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# Introduction to Machine Learning with Python

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A GUIDE FOR DATA SCIENTISTS

Andreas C. Müller & Sarah Guido

[www.it-ebooks.info](http://www.it-ebooks.info)



## Introduction to Machine Learning with Python

by Andreas C. Mueller and Sarah Guido

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# Machine Learning with Python

*Andreas C. Mueller and Sarah Guido*

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# Table of Contents

<b>1. Introduction.....</b>	<b>9</b>
Why machine learning?	9
Problems that machine learning can solve	10
Knowing your data	13
Why Python?	13
What this book will cover	13
What this book will not cover	14
Scikit-learn	14
Installing Scikit-learn	15
Essential Libraries and Tools	16
Python2 versus Python3	19
Versions Used in this Book	19
A First Application: Classifying iris species	20
Meet the data	22
Measuring Success: Training and testing data	24
First things first: Look at your data	25
Building your first model: k nearest neighbors	27
Making predictions	28
Evaluating the model	29
Summary	30
<b>2. Supervised Learning.....</b>	<b>33</b>
Classification and Regression	33
Generalization, Overfitting and Underfitting	35
Supervised Machine Learning Algorithms	37
k-Nearest Neighbor	42
k-Neighbors Classification	42
Analyzing KNeighborsClassifier	45

k-Neighbors Regression	47
Analyzing k nearest neighbors regression	50
Strengths, weaknesses and parameters	51
Linear models	51
Linear models for regression	51
Linear Regression aka Ordinary Least Squares	53
Ridge regression	55
Lasso	57
Linear models for Classification	60
Linear Models for multiclass classification	66
Strengths, weaknesses and parameters	69
Naive Bayes Classifiers	70
Strengths, weaknesses and parameters	71
Decision trees	71
Building Decision Trees	73
Controlling complexity of Decision Trees	76
Analyzing Decision Trees	77
Feature Importance in trees	78
Strengths, weaknesses and parameters	81
Ensembles of Decision Trees	82
Random Forests	82
Gradient Boosted Regression Trees (Gradient Boosting Machines)	88
Kernelized Support Vector Machines	91
Linear Models and Non-linear Features	92
The Kernel Trick	96
Understanding SVMs	97
Tuning SVM parameters	98
Preprocessing Data for SVMs	101
Strengths, weaknesses and parameters	102
Neural Networks (Deep Learning)	102
The Neural Network Model	103
Tuning Neural Networks	106
Strengths, weaknesses and parameters	115
Uncertainty estimates from classifiers	116
The Decision Function	117
Predicting probabilities	119
Uncertainty in multi-class classification	121
Summary and Outlook	123
<b>3. Unsupervised Learning and Preprocessing.....</b>	<b>127</b>
Types of unsupervised learning	127
Challenges in unsupervised learning	128

Preprocessing and Scaling	128
Different kinds of preprocessing	129
Applying data transformations	130
Scaling training and test data the same way	132
The effect of preprocessing on supervised learning	134
Dimensionality Reduction, Feature Extraction and Manifold Learning	135
Principal Component Analysis (PCA)	135
Non-Negative Matrix Factorization (NMF)	152
Manifold learning with t-SNE	157
Clustering	162
k-Means clustering	162
Agglomerative Clustering	173
DBSCAN	178
Summary of Clustering Methods	194
Summary and Outlook	195
<b>4. Summary of scikit-learn methods and usage. ....</b>	<b>197</b>
The Estimator Interface	197
Fit resets a model	198
Method chaining	199
Shortcuts and efficient alternatives	200
Important Attributes	200
Summary and outlook	201
<b>5. Representing Data and Engineering Features. ....</b>	<b>203</b>
Categorical Variables	204
One-Hot-Encoding (Dummy variables)	205
Binning, Discretization, Linear Models and Trees	210
Interactions and Polynomials	215
Univariate Non-linear transformations	222
Automatic Feature Selection	225
Univariate statistics	225
Model-based Feature Selection	227
Iterative feature selection	229
Utilizing Expert Knowledge	230
Summary and outlook	237
<b>6. Model evaluation and improvement. ....</b>	<b>239</b>
Cross-validation	240
Cross-validation in scikit-learn	241
Benefits of cross-validation	241
Stratified K-Fold cross-validation and other strategies	242

More control over cross-validation	244
Leave-One-Out cross-validation	245
Shuffle-Split cross-validation	245
Cross-validation with groups	246
Grid Search	247
Simple Grid-Search	248
The danger of overfitting the parameters and the validation set	249
Grid-search with cross-validation	251
Analyzing the result of cross-validation	255
Using different cross-validation strategies with grid-search	259
Nested cross-validation	260
Parallelizing cross-validation and grid-search	261
Evaluation Metrics and scoring	262
Keep the end-goal in mind	262
Metrics for binary classification	263
Multi-class classification	285
Regression metrics	288
Using evaluation metrics in model selection	288
Summary and outlook	290
<b>7. Algorithm Chains and Pipelines. . . . .</b>	<b>293</b>
Parameter Selection with Preprocessing	294
Building Pipelines	295
Using Pipelines in Grid-searches	296
The General Pipeline Interface	299
Convenient Pipeline creation with <code>make_pipeline</code>	300
Grid-searching preprocessing steps and model parameters	304
Summary and Outlook	306
<b>8. Working with Text Data. . . . .</b>	<b>307</b>
Types of data represented as strings	307
Example application: Sentiment analysis of movie reviews	309
Representing text data as Bag of Words	311
Bag-of-word for movie reviews	314
Stop-words	317
Rescaling the data with TFIDF	318
Investigating model coefficients	321
Bag of words with more than one word (n-grams)	322
Advanced tokenization, stemming and lemmatization	326
Topic Modeling and Document Clustering	329
Summary and Outlook	337

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# Introduction

Machine learning is about extracting knowledge from data. It is a research field at the intersection of statistics, artificial intelligence and computer science, which is also known as predictive analytics or statistical learning. The application of machine learning methods has in recent years become ubiquitous in everyday life. From automatic recommendations of which movies to watch, to what food to order or which products to buy, to personalized online radio and recognizing your friends in your photos, many modern websites and devices have machine learning algorithms at their core.

When you look at complex websites like Facebook, Amazon or Netflix, it is very likely that every part of the website you are looking at contains multiple machine learning models.

Outside of commercial applications, machine learning has had a tremendous influence on the way data driven research is done today. The tools introduced in this book have been applied to diverse scientific questions such as understanding stars, finding distant planets, analyzing DNA sequences, and providing personalized cancer treatments.

Your application doesn't need to be as large-scale or world-changing as these examples in order to benefit from machine learning. In this chapter, we will explain why machine learning became so popular, and discuss what kind of problem can be solved using machine learning. Then, we will show you how to build your first machine learning model, introducing important concepts on the way.

## Why machine learning?

In the early days of “intelligent” applications, many systems used hand-coded rules of “if” and “else” decisions to process data or adjust to user input. Think of a spam filter

whose job is to move an email to a spam folder. You could make up a black-list of words that would result in an email marked as spam. This would be an example of using an expert designed rule system to design an “intelligent” application. Designing kind of manual design of decision rules is feasible for some applications, in particular for those applications in which humans have a good understanding of how a decision should be made. However, using hand-coded rules to make decisions has two major disadvantages:

1. The logic required to make a decision is specific to a single domain and task. Changing the task even slightly might require a rewrite of the whole system.
2. Designing rules requires a deep understanding of how a decision should be made by a human expert.

One example of where this hand-coded approach will fail is in detecting faces in images. Today every smart phone can detect a face in an image. However, face detection was an unsolved problem until as recent as 2001. The main problem is that the way in which pixels (which make up an image in a computer) are “perceived by” the computer is very different from how humans perceive a face. This difference in representation makes it basically impossible for a human to come up with a good set of rules to describe what constitutes a face in a digital image.

Using machine learning, however, simply presenting a program with a large collection of images of faces is enough for an algorithm to determine what characteristics are needed to identify a face.

## Problems that machine learning can solve

The most successful kind of machine learning algorithms are those that automate a decision making processes by generalizing from known examples. In this setting, which is known as a *supervised learning* setting, the user provides the algorithm with pairs of inputs and desired outputs, and the algorithm finds a way to produce the desired output given an input.

In particular, the algorithm is able to create an output for an input it has never seen before without any help from a human.

Going back to our example of spam classification, using machine learning, the user provides the algorithm a large number of emails (which are the input), together with the information about whether any of these emails are spam (which is the desired output). Given a new email, the algorithm will then produce a prediction as to whether or not the new email is spam.

Machine learning algorithms that learn from input-output pairs are called supervised learning algorithms because a “teacher” provides supervision to the algorithm in the form of the desired outputs for each example that they learn from.



While creating a dataset of inputs and outputs is often a laborious manual process, supervised learning algorithms are well-understood and their performance is easy to measure. If your application can be formulated as a supervised learning problem, and you are able to create a dataset that includes the desired outcome, machine learning will likely be able to solve your problem.

Examples of supervised machine learning tasks include:

- **Identifying the ZIP code from handwritten digits on an envelope.** Here the input is a scan of the handwriting, and the desired output is the actual digits in the zip code. To create a data set for building a machine learning model, you need to collect many envelopes. Then you can read the zip codes yourself and store the digits as your desired outcomes.
- **Determining whether or not a tumor is benign based on a medical image.** Here the input is the image, and the output is whether or not the tumor is benign. To create a data set for building a model, you need a database of medical images. You also need an expert opinion, so a doctor needs to look at all of the images and decide which tumors are benign and which are not.
- **Detecting fraudulent activity in credit card transactions.** Here the input is a record of the credit card transaction, and the output is whether it is likely to be fraudulent or not. Assuming that you are the entity distributing the credit cards, collecting a dataset means storing all transactions, and recording if a user reports any transaction as fraudulent.

An interesting thing to note about the three examples above is that although the inputs and outputs look fairly straight-forward, the data collection process for these three tasks is vastly different.

While reading envelopes is laborious, it is easy and cheap. Obtaining medical imaging and expert opinions on the other hand not only requires expensive machinery but also rare and expensive expert knowledge, not to mention ethical concerns and privacy issues. In the example of detecting credit card fraud, data collection is much simpler. Your customers will provide you with the desired output, as they will report fraud. All you have to do to obtain the input output pairs of fraudulent and non-fraudulent activity is wait.

The other type of algorithms that we will cover in this book is unsupervised algorithms. In unsupervised learning, only the input data is known and there is no known output data given to the algorithm. While there are many successful applications of these methods as well, they are usually harder to understand and evaluate.

Examples of unsupervised learning include:

- **Identifying topics in a set of blog posts.** If you have a large collection of text data, you might want to summarize it and find prevalent themes in it. You might not know beforehand what these topics are, or how many topics there might be. Therefore, there are no known outputs.
- **Segmenting customers into groups with similar preferences.** Given a set of customer records, you might want to identify which customers are similar, and whether there are groups of customers with similar preferences. For a shopping site these might be “parents”, “bookworms” or “gamers”. Since you don’t know in advanced what these groups might be, or even how many there are, you have no known outputs.
- **Detecting abnormal access patterns to a website.** To identify abuse or bugs, it is often helpful to find access patterns that are different from the norm. Each abnormal pattern might be very different, and you might not have any recorded instances of abnormal behavior. Since in this example you only observe traffic, and you don’t know what constitutes normal and abnormal behavior, this is an unsupervised problem.

For both supervised and unsupervised learning tasks, it is important to have a representation of your input data that a computer can understand. Often it is helpful to think of your data as a table. Each data point that you want to reason about (each email, each customer, each transaction) is a row, and each property that describes that data point (say the age of a customer, the amount or location of a transaction) is a column.

You might describe users by their age, their gender, when they created an account and how often they bought from your online shop. You might describe the image of a tumor by the gray-scale values of each pixel, or maybe by using the size, shape and color of the tumor to describe it.

Each entity or row here is known as data point or *sample* in machine learning, while the columns, the properties that describe these entities, are called *features*.

We will later go into more detail on the topic of building a good representation of your data, which is called feature extraction or feature engineering. You should keep in mind however that no machine learning algorithm will be able to make a prediction on data for which it has no information. For example, if the only feature that you have for a patient is their last name, no algorithm will be able to predict their gender. This information is simply not contained in your data. If you add another feature that contains their first name, you will have much better luck, as it is often possible to tell the gender by a person’s first name.

## Knowing your data

Quite possibly the most important part in the machine learning process is understanding the data you are working with. It will not be effective to randomly choose an algorithm and throw your data at it. It is necessary to understand what is going on in your dataset before you begin building a model. Each algorithm is different in terms of what data it works best for, what kinds of data it can handle, what kind of data it is optimized for, and so on. Before you start building a model, it is important to know the answers to most of, if not all of, the following questions:

- How much data do I have? Do I need more?
- How many features do I have? Do I have too many? Do I have too few?
- Is there missing data? Should I discard the rows with missing data or handle them differently?
- What question(s) am I trying to answer? Do I think the data collected can answer that question?

The last bullet point is the most important question, and certainly is not easy to answer. Thinking about these questions will help drive your analysis.

Keeping these basics in mind as we move through the book will prove helpful, because while scikit-learn is a fairly easy tool to use, it is geared more towards those with domain knowledge in machine learning.

## Why Python?

Python has become the lingua franca for many data science applications. It combines the powers of general purpose programming languages with the ease of use of domain specific scripting languages like matlab or R.

Python has libraries for data loading, visualization, statistics, natural language processing, image processing, and more. This vast toolbox provides data scientists with a large array of general and special purpose functionality.

As a general purpose programming language, Python also allows for the creation of complex graphic user interfaces (GUIs), web services and for integration into existing systems.

## What this book will cover

In this book, we will focus on applying machine learning algorithms for the purpose of solving practical problems. We will focus on how to write applications using the machine learning library scikit-learn for the Python programming language. Impor-

tant aspects that we will cover include formulating tasks as machine learning problems, preprocessing data for use in machine learning algorithms, and choosing appropriate algorithms and algorithmic parameters.

We will focus mostly on supervised learning techniques and algorithms, as these are often the most useful ones in practice, and they are easy for beginners to use and understand.

We will also discuss several common types of input, including text data.

## What this book will not cover

This book will not cover the mathematical details of machine learning algorithms, and we will keep the number of formulas that we include to a minimum. In particular, we will not assume any familiarity with linear algebra or probability theory. As mathematics, in particular probability theory, is the foundation upon which machine learning is built, we will not be able to go into the analysis of the algorithms in great detail. If you are interested in the mathematics of machine learning algorithms, we recommend the text book “Elements of Statistical Learning” by Hastie, Tibshirani and Friedman, which is available for free at the authors website[footnote: <http://statweb.stanford.edu/~tibs/ElemStatLearn/>]. We will also not describe how to write machine learning algorithms from scratch, and will instead focus on how to use the large array of models already implemented in scikit-learn and other libraries.

We will not discuss reinforcement learning, which is about an agent learning from its interaction with an environment, and we will only briefly touch upon deep learning.

Some of the algorithms that are implemented in scikit-learn but are outside the scope of this book include Gaussian Processes, which are complex probabilistic models, and semi-supervised models, which work with supervised information on only some of the samples.

We will not also explicitly talk about how to work with time-series data, although many of techniques we discuss are applicable to this kind of data as well. Finally, we will not discuss how to do machine learning on natural images, as this is beyond the scope of this book.

## Scikit-learn

Scikit-learn is an open-source project, meaning that scikit-learn is free to use and distribute, and anyone can easily obtain the source code to see what is going on behind the scenes. The scikit-learn project is constantly being developed and improved, and has a very active user community. It contains a number of state-of-the-art machine learning algorithms, as well as comprehensive documentation about each algorithm on the website [footnote <http://scikit-learn.org/stable/documentation>]. Scikit-learn is

a very popular tool, and the most prominent Python library for machine learning. It is widely used in industry and academia, and there is a wealth of tutorials and code snippets about scikit-learn available online. Scikit-learn works well with a number of other scientific Python tools, which we will discuss later in this chapter.

While studying the book, we recommend that you also browse the scikit-learn user guide and API documentation for additional details, and many more options to each algorithm. The online documentation is very thorough, and this book will provide you with all the prerequisites in machine learning to understand it in detail.

## Installing Scikit-learn

Scikit-learn depends on two other Python packages, NumPy and SciPy. For plotting and interactive development, you should also install matplotlib, IPython and the Jupyter notebook. We recommend using one of the following pre-packaged Python distributions, which will provide the necessary packages:

- Anaconda (<https://store.continuum.io/cshop/anaconda/>): a Python distribution made for large-scale data processing, predictive analytics, and scientific computing. Anaconda comes with NumPy, SciPy, matplotlib, IPython, Jupyter notebooks, and scikit-learn. Anaconda is available on Mac OS X, Windows, and Linux.
- Enthought Canopy (<https://www.enthought.com/products/canopy/>): another Python distribution for scientific computing. This comes with NumPy, SciPy, matplotlib, and IPython, but the free version does not come with scikit-learn. If you are part of an academic, degree-granting institution, you can request an academic license and get free access to the paid subscription version of Enthought Canopy. Enthought Canopy is available for Python 2.7.x, and works on Mac, Windows, and Linux.
- Python(x,y) (<https://code.google.com/p/pythonxy/>): a free Python distribution for scientific computing, specifically for Windows. Python(x,y) comes with NumPy, SciPy, matplotlib, IPython, and scikit-learn.

If you already have a python installation set up, you can use pip to install any of these packages.

```
$ pip install numpy scipy matplotlib ipython scikit-learn
```

We do not recommended using pip to install NumPy and SciPy on Linux, as it involves compiling the packages from source. See the scikit-learn website for more detailed installation.

## Essential Libraries and Tools

Understanding what scikit-learn is and how to use it is important, but there are a few other libraries that will enhance your experience. Scikit-learn is built on top of the NumPy and SciPy scientific Python libraries. In addition to knowing about NumPy and SciPy, we will be using Pandas and matplotlib. We will also introduce the Jupyter Notebook, which is an browser-based interactive programming environment. Briefly, here is what you should know about these tools in order to get the most out of scikit-learn.

If you are unfamiliar with numpy or matplotlib, we recommend reading the first chapter of the scipy lecture notes[footnote: <http://www.scipy-lectures.org/>].

### Jupyter Notebook

The Jupyter Notebook is an interactive environment for running code in the browser. It is a great tool for exploratory data analysis and is widely used by data scientists. While Jupyter Notebook supports many programming languages, we only need the Python support. The Jupyter Notebook makes it easy to incorporate code, text, and images, and all of this book was in fact written as an IPython notebook.

All of the code examples we include can be downloaded from github [FIXME add github footnote].

### NumPy

NumPy is one of the fundamental packages for scientific computing in Python. It contains functionality for multidimensional arrays, high-level mathematical functions such as linear algebra operations and the Fourier transform, and pseudo random number generators.

The NumPy array is the fundamental data structure in scikit-learn. Scikit-learn takes in data in the form of NumPy arrays. Any data you're using will have to be converted to a NumPy array. The core functionality of NumPy is this “ndarray”, meaning it has  $n$  dimensions, and all elements of the array must be the same type. A NumPy array looks like this:

```
import numpy as np

x = np.array([[1, 2, 3], [4, 5, 6]])
x
array([[1, 2, 3],
       [4, 5, 6]])
```

## SciPy

SciPy is both a collection of functions for scientific computing in python. It provides, among other functionality, advanced linear algebra routines, mathematical function optimization, signal processing, special mathematical functions and statistical distributions. Scikit-learn draws from SciPy's collection of functions for implementing its algorithms.

The most important part of scipy for us is `scipy.sparse` which provides *sparse matrices*, which is another representation that is used for data in scikit-learn. Sparse matrices are used whenever we want to store a 2d array that contains mostly zeros:

```
from scipy import sparse

# create a 2d numpy array with a diagonal of ones, and zeros everywhere else
eye = np.eye(4)
print("Numpy array:\n%s" % eye)

# convert the numpy array to a scipy sparse matrix in CSR format
# only the non-zero entries are stored
sparse_matrix = sparse.csr_matrix(eye)
print("\nScipy sparse CSR matrix:\n%s" % sparse_matrix)
```

Numpy array:

```
[[ 1.  0.  0.  0.]
 [ 0.  1.  0.  0.]
 [ 0.  0.  1.  0.]
 [ 0.  0.  0.  1.]]
```

Scipy sparse CSR matrix:

```
(0, 0) 1.0
(1, 1) 1.0
(2, 2) 1.0
(3, 3) 1.0
```

More details on scipy sparse matrices can be found in the scipy lecture notes.

