDD. It's used when each value at the input can be mapped to 0 or more output elements.
  For example, to count the number of times that each word appears in a text, we should map each word to a key-value pair (the word would be the key, and 1 the value), producing more than one key-value element for each input line of text in this way.
- `filter(function)`: This returns a dataset composed of all the values where the function returns true.
- `sample(withReplacement, fraction, seed)`: This bootstraps the RDD, allowing you to create a sampled RDD (with or without replacement) whose length is a fraction of the input one.
- `distinct()`: This returns an RDD containing the distinct elements of the input RDD.
- `coalesce(numPartitions)`: This decreases the number of partitions in the RDD.
- `repartition(numPartitions)`: This changes the number of partitions in the RDD. This method always shuffles all the data over the network.
- `groupByKey()`: This creates an RDD in which, for each key, the value is a sequence of values that have that key in the input dataset.
- `reduceByKey(function)`: This aggregates the input RDD by key, and then applies the `reduce` function to the values of each group.
- `sortByKey(ascending)`: This sorts the elements in the RDD by key in ascending or descending order.
- `union(otherRDD)`: This merges two RDDs together.
- `intersection(otherRDD)`: This returns an RDD composed by just the values appearing both in the input and argument RDD.
- `join(otherRDD)`: This returns a dataset where the key-value inputs are joined (on the key) to the argument RDD.

Similar to the `join` function in SQL, these methods are available as well: `cartesian`, `leftOuterJoin`, `rightOuterJoin`, and `fullOuterJoin`.

Now, let's overview what the most popular actions available in PySpark are. Note that actions trigger the processing of the RDD through all the transformers in the chain:

- `reduce(function)`: This aggregates the elements of the RDD and produces an output value
- `count()`: This returns the count of the elements in the RDD
- `countByKey()`: This returns a Python dictionary, where each key is associated with the number of elements in the RDD with that key
- `collect()`: This returns all the elements in the transformed RDD locally
- `first()`: This returns the first value of the RDD
- `take(N)`: This returns the first N values in the RDD
- `takeSample(withReplacement, N, seed)`: This returns a bootstrap of N elements in the RDD with or without replacement, eventually using the random seed provided as an argument
- `takeOrdered(N, ordering)`: This returns the top N elements in the RDD after having sorted it by value (ascending or descending)
- `saveAsTextFile(path)`: This saves the RDD as a set of text files in the specified directory

There are also a few methods that are neither transformers nor actions:

- `cache()`: This caches the elements of the RDD; therefore, future computations based on the same RDD can reuse this as a starting point
- `persist(storage)`: This is the same as `cache`, but you can specify where to store the elements of RDD (memory, disk, or both)
- `unpersist()`: This undoes the `persist` or `cache` operation

Let's now try to work through an example using RDDs in order to compute some text statistics and extract the most popular word from a large text (Shakespeare's plays). With Spark, the algorithm for computing text statistics should be as follows:

1. The input file is read and parallelized on an RDD. This operation can be done with the `textFile` method provided by the `SparkContext`.
2. For each line of the input file, three key-value pairs are returned: one containing the number of chars, one the number of words, and the last the number of lines. In Spark, this is a `flatMap` operation, as three outputs are generated for each input line.

3. For each key, we sum up all the values. This can be done with the `reduceByKey` method.
4. Finally, the results are collected. In this case, we can use the `collectAsMap` method, which collects the key-value pairs in the RDD and returns a Python dictionary. Note that this is an action; therefore, the RDD chain is executed and a result is returned:

```
In: def emit_feats(line):
        return [("chars", len(line)), \
         ("words", len(line.split())), \
         ("lines", 1)]

print((sc.textFile("file:////home//jovyan//shakespeare_all.txt")
            .flatMap(emit_feats)
            .reduceByKey(lambda a,b: a+b)
            .collectAsMap()))

Out: {'chars': 5535014, 'words': 959893, 'lines': 149689}
```

To determine the most popular word in a text, follow these steps:

1. The input file is read and parallelized on an RDD with the `textFile` method.
2. For each line, all the words are extracted. For this operation, we can use the `flatMap` method and a regular expression.
3. Each word in the text (that is, each element of the RDD) is now mapped to a key-value pair: the key is the lower-case word and the value is always `1`. This is a map operation.
4. With a `reduceByKey` call, we count how many times each word (key) appears in the text (RDD). The outputs are key-value pairs, where the key is a word and the value is the number of times the word appears in the text.
5. We flip keys and values and create a new RDD. This is a map operation.
6. We sort the RDD into descending order and extract (take) the first element. This is an action and can be done in one operation with the `takeOrdered` method.

We can actually further improve the solution, collapsing the second and third steps together (`flatMap`-ing a key-value pair for each word, where the key is the lower-case word and value is the number of occurrences), and the fifth and sixth steps together (taking the first element and ordering the elements in the RDD by their value; that is, the second element of the pair):

```
In: import re
    WORD_RE = re.compile(r"[\w']+")
    print((sc.textFile("file:////home//jovyan//shakespeare_all.txt")
            .flatMap(lambda line: [(word.lower(), 1) for word in
                                   WORD_RE.findall(line)])
            .reduceByKey(lambda a,b: a+b)
            .takeOrdered(1, key = lambda x: -x[1]))

Out: [('the', 29998)]
```

Sharing variables across cluster nodes

When we're working on a distributed environment, sometimes it is required to share information across nodes so that all the nodes can operate using consistent variables. Spark handles this case by providing two kinds of variables: read-only and write-only variables. By no longer ensuring that a shared variable is both readable and writable, it also drops the consistency requirement, letting the hard work of managing this situation fall on the developer's shoulders. Usually, a solution is quickly reached, as Spark is really flexible and adaptive.

Read-only broadcast variables

Broadcast variables are variables shared by the driver node; that is, the node running the IPython notebook in our configuration, with all the nodes in the cluster. It's a read-only variable, as the variable is broadcast by one node and never read back if another node changes it.

Let's now see how it works in a simple example: we want to one-hot encode a dataset containing just gender information as a string. The dummy dataset contains just a feature that can be male `M`, female `F`, or unknown `U` (if the information is missing). Specifically, we want all the nodes to use the defined one-hot encoding, as listed in the following dictionary:

```
In: one_hot_encoding = {"M": (1, 0, 0), "F": (0, 1, 0),
                        "U": (0, 0, 1)}
```

In our solution, we first broadcast the Python dictionary (calling the `broadcast` method provided by the `SparkContext`, sc) inside the mapped function; using its value property, we can now access it. After doing this, we have a generic `map` function that can work on any one-hot map dictionary:

```
In: bcast_map = sc.broadcast(one_hot_encoding)
    def bcast_map_ohe(x, shared_ohe):
        return shared_ohe[x]
    (sc.parallelize(["M", "F", "U", "F", "M", "U"])
         .map(lambda x: bcast_map_ohe(x, bcast_map.value))
         .collect())
```

Broadcast variables are saved in-memory in all the nodes composing a cluster; therefore, they never share a large amount of data, which can fill them up and make the following processing impossible.

To remove a broadcast variable, use the `unpersist` method on the broadcast variable. This operation will free up the memory of that variable on all the nodes:

```
In: bcast_map.unpersist()
```

Write-only accumulator variables

The other variables that can be shared in a Spark cluster are accumulators. Accumulators are write-only variables that can be added together and are typically used to implement sums or counters. Only the driver node, which is the one that is running the IPython Notebook, can read its value; all the other nodes can't read this. Let's see how it works using an example: we want to process a text file and understand how many lines are empty while processing it. Of course, we can do this by scanning the dataset twice (using two Spark jobs), with the first one counting the empty lines and the second one doing the real processing, but this solution is not very effective. Following this, you will take all the steps necessary for processing a text file and counting its lines.

The steps needed are as follows:

1. First, we download a text file to be processed from the Web, *The Adventures of Sherlock Holmes* by Sir Arthur Conan Doyle, as offered by Project Gutenberg:

   ```
   In: import urllib.request
       url = "http://gutenberg.pglaf.org/1/6/6/1661/1661.txt"
       urllib.request.urlretrieve(url, "sherlock.tx")
   ```

2. We then instantiate an accumulator variable (with the initial value of `0`) and we add `1` for each empty line that we find while processing each line of the input file (with a map). At the same time, we can do some processing on each line; in the following piece of code, for example, we simply return `1` for each line, counting all the lines in the file in this way.

3. At the end of the processing, we will have two pieces of information: the first is the number of lines, from the result of the `count()` action on the transformed RDD, and the second is the number of empty lines contained in the value property of the accumulator. Remember, both of these are available after having scanned the dataset once:

```
In: accum = sc.accumulator(0)
    def split_line(line):
        if len(line) == 0:
            accum.add(1)
        return 1

    filename = 'file:////home//jovyan//sherlock.txt'
    tot_lines = (
        sc.textFile(filename)
        .map(split_line)
        .count())

    empty_lines = accum.value
    print("In the file there are %d lines" % tot_lines)
    print("And %d lines are empty" % empty_lines)

Out: In the file there are 13053 lines
     And 2666 lines are empty
```

Broadcast and accumulator variables together—an example

Although broadcast and accumulator variables are simple and very limited variables (one is read-only, and the other one is write only), they can be actively used to create very complex operations. For example, let's try to apply different machine learning algorithms on the `iris` dataset in a distributed environment. We will build a Spark job in the following way:

- The dataset is read and broadcast to all the nodes (as it's small enough to fit in-memory).
- Each node will use a different classifier on the dataset and return the classifier name and its accuracy score on the full dataset. Note that, to keep things easy in this simple example, we won't do any preprocessing, train/test splitting, or hyperparameter optimization.
- If the classifiers raise an exception, the string representation of the error, along with the classifier name, should be stored in an accumulator.

- The final output should contain a list of the classifiers that performed the classification task without errors and their accuracy score.

As the first step, we load the `iris` dataset and broadcast it to all the nodes in the cluster:

```
In: from sklearn.datasets import load_iris
    bcast_dataset = sc.broadcast(load_iris())
```

Now, let's continue coding by creating a custom accumulator. It will contain a list of tuples to store the classifier name and the exception it experienced as a string. The custom accumulator is derived using the `AccumulatorParam` class and should contain at least two methods: `zero` (which is called when it's initialized) and `addInPlace` (which is called when the add method is called on the accumulator).

The easiest way to do this is shown in the following code, followed by its initialization as an empty list. Bear in mind that the additive operation is a bit tricky: we need to combine two elements—a tuple and a list—but we don't know which element is the list and which is the tuple; therefore, we first ensure that both elements are lists, and then we can proceed to concatenate them in an easy way (by using the plus operator):

```
In: from pyspark import AccumulatorParam
    class ErrorAccumulator(AccumulatorParam):
        def zero(self, initialList):
            return initialList
        def addInPlace(self, v1, v2):
            if not isinstance(v1, list):
                v1 = [v1]
            if not isinstance(v2, list):
                v2 = [v2]
           return v1 + v2

    errAccum = sc.accumulator([], ErrorAccumulator())
```

Now, let's define the mapping function: each node should train, test, and evaluate a classifier on the broadcast `iris` dataset. As an argument, the function will receive the classifier object and should return a tuple containing the classifier name and its accuracy score contained in a list.

If an exception is raised by doing so, the classifier name and the exception, quoted as a string, are added to the accumulator, and an empty list is returned:

```
In: def apply_classifier(clf, dataset):
        clf_name = clf.__class__.name
        X = dataset.value.data
        y = dataset.value.target
        try:
            from sklearn.metrics import accuracy_score
            clf.fit(X, y)
            y_pred = clf.predict(X)
            acc = accuracy_score(y, y_pred)
            return [(clf_name, acc)]
        except Exception as e:
            errAccum.add((clf_name, str(e)))
            return []
```

Finally, we have arrived at the core of the job. We're now instantiating a few objects from scikit-learn (some of them are not classifiers, in order to test the accumulator). We will transform them into an RDD, and apply the `map` function that we created in the previous cell. As the returned value is a list, we can use `flatMap` to collect only the outputs of the mappers that didn't get caught in an exception:

```
In: from sklearn.linear_model import SGDClassifier
    from sklearn.dummy import DummyClassifier
    from sklearn.decomposition import PCA
    from sklearn.manifold import MDS

    classifiers = [DummyClassifier('most_frequent'),
                   SGDClassifier(),
                   PCA(),
                   MDS()]

    (sc.parallelize(classifiers)
     .flatMap(lambda x: apply_classifier(x, bcast_dataset))
     .collect())

Out: [('DummyClassifier', 0.33333333333333331),
      ('SGDClassifier', 0.85333333333333339)]
```

As expected, only the *real* classifiers are contained in the output. Let's see which classifiers generated an error. Unsurprisingly, here we spot the two missing ones from the preceding output:

```
In: print("The errors are:", errAccum.value)

Out: The errors are: [('PCA', "'PCA' object has no attribute 'predict'"),
     ('MDS', "'MDS' object has no attribute 'predict'")]
```

As a final step, let's clean up the broadcast dataset:

```
In: bcast_dataset.unpersist()
```

Remember that, in this example, we've used a small dataset that could be broadcast. In real-world big-data problems, you'll need to load the dataset from the HDFS and broadcast the HDFS path.

Data preprocessing in Spark

So far, we've seen how to load text data from the local filesystem and the HDFS. Text files can contain either unstructured data (like a text document) or structured data (like a CSV file). As for semi-structured data, just like files containing JSON objects, Spark has special routines that are able to transform a file into a DataFrame, similar to the DataFrame in R and the Python package pandas. DataFrames are very similar to RDBMS tables, where a schema is set.

CSV files and Spark DataFrames

We start by showing you how to read CSV files and transform them into Spark DataFrames. Just follow the steps in the following example:

1. In order to import CSV-compliant files, we need to first create a SQL context, by creating an `SQLContext` object from the local `SparkContext`:

```
In: from pyspark.sql import SQLContext
    sqlContext = SQLContext(sc)
```

2. For our example, we created a simple CSV file, which is a table with six rows and three columns, where some attributes are missing (such as the gender attribute for the user with `user_id=0`):

```
In: data = """balance,gender,user_id
    10.0,,0
    1.0,M,1
    -0.5,F,2
    0.0,F,3
    5.0,,4
    3.0,M,5
    """
    with open("users.csv", "w") as output:
    output.write(data)
```

3. Using the `read.format` method provided by `sqlContext`, we already have the table well-formatted and with all the right column names in a variable. The output variable type is a Spark DataFrame. To show the variable in a nice, formatted table, use its `show` method:

```
In: df = sqlContext.read.format('com.databricks.spark.csv')\
    .options(header='true', inferschema='true').load('users.csv')
    df.show()

Out: +-------+------+-------+
     |balance|gender|user_id|
     +-------+------+-------+
     |   10.0|  null|      0|
     |    1.0|     M|      1|
     |   -0.5|     F|      2|
     |    0.0|     F|      3|
     |    5.0|  null|      4|
     |    3.0|     M|      5|
     +-------+------+-------+
```

4. Additionally, we can investigate the schema of the DataFrame using the `printSchema` method. We realize that, while reading the CSV file, each column type is inferred by the data (in the preceding example, the `user_id` column contains long integers, the gender column is composed of strings, and the balance is a double floating point):

```
In: df.printSchema()

Out: root
     |-- balance: double (nullable = true)
     |-- gender: string (nullable = true)
     |-- user_id: long (nullable = true)
```

5. Exactly like a table in an RDBMS, we can slice and dice the data in the DataFrame, making selections of columns, and filtering the data by attributes. In this example, we want to print the `balance`, `gender`, and `user_id` of the users whose `gender` is not missing, and who have a balance that is strictly greater than `0`. For this, we can use the `filter` and `select` methods:

```
In: (df.filter(df['gender'] != 'null')
     .filter(df['balance'] > 0)
     .select(['balance', 'gender', 'user_id'])
     .show())

Out: +-------+------+-------+
     |balance|gender|user_id|
     +-------+------+-------+
     |    1.0|     M|      1|
     |    3.0|     M|      5|
     +-------+------+-------+
```

6. We can also rewrite each piece of the preceding job in a SQL-like language. In fact, the `filter` and `select` methods can accept SQL-formatted strings:

```
In: (df.filter('gender is not null')
     .filter('balance > 0').select("*").show())
```

7. We can also use just one call to the `filter` method:

```
In: df.filter('gender is not null and balance > 0').show()
```

Dealing with missing data

A common problem of data preprocessing is how to handle missing data. Spark DataFrames, which are similar to pandas DataFrames, offer a wide range of operations that you can do on them. For example, the easiest option to achieve a dataset composed of complete rows only is to discard rows containing missing information. For this, in a Spark DataFrame, we first have to access the `na` attribute of the DataFrame and then call the `drop` method. The resulting table will contain only the complete rows:

```
In: df.na.drop().show()

Out: +-------+------+-------+
     |balance|gender|user_id|
     +-------+------+-------+
     |    1.0|     M|      1|
     |   -0.5|     F|      2|
     |    0.0|     F|      3|
     |    3.0|     M|      5|
     +-------+------+-------+
```

If such an operation removes too many rows, we can always decide what columns should account for the removal of the row (as the augmented subset of the `drop` method):

```
In: df.na.drop(subset=["gender"]).show()
```

Also, if you want to set default values for each column instead of removing the line data, you can use the `fill` method, passing a dictionary composed by the column name (as the dictionary key) and the default value to substitute missing data in that column (as the value of the key in the dictionary).

As an example, if you want to ensure that the variable balance, where missing, is set to 0, and the variable gender, where missing, is set to U, you can simply do the following:

```
In: df.na.fill({'gender': "U", 'balance': 0.0}).show()

Out: +-------+------+-------+
     |balance|gender|user_id|
     +-------+------+-------+
     |   10.0|     U|      0|
     |    1.0|     M|      1|
     |   -0.5|     F|      2|
     |    0.0|     F|      3|
     |    5.0|     U|      4|
     |    3.0|     M|      5|
     +-------+------+-------+
```

Grouping and creating tables in-memory

To have a function applied to a group of rows (exactly as in the case of SQL GROUP BY), you can use two similar methods. In the following example, we want to compute the average balance per gender:

```
In:(df.na.fill({'gender': "U", 'balance': 0.0})
    .groupBy("gender").avg('balance').show())

Out: +------+------------+
     |gender|avg(balance)|
     +------+------------+
     |     F|       -0.25|
     |     M|         2.0|
     |     U|         7.5|
     +------+------------+
```

So far, we've worked with DataFrames, but, as you've seen, the distance between DataFrame methods and SQL commands is minimal. Actually, using Spark, it is possible to register the DataFrame as a SQL table to fully enjoy the power of SQL. The table is saved in memory and distributed in a way similar to an RDD. To register the table, we need to provide a name, which will be used in future SQL commands. In this case, we decide to name it users:

```
In: df.registerTempTable("users")
```

By calling the SQL method provided by the Spark SQL context, we can run any SQL-compliant table:

```
In: sqlContext.sql("""
    SELECT gender, AVG(balance)
    FROM users
    WHERE gender IS NOT NULL
    GROUP BY gender""").show()

Out: +------+------------+
     |gender|avg(balance)|
     +------+------------+
     |     F|       -0.25|
     |     M|         2.0|
     +------+------------+
```

Not surprisingly, the table output by the command (as well as the `users` table itself) is of the Spark `DataFrame` type:

```
In: type(sqlContext.table("users"))

Out: pyspark.sql.dataframe.DataFrame
```