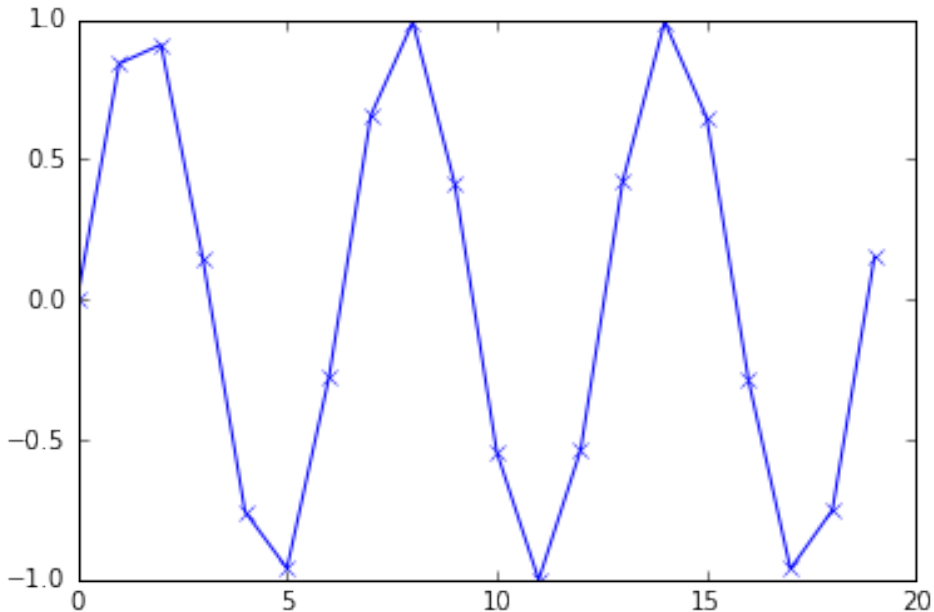
## matplotlib

Matplotlib is the primary scientific plotting library in Python. It provides function for making publication-quality visualizations such as line charts, histograms, scatter

plots, and so on. Visualizing your data and any aspects of your analysis can give you important insights, and we will be using matplotlib for all our visualizations.

```
%matplotlib inline
import matplotlib.pyplot as plt

# Generate a sequence of integers
x = np.arange(20)
# create a second array using sinus
y = np.sin(x)
# The plot function makes a line chart of one array against another
plt.plot(x, y, marker="x")
```



## Pandas

Pandas is a Python library for data wrangling and analysis. It is built around a data structure called DataFrame, that is modeled after the R DataFrame. Simply put, a Pandas DataFrame is a table, similar to an Excel Spreadsheet. Pandas provides a great range of methods to modify and operate on this table, in particular it allows SQL-like queries and joins of tables. Another valuable tool provided by Pandas is its ability to ingest from a great variety of file formats and databases, like SQL, Excel files and comma separated value (CSV) files. Going into details about the functionality of Pandas is out of the scope of this book. However, “Python for Data Analysis” by Wes McKinney provides a great guide.

Here is a small example of creating a DataFrame using a dictionary:



```
import pandas as pd

# create a simple dataset of people
data = {'Name': ["John", "Anna", "Peter", "Linda"],
        'Location': ["New York", "Paris", "Berlin", "London"],
        'Age' : [24, 13, 53, 33]
        }

data_pandas = pd.DataFrame(data)
data_pandas
```

	Age	Location	Name
0	24	New York	John
1	13	Paris	Anna
2	53	Berlin	Peter
3	33	London	Linda

## Python2 versus Python3

There are two major versions of Python that are widely used at the moment: Python2 (more precisely 2.7) and Python3 (with the latest release being 3.5 at the time of writing), which sometimes leads to some confusion. Python2 is no longer actively developed, but because Python3 contains major changes, Python2 code does usually not run without changes on Python3. If you are new to Python, or are starting a new project from scratch, we highly recommend using the latests version of Python3.

If you have a large code-base that you rely on that is written for Python2, you are excused from upgrading for now. However, you should try to migrate to Python3 as soon as possible. Writing any new code, it is for the most part quite easy to write code that runs under Python2 and Python3 [Footnote: The `six` package can be very handy for that].

All the code in this book is written in a way that works for both versions. However, the exact output might differ slightly under Python2.

## Versions Used in this Book

We are using the following versions of the above libraries in this book:

```
import pandas as pd
print("pandas version: %s" % pd.__version__)

import matplotlib
print("matplotlib version: %s" % matplotlib.__version__)

import numpy as np
print("numpy version: %s" % np.__version__)
```

```
import IPython
print("IPython version: %s" % IPython.__version__)

import sklearn
print("scikit-learn version: %s" % sklearn.__version__)

pandas version: 0.17.1

matplotlib version: 1.5.1

numpy version: 1.10.4

IPython version: 4.1.2

scikit-learn version: 0.18.dev0
```

While it is not important to match these versions exactly, you should have a version of scikit-learn that is at least as recent as the one we used.

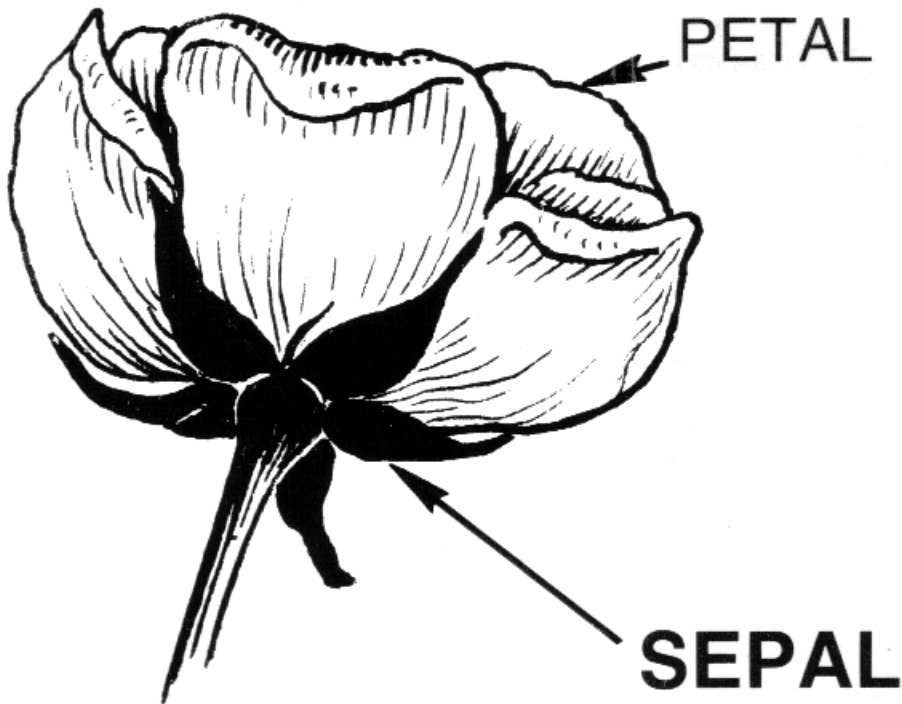
Now that we have everything set up, let's dive into our first application of machine learning.

## A First Application: Classifying iris species

In this section, we will go through a simple machine learning application and create our first model.

In the process, we will introduce some core concepts and nomenclature for machine learning.

Let's assume that a hobby botanist is interested in distinguishing what the species is of some iris flowers that she found. She has collected some measurements associated with the iris: the length and width of the petals, and the length and width of the sepal, all measured in centimeters.



She also has the measurements of some irises that have been previously identified by an expert botanist as belonging to the species *Setosa*, *Versicolor* or *Virginica*. For these measurements, she can be certain of which species each iris belongs to. Let's assume that these are the only species our hobby botanist will encounter in the wild.

Our goal is to build a machine learning model that can learn from the measurements of these irises whose species is known, so that we can predict the species for a new iris.

Since we have measurements for which we know the correct species of iris, this is a supervised learning problem. In this problem, we want to predict one of several options (the species of iris). This is an example of a *classification* problem. The possible outputs (different species of irises) are called *classes*.

Since every iris in the dataset belongs to one of three classes this problem is a three-class classification problem.

The desired output for a single data point (an iris) is the species of this flower. For a particular data point, the species it belongs to is called its *label*.

## Meet the data

The data we will use for this example is the iris dataset, a classical dataset in machine learning and statistics.

It is included in scikit-learn in the dataset module. We can load it by calling the `load_iris` function:

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

The iris object that is returned by `load_iris` is a *Bunch* object, which is very similar to a dictionary. It contains keys and values:

```
iris.keys()
dict_keys(['DESCR', 'data', 'target_names', 'feature_names', 'target'])
```

The value to the key `DESCR` is a short description of the dataset. We show the beginning of the description here. Feel free to look up the rest yourself.

```
print(iris['DESCR'][:193] + "\n...")
Iris Plants Database
=====

Notes
-----

Data Set Characteristics:

    :Number of Instances: 150 (50 in each of three classes)

    :Number of Attributes: 4 numeric, predictive att

    ...
```

The value with key `target_names` is an array of strings, containing the species of flower that we want to predict:

```
iris['target_names']
array(['setosa', 'versicolor', 'virginica'],
      dtype='<U10')
```

The `feature_names` are a list of strings, giving the description of each feature:

```
iris['feature_names']
```

```
['sepal length (cm)',  
 'sepal width (cm)',  
 'petal length (cm)',  
 'petal width (cm)']
```

The data itself is contained in the `target` and `data` fields. The `data` contains the numeric measurements of sepal length, sepal width, petal length, and petal width in a `numpy` array:

```
type(iris['data'])  
numpy.ndarray
```

The rows in the data array correspond to flowers, while the columns represent the four measurements that were taken for each flower:

```
iris['data'].shape  
(150, 4)
```

We see that the data contains measurements for 150 different flowers.

Remember that the individual items are called *samples* in machine learning, and their properties are called *features*.

The shape of the data array is the number of samples times the number of features.

This is a convention in `scikit-learn`, and your data will always be assumed to be in this shape.

Here are the feature values for the first five samples:

```
iris['data'][:5]  
array([[ 5.1,  3.5,  1.4,  0.2],  
       [ 4.9,  3. ,  1.4,  0.2],  
       [ 4.7,  3.2,  1.3,  0.2],  
       [ 4.6,  3.1,  1.5,  0.2],  
       [ 5. ,  3.6,  1.4,  0.2]])
```

The `target` array contains the species of each of the flowers that were measured, also as a `numpy` array:

```
type(iris['target'])  
numpy.ndarray
```

The `target` is a one-dimensional array, with one entry per flower:

```
iris['target'].shape  
(150,)
```

The species are encoded as integers from 0 to 2:

```
iris['target']  
array([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, 0, 0,  
       0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,  
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,  
       1, 1, 1, 1, 1, 1, 1, 1, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,  
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2,  
       2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2])
```

The meaning of the numbers are given by the `iris['target_names']` array: 0 means Setosa, 1 means Versicolor and 2 means Virginica.

## Measuring Success: Training and testing data

We want to build a machine learning model from this data that can predict the species of iris for a new set of measurements.

Before we can apply our model to new measurements, we need to know whether our model actually works, that is whether we should trust its predictions.

Unfortunately, we can not use the data we use to build the model to evaluate it. This is because our model can always simply remember the whole training set, and will therefore always predict the correct label for any point in the training set. This “remembering” does not indicate to us whether our model will *generalize* well, in other words whether it will also perform well on new data. So before we apply our model to new measurements, we will want to know whether we can trust its predictions.

To assess the models’ performance, we show the model new data (that it hasn’t seen before) for which we have labels. This is usually done by splitting the labeled data we have collected (here our 150 flower measurements) into two parts.

The part of the data is used to build our machine learning model, and is called the *training data* or *training set*. The rest of the data will be used to access how well the model works and is called *test data*, *test set* or *hold-out set*.

Scikit-learn contains a function that shuffles the dataset and splits it for you, the `train_test_split` function.

This function extracts 75% of the rows in the data as the training set, together with the corresponding labels for this data. The remaining 25% of the data, together with the remaining labels are declared as the test set.

How much data you want to put into the training and the test set respectively is somewhat arbitrary, but using a test-set containing 25% of the data is a good rule of thumb.

In scikit-learn, data is usually denoted with a capital X, while labels are denoted by a lower-case y.

Let's call `train_test_split` on our data and assign the outputs using this nomenclature:

```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(iris['data'], iris['target'],
                                                random_state=0)
```

The `train_test_split` function shuffles the dataset using a pseudo random number generator before making the split. If we would take the last 25% of the data as a test set, all the data point would have the label 2, as the data points are sorted by the label (see the output for `iris['target']` above). Using a tests set containing only one of the three classes would not tell us much about how well we generalize, so we shuffle our data, to make sure the test data contains data from all classes.

To make sure that we will get the same output if we run the same function several times, we provide the pseudo random number generator with a fixed seed using the `random_state` parameter. This will make the outcome deterministic, so this line will always have the same outcome. We will always fix the `random_state` in this way when using randomized procedures in this book.

The output of the `train_test_split` function are `X_train`, `X_test`, `y_train` and `y_test`, which are all numpy arrays. `X_train` contains 75% of the rows of the dataset, and `X_test` contains the remaining 25%:

```
X_train.shape
(112, 4)
X_test.shape
(38, 4)
```

## First things first: Look at your data

Before building a machine learning model, it is often a good idea to inspect the data, to see if the task is easily solvable without machine learning, or if the desired information might not be contained in the data.

Additionally, inspecting your data is a good way to find abnormalities and peculiarities. Maybe some of your irises were measured using inches and not centimeters, for example. In the real world, inconsistencies in the data and unexpected measurements are very common.

One of the best ways to inspect data is to visualize it. One way to do this is by using a scatter plot.

A scatter plot of the data puts one feature along the x-axis, one feature along the y-axis, and draws a dot for each data point.

Unfortunately, computer screens have only two dimensions, which allows us to only plot two (or maybe three) features at a time. It is difficult to plot datasets with more than three features this way.

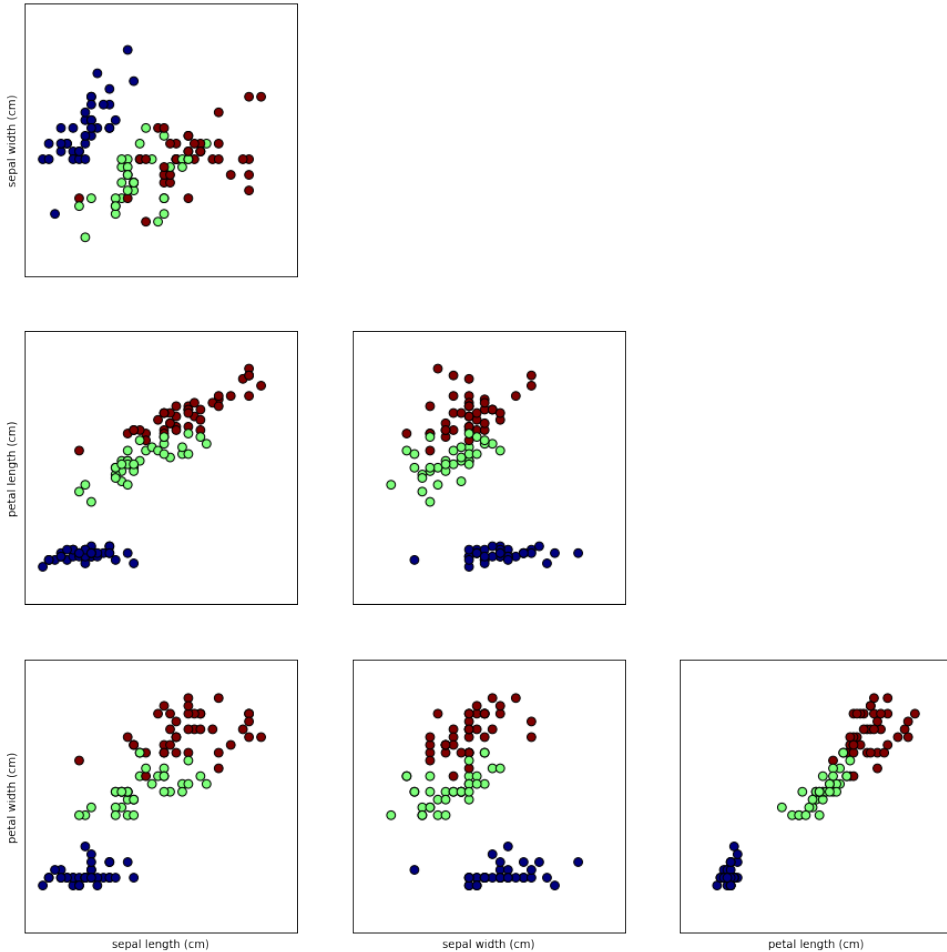
One way around this problem is to do a pair plot, which looks at all pairs of two features. If you have a small number of features, such as the four we have here, this is quite reasonable. You should keep in mind that a pair plot does not show the interaction of all of features at once, so some interesting aspects of the data may not be revealed when visualizing it this way.

Here is a pair plot of the features in the training set. The data points are colored according to the species the iris belongs to:

```
fig, ax = plt.subplots(3, 3, figsize=(15, 15))
plt.suptitle("iris_pairplot")

for i in range(3):
    for j in range(3):
        ax[i, j].scatter(X_train[:, j], X_train[:, i + 1], c=y_train, s=60)
        ax[i, j].set_xticks(())
        ax[i, j].set_yticks(())
        if i == 2:
            ax[i, j].set_xlabel(iris['feature_names'][j])
        if j == 0:
            ax[i, j].set_ylabel(iris['feature_names'][i + 1])
        if j > i:
            ax[i, j].set_visible(False)
```





From the plots, we can see that the three classes seem to be relatively well separated using the sepal and petal measurements. This means that a machine learning model will likely be able to learn to separate them.

## Building your first model: k nearest neighbors

Now we can start building the actual machine learning model. There are many classification algorithms in scikit-learn that we could use. Here we will use a k nearest neighbors classifier, which is easy to understand.

Building this model only consists of storing the training set. To make a prediction for a new data point, the algorithm finds the point in the training set that is closest to the new point. Then, it assigns the label of this closest data training point to the new data point.

The  $k$  in  $k$  nearest neighbors stands for the fact that instead of using only the closest neighbor to the new data point, we can consider any fixed number  $k$  of neighbors in the training (for example, the closest three or five neighbors). Then, we can make a prediction using the majority class among these neighbors. We will go into more details about this later.

Let's use only a single neighbor for now.

All machine learning models in scikit-learn are implemented in their own class, which are called `Estimator` classes. The  $k$  nearest neighbors classification algorithm is implemented in the `KNeighborsClassifier` class in the `neighbors` module.

Before we can use the model, we need to instantiate the class into an object. This is when we will set any parameters of the model. The single parameter of the `KNeighborsClassifier` is the number of neighbors, which we will set to one:

```
from sklearn.neighbors import KNeighborsClassifier
knn = KNeighborsClassifier(n_neighbors=1)
```

The `knn` object encapsulates the algorithm to build the model from the training data, as well the algorithm to make predictions on new data points.

It will also hold the information the algorithm has extracted from the training data. In the case of `KNeighborsClassifier`, it will just store the training set.

To build the model on the training set, we call the `fit` method of the `knn` object, which takes as arguments the numpy array `X_train` containing the training data and the numpy array `y_train` of the corresponding training labels:

```
knn.fit(X_train, y_train)

KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
                    metric_params=None, n_jobs=1, n_neighbors=1, p=2,
                    weights='uniform')
```

## Making predictions

We can now make predictions using this model on new data, for which we might not know the correct labels.

Imagine we found an iris in the wild with a sepal length of 5cm, a sepal width of 2.9cm, a petal length of 1cm and a petal width of 0.2cm. What species of iris would this be?

We can put this data into a numpy array, again with the shape number of samples (one) times number of features (four):

```
X_new = np.array([[5, 2.9, 1, 0.2]])
X_new.shape

(1, 4)
```

To make prediction we call the `predict` method of the `knn` object:

```
prediction = knn.predict(X_new)
prediction

array([0])

iris['target_names'][prediction]

array(['setosa'],

      dtype='<U10')
```

Our model predicts that this new iris belongs to the class 0, meaning its species is Setosa.

But how do we know whether we can trust our model? We don't know the correct species of this sample, which is the the whole point of building the model!

## Evaluating the model

This is where the test set that we created earlier comes in. This data was not used to build the model, but we do know what the correct species are for each iris in the test set.

We can make a prediction for an iris in the test data, and compare it against its label (the known species). We can measure how well the model works by computing the *accuracy*, which is the fraction of flowers for which the right species was predicted:

```
y_pred = knn.predict(X_test)
np.mean(y_pred == y_test)

0.97368421052631582
```

We can also use the `score` method of the `knn` object, which will compute the test set accuracy for us:

```
knn.score(X_test, y_test)

0.97368421052631582
```

For this model, the test set accuracy is about 0.97, which means we made the right prediction for 97% of the irises in the test set. Under some mathematical assumptions, this means that we can expect our model to be correct 97% of the time for new irises.

For our hobby botanist application, this high level of accuracy means that our models may be trustworthy enough to use. In later chapters we will discuss how we can improve performance, and what caveats there are in tuning a model.

## Summary

Let's summarize what we learned in this chapter. We started off formulating a task of predicting which species of iris a particular flower belongs to by using physical measurements of the flower. We used a dataset of measurements that was annotated by an expert with the correct species to build our model, making this a supervised learning task. There were three possible species, *Setosa*, *Versicolor* or *Virginica*, which made the task a three-class *classification* problem. The possible species are called *classes* in the classification problem, and the species of a single iris is called its *label*.

The dataset consists of two numpy arrays, one containing the data, which is referred to as  $X$  in scikit-learn, and one containing the correct or desired outputs, which is called  $y$ . The array  $X$  is a two-dimensional array of features, with one row per data point, and one column per feature. The array  $y$  is a one-dimensional array, which here contained one class label from 0 to 2 for each of the samples.

We split our dataset into a *training set*, to build our model, and a *test set*, to evaluate how well our model will generalize to new, unseen data.

We chose the  $k$  nearest neighbors classification algorithm, which makes predictions for a new data point by considering its closest neighbor(s) in the training set.

The algorithm is implemented in the `KNeighborsClassifier` class, which contains the algorithm to build the model, as well as the algorithm to make a prediction using the model. We instantiated the class, setting parameters. Then, we built the model by calling the `fit` method, passing the training data `X_train` and training outputs `y_train` as parameters.

We evaluated the model using the `score` method, that computes the *accuracy* of the model. We applied the `score` method to the test set data and the test set labels, and found that our model is about 97% accurate, meaning it is correct 97% of the time on the test set.

This gave us the confidence to apply the model to new data (in our example, new flower measurements), and trust that the model will be correct about 97% of the time.

Here is a summary of the code needed for the whole training and evaluation procedure:

```
X_train, X_test, y_train, y_test = train_test_split(iris['data'], iris['target'],
                                                    random_state=0)

knn = KNeighborsClassifier(n_neighbors=1)
knn.fit(X_train, y_train)

knn.score(X_test, y_test)

0.97368421052631582
```

This snippet contains the core code for applying any machine learning algorithms using scikit-learn. The `fit`, `predict` and `score` methods are the common interface to supervised models in scikit-learn, and with the concepts introduced in this chapter, you can apply these models to many machine learning tasks.

In the next chapter, we will go into more depth about the different kinds of supervised models in scikit-learn, and how to apply them successfully.



---

# Supervised Learning

As we mentioned in the introduction, supervised machine learning is one of the most commonly used and successful types of machine learning. In this chapter, we will describe supervised learning in more detail, and explain several popular supervised learning algorithms.

We already saw an application of supervised machine learning in the last chapter: classifying iris flowers into several species using physical measurements of the flowers.

Remember that supervised learning is used whenever we want to predict a certain outcome from a given input, and we have examples of input-output pairs. We build a machine learning model from these input-output pairs, which comprise our training set. Our goal is to make accurate predictions to new, never-before seen data.

Supervised learning often requires human effort to build the training set, but afterwards automates and often speeds up an otherwise laborious or infeasible task.

## Classification and Regression

There are two major types of supervised machine learning algorithms, called *classification* and *regression*.

In classification, the goal is to predict a *class label*, which is a choice from a predefined list of possibilities. In Chapter 1 (Introduction) we used the example of classifying irises into one of three possible species. Classification is sometimes separated into *binary classification*, which is the special case of distinguishing between exactly two classes, and *multi-class classification* which is classification between more than two classes. You can think of binary classification as trying to answer a “yes” or “no” question.

Classifying emails into either spam or not spam is an example of a binary classification problem. In this binary classification task, the yes or no question being asked would be “Is this email spam?”

[info box] In binary classification we often speak of one class being the *positive* class and the other class being the *negative* class. Here, positive don't represent benefit or value, but rather what the object of study is. So when looking for spam, “positive” could mean the spam class. Which of the two classes is called positive is often a subjective manner, and specific to the domain.FI

[/info box]

The iris example on the other hand is an example of a multi-class classification problem.

Another example of a multi-class classification problem is predicting what language a website is in from the text on the website. The classes here would be a pre-defined list of possible languages.

For regression tasks, the goal is to predict a continuous number, or a *floating point number* in programming terms (a real number in mathematical terms). Predicting a person's annual income from their education, their age and where they live, is a[n example of a] regression task. When predicting income, the predicted value is an *amount*, and can be any number in a given range. Another example of a regression task is predicting the yield of a corn farm, given attributes such as previous yields, weather and number of employees working on the farm. The yield again can be an arbitrary number.

An easy way to distinguish between classification and regression tasks is to ask whether there is some kind of ordering or continuity in the output. If there is an ordering, or a continuity between possible outcomes, then the problem is a regression problem.

Think about predicting annual income. There is a clear ordering of “making more money” or “making less money”. There is a natural understanding that 40.000\$ per year is *between* 50.000\$ per year and 30.000\$ per year. There is also a continuity in the output. Whether a person makes 40,000\$ or 40,001\$ a year does not make a tangible difference, even though they are different amounts of money. So if our algorithm predicts 39,999\$ or 40,001\$ when it should have predicted 40,000\$, we don't mind that much.

Contrastively, for the task of recognizing the language of a website (which is a classification problem), there is no matter of degree. A website is in one language, or it is in another. There is no continuity between languages, and there is no language that is *between* English and French [footnote: We ask linguists to excuse the simplified presentation of languages as distinct and fixed entities].



# Generalization, Overfitting and Underfitting

In supervised learning, we want to build a model on the training data, and then be able to make accurate predictions on new, unseen data, that has the same characteristics as the training set that we used. If a model is able to make accurate predictions on unseen data, we say it is able to *generalize* from the training set to the test set.

We want to build a model that is able to generalize as well as possible.

Usually we build a model in such a way that it can make accurate predictions on the training set. If the training and test set have enough in common, we expect the model to also be accurate on the test set.

However, there are some cases where this can go wrong. For example, if we allow ourselves to build very complex models, we can always be as accurate as we like on the training set.

Let's take a look at a made-up example. Say a novice data scientist wants to predict a person's salary, and for each person, the only characteristic he has is the date of birth. The dataset might look like this:

```
|Date of Birth|Annual salary ($)|
|-|-|
|30/4/1950|50500|
|05/8/1964|41000|
|09/2/2001|35200|
|17/5/1989|36000|
```

Because our novice data scientist knows he needs to present a machine learning algorithm with numbers, he replaces the date of birth with each person's age at the time of analysis, in 2016. That seems very little to go by, so our novice data scientist also adds the last four digits of their social security number, their house number, their zip code, and the number of their children.

Now the data looks like this:

```
|Age|SSN|House|ZIP|Children|Annual salary ($)|
|-|-|-|-|-|-|
|66|1882|19|10030|2|50500|
|52|1337|2|10028|0|41000|
|22|3467|8|10041|1|35200|
|25|8391|27|10009|4|36000|
```

Now he builds a machine learning model using the first three rows as a training set. Let's save how the algorithm works for later. The algorithm produces the following formula for the annual salary:

$$\text{salary} = 333 * x[0] + 1 * x[1] + 237 * x[2] - 20 * x[3] + 26 * x[4] + 225866$$

Here  $x[0]$  to  $x[4]$  contain the age, last digits of the SSN, the house number, ZIP code and number of children.

The formula works very well on the training set, the first three rows of the dataset. The predictions for the training set are 53681, 44433 and 37761 which are very close to the true values.

However, the prediction the formula makes for the fourth point in the dataset, which was not part of the training set, is 48905, which is quite far from the 36000 which was the desired output.

So what happened here? The data scientist allowed his machine learning algorithm to build a relatively complex interaction between the five features and the output (the annual salary) without a lot of support for this model in the data. The result is a model that doesn't reflect a real world relationship. For example, this model predicts that you would make \$237 more if you move to the house next door (237 is the coefficient for  $x[2]$ !

Building a complex model that does well on the training set but does not generalize to new data is known as *overfitting*, because we are focusing too much on the particularities of the training data. Avoiding overfitting is a crucial aspect of building a successful machine learning model. A good way to avoid overfitting is to restrict ourselves to building very simple models.

A much simpler model for the salary prediction task is to always predict the average salary of the three people in the training set, which is

Predicting that everybody's salary is 42233 is clearly too simple, and does not capture the variation in our training set very well. Using too simple a model is called *underfitting*, because we don't explain the target output for the training data well enough.

A middle ground for the salary prediction would be to use age as a single feature, which restricts us to very simple models, but still allows us to capture some trends in our data.

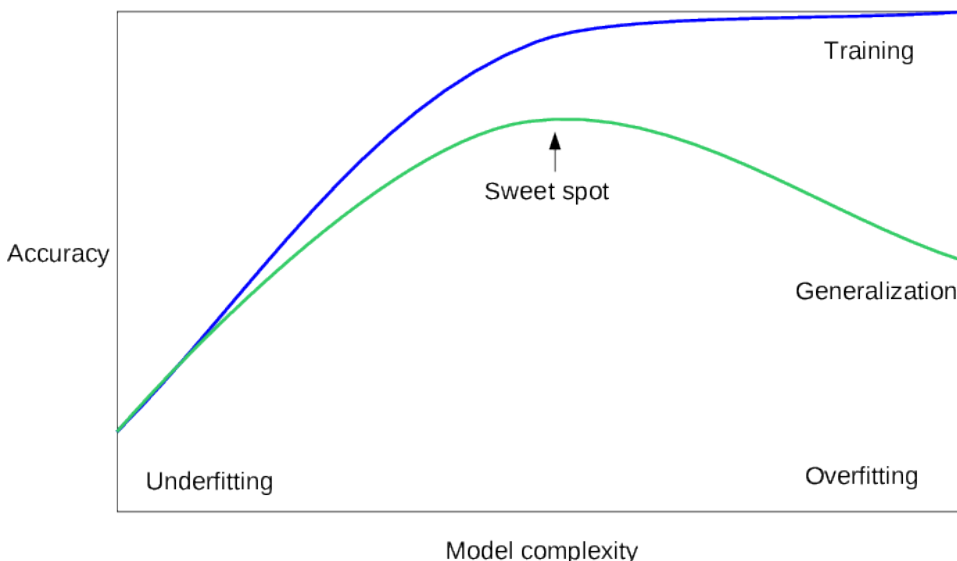
A model only including the age feature is:

$$\text{salary} = 323 * \text{age} + 27146$$

This model makes predictions of 48464, 43942, and 34252 for the training set, which is not as good as our previous model.

However, it generalizes much better to the test set when compared to the complex model we used before. It predicts 35221 for the fourth row in the table.

The trade-off between overfitting and underfitting is illustrated in Figure model\_complexity.



If we choose use a model that is too simple, we will do badly on the training set, and similarly badly on the test set, as we would using only the mean prediction.

The more complex we allow our model to be, the better we will be able to predict on the training data. However, if our model becomes too complex, we start focusing too much on the particularities of our training set, and the model will not generalize well to new data.

There is a sweet spot in between, which will yield the best generalization performance. This is the model we want to find.

Understanding the implications of model complexity is hard, and has different implications for each kind of machine learning model.

## Supervised Machine Learning Algorithms

We will now go through the most popular machine learning algorithms and explain how they learn from data and how they make predictions. We will also discuss how the concept of model complexity plays out for each of these models.

While an in-depth discussion of each algorithm is beyond the scope of this book, we will try to give some intuition about how each algorithm builds a model.

We will also discuss strength and weaknesses of each algorithm, and what kind of data they can be best applied to. We will also explain the meaning of the most important parameters and options. Discussing all of them is beyond the scope of the book, and we refer you to the scikit-learn documentation for more details.

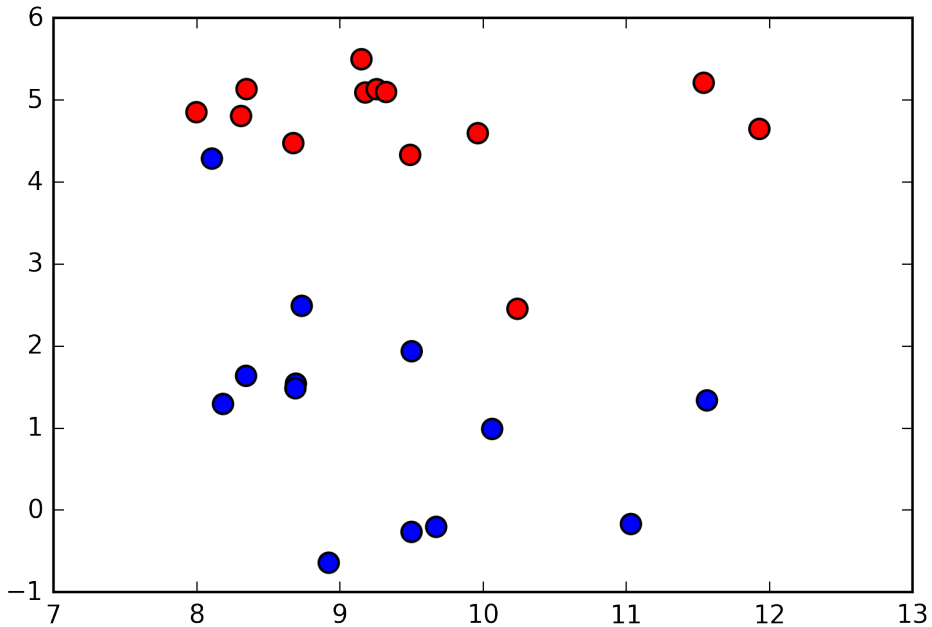
Many algorithms have a classification and a regression variant, and we will describe both.

It is not necessary to read through the description of each algorithm in detail, but understanding the models will give you a better feeling for the different ways machine learning algorithms can work. This chapter can also be used as a reference guide, and you can come back to it when you are unsure about the workings of any of the algorithms.

We will use several datasets to illustrate the different algorithms. Some of the datasets will be small synthetic (meaning made-up) datasets, designed to highlight particular aspects of the algorithms. Other datasets will be larger, real world examples datasets.

An example of a synthetic two-class classification dataset is the `forge` dataset, which has two features. Below is a scatter plot visualizing all of the data points in this dataset. The plot has the first feature on the x-axis and the second feature on the y-axis. As is always the case in scatter plots, each data point is represented as one dot. The color of the dot indicates its class, with red meaning class 0 and blue meaning class 1.

```
X, y = mglearn.datasets.make_forge()
plt.scatter(X[:, 0], X[:, 1], c=y, s=60, cmap=mglearn.cm2)
print("X.shape: %s" % (X.shape,))
```



`X.shape: (26, 2)`

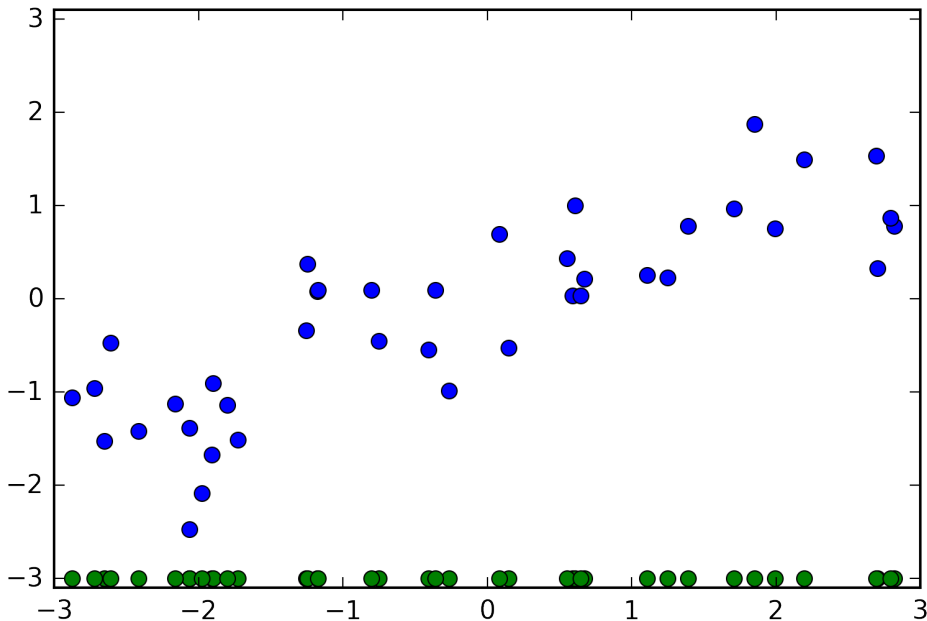
As you can see from `X.shape`, this dataset consists of 26 data points, with 2 features.

To illustrate regression algorithms, we will use the synthetic wave dataset shown below. The `wave` dataset only has a single input feature, and a continuous target variable (or *response*) that we want to model.

The plot below is showing the single feature on the x-axis, with the data points as green dots. For each data point, the target output is plotted in blue on the y-axis.

```
X, y = mglearn.datasets.make_wave(n_samples=40)
```

```
plt.plot(X, y, 'o')
plt.plot(X, -3 * np.ones(len(X)), 'o')
plt.ylim(-3.1, 3.1)
```



We are using these very simple, low-dimensional datasets as we can easily visualize them -- a computer monitor has two dimensions, so data with more than two features is hard to show. Any intuition derived from datasets with few features (also called *low-dimensional* datasets) might not hold in datasets with many features (*high dimensional* datasets). As long as you keep that in mind, inspecting algorithms on low-dimensional datasets can be very instructive.

We will complement these small synthetic dataset with two real-world datasets that are included in scikit-learn. One is the Wisconsin breast cancer dataset (or cancer for short), which records clinical measurements of breast cancer tumors. Each tumor is labeled as “benign” (for harmless tumors) or “malignant” (for cancerous tumors), and the task is to learn to predict whether a tumor is malignant based on the measurements of the tissue.

The data can be loaded using the `load_breast_cancer` from scikit-learn. Datasets that are included in scikit-learn are usually stored as Bunch objects, which contain some information about the dataset as well as the actual data.

All you need to know about Bunch objects is that they behave like dictionaries, with the added benefit that you can access values using a dot (as in `bunch.key` instead of `bunch['key']`).

```

from sklearn.datasets import load_breast_cancer
cancer = load_breast_cancer()
cancer.keys()

dict_keys(['DESCR', 'target_names', 'data', 'target', 'feature_names'])

```

The dataset consists of 569 data points, with 30 features each:

```

print(cancer.data.shape)

(569, 30)

```

Of these 569 data points, 212 are labeled as malignant, and 357 as benign:

```

print(cancer.target_names)
np.bincount(cancer.target)

array([212, 357])

['malignant' 'benign']

```

To get a description of the semantic meaning of each feature, we can have a look at the `feature_names` attribute:

```

cancer.feature_names

array(['mean radius', 'mean texture', 'mean perimeter', 'mean area',
      'mean smoothness', 'mean compactness', 'mean concavity',
      'mean concave points', 'mean symmetry', 'mean fractal dimension',
      'radius error', 'texture error', 'perimeter error', 'area error',
      'smoothness error', 'compactness error', 'concavity error',
      'concave points error', 'symmetry error', 'fractal dimension error',
      'worst radius', 'worst texture', 'worst perimeter', 'worst area',
      'worst smoothness', 'worst compactness', 'worst concavity',
      'worst concave points', 'worst symmetry', 'worst fractal dimension'],
      dtype='<U23')

```

You can find out more about the data by reading `cancer.DESCR` if you are interested.

We will also be using a real-world regression dataset, the Boston Housing dataset. The task associated with this dataset is to predict the median value of homes in several Boston neighborhoods in the 1970s, using information about the neighborhoods such as crime rate, proximity to the Charles River, highway accessibility and so on.

The datasets contains 506 data points, described by 13 features:

```
from sklearn.datasets import load_boston
boston = load_boston()
print(boston.data.shape)

(506, 13)
```

Again, you can get more information about the dataset by reading the `DESCR` attribute of `boston`.

For our purposes here, we will actually expand this dataset, by not only considering these 13 measurements as input features, but also looking at all products (also called *interactions*) between features.

In other words, we will not only consider crime rate and highway accessibility as a feature, but also the product of crime rate and highway accessibility. Including derived feature like these is called *feature engineering*, which we will discuss in more detail in Chapter 5 (Representing Data).

This derived dataset can be loaded using the `load_extended_boston` function:

```
X, y = mglearn.datasets.load_extended_boston()
print(X.shape)

(506, 105)
```

The resulting 105 features are the 13 original features, the 13 choose 2 = 91 (Footnote: the number of ways to pick 2 elements out of 13 elements) features that are product of two features, and one constant feature.

We will use these datasets to explain and illustrate the properties of the different machine learning algorithms. But for now, let's get to the algorithms themselves. First, we will revisit the k-Nearest Neighbor algorithm, that we already saw in the last chapter.

## k-Nearest Neighbor

The k-Nearest Neighbors (kNN) algorithm is arguably the simplest machine learning algorithm. Building the model only consists of storing the training dataset. To make a prediction for a new data point, the algorithm finds the closest data points in the training dataset, it “nearest neighbors”.

### k-Neighbors Classification

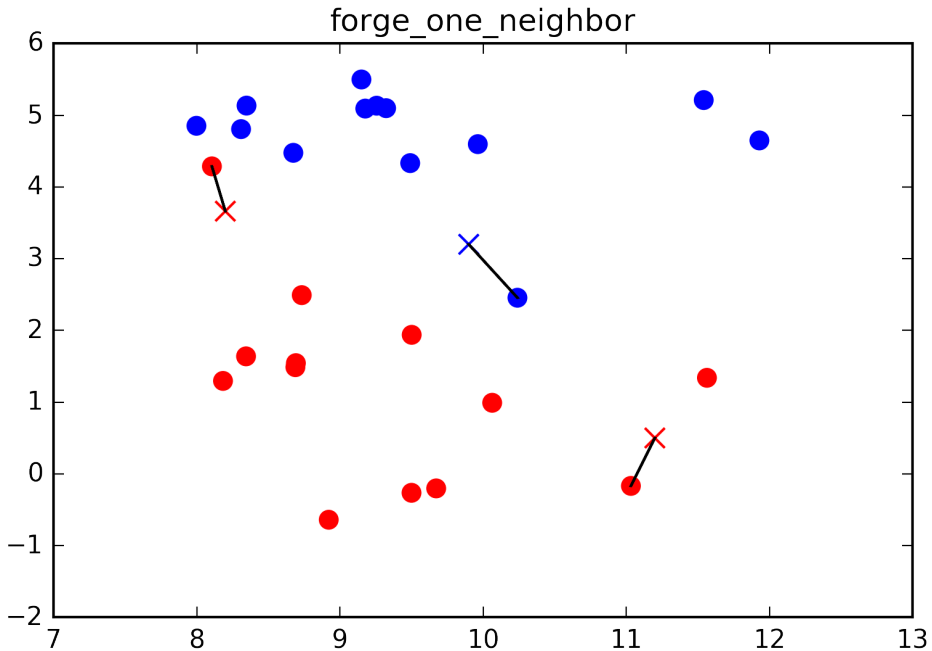
In its simplest version, the algorithm only considers exactly one nearest neighbor, which is the closest training data point to the point we want to make a prediction for.