DataFrames, tables, and RDDs are intimately connected, and RDD methods can be used on a DataFrame. Remember that each row of the DataFrame is an element of the RDD. Let's see this in detail, and first collect the whole table:

```
In: sqlContext.table("users").collect()

Out: [Row(balance=10.0, gender=None, user_id=0),
      Row(balance=1.0, gender='M', user_id=1),
      Row(balance=-0.5, gender='F', user_id=2),
      Row(balance=0.0, gender='F', user_id=3),
      Row(balance=5.0, gender=None, user_id=4),
      Row(balance=3.0, gender='M', user_id=5)]

In: a_row = sqlContext.sql("SELECT * FROM users").first()
    print(a_row)

Out: Row(balance=10.0, gender=None, user_id=0)
```

The output is a list of `Row` objects (they look like Python's `namedtuple`). Let's dig deeper into this. A `Row` contains multiple attributes, and it's possible to access them as a property or dictionary key; that is, to get the `balance` from the first row, we can choose between the two following ways:

```
In: print(a_row['balance'])
    print(a_row.balance)

Out: 10.0
     10.0
```

Also, `Row` can be collected as a Python dictionary using the `asDict` method for `Row`. The result contains the property names as key and property values (as dictionary values):

```
In: a_row.asDict()

Out: {'balance': 10.0, 'gender': None, 'user_id': 0}
```

Writing the preprocessed DataFrame or RDD to disk

To write a DataFrame or RDD to disk, we can use the `write` method. We have a selection of formats we can use; in this case, we will save it as a CSV file on the local machine:

```
In: (df.na.drop().write
     .save("file:////home//jovyan//complete_users.csv", format='csv'))
```

Checking the output on the local filesystem, we immediately see that something is different from what we expected: this operation creates multiple files (`part-r-…`). Each of them contains some rows serialized as JSON objects, and merging them together will create the comprehensive output. As Spark is made to process large and distributed files, the `write` operation is tuned for that, and each node writes part of the full RDD:

```
In: !ls -als ./complete_users.json

Out: total 20
     4 drwxr-sr-x  2 jovyan users 4096 Jul 21 19:48 .
     4 drwsrwsr-x 20 jovyan users 4096 Jul 21 19:48 ..
     4 -rw-r--r--  1 jovyan users   33 Jul 21 19:48
     part-00000-bc9077c5-67de-46b2-9ab7-c1da67ffcadd-c000.csv
     4 -rw-r--r--  1 jovyan users   12 Jul 21 19:48
     .part-00000-bc9077c5-67de46b2-9ab7-c1da67ffcadd-c000.csv.crc
     0 -rw-r--r--  1 jovyan users    0 Jul 21 19:48 _SUCCESS
     4 -rw-r--r--  1 jovyan users    8 Jul 21 19:48 ._SUCCESS.crc
```

In order to read it back, we don't have to create a standalone file—even multiple pieces are fine in the read operation. A CSV file can also be read in the `FROM` clause of a SQL query. Let's now try to print the CSV that we've just written to disk without creating an intermediate DataFrame:

```
In: sqlContext.sql("""SELECT * FROM
    csv.`file:////home//jovyan//complete_users.csv`""").show()

Out: +----+---+---+
     | _c0|_c1|_c2|
     +----+---+---+
     | 1.0|  M|  1|
     |-0.5|  F|  2|
     | 0.0|  F|  3|
     | 3.0|  M|  5|
     +----+---+---+
```

Beyond JSON, there is another format that's very popular when dealing with structured, big datasets: Parquet format. Parquet is a columnar storage format that's available in the Hadoop ecosystem. It compresses and encodes the data, and can work with nested structures; all these qualities make it very efficient. Saving and loading are very similar to CSV, and, even in this case, this operation produces multiple files written to disk:

```
In: (df.na.drop().write
    .save("file:////home//jovyan//complete_users.parquet",
          format='parquet'))
```

Working with Spark DataFrames

So far, we've described how to load DataFrames from CSV and Parquet files, but not how to create them from an existing RDD. In order to do so, you just need to create one `Row` object for each record in the RDD and call the `createDataFrame` method of the SQL context. Finally, you can register it as a `temp` table to use the power of the SQL syntax fully:

```
In: from pyspark.sql import Row
    rdd_gender = \
    sc.parallelize([Row(short_gender="M", long_gender="Male"),
    Row(short_gender="F", long_gender="Female")])
    (sqlContext.createDataFrame(rdd_gender)
     .registerTempTable("gender_maps"))

    sqlContext.table("gender_maps").show()

Out: +-----------+------------+
     |long_gender|short_gender|
     +-----------+------------+
     |       Male|           M|
     |     Female|           F|
     +-----------+------------+
```

TIP: This is also the preferred way to operate with CSV files. First, the file is read with `sc.textFile`; then, the final DataFrame is created with the `split` method, the `Row` constructor, and the `createDataFrame` method.

When you have multiple DataFrames in-memory, or that can be loaded from disk, you can join and use all the operations available in a classic RDBMS. In this example, we can join the DataFrame we've created from the RDD with the `users` dataset contained in the Parquet file that we've stored. The result is astonishing:

```
In: sqlContext.sql("""
    SELECT balance, long_gender, user_id
    FROM parquet.`file:////home//jovyan//complete_users.parquet`
    JOIN gender_maps ON gender=short_gender""").show()

Out: +-------+-----------+-------+
     |balance|long_gender|user_id|
     +-------+-----------+-------+
     |    3.0|       Male|      5|
     |    1.0|       Male|      1|
     |    0.0|     Female|      3|
     |   -0.5|     Female|      2|
     +-------+-----------+-------+
```

As the tables are in-memory, so the last thing to do is to clean up by releasing the memory used to keep them. By calling the `tableNames` method, provided by the `sqlContext`, we get the list of all the tables that we currently have in memory. Then, to free them up, we can use `dropTempTable` with the name of the table as an argument. Beyond this point, any further reference to these tables will return an error:

```
In: sqlContext.tableNames()

Out: ['gender_maps', 'users']

In: for table in sqlContext.tableNames():
        sqlContext.dropTempTable(table)
```

Since Spark 1.3, DataFrame has been the preferred way to operate on a dataset when doing datascience operations.

Machine learning with Spark

At this point in the chapter, we arrived at the main task of your job: creating a model to predict one or multiple attributes being missing in the dataset. For this task, we can use some machine learning modeling, and Spark can give us a big hand in this context.

MLlib is the Spark machine learning library; although it is built in Scala and Java, its functions are also available in Python. It contains classification, regression, recommendation algorithms, some routines for dimensionality reduction and feature selection, and it has lots of functionalities for text processing. All of them are able to cope with huge datasets, and use the power of all the nodes in the cluster to achieve their goal.

As of now, it's composed of two main packages: MLlib, which operates on RDDs, and ML, which operates on DataFrames. As the latter performs well and is the most popular way to represent data in data science, developers have chosen to contribute and improve the ML branch, letting the former remain, but without further developments. MLlib seems to be a complete library at first sight, but, after having started using Spark, you will notice that there's neither a statistic nor numerical library in the default package. Here, SciPy and NumPy come to your help, and, once again, they're essential for data science.

In this section, we will try to explore the functionalities of the `pyspark.ml` package; as of now, it's still in the early stages compared to the state-of-the-art scikit-learn library, but it definitely has a lot of potential for the future.

Spark is a high-level, distributed, and complex piece of software that should be used only on big data and with a cluster of multiple nodes; in fact, if the dataset can fit in-memory, it's more convenient to use other libraries such as scikit-learn or similar, which focus just on the data science side of the problem. Running Spark on a single node on a small dataset can be five times slower than the scikit-learn-equivalent algorithm.

Spark on the KDD99 dataset

Let's conduct this exploration using a real-world dataset: the KDD99 dataset. The goal of the competition was to create a network-intrusion-detection system that is able to recognize which network flow is malicious and which is not. Moreover, many different attacks are in the dataset; the goal is to accurately predict them using the features of the flow of packets contained in the dataset.

As a side note on the dataset, it has been extremely useful for developing great solutions for **intrusion-detection systems** (**IDS**) in the first few years after its release. Nowadays, as an outcome of this, all the attacks included in the dataset are very easy to detect, and so it's not used in IDS development anymore. The features include the protocol (`tcp`, `icmp`, and `udp`), service (`http`, `smtp`, and so on), size of the packets, flags active in the protocol, number of attempts to become root, and so on.

More information about the KDD99 challenge and datasets is available at `http://kdd.ics.uci.edu/databases/kddcup99/kddcup99.html`.

Although this is a classic multiclass classification problem, we will dig into it to show you how to perform this task in Spark.

Reading the dataset

First of all, let's download and decompress the dataset. We will be very conservative and use just 10% of the original training dataset (75 MB, uncompressed), as all our analysis is run on a small virtual machine. If you want to give it a try, you can uncomment the lines in the following snippet of code and download the full training dataset (750 MB uncompressed). We download the training dataset, testing (47 MB), and feature names, using bash commands:

```
In: !mkdir datasets
    !rm -rf ./datasets/kdd*
    # !wget -q -O datasets/kddtrain.gz \
    # http://kdd.ics.uci.edu/databases/kddcup99/kddcup.data.gz
    !wget -q -O datasets/kddtrain.gz \
    http://kdd.ics.uci.edu/databases/kddcup99/kddcup.data_10_percent.gz
    !wget -q -O datasets/kddtest.gz \
    http://kdd.ics.uci.edu/databases/kddcup99/corrected.gz
    !wget -q -O datasets/kddnames \
    http://kdd.ics.uci.edu/databases/kddcup99/kddcup.names
    !gunzip datasets/kdd*gz
```

Now, print the first few lines to have an understanding of the format. It is clear that it's a classic CSV without a header, containing a dot at the end of each line. Also, we can see that some fields are numeric, but a few of them are textual, and the target variable is contained in the last field:

```
In: !head -3 datasets/kddtrain

Out:
```

```
0,tcp,http,SF,181,5450,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,8,8,0.00,0.00,0.00,0
.00,1.00,0.00,0.00,9,9,1.00,0.00,0.11,0.00,0.00,0.00,0.00,0.00,normal.
0,tcp,http,SF,239,486,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,8,8,0.00,0.00,0.00,0.
00,1.00,0.00,0.00,19,19,1.00,0.00,0.05,0.00,0.00,0.00,0.00,0.00,normal.
0,tcp,http,SF,235,1337,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,8,8,0.00,0.00,0.00,0
.00,1.00,0.00,0.00,29,29,1.00,0.00,0.03,0.00,0.00,0.00,0.00,0.00,normal.
```

To create a DataFrame with named fields, we should first read the header included in the `kddnames` file. The target field will be simply named `target`. After having read and parsed the file, we print the number of features of our problem (remember that the target variable is not a feature) and their first ten names:

```
In: with open('datasets/kddnames', 'r') as fh:
        header = [line.split(':')[0]
                  for line in fh.read().splitlines()][1:]
        header.append('target')

    print("Num features:", len(header)-1)
    print("First 10:", header[:10])

Out: Num features: 41
     First 10: ['duration', 'protocol_type', 'service', 'flag',
     'src_bytes', 'dst_bytes', 'land', 'wrong_fragment', 'urgent', 'hot']
```

Now, let's create two separate RDDs—one for the training data and the other for the testing data:

```
In: train_rdd = sc.textFile('file:////home//jovyan//datasets//kddtrain')
    test_rdd = sc.textFile('file:////home//jovyan//datasets//kddtest')
```

Now, we need to parse each line of each file to create a DataFrame. First, we split each line of the CSV file into separate fields, and then we cast each numerical value to a floating point and each text value to a string. Finally, we remove the dot at the end of each line.

As the last step, by using the `createDataFrame` method provided by `sqlContext`, we can create two Spark DataFrames with named columns for both the training and testing datasets:

```
In: def line_parser(line):
        def piece_parser(piece):
             if "." in piece or piece.isdigit():
                 return float(piece)
             else:
                 return piece
    return [piece_parser(piece) for piece in line[:-1].split(',')]

    train_df =
sqlContext.createDataFrame(train_rdd.map(line_parser),header)
    test_df = sqlContext.createDataFrame(test_rdd.map(line_parser), header)
```

So far, we've written just RDD transformers; let's introduce an action to see how many observations we have in the datasets, and, at the same time, check the correctness of the previous code:

```
In: print("Train observations:", train_df.count())
    print("Test observations:", test_df.count())

Out: Train observations: 494021
     Test observations: 311029
```

Although we're using a tenth of the full KDD99 dataset, we are still working on half a million observations. Multiplied by the number of features, `41`, we can clearly see that we'll be training our classifier on an observation matrix containing more than 20 million values. This is not such a big dataset for Spark (and neither is the full KDD99); developers around the world are already using it on petabytes and billions of records. Don't be scared if the numbers seem big: Spark is designed to cope with them.
Now, let's see how it looks on the schema of the DataFrame. Specifically, we want to identify which fields are numeric and which contain strings (note that the result has been truncated for brevity):

```
In: train_df.printSchema()

Out: root
      |-- duration: double (nullable = true)
      |-- protocol_type: string (nullable = true)
      |-- service: string (nullable = true)
      |-- flag: string (nullable = true)
      |-- src_bytes: double (nullable = true)
      |-- dst_bytes: double (nullable = true)
      ...
      |-- target: string (nullable = true
```

Feature engineering

From a visual analysis, only four fields are strings: `protocol_type`, `service`, `flag`, and `target` (which is the multiclass target label, as expected).
As we will use a tree-based classifier, we want to encode the text of each level to a number for each variable. With scikit-learn, this operation can be done with a `sklearn.preprocessing.LabelEncoder` object. It's equivalent in Spark is the `StringIndexer` of the `pyspark.ml.feature` package.
We need to encode four variables with Spark, and then we have to chain four `StringIndexer` objects together in a cascade: each of them will operate on a specific column of the DataFrame, outputting a DataFrame with an additional column (similar to a `map` operation). The mapping is automatic, ordered by frequency: Spark ranks the count of each level in the selected column, mapping the most popular level to `0`, the next to `1`, and so on. Note that, with this operation, you will traverse the dataset once to count the occurrences of each level; if you already know the mapping, it will be more effective to broadcast it and use a `map` operation, as shown at the beginning of this chapter.

More generically, all the classes contained in the `pyspark.ml.feature` package are used to extract, transform, and select features from a DataFrame. All of them read some columns and create some other columns in the DataFrame.

Similarly, we could have used a one-hot encoder to generate a numerical observation matrix. In the case of a one-hot encoder, we would have had multiple output columns in the DataFrame, one for each level of each categorical feature. For this, Spark offers the `pyspark.ml.feature.OneHotEncoderEstimator` class.

As of Spark 2.3.1, the feature operations available in Python are contained in the following exhaustive list: `https://spark.apache.org/docs/latest/ml-features.html` (all of them can be found in the `pyspark.ml.feature` package). Names should be intuitive, except for a couple of them, which will be explained inline or later in the text.

Going back to the example, we now want to encode the levels in each categorical variable as discrete numbers. As we've explained, for this, we will use a `StringIndexer` object for each variable. Moreover, we can use an ML pipeline and set them as stages of it.

Then, to fit all the indexers, you just need to call the `fit` method of the pipeline. Internally, it will fit all the staged objects sequentially. When it has completed the fit operation, a new object is created, and we can refer to it as the fitted pipeline. Calling the `transform` method of this new object will sequentially call all the staged elements (which are already fitted), each being called after the previous one is completed. In the following snippet of code, you'll see the pipeline in action. Note that transformers compose the pipeline. Therefore, as no actions are present, nothing is actually executed. In the output DataFrame, you'll note four additional columns named the same as the original categorical ones, but with the `_cat` suffix:

```
In: from pyspark.ml import Pipeline
    from pyspark.ml.feature import StringIndexer

    cols_categorical = ["protocol_type", "service", "flag","target"]
    preproc_stages = []
    for col in cols_categorical:
        out_col = col + "_cat"
        preproc_stages.append(
            StringIndexer(
                inputCol=col, outputCol=out_col, handleInvalid="skip"))

    pipeline = Pipeline(stages=preproc_stages)
    indexer = pipeline.fit(train_df)
    train_num_df = indexer.transform(train_df)
    test_num_df = indexer.transform(test_df)
```

Let's investigate the pipeline a bit more. Here, we will see the stages in the pipeline: unfit pipeline and fitted pipeline. Note that there's a big difference between Spark and scikit-learn: in scikit-learn, fit and transform are called on the same object, and, in Spark, the `fit` method produces a new object (typically, its name is added with a `Model` suffix, just as for `Pipeline` and `PipelineModel`), where you'll be able to call the `transform` method. This difference is derived from closures—a fitted object is easy to distribute across processes and the cluster:

```
In: print(pipeline.getStages(), '\n')
    print(pipeline)
    print(indexer)

Out: [StringIndexer_44f6bd05e502a8ace0aa,
      StringIndexer_414084eb873c15c387cd,
      StringIndexer_4ca38a4ad6ffeb6ddc95,
      StringIndexer_489c92cd030c80c6f677]

      Pipeline_46a68853ff9dcdece078
      PipelineModel_4f61afaf96ccc4be4b02
```

Extracting some columns from the DataFrame is as easy as using `SELECT` in a SQL query. Now, let's build a list of names for all the numerical features. Starting with the names found in the header, we remove the categorical ones and replace them with
the numerically derived ones. Finally, as we want only the features, we remove the target variable and its numerically derived equivalent:

```
In: features_header = set(header) \
    - set(cols_categorical) \
    | set([c + "_cat" for c in cols_categorical]) \
    - set(["target", "target_cat"])
    features_header = list(features_header)
    print(features_header)
    print("Total numerical features:", len(features_header))

Out: ['flag_cat', 'count', 'land', 'serror_rate', 'num_compromised',
     'num_access_files', 'dst_host_srv_serror_rate', 'src_bytes',
     'num_root', 'srv_serror_rate', 'num_shells', 'diff_srv_rate',
     'dst_host_serror_rate',
     'rerror_rate', 'num_file_creations', 'same_srv_rate',
     'service_cat',
     'num_failed_logins', 'duration', 'dst_host_diff_srv_rate', 'hot',
     'is_guest_login', 'dst_host_same_srv_rate', 'num_outbound_cmds',
     'su_attempted', 'dst_host_count', 'dst_bytes',
     'srv_diff_host_rate',
     'dst_host_srv_count', 'srv_count', 'root_shell',
     'srv_rerror_rate',
     'wrong_fragment', 'dst_host_rerror_rate', 'protocol_type_cat',
     'urgent',
     'dst_host_srv_rerror_rate', 'dst_host_srv_diff_host_rate',
     'logged_in',
     'is_host_login', 'dst_host_same_src_port_rate']
     Total numerical features: 41
```

Here, the `VectorAssembler` class comes to our help to build the feature matrix. We just need to pass the columns to be selected as arguments and the new column to be created in the DataFrame. We decide that the output column will be simply named `features`. We apply this transformation to both training and testing datasets, and then we select just the two columns that we're interested in—`features` and `target_cat`:

```
In: from pyspark.ml.feature import VectorAssembler

    assembler = VectorAssembler(
        inputCols=features_header,
        outputCol="features")
    Xy_train = (assembler
                .transform(train_num_df)
                .select("features", "target_cat"))
    Xy_test = (assembler
               .transform(test_num_df)
               .select("features", "target_cat"))
```