The prediction is then simply the known output for this training point.

Figure `forge_one_neighbor` illustrates this for the case of classification on the `forge` dataset.



```
mglearn.plots.plot_knn_classification(n_neighbors=1)
plt.title("forge_one_neighbor");
```

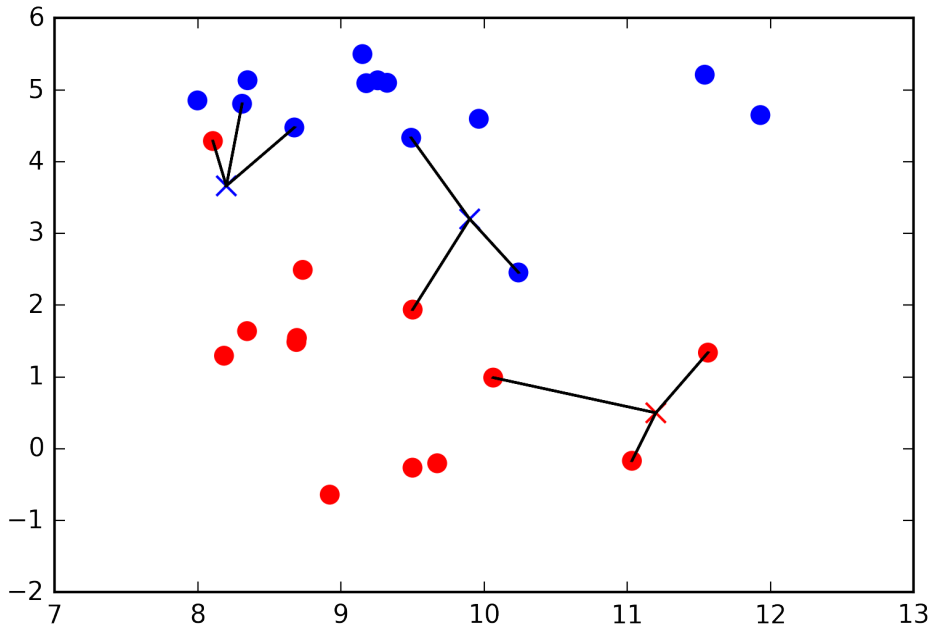


Here, we added three new data points, shown as crosses. For each of them, we marked the closest point in the training set. The prediction of the one-nearest-neighbor algorithm is the label of that point (shown by the color of the cross).

Instead of considering only the closest neighbor, we can also consider an arbitrary number  $k$  of neighbors. This is where the name of the  $k$  neighbors algorithm comes from. When considering more than one neighbor, we use *voting* to assign a label. This means, for each test point, we count how many neighbors are red, and how many neighbors are blue. We then assign the class that is more frequent: in other words, the majority class among the  $k$  neighbors.

Below is an illustration using the three closest neighbors. Again, the prediction is shown as the color of the cross. You can see that the prediction changed for the point in the top left from using only one neighbor.

```
mglearn.plots.plot_knn_classification(n_neighbors=3)
```



While this illustration is for a binary classification problem, you can imagine this working with any number of classes. For more classes, we count how many neighbors belong to each class, and again predict the most common class.

Now let's look at how we can apply the  $k$  nearest neighbors algorithm using scikit-learn.

First, we split our data into a training and a test set, so we can evaluate generalization performance, as discussed in Chapter 1 (Introduction).

```
from sklearn.model_selection import train_test_split
X, y = mglearn.datasets.make_forge()
```

```
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
```

Next we import and instantiate the class. This is when we can set parameters, like the number of neighbors to use. Here, we set it to three.

```
from sklearn.neighbors import KNeighborsClassifier
clf = KNeighborsClassifier(n_neighbors=3)
```

Now, we fit the classifier using the training set. For `KNeighborsClassifier` this means storing the dataset, so we can compute neighbors during prediction.

```
clf.fit(X_train, y_train)
KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='minkowski',
```

```
metric_params=None, n_jobs=1, n_neighbors=3, p=2,
weights='uniform')
```

To make predictions on the test data, we call the `predict` method. This computes the nearest neighbors in the training set and finds the most common class among these:

```
clf.predict(X_test)
array([1, 0, 1, 0, 1, 0, 0])
```

To evaluate how well our model generalizes, we can call the `score` method with the test data together with the test labels:

```
clf.score(X_test, y_test)
0.8571428571428571
```

We see that our model is about 86% accurate, meaning the model predicted the class correctly for 85% of the samples in the test dataset.

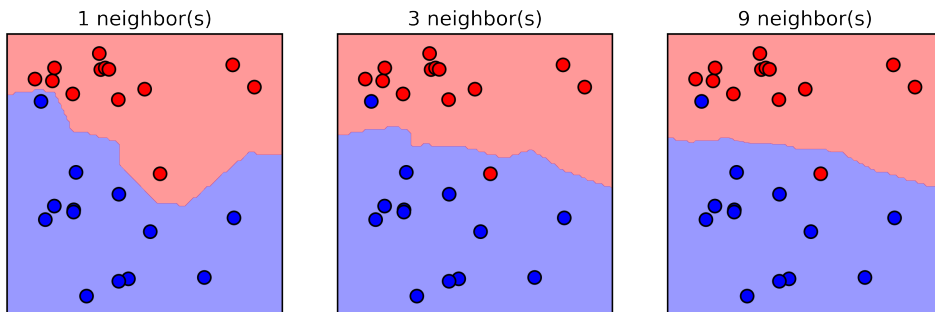
## Analyzing KNeighborsClassifier

For two-dimensional datasets, we can also illustrate the prediction for all possible test point in the *xy*-plane. We color the plane red in regions where points would be assigned the red class, and blue otherwise. This lets us view the *decision boundary*, which is the divide between where the algorithm assigns class red versus where it assigns class blue.

Here is a visualization of the decision boundary for one, three and five neighbors:

```
fig, axes = plt.subplots(1, 3, figsize=(10, 3))

for n_neighbors, ax in zip([1, 3, 9], axes):
    clf = KNeighborsClassifier(n_neighbors=n_neighbors).fit(X, y)
    mglearn.plots.plot_2d_separator(clf, X, fill=True, eps=0.5, ax=ax, alpha=.4)
    ax.scatter(X[:, 0], X[:, 1], c=y, s=60, cmap=mglearn.cm2)
    ax.set_title("%d neighbor(s)" % n_neighbors)
```



As you can see in the left figure, using a single neighbor results in a decision boundary that follows the training data closely. Considering more and more neighbors leads to a smoother decision boundary. A smoother boundary corresponds to a simple model. In other words, using few neighbors corresponds to high model complexity (as shown on the right side of Figure model\_complexity), and using many neighbors corresponds to low model complexity (as shown on the left side of Figure model\_complexity).

Let's investigate whether we can confirm the connection between model complexity and generalization that we discussed above.

We will do this on the real world breast cancer dataset.

We begin by splitting the dataset into a training and a test set. Then we will evaluate training and test set performance with different numbers of neighbors.

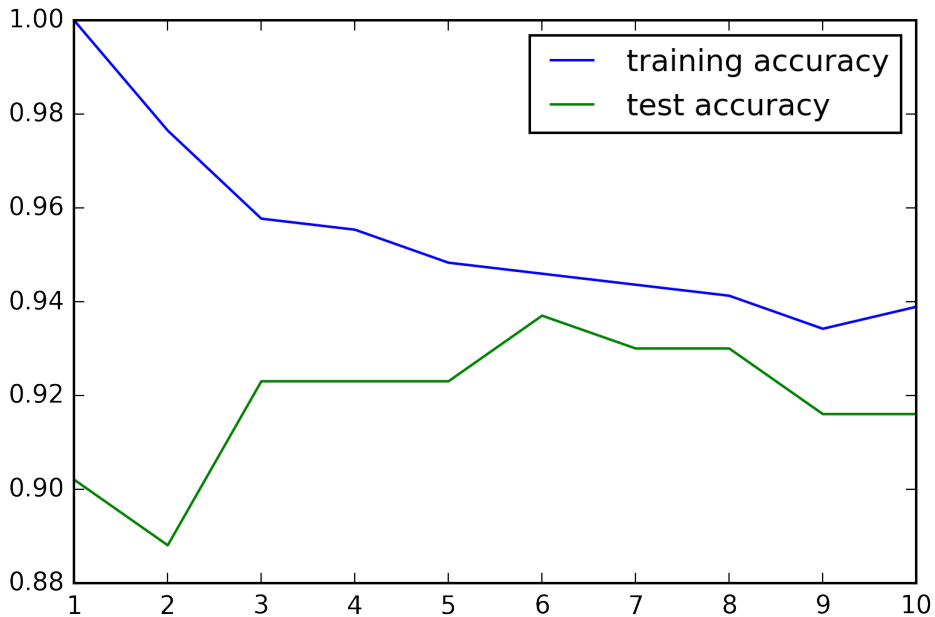
```
from sklearn.datasets import load_breast_cancer

cancer = load_breast_cancer()
X_train, X_test, y_train, y_test = train_test_split(
    cancer.data, cancer.target, stratify=cancer.target, random_state=66)

training_accuracy = []
test_accuracy = []
# try n_neighbors from 1 to 10.
neighbors_settings = range(1, 11)

for n_neighbors in neighbors_settings:
    # build the model
    clf = KNeighborsClassifier(n_neighbors=n_neighbors)
    clf.fit(X_train, y_train)
    # record training set accuracy
    training_accuracy.append(clf.score(X_train, y_train))
    # record generalization accuracy
    test_accuracy.append(clf.score(X_test, y_test))

plt.plot(neighbors_settings, training_accuracy, label="training accuracy")
plt.plot(neighbors_settings, test_accuracy, label="test accuracy")
plt.legend()
```



The plot shows the training and test set accuracy on the y axis against the setting of `n_neighbors` on the x axis. While the real world plots are rarely very smooth, we can still recognize some of the characteristics of overfitting and underfitting. As considering fewer neighbors corresponds to a more complex model, the plot is horizontally flipped relative to the illustration in Figure `model_complexity`.

Considering a single nearest neighbor, the prediction on the training set is perfect. Considering more neighbors, the model becomes more simple, and the training accuracy drops.

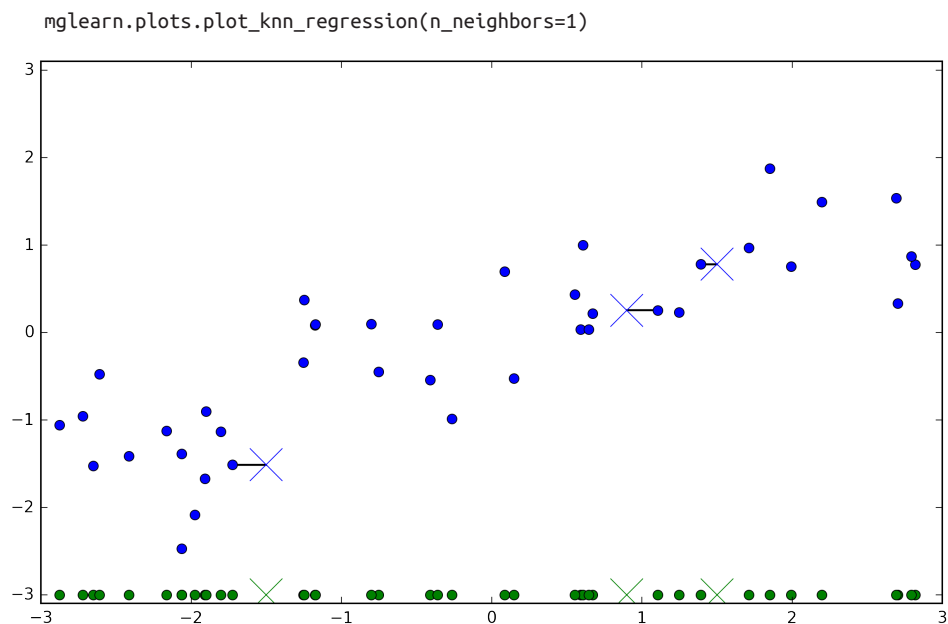
The test set accuracy for using a single neighbor is lower than when using more neighbors, indicating that using a single nearest neighbor leads to a model that is too complex. On the other hand, when considering 10 neighbors, the model is too simple, and performance is even worse. The best performance is somewhere in the middle, around using six neighbors.

Still, it is good to keep the scale of the plot in mind. The worst performance is around 88% accuracy, which might still be acceptable.

## k-Neighbors Regression

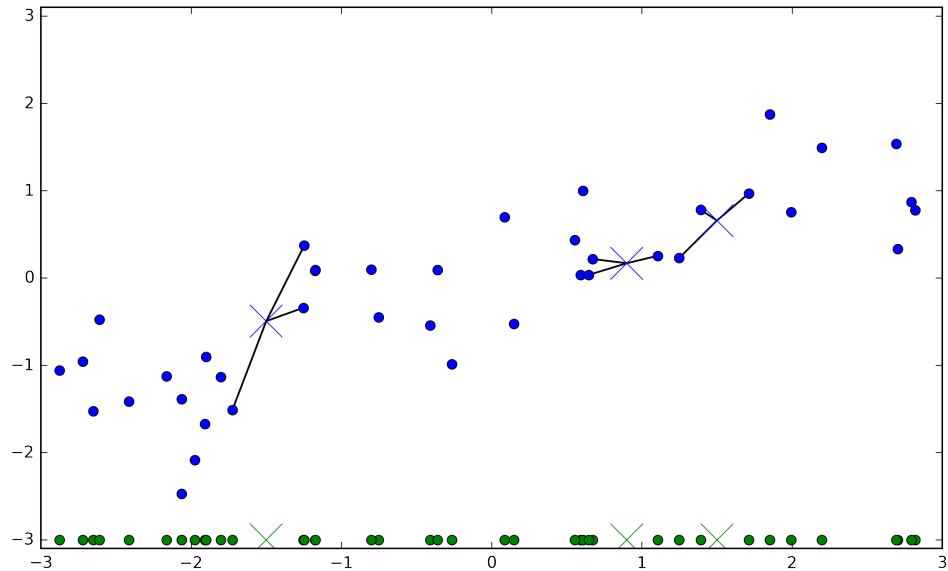
There is also a regression variant of the k-nearest neighbors algorithm. Again, let's start by using a single nearest neighbor, this time using the wave dataset. We added three test data points as green crosses on the x axis.

The prediction using a single neighbor is just the target value of the nearest neighbor, shown as the blue cross:



Again, we can also use more than one nearest neighbor for regression. When using multiple nearest neighbors for regression, the prediction is the average (or mean) of the relevant neighbors:

```
mglearn.plots.plot_knn_regression(n_neighbors=3)
```



The k nearest neighbors algorithm for regression is implemented in the `KNeighborsRegressor` class in scikit-learn.

Using it looks much like the `KNeighborsClassifier` above:

```
from sklearn.neighbors import KNeighborsRegressor

X, y = mglearn.datasets.make_wave(n_samples=40)

# split the wave dataset into a training and a test set
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)

# Instantiate the model, set the number of neighbors to consider to 3:
reg = KNeighborsRegressor(n_neighbors=3)
# Fit the model using the training data and training targets:
reg.fit(X_train, y_train)

KNeighborsRegressor(algorithm='auto', leaf_size=30, metric='minkowski',
                    metric_params=None, n_jobs=1, n_neighbors=3, p=2,
                    weights='uniform')
```

Now, we can make predictions on the test set:

```
reg.predict(X_test)
array([-0.05396539,  0.35686046,  1.13671923, -1.89415682, -1.13881398,
        -1.63113382,  0.35686046,  0.91241374, -0.44680446, -1.13881398])
```

We can also evaluate the model using the score method, which for regressors returns the  $R^2$  score.

The  $R^2$  score, also known as coefficient of determination, is a measure of goodness of a prediction for a regression model, and yields a score up to 1. A value of 1 corresponds to a perfect prediction, and a value of 0 corresponds to a constant model that just predicts the mean of the training set responses  $y_{train}$ .

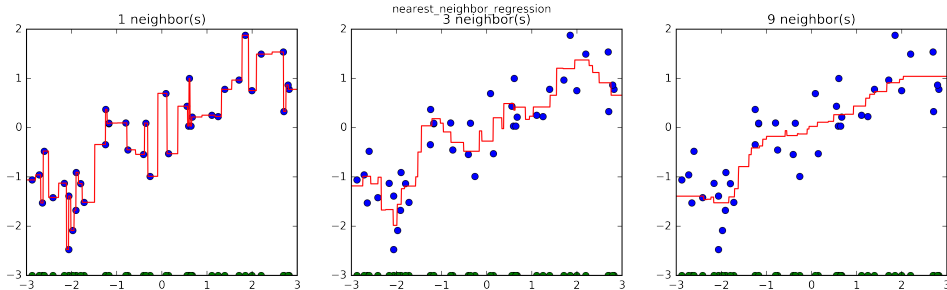
```
reg.score(X_test, y_test)
0.83441724462496036
```

Here, the score is 0.83 which indicates a relatively good model fit.

## Analyzing $k$ nearest neighbors regression

For our one-dimensional dataset, we can see what the predictions look like for all possible feature values. To do this, we create a test-dataset consisting of many points on the line.

```
fig, axes = plt.subplots(1, 3, figsize=(15, 4))
# create 1000 data points, evenly spaced between -3 and 3
line = np.linspace(-3, 3, 1000).reshape(-1, 1)
plt.suptitle("nearest_neighbor_regression")
for n_neighbors, ax in zip([1, 3, 9], axes):
    # make predictions using 1, 3 or 9 neighbors
    reg = KNeighborsRegressor(n_neighbors=n_neighbors).fit(X, y)
    ax.plot(X, y, 'o')
    ax.plot(X, -3 * np.ones(len(X)), 'o')
    ax.plot(line, reg.predict(line))
    ax.set_title("%d neighbor(s)" % n_neighbors)
```



In the plots above, the blue points are again the responses for the training data, while the red line is the prediction made by the model for all points on the line.

Using only a single neighbor, each point in the training set has an obvious influence on the predictions, and the predicted values go through all of the data points. This leads to a very unsteady prediction. Considering more neighbors leads to smoother predictions, but these do not fit the training data as well.



## Strengths, weaknesses and parameters

In principal, there are two important parameters to the KNeighbors classifier: the number of neighbors and how you measure distance between data points. In practice, using a small number of neighbors like 3 or 5 often works well, but you should certainly adjust this parameter. Choosing the right distance measure is somewhat beyond the scope of this book. By default, Euclidean distance is used, which works well in many settings.

One of the strengths of nearest neighbors is that the model is very easy to understand, and often gives reasonable performance without a lot of adjustments. Using nearest neighbors is a good baseline method to try before considering more advanced techniques. Building the nearest neighbors model is usually very fast, but when your training set is very large (either in number of features or in number of samples) prediction can be slow.

When using nearest neighbors, it's important to preprocess your data (see Chapter 3 Unsupervised Learning). Nearest neighbors often does not perform well on dataset with very many features, in particular sparse datasets, a common type of data in which there are many features, but only few of the features are non-zero for any given data point.

So while the nearest neighbors algorithm is easy to understand, it is not often used in practice, due to prediction being slow, and its inability to handle many features. The method we discuss next has neither of these drawbacks.

## Linear models

Linear models are a class of models that are widely used in practice, and have been studied extensively in the last few decades, with roots going back over a hundred years.

Linear models are models that make a prediction that using a *linear function* of the input features, which we will explain below.