Also, the default behavior of `VectorAssembler` is to produce either `DenseVectors` or `SparseVectors`. In this case, as the vector of features contains many zeros, it returns a sparse vector. To see what's inside the output, we can print the first line. Note that this is an action. Consequently, the job is executed before getting the result printed:

```
In: Xy_train.first()

Out: Row(features=SparseVector(41, {1: 8.0, 7: 181.0, 15: 1.0, 16: 2.0, 22:
       1.0, 25: 9.0, 26: 5450.0, 28: 9.0, 29: 8.0, 34: 1.0, 38: 1.0,
       40: 0.11}), target_cat=2.0)
```

Training a learner

Finally, we arrive at the hot piece of the task: training a classifier. Classifiers are contained in the `pyspark.ml.classification` package, and, for this example, we're using a random forest. For Spark 2.3.1, you can find the extensive list of algorithms that are available at `https://spark.apache.org/docs/2.3.1/ml-classification-regression.html`. The list of algorithms is quite complete, comprising linear models, SVM, Naive Bayes, and tree ensembles. Note that not all of them are capable of operating on multiclass problems, and may have different parameters; always check the documentation related to the version in use. Beyond classifiers, the other learners implemented in Spark 2.3.1 with a Python interface are as follows:

- Clustering (the `pyspark.ml.clustering` package): KMeans
- Recommender (the `pyspark.ml.recommendation` package): ALS (a collaborative filtering recommender, based on alternating least squares)

Let's go back to the goal of the KDD99 challenge. Now, it's time to instantiate a random forest classifier and set its parameters. The parameters to set are `featuresCol` (the column containing the feature matrix), `labelCol` (the column of the DataFrame containing the target label), `seed` (the random seed to make the experiment replicable), and `maxBins` (the maximum number of bins to use for the splitting point in each node of the tree). The default value for the number of trees in the forest is `20`, and each tree is a maximum of five levels deep. Moreover, by default, this classifier creates three output columns in the DataFrame: `rawPrediction` (to store the prediction score for each possible label), `probability` (to store the likelihood of each label), and `prediction` (the most probable label):

```
In: from pyspark.ml.classification import RandomForestClassifier
    clf = RandomForestClassifier(
        labelCol="target_cat", featuresCol="features",
        maxBins=100, seed=101)
    fit_clf = clf.fit(Xy_train)
```

Even in this case, the trained classifier is a different object. Exactly as before, the trained classifier is named the same as the classifier with the `Model` suffix:

```
In: print(clf)
    print(fit_clf)
Out: RandomForestClassifier_4c47a18a99f683bec69e
     RandomForestClassificationModel
     (uid=RandomForestClassifier_4c47a18a99f683bec69e) with 20 trees
```

On the trained `classifier` object (that is, `RandomForestClassificationModel`), it's possible to call the `transform` method. We predict the label on both the training and `test` datasets and print the first line of the `test` dataset. As defined in the classifier, the predictions will be found in the column named `prediction`:

```
In: Xy_pred_train = fit_clf.transform(Xy_train)
    Xy_pred_test = fit_clf.transform(Xy_test)
    print("First observation after classification stage:")
    print(Xy_pred_test.first())

Out: First observation after classification stage:
     Row(features=SparseVector(41, {1: 1.0, 7: 105.0, 15: 1.0, 16: 1.0, 19:
     0.01, 22: 1.0, 25: 255.0, 26: 146.0, 28: 254.0, 29: 1.0, 34: 2.0}),
     target_cat=2.0, rawPrediction=DenseVector([0.0152, 0.0404, 19.6276,
     0.0381, 0.0087, 0.0367, 0.034, 0.1014, 0.0641, 0.0051, 0.0105, 0.0053,
     0.002, 0.0005, 0.0026, 0.0009, 0.0018, 0.0009, 0.0009, 0.0006, 0.0013,
     0.0006, 0.0008]), probability=DenseVector([0.0008, 0.002, 0.9814,
     0.0019,
     0.0004, 0.0018, 0.0017, 0.0051, 0.0032, 0.0003, 0.0005, 0.0003,
     0.0001,
     0.0, 0.0001, 0.0, 0.0001, 0.0, 0.0, 0.0, 0.0001, 0.0, 0.0]),
     prediction=2.0)
```

Evaluating a learner's performance

The next step in any datascience task is to check the performance of the learner on the training and testing datasets. For this task, we will use the `F1-score` as it's a good metric that merges precision and recall performances. Evaluation metrics are enclosed in the `pyspark.ml.evaluation` package; among the few choices we have, we're using the one to evaluate multiclass classifiers: `MulticlassClassificationEvaluator`. As parameters, we're providing the metric (`precision`, `recall`, `accuracy`, `F1-score`, and so on) and the name of the columns containing the true label and predicted label:

```
In: from pyspark.ml.evaluation import MulticlassClassificationEvaluator
    evaluator = MulticlassClassificationEvaluator(
        labelCol="target_cat",
        predictionCol="prediction",
        metricName="f1")
    f1_train = evaluator.evaluate(Xy_pred_train)
    f1_test = evaluator.evaluate(Xy_pred_test)
    print("F1-score train set: %0.3f" % f1_train)
    print("F1-score test set: %0.3f" % f1_test)

Out: F1-score train set: 0.993
     F1-score test set: 0.968
```

The obtained values are pretty high, and there's a big difference between the performance on the training dataset and the testing dataset. Beyond the evaluator for multiclass classifiers, an evaluator object for the regressor (where the metric can be MSE, RMSE, R2, or MAE) and binary classifiers are available in the same package.

The power of the machine learning pipeline

So far, we've built and displayed the output, piece by piece. It's also possible to put all the operations in a cascade and set them as stages of a pipeline. In fact, we can chain together what we've seen so far (the four label encoders, vector builder, and classifier) in a standalone pipeline, fit it to the training dataset, and finally use it on the test dataset to obtain the predictions.

This way to operate is more effective, but you'll lose the exploratory power of the step-by-step analysis. Readers who are data scientists are advised to use end-to-end pipelines only when they are completely sure of what's going on inside, and only to build production models. To show that the pipeline is equivalent to what we've seen so far, we compute the `F1-score` on the test dataset and print it. Unsurprisingly, it's exactly the same value:

```
In: full_stages = preproc_stages + [assembler, clf]
    full_pipeline = Pipeline(stages=full_stages)
    full_model = full_pipeline.fit(train_df)
    predictions = full_model.transform(test_df)
    f1_preds = evaluator.evaluate(predictions)
    print("F1-score test set: %0.3f" % f1_preds)

Out: F1-score test set: 0.968
```

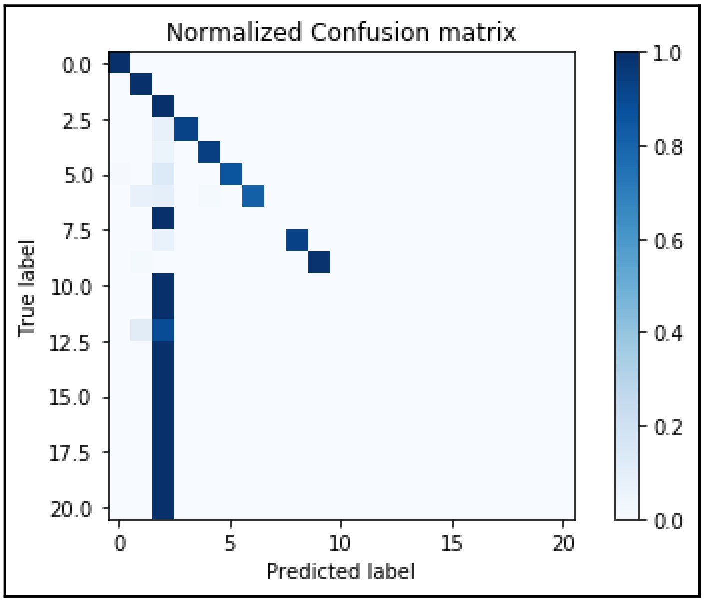
On the driver node, the one running the IPython notebook, we can also use the `matplotlib` library to visualize the results of our analysis. For example, to show a normalized confusion matrix of the classification results (normalized by the support of each class), we can create the following function:

```
In: import numpy as np
    import matplotlib.pyplot as plt
    %matplotlib inline

    def plot_confusion_matrix(cm):
        cm_normalized = \
        cm.astype('float') / cm.sum(axis=1)[:, np.newaxis]
        plt.imshow(
            cm_normalized, interpolation='nearest', cmap=plt.cm.Blues)
        plt.title('Normalized Confusion matrix')
        plt.colorbar()
        plt.tight_layout()
        plt.ylabel('True label')
        plt.xlabel('Predicted label')
```

Spark is able to build a `confusion` matrix, but that method is in the `pyspark.mllib` package. In order to be able to use the methods in this package, we have to transform the DataFrame into an RDD using the `.rdd` method:

```
In: from pyspark.mllib.evaluation import MulticlassMetrics

    metrics = MulticlassMetrics(
        predictions.select("prediction", "target_cat").rdd)
    conf_matrix = metrics.confusionMatrix()toArray()
    plot_confusion_matrix(conf_matrix)
```

Here is the plotted confusion matrix, resulting from the previous code snippet:



Manual tuning

Although the `F1-score` was close to `0.97`, the normalized confusion matrix shows that the classes are strongly unbalanced, and that the classifier has just learned how to classify the most popular ones properly. To improve the results, we can re-sample each class which will, in effect, to try to balance the training dataset better.