### Linear models for regression

For regression, the general prediction formula for a linear model looks as follows:

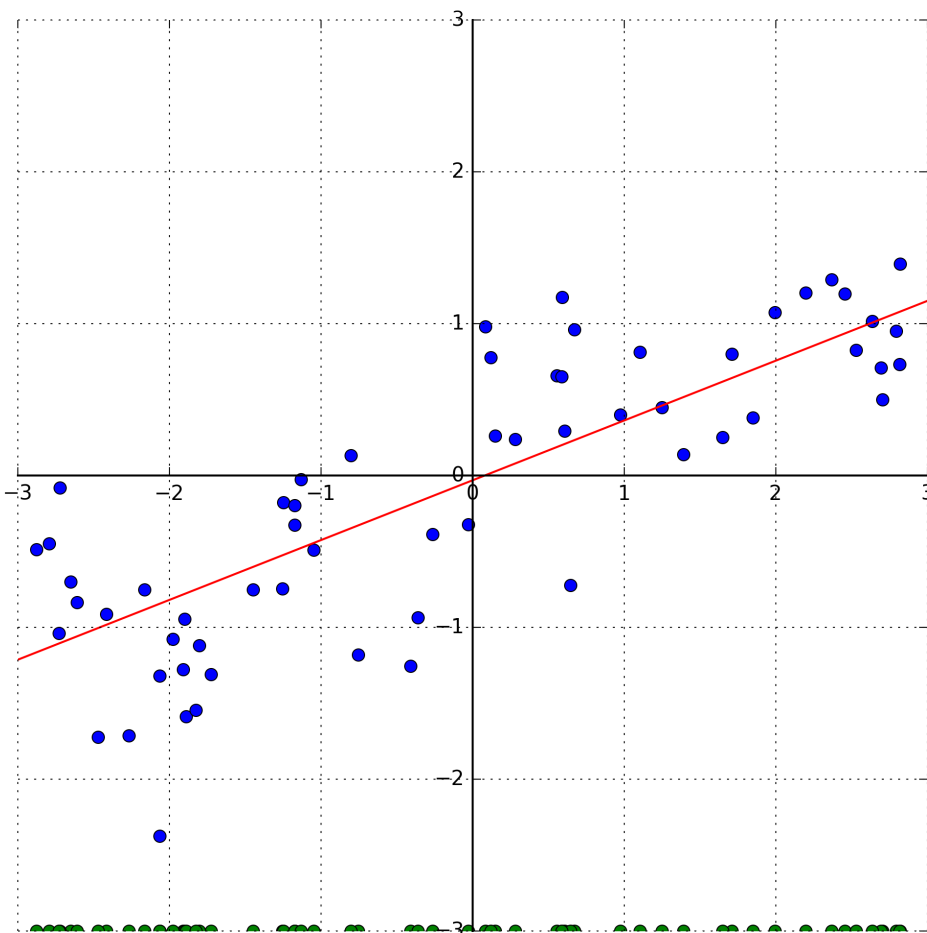
$$\begin{aligned} \hat{y} &= w[0] x[0] + w[1] x[1] + \dots + w[p] x[p] + b \end{aligned} \text{ (1) linear regression}$$

Here,  $x[0]$  to  $x[p]$  denotes the features (here the number of features is  $p$ ) of a single data point,  $w$  and  $b$  are parameters of the model that are learned, and  $\hat{y}$  is the prediction the model makes. For a dataset with a single feature, this is

which you might remember as the equation for a line from high school mathematics. Here,  $w[0]$  is the slope, and  $b$  is the y-axis offset. For more features,  $w$  contains the slopes along each feature axis. Alternatively, you can think of the predicted response as being a weighted sum of the input features, with weights (which can be negative) given by the entries of  $w$ .

Trying to learn the parameters  $w[0]$  and  $b$  on our one-dimensional wave dataset might lead to the following line:

```
mglearn.plots.plot_linear_regression_wave()
```



```
w[0]: 0.393906  b: -0.031804
```

We added a coordinate cross into the plot to make it easier to understand the line. Looking at  $w[0]$  we see that the slope should be roughly around .4, which we can confirm visually in the plot above. The intercept is where the prediction line should cross the  $y$ -axis, which is slightly below 0, which you can also confirm in the image.

Linear models for regression can be characterized as regression models for which the prediction is a line for a single feature, a plane when using two features, or a hyper-plane in higher dimensions (that is when having more features).

If you compare the predictions made by the red line with those made by the `KNeighborsRegressor` in Figure `nearest_neighbor_regression`, using a straight line to make predictions seems very restrictive. It looks like all the fine details of the data are lost. In a sense this is true. It is a strong (and somewhat unrealistic) assumption that our target  $y$  is a linear combination of the features. But looking at one-dimensional data gives a somewhat skewed perspective. For datasets with many features, linear models can be very powerful. In particular, if you have more features than training data points, any target  $y$  can be perfectly modeled (on the training set) as a linear function (FOOTNOTE This is easy to see if you know some linear algebra).

There are many different linear models for regression. The difference between these models is how the model parameters  $w$  and  $b$  are learned from the training data, and how model complexity can be controlled. We will now go through the most popular linear models for regression.

## Linear Regression aka Ordinary Least Squares

Linear regression or *Ordinary Least Squares* (OLS) is the simplest and most classic linear method for regression.

Linear regression finds the parameters  $w$  and  $b$  that minimize the *mean squared error* between predictions and the true regression targets  $y$  on the training set. The mean squared error is the sum of the squared differences between the predictions and the true values. Linear regression has no parameters, which is a benefit, but it also has no way to control model complexity.

Here is the code that produces the model you can see in figure XX.

```
from sklearn.linear_model import LinearRegression
X, y = mglearn.datasets.make_wave(n_samples=60)
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=42)

lr = LinearRegression().fit(X_train, y_train)
```

The “slope” parameters  $w$ , also called weights or *coefficients* are stored in the `coef_` attribute, while the offset or *intercept*  $b$  is stored in the `intercept_` attribute. [Footnote: you might notice the strange-looking trailing underscore. Scikit-learn always

stores anything that is derived from the training data in attributes that end with a trailing underscore. That is to separate them from parameters that are set by the user.]

```
print("lr.coef_: %s" % lr.coef_)
print("lr.intercept_: %s" % lr.intercept_)

lr.coef_: [ 0.39390555]

lr.intercept_: -0.0318043430268
```

The `intercept_` attribute is always a single float number, while the `coef_` attribute is a numpy array with one entry per input feature. As we only have a single input feature in the wave dataset, `lr.coef_` only has a single entry.

Let's look at the training set and test set performance:

```
print("training set score: %f" % lr.score(X_train, y_train))
print("test set score: %f" % lr.score(X_test, y_test))

training set score: 0.670089

test set score: 0.659337
```

An  $R^2$  of around .66 is not very good, but we can see that the score on training and test set are very close together. This means we are likely underfitting, not overfitting. For this one-dimensional dataset, there is little danger of overfitting, as the model is very simple (or restricted).

However, with higher dimensional datasets (meaning a large number of features), linear models become more powerful, and there is a higher chance of overfitting.

Let's take a look at how `LinearRegression` performs on a more complex dataset, like the Boston Housing dataset. Remember that this dataset has 506 samples and 105 derived features.

We load the dataset and split it into a training and a test set. Then we build the linear regression model as before:

```
X, y = mglearn.datasets.load_extended_boston()

X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
lr = LinearRegression().fit(X_train, y_train)
```

When comparing training set and test set score, we find that we predict very accurately on the training set, but the  $R^2$  on the test set is much worse:

```
print("training set score: %f" % lr.score(X_train, y_train))
print("test set score: %f" % lr.score(X_test, y_test))

training set score: 0.952353

test set score: 0.605775
```

This is a clear sign of overfitting, and therefore we should try to find a model that allows us to control complexity.

One of the most commonly used alternatives to standard linear regression is *Ridge regression*, which we will look into next.

## Ridge regression

Ridge regression is also a linear model for regression, so the formula it uses to make predictions is still Formula (1), as for ordinary least squares. In Ridge regression, the coefficients  $w$  are chosen not only so that they predict well on the training data, but there is an additional constraint. We also want the magnitude of coefficients to be as small as possible; in other words, all entries of  $w$  should be close to 0.

Intuitively, this means each feature should have as little effect on the outcome as possible (which translates to having a small slope), while still predicting well.

This constraint is an example of what is called *regularization*. Regularization means explicitly restricting a model to avoid overfitting. The particular kind used by Ridge regression is known as  $l_2$  regularization. [footnote: Mathematically, Ridge penalizes the  $l_2$  norm of the coefficients, or the Euclidean length of  $w$ .]

Ridge regression is implemented in `linear_model.Ridge`. Let's see how well it does on the extended Boston dataset:

```
from sklearn.linear_model import Ridge

ridge = Ridge().fit(X_train, y_train)
print("training set score: %f" % ridge.score(X_train, y_train))
print("test set score: %f" % ridge.score(X_test, y_test))

training set score: 0.886058

test set score: 0.752714
```

As you can see, the training set score of Ridge is *lower* than for LinearRegression, while the test set score is *higher*. This is consistent with our expectation. With linear regression, we were overfitting to our data. Ridge is a more restricted model, so we are less likely to overfit. A less complex model means worse performance on the training set, but better generalization.

As we are only interested in generalization performance, we should choose the Ridge model over the LinearRegression model.

The Ridge model makes a trade-off between the simplicity of the model (near zero coefficients) and its performance on the training set. How much importance the model places on simplicity versus training set performance can be specified by the user, using the `alpha` parameter. Above, we used the default parameter `alpha=1.0`. There is no reason why this would give us the best trade-off, though. Increasing `alpha`

forces coefficients to move more towards zero, which decreases training set performance, but might help generalization.

```
ridge10 = Ridge(alpha=10).fit(X_train, y_train)
print("training set score: %f" % ridge10.score(X_train, y_train))
print("test set score: %f" % ridge10.score(X_test, y_test))

training set score: 0.788346

test set score: 0.635897
```

Decreasing alpha allows the coefficients to be less restricted, meaning we move right on the figure XXX.

For very small values of alpha, coefficients are barely restricted at all, and we end up with a model that resembles LinearRegression.

```
ridge01 = Ridge(alpha=0.1).fit(X_train, y_train)
print("training set score: %f" % ridge01.score(X_train, y_train))
print("test set score: %f" % ridge01.score(X_test, y_test))

training set score: 0.928578

test set score: 0.771793
```

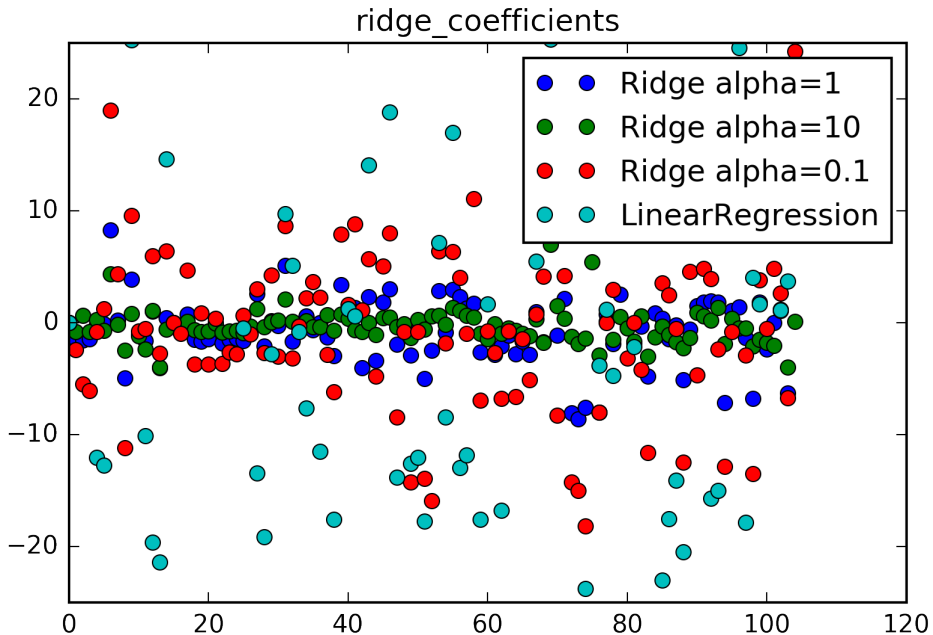
Here,  $\alpha=0.1$  seems to be working well. We could try decreasing alpha even more to improve generalization. For now, notice how the parameter alpha corresponds to the model complexity as shown in Figure model\_complexity. We will discuss methods to properly select parameters in Chapter 6 (Model Selection).

We can also get a more qualitative insight into how the alpha parameter changes the model by inspecting the `coef_` attribute of models with different values of alpha. A higher alpha means a more restricted model, so we expect that the entries of `coef_` have smaller magnitude for a high value of alpha than for a low value of alpha.

This is confirmed in the plot below:

```
plt.title("ridge_coefficients")
plt.plot(ridge.coef_, 'o', label="Ridge alpha=1")
plt.plot(ridge10.coef_, 'o', label="Ridge alpha=10")
plt.plot(ridge01.coef_, 'o', label="Ridge alpha=0.1")

plt.plot(lr.coef_, 'o', label="LinearRegression")
plt.ylim(-25, 25)
plt.legend()
```



Here, the x-axis enumerates the entries of `coef_`:  $x=0$  shows the coefficient associated with the first feature,  $x=1$  the coefficient associated with the second feature, and so on up to  $x=100$ . The y-axis shows the numeric value of the corresponding value of the coefficient. The main take-away here is that for  $\alpha=10$  (as shown by the green dots), the coefficients are mostly between around -3 and 3. The coefficients for the ridge model with  $\alpha=1$  (as shown by the blue dots), are somewhat larger. The red dots have larger magnitude still, and many of the teal dots, corresponding to linear regression without any regularization (which would be  $\alpha=0$ ) are so large they are even outside of the chart.

## Lasso

An alternative to Ridge for regularizing linear regression is the *Lasso*. The lasso also restricts coefficients to be close to zero, similarly to Ridge regression, but in a slightly different way, called “l1” regularization.[footnote: The Lasso penalizes the l1 norm of the coefficient vector, or in other words the sum of the absolute values of the coefficients].

The consequence of l1 regularization is that when using the Lasso, some coefficients are *exactly zero*. This means some features are entirely ignored by the model. This can be seen as a form of automatic *feature selection*. Having some coefficients be exactly zero often makes a model easier to interpret, and can reveal the most important features of your model.

Let's apply the lasso to the extended Boston housing dataset:

```
from sklearn.linear_model import Lasso

lasso = Lasso().fit(X_train, y_train)
print("training set score: %f" % lasso.score(X_train, y_train))
print("test set score: %f" % lasso.score(X_test, y_test))
print("number of features used: %d" % np.sum(lasso.coef_ != 0))

training set score: 0.293238

test set score: 0.209375

number of features used: 4
```

As you can see, the Lasso does quite badly, both on the training and the test set. This indicates that we are

underfitting. We find that it only used four of the 105 features. Similarly to Ridge, the Lasso also has a regularization parameter  $\alpha$  that controls how strongly coefficients are pushed towards zero. Above, we used the default of  $\alpha=1.0$ . To diminish underfitting, let's try decreasing  $\alpha$ :

```
lasso001 = Lasso(alpha=0.01).fit(X_train, y_train)
print("training set score: %f" % lasso001.score(X_train, y_train))
print("test set score: %f" % lasso001.score(X_test, y_test))
print("number of features used: %d" % np.sum(lasso001.coef_ != 0))
```

```
/home/andy/checkout/scikit-learn/sklearn/linear_model/coordinate_descent.py:474: ConvergenceWarning)
ConvergenceWarning)
```

A lower  $\alpha$  allowed us to fit a more complex model, which worked better on the training and the test data. The performance is slightly better than using Ridge, and we are using only 32 of the 105 features. This makes this model potentially easier to understand.

If we set  $\alpha$  too low, we again remove the effect of regularization and end up with a result similar to LinearRegression.

```
lasso00001 = Lasso(alpha=0.0001).fit(X_train, y_train)
print("training set score: %f" % lasso00001.score(X_train, y_train))
print("test set score: %f" % lasso00001.score(X_test, y_test))
print("number of features used: %d" % np.sum(lasso00001.coef_ != 0))
```

```
/home/andy/checkout/scikit-learn/sklearn/linear_model/coordinate_descent.py:474: ConvergenceWarning)
ConvergenceWarning)
```

Again, we can plot the coefficients of the different models, similarly to Figure `ridge_coefficients`.

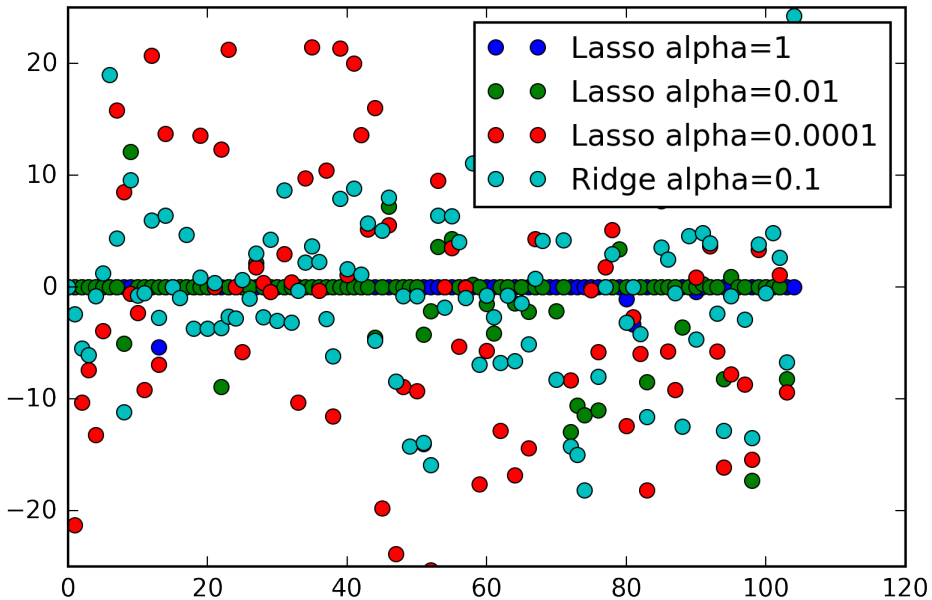


For  $\alpha=1$ , with coefficients shown as blue dots, we not only see that most of the coefficients are zero (which we already knew), but that the remaining coefficients are also small in magnitude. Decreasing  $\alpha$  to 0.01 we obtain the solution shown as the green dots, which causes most features be exactly zero. Using  $\alpha=0.00001$ , we get a model that is quite unregularized, with most coefficients nonzero and of large magnitude.

For comparison, the best Ridge solution is shown in teal. The ridge model with  $\alpha=0.1$  has similar predictive performance as the lasso model with  $\alpha=0.01$ , but using Ridge, all coefficients are non-zero.

```
plt.plot(lasso.coef_, 'o', label="Lasso alpha=1")
plt.plot(lasso001.coef_, 'o', label="Lasso alpha=0.01")
plt.plot(lasso00001.coef_, 'o', label="Lasso alpha=0.00001")

plt.plot(ridge01.coef_, 'o', label="Ridge alpha=0.1")
plt.ylim(-25, 25)
plt.legend()
```



In practice, Ridge regression is usually the first choice between these two models. However, if you have a large amount of features and expect only a few of them to be important, Lasso might be a better choice. Similarly, if you would like to have a model that is easy to interpret, Lasso will provide a model that is easier to understand, as it will select only a subset of the input features.

## Linear models for Classification

Linear models are also extensively used for classification. Let's look at binary classification first. In this case, a prediction is made using the following formula:

```
\begin{align*}
&\hat{y} = w[0] x[0] + w[1] x[1] + \dots + w[p] * x[p] + b > 0 \text{ (2) linear} \\
&\text{binary classification} \\
\end{align*}
```

The formula looks very similar to the one for linear regression, but instead of just returning the weighted sum of the features, we threshold the predicted value at zero. If the function was smaller than zero, we predict the class -1, if it was larger than zero, we predict the class +1.

This prediction rule is common to all linear models for classification. Again, there are many different ways to find the coefficients  $w$  and the intercept  $b$ .

For linear models for regression, the output  $y$  was a linear function of the features: a line, plane, or hyperplane (in higher dimensions). For linear models for classification, the *decision boundary* is a linear function of the input. In other words, a (binary) linear classifier is a classifier that separates two classes using a line, a plane or a hyperplane. We will see examples of that below.

There are many algorithms for learning linear models. These algorithms all differ in the following two ways:

1. How they measure how well a particular combination of coefficients and intercept fits the training data.
1. If and what kind of regularization they use.

Different algorithms choose different ways to measure what “fitting the training set well” means in 1. For technical mathematical reasons, it is not possible to adjust  $w$  and  $b$  to minimize the number of misclassifications the algorithms produce, as one might hope. For our purposes, and many applications, the different choices for 1. (called *loss function*) is of little significance.

The two most common linear classification algorithms are logistic regression, implemented in `linear_model.LogisticRegression` and linear support vector machines (linear SVMs), implemented in `svm.LinearSVC` (SVC stands for Support Vector Classifier). Despite its name, `LogisticRegression` is a classification algorithm and not a regression algorithm, and should not be confused with `LinearRegression`.

We can apply the `LogisticRegression` and `LinearSVC` models to the `forge` dataset, and visualize the decision boundary as found by the linear models:

```

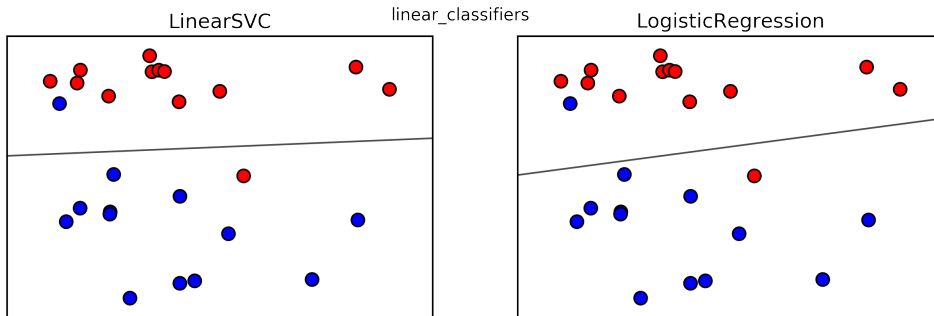
from sklearn.linear_model import LogisticRegression
from sklearn.svm import LinearSVC

X, y = mglearn.datasets.make_forge()

fig, axes = plt.subplots(1, 2, figsize=(10, 3))
plt.suptitle("linear_classifiers")

for model, ax in zip([LinearSVC(), LogisticRegression()], axes):
    clf = model.fit(X, y)
    mglearn.plots.plot_2d_separator(clf, X, fill=False, eps=0.5, ax=ax, alpha=.7)
    ax.scatter(X[:, 0], X[:, 1], c=y, s=60, cmap=mglearn.cm2)
    ax.set_title("%s" % clf.__class__.__name__)

```



In this figure, we have the first feature of the forge dataset on the x axis and the second feature on the y axis as before. We display the decision boundaries found by LinearSVC and LogisticRegression respectively as straight lines, separating the area classified as blue on the top from the area classified as red on the bottom.