First, let's count how many cases there are in the training dataset for each class:

```
In: train_composition = (train_df.groupBy("target")
                          .count()
                          .rdd
                          .collectAsMap())
    print(train_composition)

Out: {'neptune': 107201,
      'nmap': 231,
      'portsweep': 1040,
      'back': 2203,
      'warezclient': 1020,
      'normal': 97278,
      ...
```

```
        'loadmodule': 9,
        'phf': 4}
```

This is clear evidence of a strong imbalance. We can try to improve the performance by oversampling rare classes and subsampling too-popular classes. In this example, we will create a training dataset, where each class is represented at least 1,000 times, but up to 25,000 times. For this, we go through the following steps:

1. Let's first create the subsampling/oversampling rate and broadcast it throughout the cluster, and then `flatMap` each line of the training dataset to resample it properly:

```
In: def set_sample_rate_between_vals(cnt, the_min, the_max):
        if the_min <= cnt <= the_max:
            # no sampling
            return 1
        elif cnt < the_min:
            # Oversampling: return many times the same observation
            return the_min/float(cnt)
        else:
            # Subsampling: sometime don't return it
            return the_max/float(cnt)
    sample_rates = {k:set_sample_rate_between_vals(v, 1000, 25000)
                    for k,v in train_composition.items()}
    sample_rates

Out: {'neptune': 0.23320677978750198,
      'nmap': 4.329004329004329,
      'portsweep': 1,
      'back': 1,
      'warezclient': 1,
      'normal': 0.2569954152017928,
      ...
      'loadmodule': 111.11111111111111,
      'phf': 250.0}

In: bc_sample_rates = sc.broadcast(sample_rates)

    def map_and_sample(el, rates):
        rate = rates.value[el['target']]
        if rate > 1:
            return [el]*int(rate)
        else:
            import random
            return [el] if random.random() < rate else []

    sampled_train_df = (train_df
                        .rdd
                        .flatMap(
                         lambda x: map_and_sample(x,
                                       bc_sample_rates))
                        .toDF()
                        .cache())
```

2. These sampled dataset in the `sampled_train_df` DataFrame variable is also cached; we will use it many times during the hyperparameter optimization step. It should easily fit in memory, as the number of lines is lower than the original number:

```
In: sampled_train_df.count()

Out: 96559
```

3. To get an idea of what's inside, we can print the first line. Pretty quick to print the value, isn't it? Of course, that's quite fast and nice because it has been cached:

```
In: sampled_train_df.first()

Out: Row(duration=0.0, protocol_type='tcp', service='http',
     flag='SF',
     src_bytes=210.0, dst_bytes=624.0, land=0.0,
     wrong_fragment=0.0,
     urgent=0.0, hot=0.0, num_failed_logins=0.0, logged_in=1.0,
     num_compromised=0.0, root_shell=0.0, su_attempted=0.0,
     num_root=0.0,
     num_file_creations=0.0, num_shells=0.0, num_access_files=0.0,
     num_outbound_cmds=0.0, is_host_login=0.0, is_guest_login=0.0,
     count=18.0,
     srv_count=18.0, serror_rate=0.0, srv_serror_rate=0.0,
     rerror_rate=0.0,
     srv_rerror_rate=0.0, same_srv_rate=1.0, diff_srv_rate=0.0,
     srv_diff_host_rate=0.0, dst_host_count=18.0,
     dst_host_srv_count=109.0,
     dst_host_same_srv_rate=1.0, dst_host_diff_srv_rate=0.0,
     dst_host_same_src_port_rate=0.06,
     dst_host_srv_diff_host_rate=0.05,
     dst_host_serror_rate=0.0, dst_host_srv_serror_rate=0.0,
     dst_host_rerror_rate=0.0, dst_host_srv_rerror_rate=0.0,
     target='normal')
```

4. Let's now use the pipeline that we created to make some predictions and print the `F1-score` of this new solution:

```
In:  full_model = full_pipeline.fit(sampled_train_df)
     predictions = full_model.transform(test_df)
     f1_preds = evaluator.evaluate(predictions)
     print("F1-score test set: %0.3f" % f1_preds)

Out: F1-score test set: 0.967
```

5. Test it on a classifier of `50` trees. To do so, we can build another pipeline (named `refined_pipeline`) and substitute the final stage with the new classifier. Performances seem the same, even if the training dataset has been slashed in size:

```
In: clf = RandomForestClassifier(
        numTrees=50, maxBins=100, seed=101,
        labelCol="target_cat", featuresCol="features")
    stages = full_pipeline.getStages()[:-1]
    stages.append(clf)
    refined_pipeline = Pipeline(stages=stages)
    refined_model = refined_pipeline.fit(sampled_train_df)
    predictions = refined_model.transform(test_df)
    f1_preds = evaluator.evaluate(predictions)
    print ("F1-score test set: %0.3f" % f1_preds )

Out: F1-score test set: 0.968
```

This concludes our example about tuning models on Spark. This final test provides us with a fair estimate about how effective our model could be in production.

Cross-validation

We can go forward with manual optimization and find the right model after having exhaustively tried many different configurations. Doing that would lead to both an immense waste of time (and reusability of the code) and will overfit the test dataset. Cross-validation is instead the correct key to run the hyperparameter optimization. Let's now see how Spark performs this crucial task.

First of all, as the training will be used many times, we can `cache` it. Therefore, let's `cache` it after all the transformations:

```
In: pipeline_to_clf = Pipeline(
        stages=preproc_stages + [assembler]).fit(sampled_train_df)
    train = pipeline_to_clf.transform(sampled_train_df).cache()
    test = pipeline_to_clf.transform(test_df)
```

The useful classes for hyperparameter optimization with cross-validation are contained in the `pyspark.ml.tuning` package. Two elements are essential: a grid map of parameters (which can be built with `ParamGridBuilder`) and the actual cross-validation procedure (run by the `CrossValidator` class).

In this example, we want to set some parameters of our classifier that won't change throughout the cross-validation. Exactly as with scikit-learn, they're set when the `classification` object is created (in this case, column names, seed, and the maximum number of bins).

Then, thanks to the grid builder, we decide which arguments should be changed for each iteration of the cross-validation algorithm. In this example, we want to check the classification performance changes the maximum depth of each tree in the forest from `3` to `12` (incrementing by 3) and the number of trees in the forest from 20 or 50. Finally, we launch the cross-validation (with the `fit` method) after having set the grid map, the classifier that we want to test, and the number of folds. The parameter evaluator is essential: it will tell us which is the best model to keep after the cross-validation. Note that this operation may take 15-20 minutes to run (under the hood, *4*2*3=24* models are trained and tested):

```
In: from pyspark.ml.tuning import ParamGridBuilder, CrossValidator

    rf = RandomForestClassifier(
        cacheNodeIds=True, seed=101, labelCol="target_cat",
        featuresCol="features", maxBins=100)
    grid = (ParamGridBuilder()
            .addGrid(rf.maxDepth, [3, 6, 9, 12])
            .addGrid(rf.numTrees, [20, 50])
            .build())
    cv = CrossValidator(
        estimator=rf, estimatorParamMaps=grid,
        evaluator=evaluator, numFolds=3)
    cvModel = cv.fit(train)
```

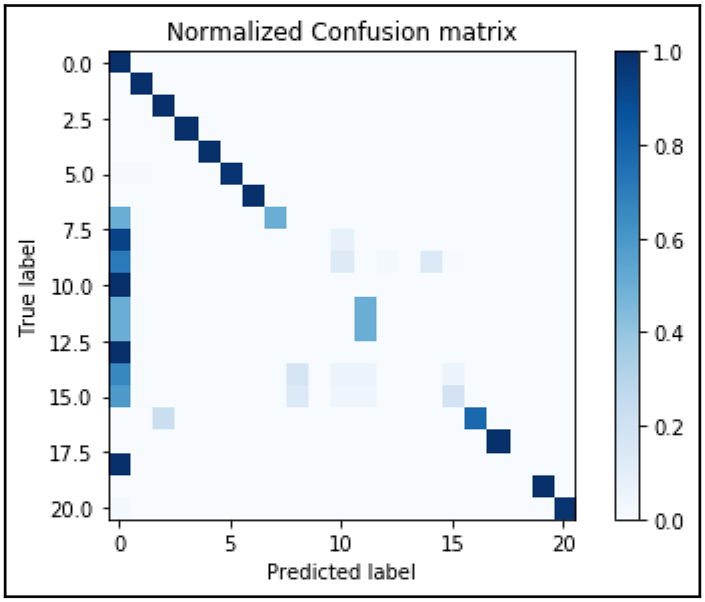
In the end, we can predict the label using the cross-validated model, as we're using a pipeline or classifier by itself. In this case, the performances of the classifier chosen with cross-validation are slightly better than in the previous case, and allow us to beat the `0.97` barriers:

```
In: predictions = cvModel.transform(test)
    f1_preds = evaluator.evaluate(predictions)
    print("F1-score test set: %0.3f" % f1_preds)

Out: F1-score test set: 0.970
```

Furthermore, by plotting the normalized confusion matrix, you immediately realize that this solution is able to discover a wider variety of attacks, even the less popular ones:

```
In: metrics = MulticlassMetrics(
        predictions.select("prediction", "target_cat").rdd)
    conf_matrix = metrics.confusionMatrix().toArray()
    plot_confusion_matrix(conf_matrix)
```

This time, the output is the normalized confusion matrix, showing where misplacement in predictions happens the most:



Final cleanup

Here, we are at the end of the classification task. Remember to remove all the variables that you've used and the temporary table that you've created from the `cache`:

```
In: bc_sample_rates.unpersist()
    sampled_train_df.unpersist()
    train.unpersist()
```

After the Spark memory is cleared, we can turn off the Jupyter notebook.

Summary

In this chapter, we have introduced you to the Hadoop ecosystem, including the architecture, HDFS, and PySpark. After this introduction, we started setting up your local Spark instance, and after sharing variables across cluster nodes, we went through data processing in Spark using both RDDs and DataFrames.

Later on in this chapter, we learned about machine learning with Spark, which included reading a dataset, training a learner, the power of the machine learning pipeline, cross-validation, and even testing what we learned with an example dataset.