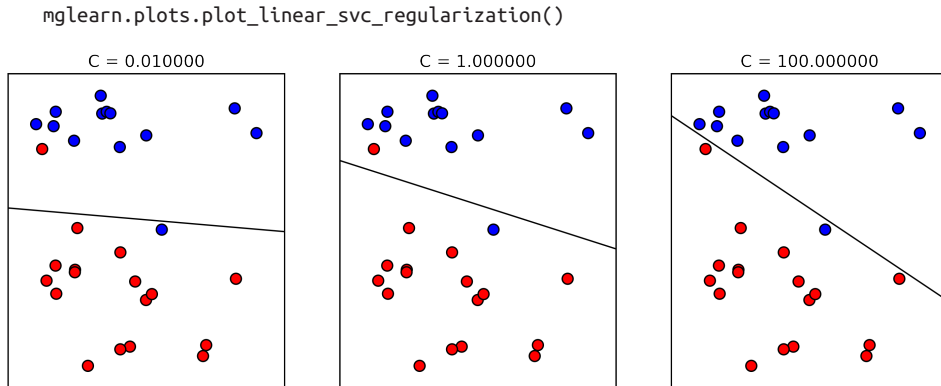
In other words, any new data point that lies above the black line will be classified as blue by the respective classifier, while any point that lies below the black line will be classified as red.

The two models come up with similar decision boundaries. Note that both misclassify two of the points. By default, both models apply an  $\ell_2$  regularization, in the same way that Ridge does for regression.

For LogisticRegression and LinearSVC the trade-off parameter that determines the strength of the regularization is called  $C$ , and higher values of  $C$  correspond to *less* regularization. In other words, when using a high value of the parameter  $C$ , LogisticRegression and LinearSVC try to fit the training set as best as possible, while with low values of the parameter  $C$ , the model put more emphasis on finding a coefficient vector  $w$  that is close to zero.

There is another interesting intuition of how the parameter  $C$  acts. Using low values of  $C$  will cause the algorithms try to adjust to the “majority” of data points, while

using a higher value of  $C$  stresses the importance that each individual data point be classified correctly. Here is an illustration using `LinearSVC`.



On the left hand side, we have a very small  $C$  corresponding to a lot of regularization. Most of the blue points are at the top, and most of the red points are at the bottom. The strongly regularized model chooses a relatively horizontal line, misclassifying two points.

In the center plot,  $C$  is slightly higher, and the model focuses more on the two misclassified samples, tilting the decision boundary. Finally, on the right hand side, a very high value of  $C$  in the model tilts the decision boundary a lot, now correctly classifying all red points. One of the blue points is still misclassified, as it is not possible to correctly classify all points in this dataset using a straight line. The model illustrated on the right hand side tries hard to correctly classify all points, but might not capture the overall layout of the classes well. In other words, this model is likely overfitting.

Similarly to the case of regression, linear models for classification might seem very restrictive in low dimensional spaces, only allowing for decision boundaries which are straight lines or planes. Again, in high dimensions, linear models for classification become very powerful, and guarding against overfitting becomes increasingly important when considering more features.

Let's analyze `LinearLogistic` in more detail on the `breast_cancer` dataset:

```
from sklearn.datasets import load_breast_cancer
cancer = load_breast_cancer()
X_train, X_test, y_train, y_test = train_test_split(
    cancer.data, cancer.target, stratify=cancer.target, random_state=42)
logisticregression = LogisticRegression().fit(X_train, y_train)
print("training set score: %f" % logisticregression.score(X_train, y_train))
print("test set score: %f" % logisticregression.score(X_test, y_test))
```

```
training set score: 0.953052
```

```
test set score: 0.958042
```

The default value of  $C=1$  provides quite good performance, with 95% accuracy on both the training and the test set. As training and test set performance are very close, it is likely that we are underfitting. Let's try to increase  $C$  to fit a more flexible model.

```
logisticregression100 = LogisticRegression(C=100).fit(X_train, y_train)
print("training set score: %f" % logisticregression100.score(X_train, y_train))
print("test set score: %f" % logisticregression100.score(X_test, y_test))
```

```
training set score: 0.971831
```

```
test set score: 0.965035
```

Using  $C=100$  results in higher training set accuracy, and also a slightly increased test set accuracy, confirming our intuition that a more complex model should perform better.

We can also investigate what happens if we use an even more regularized model than the default of  $C=1$ , by setting  $C=0.01$ .

```
logisticregression001 = LogisticRegression(C=0.01).fit(X_train, y_train)
print("training set score: %f" % logisticregression001.score(X_train, y_train))
print("test set score: %f" % logisticregression001.score(X_test, y_test))
```

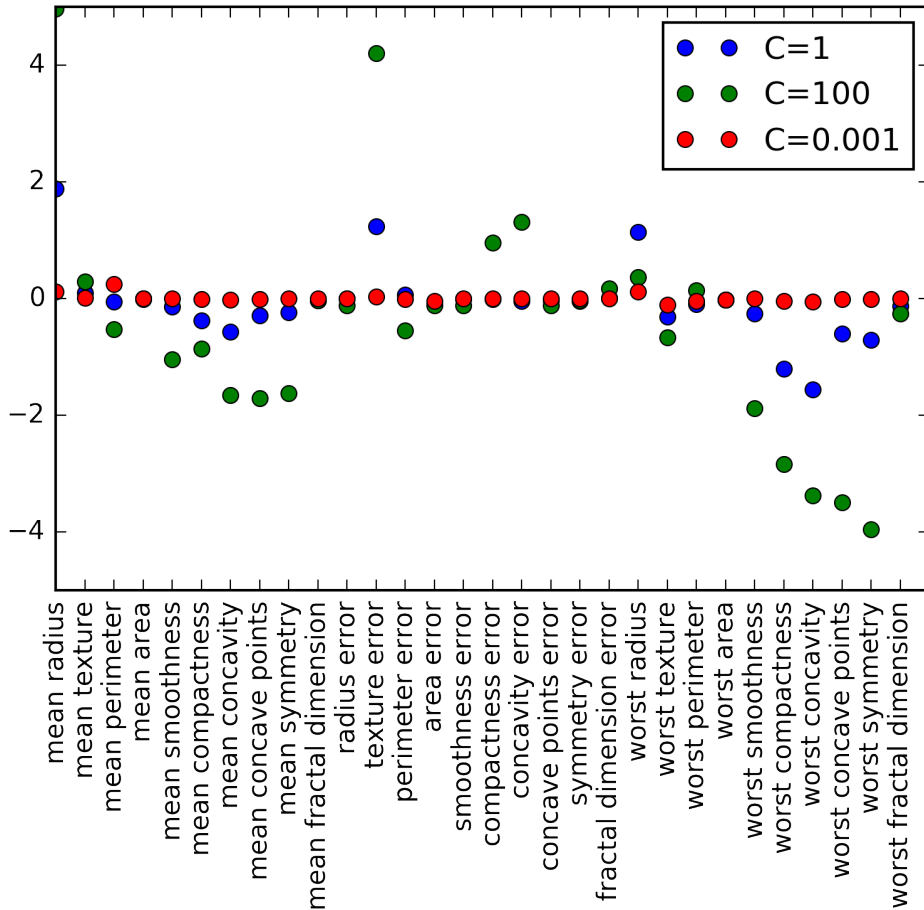
```
training set score: 0.934272
```

```
test set score: 0.930070
```

As expected, when moving more to the left in Figure `model_complexity` from an already underfit model, both training and test set accuracy decrease relative to the default parameters.

Finally, let's look at the coefficients learned by the models with the three different settings of the regularization parameter  $C$ .

```
plt.plot(logisticregression.coef_.T, 'o', label="C=1")
plt.plot(logisticregression100.coef_.T, 'o', label="C=100")
plt.plot(logisticregression001.coef_.T, 'o', label="C=0.001")
plt.xticks(range(cancer.data.shape[1]), cancer.feature_names, rotation=90)
plt.ylim(-5, 5)
plt.legend()
```



As LogisticRegression applies an L2 regularization by default, the result looks similar to Ridge in Figure ridge\_coefficients. Stronger regularization pushes coefficients more and more towards zero, though coefficients never become exactly zero.

Inspecting the plot more closely, we can also see an interesting effect in the third coefficient, for “mean perimeter”. For C=100 and C=1, the coefficient is negative, while for C=0.001, the coefficient is positive, with a magnitude that is even larger as for C=1. Interpreting a model like this, one might think the coefficient tells us which class a feature is associated with. For example, one might think that a high “texture error” feature is related to a sample being “malignant”. However, the change of sign in the coefficient for “mean perimeter” means that depending on which model we look at, high “mean perimeter” could be either taken as being indicative of “benign” or indicative of “malignant”. This illustrates that interpretations of coefficients of linear models should always be taken with a grain of salt.

If we desire a more interpretable model, using L1 regularization might help, as it limits the model to only using a few features. Here is the coefficient plot and classification accuracies for L1 regularization:

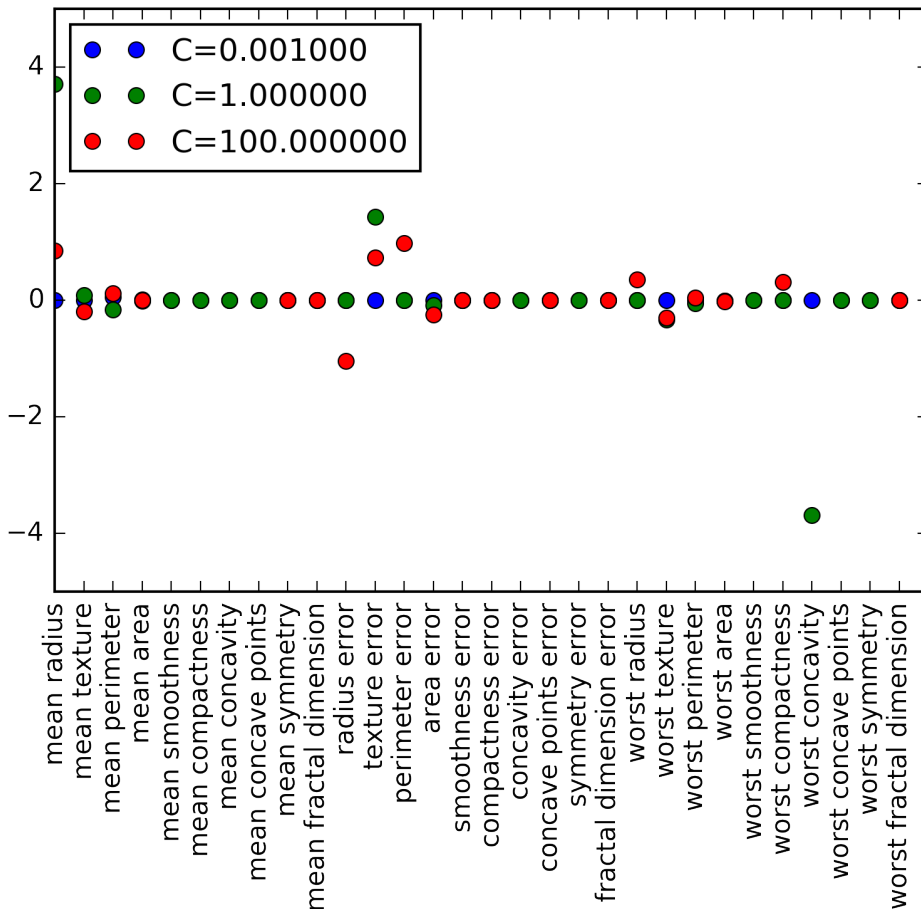
```

for C in [0.001, 1, 100]:
    lr_l1 = LogisticRegression(C=C, penalty="l1").fit(X_train, y_train)
    print("training accuracy of L1 logreg with C=%f: %f"
          % (C, lr_l1.score(X_train, y_train)))
    print("test accuracy of L1 logreg with C=%f: %f"
          % (C, lr_l1.score(X_test, y_test)))
    plt.plot(lr_l1.coef_.T, 'o', label="C=%f" % C)

plt.xticks(range(cancer.data.shape[1]), cancer.feature_names, rotation=90)

plt.ylim(-5, 5)
plt.legend(loc=2)

```



```

training accuracy of L1 logreg with C=0.001000: 0.913146
test accuracy of L1 logreg with C=0.001000: 0.923077
training accuracy of L1 logreg with C=1.000000: 0.960094
test accuracy of L1 logreg with C=1.000000: 0.958042
training accuracy of L1 logreg with C=100.000000: 0.985915
test accuracy of L1 logreg with C=100.000000: 0.979021

```

## Linear Models for multiclass classification

Many linear classification models are binary models, and don't extend naturally to the multi-class case (with the exception of Logistic regression). A common technique to extend a binary classification algorithm to a multi-class classification algorithm is the *one-vs-rest* approach. In the one-vs-rest approach, a binary model is learned for each class, which tries to separate this class from all of the other classes, resulting in as many binary models as there are classes.

To make a prediction, all binary classifiers are run on a test point. The classifier that has the highest score on its single class "wins" and this class label is returned as prediction.

Having one binary classifier per class results in having one vector of coefficients  $w$  and one intercept  $b$  for each class. The class for which the result of formula

```

\begin{align*}
& w[0] x[0] + w[1] x[1] + \dots + w[p] * x[p] + b \quad \text{(3) classification confidence} \\
\end{align*}

```

is highest is the assigned class label.

The mathematics behind logistic regression are somewhat different from the one-vs-rest approach, but they also result in one coefficient vector and intercept per class, and the same method of making a prediction is applied.

Let's apply the one-vs-rest method to a simple three-class classification dataset.

We use a two-dimensional dataset, where each class is given by data sampled from a Gaussian distribution.

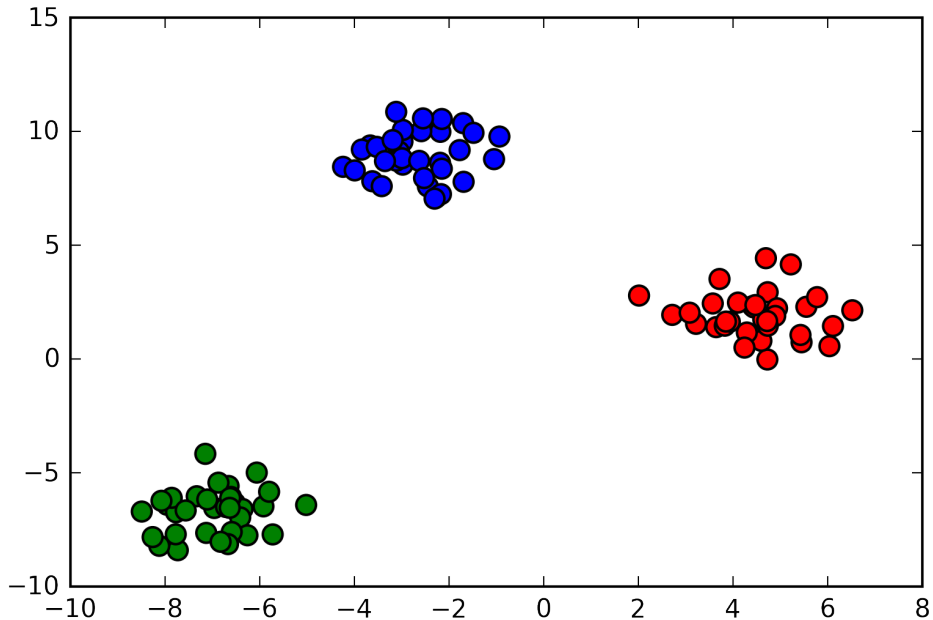
```

from sklearn.datasets import make_blobs

X, y = make_blobs(random_state=42)
plt.scatter(X[:, 0], X[:, 1], c=y, s=60, cmap=mglearn.cm3)

```





Now, we train a LinearSVC classifier on the dataset.

```
linear_svm = LinearSVC().fit(X, y)
print(linear_svm.coef_.shape)
print(linear_svm.intercept_.shape)
```

```
(3, 2)
```

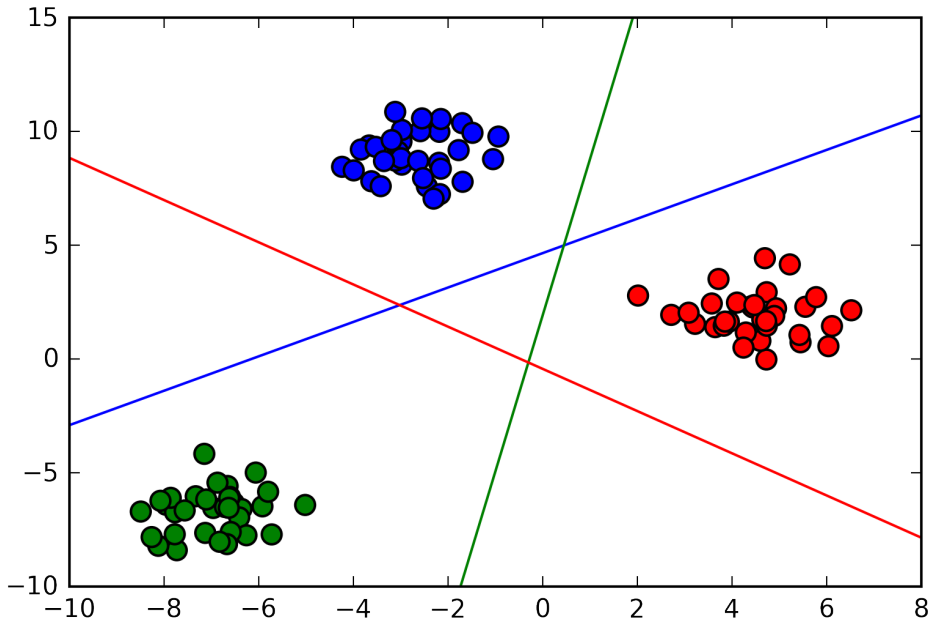
```
(3,)
```

We see that the shape of the `coef_` is (3, 2), meaning that each row of `coef_` contains the coefficient vector for one of the three classes. Each row has two entries, corresponding to the two features in the dataset.

The `intercept_` is now a one-dimensional array, storing the intercepts for each class.

Let's visualize the lines given by the three binary classifiers:

```
plt.scatter(X[:, 0], X[:, 1], c=y, s=60, cmap=mglearn.cm3)
line = np.linspace(-15, 15)
for coef, intercept in zip(linear_svm.coef_, linear_svm.intercept_):
    plt.plot(line, -(line * coef[0] + intercept) / coef[1])
plt.ylim(-10, 15)
plt.xlim(-10, 8)
```



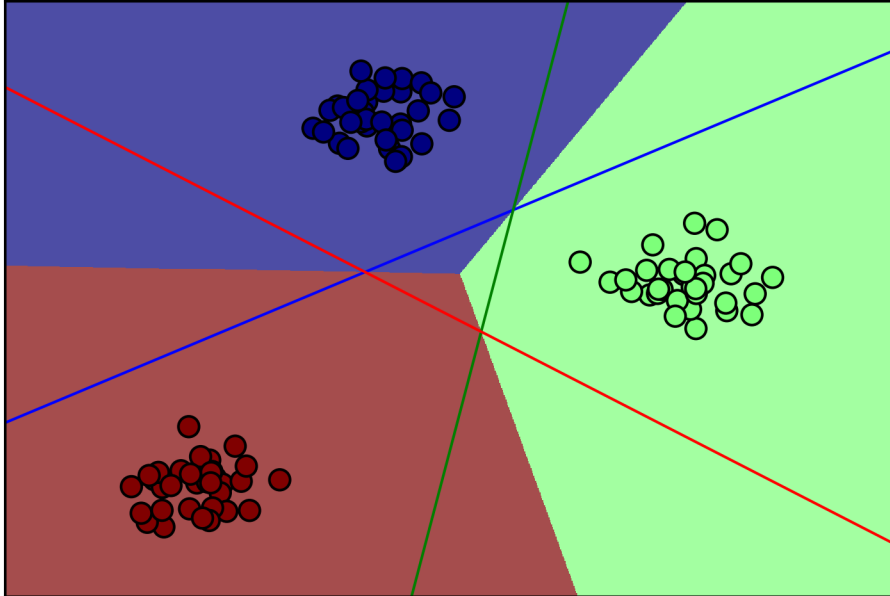
The red line shows the decision boundary for the binary classifier for the red class, and so on.

You can see that all the red points in the training data are below the red line, which means they are on the “red” side of this binary classifier. The red points are left of the green line, which means they are classified as “rest” by the binary classifier for the green class. The red points are below the blue line, which means the binary classifier for the blue class also classifies them as “rest”. Therefore, any point in this area will be classified as red by the final classifier (Formula (3) of the red classifier is greater than zero, while it is smaller than zero for the other two classes).

But what about the triangle in the middle of the plot? All three binary classifiers classify points there as “rest”. Which class would a point there be assigned to? The answer is the one with the highest value in Formula (3): the class of the closest line.

The following figure shows the prediction shown for all regions of the 2d space:

```
mglearn.plots.plot_2d_classification(linear_svm, X, fill=True, alpha=.7)
plt.scatter(X[:, 0], X[:, 1], c=y, s=60)
line = np.linspace(-15, 15)
for coef, intercept in zip(linear_svm.coef_, linear_svm.intercept_):
    plt.plot(line, -(line * coef[0] + intercept) / coef[1])
```



## Strengths, weaknesses and parameters

The main parameter of linear models is the regularization parameter, called  $\alpha$  in the regression models and  $C$  in `LinearSVC` and `LogisticRegression`. Large  $\alpha$  or small  $C$  mean simple models. In particular for the regression models, tuning this parameter is quite important. Usually  $C$  and  $\alpha$  are searched for on a logarithmic scale.

The other decision you have to make is whether you want to use L1 regularization or L2 regularization. If you assume that only few of your features are actually important, you should use L1. Otherwise, you should default to L2.

L1 can also be useful if interpretability of the model is important. As L1 will use only a few features, it is easier to explain which features are important to the model, and what the effect of these features is.

Linear models are very fast to train, and also fast to predict. They scale to very large datasets and work well with sparse data. If your data consists of hundreds of thousands or millions of samples, you might want to investigate `SGDClassifier` and `SGDRegressor`, which implement even more scalable versions of the linear models described above.

Another strength of linear models is that they make it relatively easy to understand how a prediction is made, using Formula (1) for regression and Formula (2) for clas-

sification. Unfortunately, it is often not entirely clear why coefficients are the way they are. This is particularly true if your dataset has highly correlated features; in these cases, the coefficients might be hard to interpret.

Linear models often perform well when the number of features is large compared to the number of samples. They are also often used on very large datasets, simply because other models are not feasible to train. However, on smaller dataset, other models might yield better generalization performance.

## Naive Bayes Classifiers

Naive Bayes classifiers are a family of classifiers that are quite similar to the linear models discussed above. However, they tend to be even faster in training. The price paid for this efficiency is that naive Bayes models often provide generalization performance that is slightly worse than linear classifiers like `LogisticRegression` and `LinearSVC`.

The reason that naive Bayes models are so efficient is that they learn parameters by looking at each feature individually, and collect simple per-class statistics from each feature.

There are three kinds of naive Bayes classifiers implemented in `scikit-learn`, `GaussianNB`, `BernoulliNB` and `MultinomialNB`.

`GaussianNB` can be applied to any continuous data, while `BernoulliNB` assumes binary data and `MultinomialNB` assumes count data (that is each feature represents an integer count of something, like how often a word appears in a sentence). `BernoulliNB` and `MultinomialNB` are mostly used in text data classification, and we will revisit them in Chapter 7 (Text Data).

The `BernoulliNB` classifier counts how often every feature of each class is not zero. This is most easily understood with an example:

```
x = np.array([[0, 1, 0, 1],
              [1, 0, 1, 1],
              [0, 0, 0, 1],
              [1, 0, 1, 0]])
y = np.array([0, 1, 0, 1])
```

Here, we have four data points, with four binary features each. There are two classes, 0 and 1.

For class 0 (the first and third data point), the first feature is zero 2 times and non-zero 0 times, the second features is zero 1 time and non-zero 1 time, and so on.

These same counts are then calculated for the data points in the second class.

Counting the non-zero entries per class in essence looks like this:

```

counts = {}
for label in np.unique(y):
    # iterate over each class
    # count (sum) entries of 1 per feature
    counts[label] = X[y == label].sum(axis=0)
print(counts)

{0: array([0, 1, 0, 2]), 1: array([2, 0, 2, 1])}

```

The other two naive Bayes models, `MultinomialNB` and `GaussianNB` are slightly different in what kind of statistics they compute. `MultinomialNB` takes into account the average value of each feature for each class, while `GaussianNB` stores the average value as well as the standard deviation of each feature for each class.

To make a prediction, a data point is compared to the statistics for each of the classes, and the best matching class is predicted. Interestingly, for `MultinomialNB` and `BernoulliNB`, this leads to a prediction formula that is of the same form as in the linear models (Formula (2)). Unfortunately, `coef_` for the naive Bayes models has a slightly different meaning than in the linear models, in that `coef_` is not the same as  $w$ .

## Strengths, weaknesses and parameters

The `MultinomialNB` and `BernoulliNB` have a single parameter `alpha`, which controls model complexity. The way `alpha` works is that the algorithm adds `alpha` many virtual data points to the data, that have positive values for all the features. This results in a “smoothing” of the statistics. A large `alpha` means more smoothing, resulting in less complex models. The algorithms performance is relatively robust to the setting of `alpha`, meaning that setting `alpha` is not critical for good performance. However, tuning it usually improves accuracy somewhat.

The `GaussianNB` model seems to be rarely used by practitioners, while the other two variants of naive Bayes are widely used for sparse count data such as text. `MultinomialNB` usually performs better than `BinaryNB`, in particular on datasets with a relatively large number of non-zero features (i.e. large documents).

The naive Bayes models share many of the strengths and weaknesses of the linear models. They are very fast to train and to predict, and the training procedure is easy to understand. The models work very well with high-dimensional sparse data, and are relatively robust to the parameters. Naive Bayes models are great baseline models, and are often used on very large datasets, where training even a linear model might take too long.

## Decision trees

Decision trees are a widely used models for classification and regression tasks.

Essentially, they learn a hierarchy of “if-else” questions, leading to a decision.

These questions are similar to the questions you might ask in a game of twenty questions.

Imagine you want to distinguish between the following four animals: bears, hawks, penguins and dolphins.

Your goal is to get to the right answer b] asking as few if-else questions as possible.

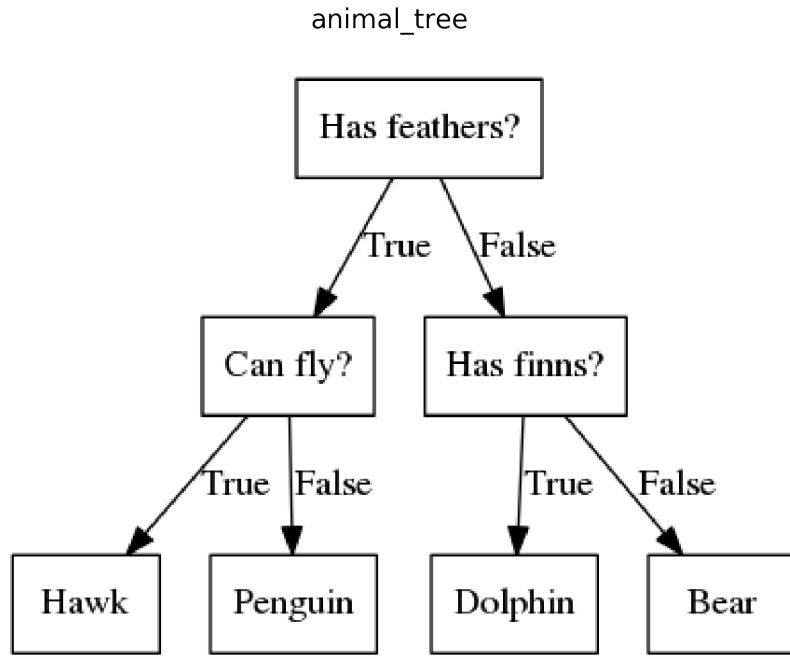
You might start off by asking whether the animal has feathers, a question that narrows down your possible animals to just two animals.

If the answer is yes, you can ask another question that could help you distinguish between hawks and penguins. For example, you could ask whether or not the animal can fly. If the animal doesn't have feathers, your possible animal choices are dolphins and bears, and you will need to ask a question to distinguish between these two animals, for example, asking whether the animal has fins.

This series of questions can be expressed as a decision tree, as shown in Figure animal\_tree.

In this illustration, each node in the tree either represents a question, or a terminal node (also called a *leaf*) which contains the answer. The edges connect the answers to a question with the next question you would ask.

```
mglearn.plots.plot_animal_tree()  
plt.suptitle("animal_tree");
```



In machine learning parlance, we built a model to distinguish between four classes of animals (hawks, penguins, dolphins and bears) using the three features “has feathers”, “can fly” and “has fins”.

Instead of building these models by hand, we can learn them from data using supervised learning.

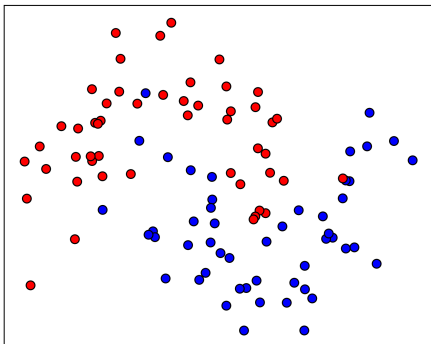
## Building Decision Trees

Let’s go through the process of building a decision tree for the 2d classification dataset shown at the top of Figure tree\_building. The dataset consists of two half-moon shapes of blue and red points, consisting of 75 data points each. We will refer to this dataset as two\_moons.

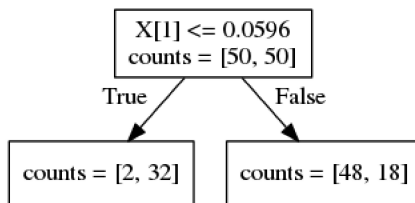
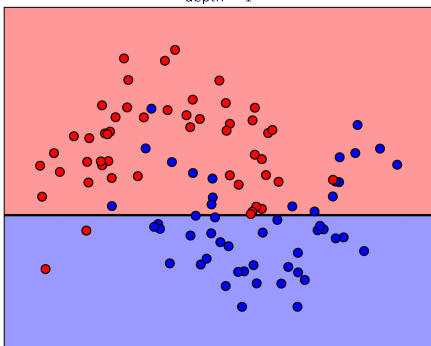
```

mglearn.plots.plot_tree_progressive()
plt.suptitle("tree_building");

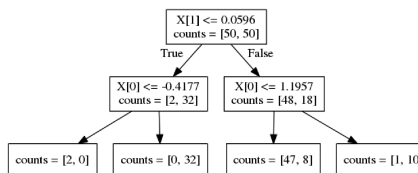
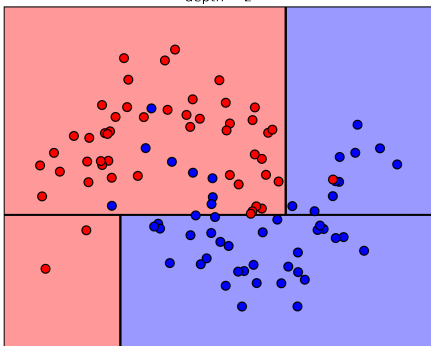
```



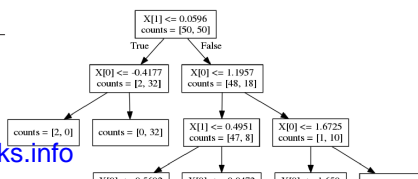
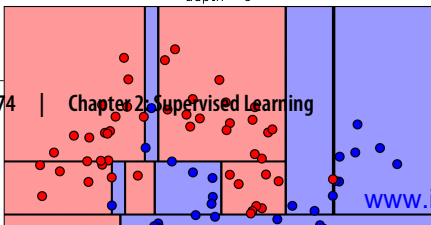
depth = 1



depth = 2



depth = 9





Learning a decision tree means learning a sequence of if/else questions that gets us to the true answer most quickly.

In the machine learning setting, these questions are called *tests* (not to be confused with the test set, which is the data we use to test to see how generalizable our model is).

Usually data does not come in the form of binary yes/no features as in the animal example, but is instead represented as continuous features such as in the 2d dataset shown in the figure. The tests that are used on continuous data are of the form “is feature  $i$  larger than value  $a$ ”.

To build a tree, the algorithm searches over all possible tests, and finds the one that is most informative about the target variable.

The second row in Figure `tree_building` shows the first test that is picked. Splitting the dataset vertically at  $x[1]=0.2372$  yields the most information; it best separates the blue points from the red points. The top node, also called the *root*, represents the whole dataset, consisting of 75 red and 75 blue points. The split is done by testing whether  $x[1] \leq 0.2372$ , indicated by a black line. If the test is true, a point is assigned to the left node, which contains 8 blue points and 58 red points. Otherwise the point is assigned to the right node, which contains 67 red points and 17 blue points. These two nodes correspond to the top and bottom region shown in Figure `tree_building`.

Even though the first split did a good job of separating the blue and red points, the bottom region still contains blue points, and the top region still contains red points.

We can build a more accurate model by repeating the process of looking for the best test in both regions.

Figure `tree_building` shows that the most informative next split for the left and the right region are based on  $x[0]$ .

This recursive process yields a binary tree of decisions, with each node containing a test.

Alternatively, you can think of each test as splitting the part of the data that is currently considered along one axis. This yields a view of the algorithm as building a hierarchical partition. As each test concerns only a single feature, the regions in the resulting partition always have axis-parallel boundaries.

Figure `tree_building` illustrates the partitioning of the data in the left hand column, and the resulting tree in the right hand column.

The recursive partitioning of the data is usually repeated until each region in the partition (each leaf in the decision tree) only contains a single target value (a single class

or a single regression value). A leaf of the tree containing only one target value is called *pure*.

A prediction on a new data point is made by checking which region of the partition of the feature space the point lies in, and then predicting the majority target (or the single target in the case of pure leaves) in that region. The region can be found by traversing the tree from the root and going left or right, depending on whether the test is fulfilled or not.

## Controlling complexity of Decision Trees

Typically, building a tree as described above, and continuing until all leaves are pure leads to models that are very complex and highly overfit to the training data. The presence of pure leaves mean that a tree is 100% accurate on the training set; each data point in the training set is in a leaf that has the correct majority class. The overfitting can be seen on the left of Figure `tree_building` in the bottom column. You can see the regions determined to be red in the middle of all the blue points. On the other hand, there is a small strip of blue around the single blue point to the very right. This is not how one would imagine the decision boundary to look, and the decision boundary focuses a lot on single outlier points that are far away from the other points in that class.

There are two common strategies to prevent overfitting: stopping the creation of the tree early, also called *pre-pruning*, or building the tree but then removing or collapsing nodes that contain little information, also called *post-pruning* or just *pruning*. Possible criteria for pre-pruning include limiting the maximum depth of the tree, limiting the maximum number of leaves, or requiring a minimum number of points in a node to keep splitting it.

Decision trees in scikit-learn are implemented in the `DecisionTreeRegressor` and `DecisionTreeClassifier` classes. Scikit-learn only implements *pre-pruning*, not *post-pruning*.

Let's look at the effect of pre-pruning in more detail on the breast cancer dataset.

As always, we import the dataset and split it into a training and test part.

Then we build a model using the default setting of fully developing the tree (growing the tree until all leaves are pure). We fix the `random_state` in the tree, which is used for tie-breaking internally.

```
from sklearn.tree import DecisionTreeClassifier

cancer = load_breast_cancer()
X_train, X_test, y_train, y_test = train_test_split(
    cancer.data, cancer.target, stratify=cancer.target, random_state=42)
tree = DecisionTreeClassifier(random_state=0)
tree.fit(X_train, y_train)
```

```

print("accuracy on training set: %f" % tree.score(X_train, y_train))
print("accuracy on test set: %f" % tree.score(X_test, y_test))

accuracy on training set: 1.000000

accuracy on test set: 0.937063

```

As expected, the accuracy on the training set is 100% as the leaves are pure.

The test-set accuracy is slightly worse than the linear models above, which had around 95% accuracy.

Now let's apply pre-pruning to the tree, which will stop developing the tree before we perfectly fit to the training data.

One possible way is to stop building the tree after a certain depth has been reached. Here we set `max_depth=4`, meaning only four consecutive questions can be asked (cf. Figure `tree_building`).

```

tree = DecisionTreeClassifier(max_depth=4, random_state=0)
tree.fit(X_train, y_train)

print("accuracy on training set: %f" % tree.score(X_train, y_train))
print("accuracy on test set: %f" % tree.score(X_test, y_test))

accuracy on training set: 0.988263

accuracy on test set: 0.951049

```

Limiting the depth of the tree decreases overfitting. This leads to a lower accuracy on the training set, but an improvement on the test set.

## Analyzing Decision Trees

We can visualize the tree using the `export_graphviz` function from the `tree` module.

This writes a file in the dot file format, which is a text file format for storing graphs.

We set an option to color the nodes to reflect the majority class in each node and pass the class and features names so the tree can be properly labeled.

```

from sklearn.tree import export_graphviz
export_graphviz(tree, out_file="mytree.dot", class_names=["malignant", "benign"],
                feature_names=cancer.feature_names, impurity=False, filled=True)

```

We can read this file and visualize it using the `graphviz` module (or you can use any program that can read dot files):

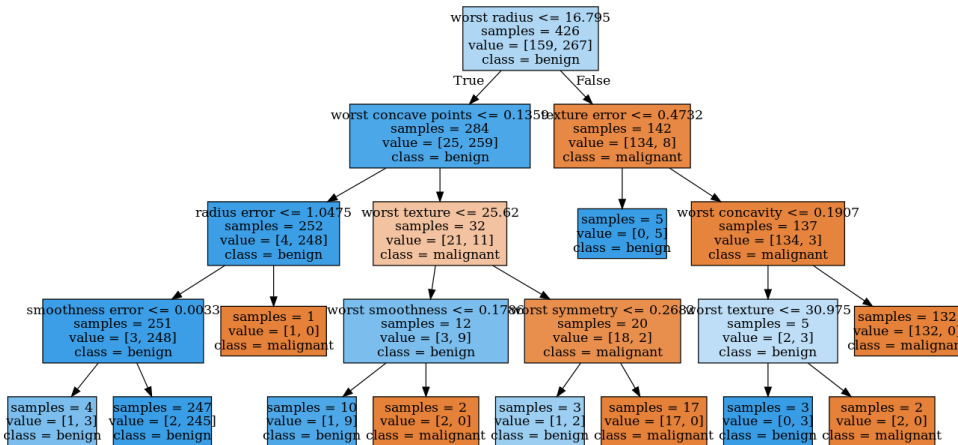
```

import graphviz

with open("mytree.dot") as f:

```

```
dot_graph = f.read()
graphviz.Source(dot_graph)
```



The visualization of the tree provides a great in-depth view of how the algorithm makes predictions, and is a good example of a machine learning algorithm that is easily explained to non-experts. However, even with a tree of depth four, as seen here, the tree can become a bit overwhelming. Deeper trees (depth ten is not uncommon) are even harder to grasp.

One method of inspecting the tree that may be helpful is to find out which path most of the data actually takes.

The `n_samples` shown in each node in the figure gives the number of samples in each node, while `value` provides the number of samples per class.

Following the branches to the right, we see that `texture_error <= 0.4732` creates a node that only contains 8 benign but 134 malignant samples. The rest of this side of the tree then uses some finer distinctions to split off these 8 remaining benign samples. Of the 142 samples that went to the right in the initial split, nearly all of them (132) end up in the leaf to the very right.

Taking a left at the root, for `texture_error > 0.4732`, we end up with 25 malignant and 259 benign samples.

Nearly all of the benign samples end up in the second leaf from the right, with most of the other leaves only containing very few samples.

## Feature Importance in trees

Instead of looking at the whole tree, which can be taxing, there are some useful statistics that we can derive properties that we can derive to summarize the workings of the tree. The most commonly used summary is *feature importance*, which rates how

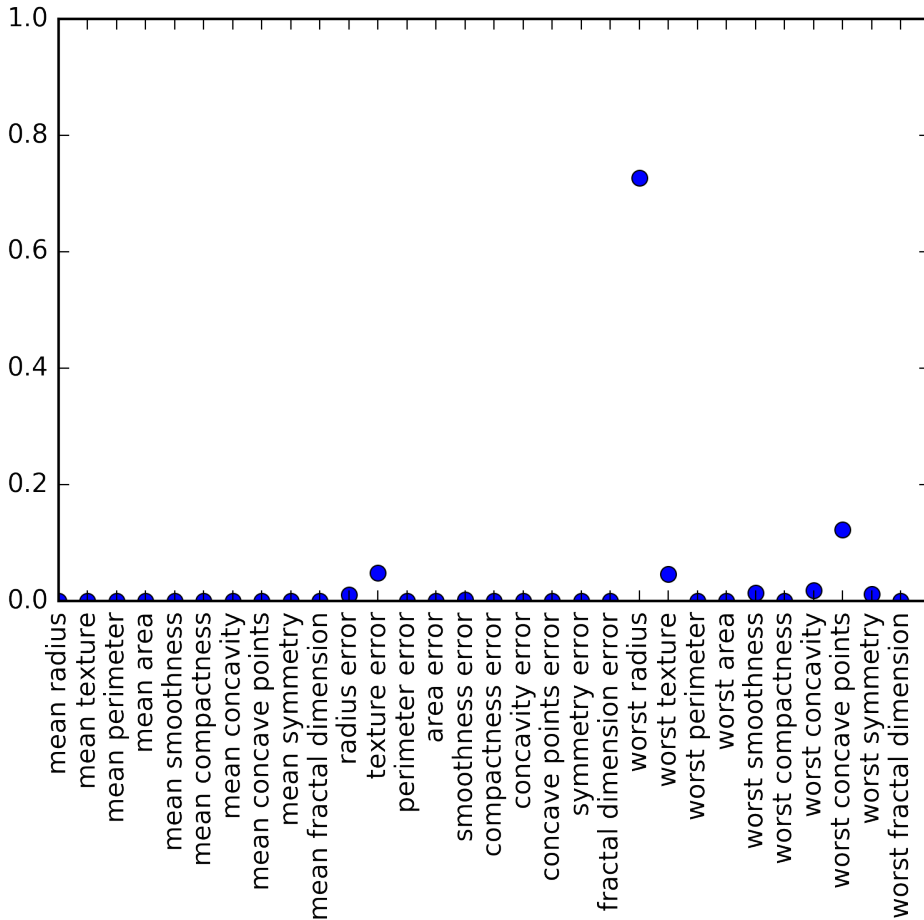
important each feature is for the decision a tree makes. It is a number between 0 and 1 for each feature, where 0 means “not used at all” and 1 means “perfectly predicts the target”.