This concludes our journey around the essentials in data science with Python, and the next chapter is just an appendix to refresh and strengthen your Python foundations. In conclusion, through all the chapters of this book, we have completed our tour of a data science project, touching on all the key steps of a project and presenting you with all the essential tools to successfully operate your own projects using Python. As a learning tool, the book accompanied you through all the phases of data science, from data loading to machine learning and visualization, illustrating the best practices and ways to avoid common pitfalls, no matter whether your data is small or big. As a reference, this book touched upon a variety of commands and packages, providing you with simple, clear instructions and examples that, if reused in your projects, could save you a lot of time during your work.

From here on, Python will surely play an even larger role in your project developments, and we were glad to have accompanied you so far in your path toward mastering Python for data science.

Strengthen Your Python Foundations

The code examples that are provided along with these chapters don't require you to master Python. However, they will assume that you've previously obtained a working knowledge of at least the basics of Python scripting. They will also assume, in particular, that you know about data structures, such as lists and dictionaries, and that you have an idea about how to make class objects work.

If you don't feel confident about the aforementioned subject or have minimal knowledge of the Python language, we suggest that before you start reading this book, you should take an online tutorial, such as the Code Academy course at `http://www.codecademy.com/en/tracks/python`, Google's Python class at `https://developers.google.com/edu/python/`, or the course offered by Kaggle at `https://www.kaggle.com/learn/python`. All the courses are free, and in a matter of a few hours of study, they should provide you with all the building blocks that will ensure that you enjoy this book to the fullest. If you prefer studying Python basics in a written book, you could read the *Whirlwind Tour of Python* by Jake Vanderplas (`https://github.com/jakevdp/WhirlwindTourOfPython`) and gain all the basic knowledge of Python you need: from variable assignment to importing packages. We have also prepared a few notes, which are arranged in this brief but challenging bonus chapter, in order to highlight the importance and strengthen your knowledge of all the aspects of the Python language that are critical for data science usage. In this bonus chapter, you will learn the following:

- What you should know about Python to be an effective data scientist
- The best resources for learning Python by watching videos
- The best resources for learning Python by directly writing and testing code
- The best resources for learning Python by reading

Your learning list

Here are the basic Python data structures that you need to learn to be as proficient as a data scientist. Leaving aside the real basics (numbers, arithmetic, strings, Booleans, variable assignments, and comparisons), the list is indeed short. We will briefly deal with it by touching upon only the recurrent structures in data science projects. Remember that the topics are quite challenging, but they are necessary to master if you want to write effective code:

- Lists
- Dictionaries
- Classes, objects, and object-oriented programming
- Exceptions
- Iterators and generators
- Conditionals
- Comprehensions
- Functions

Take it as a refresher or a learning list depending on your actual knowledge of the Python language. However, examine all the proposed examples because you will come across them again during the course of this book.

Lists

Lists are collections of elements. Elements can be integers, floats, strings, or generically, objects. Moreover, you can mix different types together. Besides, lists are more flexible than arrays because arrays allow only a single datatype. To create a list, you can either use the square brackets or the `list()` constructor, as follows:

```
a_list = [1, 2.3, 'a', True]
an_empty_list = list()
```

The following are some handy methods that you will need to remember while working with lists:

- To access the ith element, use the `[]` notation:

> Remember that lists are indexed from 0 (zero); that is, the first element is in position 0.

```
a_list[1]
# prints 2.3
a_list[1] = 2.5
# a_list is now [1, 2.5, 'a', True]
```

- You can slice lists by pointing out a starting and ending point (the ending point is not included in the resulting slice), as follows:

```
a_list[1:3]
# prints [2.3, 'a']
```

- You can slice with skips by using a colon-separated `start:end:skip` notation so that you can get an element for every skip value, as follows:

```
a_list[::2]
# returns only odd elements: [1, 'a']
a_list[::-1]
# returns the reverse of the list: [True, 'a', 2.3, 1]
```

- To append an element at the end of the list, you can use `append()`:

```
a_list.append(5)
# a_list is now [1, 2.5, 'a', True, 5]
```

- To get the length of the list, use the `len()` function, as follows:

```
len(a_list)
# prints 5
```

- To delete an element, use the `del` statement followed by the element that you wish to remove:

```
del a_list[0]
# a_list is now [2.5, 'a', True, 5]
```

- To concatenate two lists, use +, as follows:

```
a_list += [1, 'b']
# a_list is now [2.5, 'a', True, 5, 1, 'b']
```

- You can unpack lists by assigning lists to a list (or simply a sequence) of variables instead of a single variable:

```
a, b, c, d, e, f = [2.5, 'a', True, 5, 1, 'b']
# a now is 2.5, b is 'a' and so on
```

Remember that lists are mutable data structures; you can always append, remove, and modify elements. Immutable lists are called tuples and are denoted by round parentheses, `(` and `)`, instead of the square brackets as in the list, `[` and `]`:

```
tuple(a_list)
# prints (2.5, 'a', True, 5, 1, 'b')
```

Dictionaries

Dictionaries are tables that can find stuff very quickly because each key is associated with a value. It is really like using the index of a book to jump immediately to the content you need. Keys and values can belong to different data types. The only prerequisite for keys is that they should be hashable (that's a fairly complex concept; simply keep the keys as simple as possible and, therefore, don't try to use a dictionary or a list as a key). To create a dictionary, you can use curly brackets, as follows:

```
b_dict = {1: 1, '2': '2', 3.0: 3.0}
```

The following are some handy methods that you can remember while working with dictionaries:

- To access the value indexed by the `k` key, use the `[]` notation, as follows:

```
b_dict['2']
# prints '2'
b_dict['2'] = '2.0'
# b_dict is now {1: 1, '2': '2.0', 3.0: 3.0}
```

- To insert or replace a value for a key, use the `[]` notation again:

```
b_dict['a'] = 'a'
# b_dict is now {3.0: 3.0, 1: 1, '2': '2.0', 'a': 'a'}
```

- To get the number of elements in the dictionary, use the `len()` function, as follows:

  ```
  len(b_dict)
  # prints 4
  ```

- To delete an element, use the `del` statement followed by the element that you wish to remove:

  ```
  del b_dict[3.0]
  # b_dict is now {1: 1, '2': '2.0', 'a': 'a'}
  ```

Remember that dictionaries, like lists, are mutable data structures. Also remember that if you try to access an element whose key doesn't exist, a `KeyError` exception will be raised:

```
b_dict['a_key']

Traceback (most recent call last): File "<stdin>", line 1, in <module>
KeyError: 'a_key'
```

The obvious solution to this is to always check first whether an element is in the dictionary:

```
if 'a_key' in b_dict:
 b_dict['a_key']
else:
 print("'a_key' is not present in the dictionary")
```

Otherwise, you can use the `.get` method. If the key is in the dictionary, it returns its value; otherwise, it returns none:

```
b_dict.get('a_key')
```

Finally, you can use a data structure from the collections module, called `defaultdict`, and it will never raise `KeyError` because but it is instantiated by a function taking no arguments and providing the default value for any nonexistent key it may want you to require:

```
from collections import defaultdict
c_dict = defaultdict(lambda: 'empty')
c_dict['a_key']
# requiring a nonexistent key will always return the string 'empty'
```

The `default` function to be used by `defaultdict` can be defined using a `def` or `lambda` command, as described in the following section.

Defining functions

Functions are ensembles of instructions that usually receive specific inputs from you and provide a set of specific outputs related to these inputs. You can define them as one-liners, as follows:

```
def half(x):
    return x/2.0
```

You can also define them as a set of many instructions in the following way:

```
import math
def sigmoid(x):
    try:
        return 1.0 / (1 + math.exp(-x))
    except:
        if x < 0:
             return 0.0
        else:
             return 1.0
```

Finally, you can create an anonymous function by using a `lambda` function. Think of anonymous functions as simple functions that you can define inline everywhere in the code, without using the `verbose` constructor for functions (the one starting with `def`). Just call `lambda` followed by its input parameters; then, a colon will signal the beginning of the commands to be executed by the `lambda` function, which necessarily have to be on the same line. (No `return` command! The commands are what will be returned from the `lambda` function.) You can use a `lambda` function as a parameter in another function, as seen previously for `defaultdict`, or you can use it in order to express a function in one line. This is the case in our example, where we define a function by returning a `lambda` function, incorporating the parameters of the first one:

```
def sum_a_const(c):
    return lambda x: x+c

sum_2 = sum_a_const(2)
sum_3 = sum_a_const(3)
print(sum_2(2))
print(sum_3(2))
# prints 4 and 5
```

To invoke a function, write the function name, followed by its parameters within the parentheses:

```
half(10)
# prints 5.0
sigmoid(0)
# prints 0.5
```

By using functions, you ensemble repetitive procedures by formalizing their inputs and outputs without letting their calculation interfere in any way with the execution of the main program. In fact, unless you declare that a variable is a global one, all the variables you have used inside your function will be disposed of, and your main program will receive only what has been returned by the `return` command.

By the way, please be aware that if you pass a list to a function-only a list, which won't happen with variables-this will be modified, even if not returned, unless you copy it. In order to make a duplicate of a list, you can use the copy or deep copy functions (to be imported from the copy package) or simply the operator [:] applied to your list.

Why does this happen? Because lists are, in particular, data structures that are referenced by an address and not by the entire object. So, when you pass a list to a function, you are just passing an address to the memory of your computer, and the function will operate on that address by modifying your actual list:

```
a_list = [1,2,3,4,5]

def modifier(L):
    L[0] = 0

def unmodifier(L):
    M = L[:] # Here we are copying the list
    M[0] = 0

unmodifier(a_list)
print(a_list)
# you still have the original list, [1, 2, 3, 4, 5]

modifier(a_list)
print(a_list)
# your list have been modified: [0, 2, 3, 4, 5]
```

Classes, objects, and object-oriented programming

Classes are collections of methods and attributes. Briefly, attributes are variables of the object (for example, each instance of the `Employee` class has its own `name`, `age`, `salary`, and `benefits`; all of them are attributes).

Methods are simply functions that modify attributes (for example, to set the employee name, to set his/her age, and also to read this information from a database or from a CSV list). To create a class, use the `class` keyword.

In the following example, we will create a class for an incrementer. The purpose of this object is to keep track of the value of an integer and eventually increase it by 1:

```
class Incrementer(object):
 def __init__(self):
 print ("Hello world, I'm the constructor")
 self._i = 0
```

Everything within the `def` indentation is a `class` method. In this case, the method named `__init__` sets the `i` internal variable to zero (it looks exactly like a function described in the previous chapter). Look carefully at the method's definition. Its argument is `self` (this is the object itself), and every internal variable's access is made through `self`:

1. `__init__` is not just a method; it's the constructor (it's called when the object is created). In fact, when we build an `Increment` object, this method is automatically called, as follows:

```
i = Incrementer()
# prints "Hello world, I'm the constructor"
```

2. Now, let's create the `increment()` method, which increments the `i` internal counter and returns the status. Within the class definition, including the method:

```
def increment(self):
    self._i += 1
    return self._i
```

3. Then, run the following code:

```
i = Incrementer()
print (i.increment())
print (i.increment())
print (i.increment())
```

4. The preceding code results in the following output:

```
Hello world, I'm the constructor
1
2
3
```

Finally, let's see how we can create methods that accept parameters. We will now create the `set_counter` method, which sets the `_i` internal variable:

1. Within the class definition, add the following code:

```
def set_counter(self, counter):
 self._i = counter
```

2. Then, run the following code:

```
i = Incrementer()
i.set_counter(10)
print (i.increment())
print (i._i)
```

3. The preceding code gives this output:

```
Hello world, I'm the constructor
11
11
```

Note the last line of the preceding code, where you access the internal variable. Remember that, in Python, all the internal attributes of the objects are public by default, and they can be read, written, and changed externally.

Exceptions

Exceptions and errors are strongly correlated, but they are different things. An exception, for example, can be gracefully handled. Here are some examples of exceptions:

```
0/0

Traceback (most recent call last): File "<stdin>", line 1, in <module>
ZeroDivisionError: integer division or modulo by zero

len(1, 2)

Traceback (most recent call last): File "<stdin>", line 1, in <module>
```

```
TypeError: len() takes exactly one argument (2 given)

pi * 2

Traceback (most recent call last): File "<stdin>", line 1, in <module>
NameError: name 'pi' is not defined
```

In this example, three different exceptions have been raised (see the last line of each block). To handle exceptions, you can use a `try...except` block in the following way:

```
try:
 a = 10/0
except ZeroDivisionError:
 a = 0
```

You can use more than one except clause to handle more than one exception. You can eventually use a final `all-the-other` exception case handle. In this case, the structure is as follows:

```
try:
    <code which can raise more than one exception>
except KeyError:
    print ("There is a KeyError error in the code")
except (TypeError, ZeroDivisionError):
    print ("There is a TypeError or a ZeroDivisionError error in the code")
except:
    print ("There is another error in the code")
```

Finally, it is important to mention that there is the final clause, `finally`, that will be executed in all circumstances. It's very handy if you want to clean up the code (closing files, de-allocating resources, and so on). These are the things that should be done independently, regardless of whether an error has occurred or not. In this case, the code assumes the following shape:

```
try:
    <code that can raise exceptions>
except:
    <eventually more handlers for different exceptions>
finally:
    <clean-up code>
```

Iterators and generators

Looping through a list or a dictionary is very simple. Note that, with dictionaries, the iteration is key-based, which is demonstrated in the following example:

```
for entry in ['alpha', 'bravo', 'charlie', 'delta']:
    print (entry)

# prints the content of the list, one entry for line

a_dict = {1: 'alpha', 2: 'bravo', 3: 'charlie', 4: 'delta'}
for key in a_dict:
    print (key, a_dict[key])

# Prints:
# 1 alpha
# 2 bravo
# 3 charlie
# 4 delta
```

On the other hand, if you need to iterate through a sequence and generate objects on the fly, you can use a generator. A great advantage of doing this is that you don't have to create and store the complete sequence at the beginning. Instead, you build every object every time the generator is called. As a simple example, let's create a generator for a number sequence without storing the complete list in advance:

```
def incrementer():
    i = 0
    while i<5:
        yield(i)
        i +=1

for i in incrementer():
     print (i)

# Prints:
# 0
# 1
# 2
# 3
# 4
```

Conditionals

Conditionals are often used in data science since you can branch the program. The most frequently used one is the `if` statement. It works more or less the same as in other programming languages. Here's an example of it:

```
def is_positive(val):
 if val< 0:
 print ("It is negative")
 elif val> 0:
 print ("It is positive")
 else:
 print ("It is exactly zero!")

is_positive(-1)
is_positive(1.5)
is_positive(0)

# Prints:
# It is negative
# It is positive
# It is exactly zero!
```

The first condition is checked with `if`. If there are any other conditions, they are defined with `elif` (this stands for `else...if`). Finally, the default behavior is handled by `else`.

Note that `elif` and `else` are not essentials.

Comprehensions for lists and dictionaries

Use comprehensions, lists, and dictionaries that are built as one-liners with the use of an iterator and a conditional when necessary:

```
a_list = [1,2,3,4,5]
a_power_list = [value**2 for value in a_list]
# the resulting list is [1, 4, 9, 16, 25]

filter_even_numbers = [value**2 for value in a_list if value % 2 == 0]
# the resulting list is [4, 16]
```

```
another_list = ['a','b','c','d','e']
a_dictionary = {key:value for value, key in zip(a_list, another_list)}
# the resulting dictionary is {'a': 1, 'c': 3, 'b': 2, 'e': 5, 'd': 4}
```

`zip` is a function that takes, as input, multiple lists of the same length and iterates through each element with the same index at the same time, so you can match the first elements of every list together, and so on.

Comprehensions are a fast way to filter and transform data that is present in an iterator.

Learn by watching, reading, and doing

What if the refresher courses and our learning list are not enough and you need more support to strengthen your knowledge of Python? We will recommend further resources that are available free on the web. By watching tutorial videos, you can try out complex and different examples and challenge yourself with a difficult task that requires you to interact with other data scientists and Python experts.

Massive open online courses (MOOCs)

MOOCs have become increasingly popular in recent years, offering some of the best courses from the best universities and experts from around the world for free on their online platforms. You will find Python courses on Coursera (`https://www.coursera.org/`), Edx (`https://www.edx.org/`), and Udacity (`https://www.udacity.com`). Another great source is the MIT open courseware, which is easily accessible (`ocw.mit.edu/courses/electrical-engineering-and-computer-science/6-00sc-introduction-to-computer-science-and-programming-spring-2011`).

When you consult each of these sites, you may find different active courses on Python. We recommend a free, always available, and do-it-at-your-own pace course by Peter Norvig, the Director of Research at Google Inc. This course aims to take your knowledge of Python to a higher level of proficiency.

PyCon and PyData

The **Python Conference** (**PyCon**) is an annual convention organized at various locations around the world with the purpose of promoting the usage and diffusion of the Python language. During such conventions, tutorials, hands-on demonstrations, and training sessions are commonly held. You can check out `http://www.pycon.org/` to find out where and when the next PyCon will be held near you. If you cannot attend it, you can still perform a search on `www.youtube.com` because most of the interesting sessions are recorded and uploaded there. Attending and watching the real demonstration is a different thing anyway, so we warmly suggest you attend such conventions, because it really is worth it.

Similarly, **PyData**, a community of Python developers and users devoted to data analysis, organize many events around the world. You can check out `pydata.org/events.html` for upcoming events and check whether any past events may have been of interest to you. As with PyCon, presentations are often available on YouTube, on dedicated channels such as PyDataTV.

Interactive Jupyter

Sometimes, you need some written explanations and the opportunity to test some sample code by yourself. Jupyter, an open tool like Python itself, offers you all of this via its notebooks—interactive web pages where you will find both explanations and example code that can be tested directly. We devote explanations about Jupyter and its kernels throughout the is book because it is a real data science workhorse. It allows you to easily run Python scripts and evaluate their effects on the data that you are work on.

The GitHub location of the IPython kernel (the Python kernel of Jupyter, since Jupyter can run many different programming languages) offers a complete list of example notebooks. You can check it out at `github.com/ipython/ipython/wiki/A-gallery-of-interesting-IPython-Notebooks`. In particular, a section of the list is about **General Python Programming**, whereas another one is about **Statistics, Machine Learning and Data Science**, where you will find quite a lot of examples of Python scripts that you can take inspiration from in your learning.

Don't be shy, take a real challenge

If you want to do something that can take your Python coding ability to a different level, we suggest you go and take a challenge on Kaggle. **Kaggle** (`www.kaggle.com`) is a platform for predictive modeling and analytics competitions, which applies the idea of competitive programming (participants try to program according to the provided specifications) in data science by proposing challenging data problems to participants and asking them to provide possible solutions that are evaluated on a test set. The results of the test set are partly public, partly private.

The most interesting part for a Python learner is the opportunity to take part in a real problem with no obvious solution, which requires you to code something to propose possible solutions to the problem, even something simple or naive (which we suggest you start with first before getting involved in complex solutions). By doing so, the learner will come across interesting tutorials, beat-the-benchmark codes, helpful communities of data scientists, and some very smart solutions proposed by other data scientists or Kaggle itself in its blog, *no free hunch* (`blog.kaggle.com`).

You may wonder how to find the right challenge for yourself. Just have a look at the past and present competitions at `www.kaggle.com/competitions` and look for every competition that has knowledge as a reward. You will be surprised to find an ideal stage to learn about how other data scientists code in Python, and you can immediately apply what you learn from this book.

Other Books You May Enjoy

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