The feature importances always sum to one.

```
tree.feature_importances_  
array([ 0.          ,  0.          ,  0.          ,  0.          ,  0.          ,  
        0.          ,  0.          ,  0.          ,  0.          ,  0.          ,  
        0.01019737,  0.04839825,  0.          ,  0.          ,  0.0024156 ,  
        0.          ,  0.          ,  0.          ,  0.          ,  0.          ,  
        0.72682851,  0.0458159 ,  0.          ,  0.          ,  0.0141577 ,  
        0.          ,  0.018188 ,  0.1221132 ,  0.01188548,  0.          ])
```

We can visualize the feature importances in a way that is similar to the way we visualize the coefficients in the linear model.

```
plt.plot(tree.feature_importances_, 'o')  
plt.xticks(range(cancer.data.shape[1]), cancer.feature_names, rotation=90)  
plt.ylim(0, 1)
```



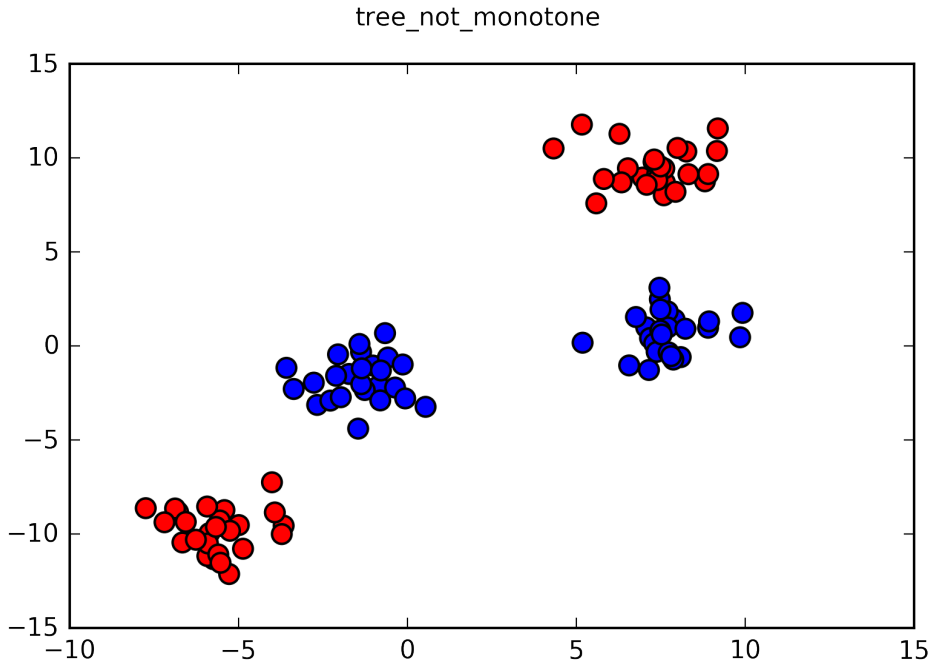
Here, we see that the feature used at the top split (“worst radius”) is by far the most important feature. This confirms our observation in analyzing the tree, that the first level already separates the two classes fairly well.

However, if a feature has a low `feature_importance`, it doesn’t mean that this feature is uninformative. It only means that this feature was not picked by the tree, likely because another feature encodes the same information.

In contrast to the coefficients in linear models, feature importances are always positive, and don’t encode which class a feature is indicative of. The feature importances tell us that `worst radius` is important, but it does not tell us whether a high radius is indicative of a sample being “benign” or “malignant”. In fact, there might not be such a simple relationship between features and class, as you can see in the example below:

```
tree = mglearn.plots.plot_tree_not_monotone()
plt.suptitle("tree_not_monotone")
```

tree



Feature importances: [ 0. 1.]

The plot shows a dataset with two features and two classes. Here, all the information is contained in  $X[1]$ , and  $X[0]$  is not used at all. But the relation between  $X[1]$  and the output class is not monotonous, meaning we cannot say “a high value of  $X[0]$  means class red, and a low value means class blue” or the other way around.

While we focus our discussion here on decision trees for classification, all that was said is similarly true for decision trees for regression, as implemented in `DecisionTreeRegressor`. Both the usage and the analysis of regression trees are very similar to classification trees, so we won't go into any more detail here.

## Strengths, weaknesses and parameters

As discussed above, the parameters that control model complexity in decision trees are the pre-pruning parameters that stop the building of the tree before it is fully developed. Usually picking one of the pre-pruning strategies, either setting `min_depth`, `max_leaf_nodes` or `min_samples_leaf` is to prevent overfitting.

Decision trees have two advantages over many of the algorithms we discussed so far: The resulting model can easily be visualized and understood by non-experts (at least for smaller trees), and the algorithm is completely invariant to scaling of the data: As each feature is processed separately, and the possible splits of the data don't depend on scaling, no preprocessing like normalization or standardization of features is needed for decision tree algorithms.

In particular, decision trees work well when you have features that are on completely different scales, or a mix of binary and continuous features.

The main down-side of decision trees is that even with the use of pre-pruning, decision trees tend to overfit, and provide poor generalization performance. Therefore, in most applications, the ensemble methods we discuss below are usually used in place of a single decision tree.

## Ensembles of Decision Trees

Ensembles are methods that combine multiple machine learning models to create more powerful models.

There are many models in the machine learning literature that belong to this category, but there are two ensemble models that have proven to be effective on a wide range of datasets for classification and regression, both of which use decision trees as their building block: Random Forests and Gradient Boosted Decision Trees.

### Random Forests

As observed above, a main drawback of decision trees is that they tend to overfit the training data. Random forests

are one way to address this problem. Random forests are essentially a collection of decision trees, where each tree is slightly different from the others.

The idea of random forests is that each tree might do a relatively good job of predicting, but will likely overfit on part of the data.

If we build many trees, all of which work well and overfit in different ways, we can reduce the amount of overfitting by averaging their results. This reduction in overfitting, while retaining the predictive power of the trees, can be shown using rigorous mathematics.

To implement this strategy, we need to build many decision trees. Each tree should do an acceptable job of predicting the target, and should also be different from the other trees. Random forests get their name from injecting randomness into the tree building to ensure each tree is different. There are two ways in which the trees in a random



forest are randomized: by selecting the data points used to build a tree and by selecting the features in each split test. Let's go into this process in more detail.

## Building Random Forests

To build a random forest model, you need to decide on the number of trees to build (the `n_estimator` parameter of `RandomForestRegressor` or `RandomForestClassifier`). Lets say we want to build ten trees. These trees will be built completely independent from each other, and [will?] make random choices to make sure they are distinct [the trees make random choices?].

To build a tree, we first take what is called a *bootstrap* sample of our data. A bootstrap sample means from our `n_samples` data points, we repeatedly draw an example randomly with replacement (i.e. the same sample can be picked multiple times), `n_samples` times. This will create a dataset that is as big as the original dataset, but some data points will be missing from it, and some will be repeated.

To illustrate, lets say we want to create a bootstrap sample of the list ['a', 'b', 'c', 'd']. A possible bootstrap sample would be ['b', 'd', 'd', 'c']. Another possible sample would be ['d', 'a', 'd', 'a'].

Next, a decision tree is built based on this newly created dataset. However, the algorithm we described for the decision tree is slightly modified. Instead of looking for the best test for each node, in each node the algorithm randomly selects a subset of the features, and looks for the best possible test involving one of these features. The amount of features that is selected is controlled by the `max_features` parameter.

This selection of a subset of features is repeated separately in each node, so that each node in a tree can make a decision using a different subset of the features.

The bootstrap sampling leads to each decision tree in the random forest being built on a slightly different dataset. Because of the selection of features in each node, each split in each tree operates on a different subset of features. Together these two mechanisms ensure that all the trees in the random forests are different.

A critical parameter in this process is `max_features`. If we set `max_features` to `n_features`, that means that each split can look at all features in the dataset, and no randomness will be injected. If we set `max_features` to one, that means that the splits have no choice at all on which feature to test, and can only search over different thresholds for the feature that was selected randomly.

Therefore, a high `max_features` means that the trees in the random forest will be quite similar, and they will be able to fit the data easily, using the most distinctive features. A low `max_features` means that the trees in the random forest will be quite different, and that each tree might need to be very deep in order to fit the data well.

To make a prediction using the random forest, the algorithm first makes a prediction for every tree in the forest. For regression, we can average these results to get our final prediction. For classification, a “soft voting” strategy is used. This means each algorithm makes a “soft” prediction, providing a probability for each possible output label. The probabilities predicted by all the trees are averaged, and the class with the highest label is predicted.

## Analyzing Random Forests

Let’s apply a random forest consisting of five trees to the `two_moon` data we studied above.

```
from sklearn.ensemble import RandomForestClassifier
from sklearn.datasets import make_moons

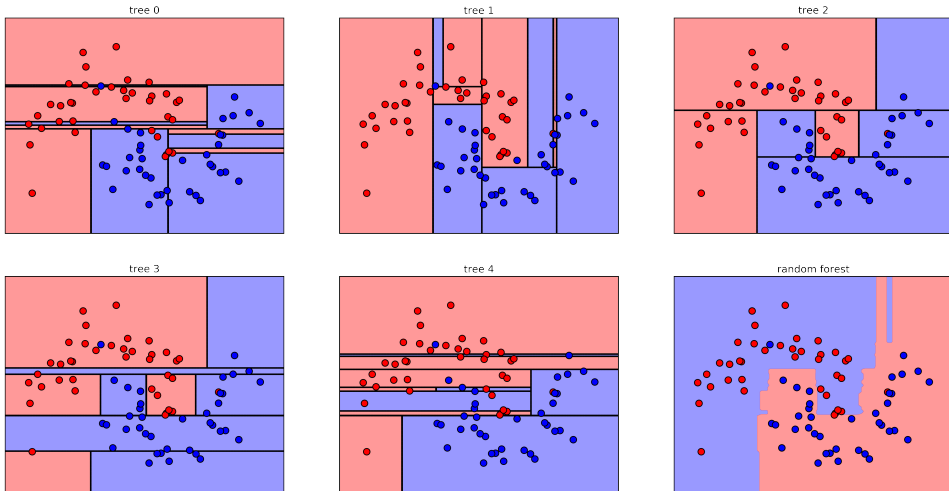
X, y = make_moons(n_samples=100, noise=0.25, random_state=3)
X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y, random_state=42)

forest = RandomForestClassifier(n_estimators=5, random_state=2)
forest.fit(X_train, y_train)

RandomForestClassifier(bootstrap=True, class_weight=None, criterion='gini',
                        max_depth=None, max_features='auto', max_leaf_nodes=None,
                        min_samples_leaf=1, min_samples_split=2,
                        min_weight_fraction_leaf=0.0, n_estimators=5, n_jobs=1,
                        oob_score=False, random_state=2, verbose=0, warn_start=False)
```

The trees that are built as part of the random forest are stored in the `estimator_` attribute. Let’s visualize the decision boundaries learned by each tree, together with their aggregate prediction, as made by the forest.

```
fig, axes = plt.subplots(2, 3, figsize=(20, 10))
for i, (ax, tree) in enumerate(zip(axes.ravel(), forest.estimators_)):
    ax.set_title("tree %d" % i)
    mglearn.plots.plot_tree_partition(X_train, y_train, tree, ax=ax)
mglearn.plots.plot_2d_separator(forest, X_train, fill=True, ax=axes[-1, -1], alpha=.4)
axes[-1, -1].set_title("random forest")
plt.scatter(X_train[:, 0], X_train[:, 1], c=np.array(['r', 'b'])[y_train], s=60)
```



You can clearly see that the decisions learned by the five trees are quite different. Each of them makes some mistakes, as some of the training points that are plotted here were not actually included in the training set of the tree, due to the bootstrap sampling.

The random forest overfit less than any of the trees individually, and provides a much more intuitive decision boundary. In any real application, we would use many more trees (often hundreds or thousands), leading to even smoother boundaries.

Let's apply a random forest consisting of 100 trees on the breast cancer dataset:

```
X_train, X_test, y_train, y_test = train_test_split(
    cancer.data, cancer.target, random_state=0)
forest = RandomForestClassifier(n_estimators=100, random_state=0)
forest.fit(X_train, y_train)

print("accuracy on training set: %f" % forest.score(X_train, y_train))
print("accuracy on test set: %f" % forest.score(X_test, y_test))

accuracy on training set: 1.000000

accuracy on test set: 0.972028
```

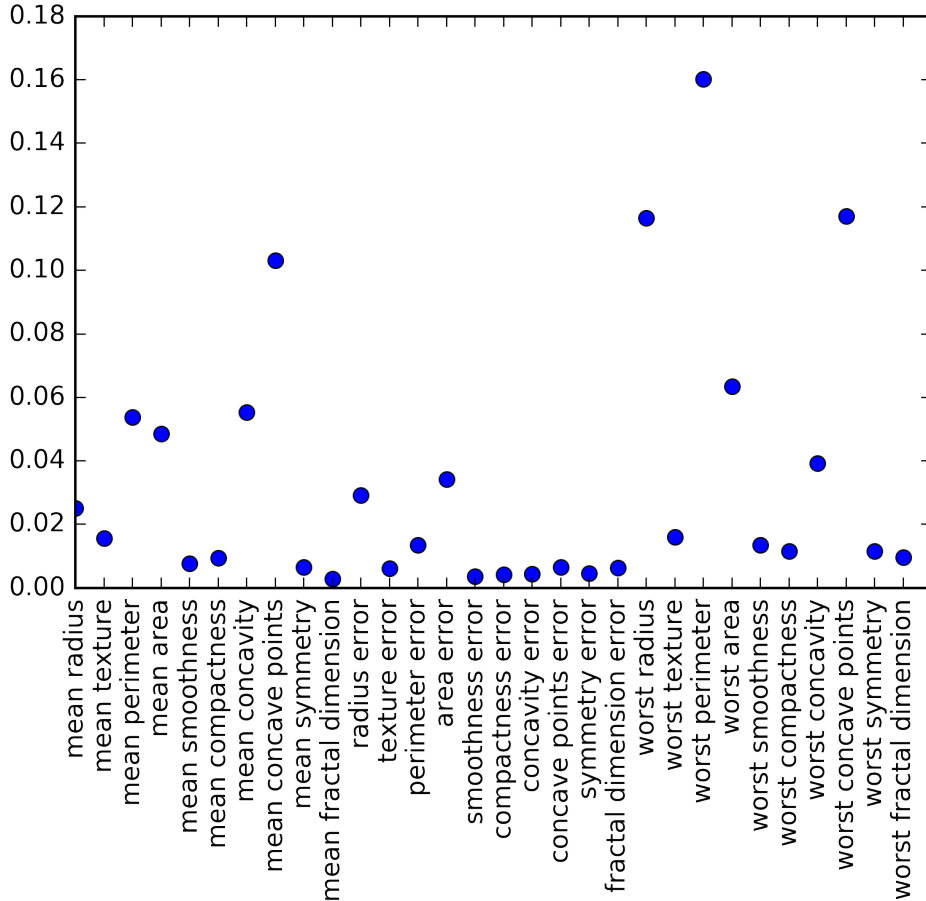
The random forest gives us an accuracy of 97%, better than the linear models or a single decision tree, without tuning any parameters. We could adjust the `max_features` setting, or apply pre-pruning as we did for the single decision tree.

However, often the default parameters of the random forest already work quite well.

Similarly to the decision tree, the random forest provides feature importances, which are computed by aggregating the feature importances over the trees in the forest. Typ-

ically the feature importances provided by the random forest are more reliable than the ones provided by a single tree.

```
plt.plot(forest.feature_importances_, 'o')
plt.xticks(range(cancer.data.shape[1]), cancer.feature_names, rotation=90);
```



As you can see, the random forest gives non-zero importance to many more features than the single tree. Similarly to the single decision tree, the random forest also gives a lot of importance to the “worst radius”, but it actually chooses “worst perimeter” to be the most informative feature overall. The randomness in building the random forest forces the algorithm to consider many possible explanations, the result of which being that the random forest captures a much broader picture of the data than a single tree.

## Strengths, weaknesses and parameters

Random forests for regression and classification are currently among the most widely used machine learning methods.

They are very powerful, often work well without heavy tuning of the parameters, and don't require scaling of the data.

Essentially, random forests share all of the benefits of decision trees, while making up for some of their deficiencies.

One reason to still use decision trees is if you need a compact representation of the decision making process. It is basically impossible to interpret tens or hundreds of trees in detail, and trees in random forests tend to be deeper than decision trees (because of the use of feature subsets). Therefore, if you need to summarize the prediction making in a visual way to non-experts, a single decision tree might be a better choice.

While building random forests on large dataset might be somewhat time-consuming, it can be parallelized across multiple CPU cores within a computer easily. If you are using a multi-core processor (as nearly all modern computers do), you can use the `n_jobs` parameter to adjust the number of cores to use. Using more CPU cores will result in linear speed-ups (using two cores, the training of the random forest will be twice as fast), but specifying `n_jobs` larger than the number of cores will not help. You can set `n_jobs=-1` to use all the cores in your computer.

You should keep in mind that random forests, by their nature, are random, and setting different random states (or not setting the `random_state` at all) can drastically change the model that is built. The more trees there are in the forest, the more robust it will be against the choice of random state. If you want to have reproducible results, it is important to fix the `random_state`.

Random forests don't tend to perform well on very high dimensional, sparse data, such as text data. For this kind of data, linear models might be more appropriate.

Random forests usually work well even on very large datasets, and training can easily be parallelized over many CPU cores within a powerful computer. However, random forests require more memory and are slower to train and to predict than linear models. If time and memory are important in an application, it might make sense to use a linear model instead.

The important parameters to adjust are `n_estimators`, `max_features` and possibly pre-pruning options like `max_depth`. For `n_estimators`, larger is always better. Averaging more trees will yield a more robust ensemble. However, there are diminishing returns, and more trees need more memory and more time to train. A common rule of thumb is to build "as many as you have time / memory for".

As described above `max_features` determines how random each tree is, and a smaller `max_features` reduces overfitting. The default values, and a good rule of thumb, are `max_features=sqrt(n_features)` for classification and `max_features=log2(n_features)` for regression.

Adding `max_features` or `max_leaf_nodes` might sometimes improve performance. It can also drastically reduce space and time requirements for training and prediction.

## Gradient Boosted Regression Trees (Gradient Boosting Machines)

Gradient boosted regression trees is another ensemble method that combines multiple decision trees to a more powerful model. Despite the “regression” in the name, these models can be used for regression and classification.

In contrast to random forests, gradient boosting works by building trees in a serial manner, where each tree tries to correct the mistakes of the previous one. There is no randomization in gradient boosted regression trees; instead, strong pre-pruning is used. Gradient boosted trees often use very shallow trees, of depth one to five, often making the model smaller in terms of memory, and making predictions faster.

The main idea behind gradient boosting is to combine many simple models (in this context known as *weak learners*), like shallow trees. Each tree can only provide good predictions on part of the data, and so more and more trees are added to iteratively improve performance.

Gradient boosted trees are frequently the winning entries in machine learning competitions, and are widely used in industry. They are generally a bit more sensitive to parameter settings than random forests, but can provide better accuracy if the parameter are set correctly.

Apart from the pre-pruning and the number of trees in the ensemble, another important parameter of gradient boosting is the `learning_rate` which controls how strongly each tree tries to correct the mistakes of the previous trees. A higher learning rate means each tree can make stronger corrections, allowing for more complex models. Similarly, adding more trees to the ensemble, which can be done by increasing `n_estimators`, also increases the model complexity, as the model has more chances to correct mistakes on the training set.

Here is an example of using `GradientBoostingClassifier` on the breast cancer dataset.

By default, 100 trees of maximum depth three are used, with a learning rate of 0.1.

```
from sklearn.ensemble import GradientBoostingClassifier

X_train, X_test, y_train, y_test = train_test_split(
    cancer.data, cancer.target, random_state=0)
```

```

gbrt = GradientBoostingClassifier(random_state=0)
gbrt.fit(X_train, y_train)

print("accuracy on training set: %f" % gbrt.score(X_train, y_train))
print("accuracy on test set: %f" % gbrt.score(X_test, y_test))

accuracy on training set: 1.000000

accuracy on test set: 0.958042

```

As the training set accuracy is 100%, we are likely to be overfitting. To reduce overfitting, we could either apply stronger pre-pruning by limiting the maximum depth or lower the learning rate:

```

gbrt = GradientBoostingClassifier(random_state=0, max_depth=1)
gbrt.fit(X_train, y_train)

print("accuracy on training set: %f" % gbrt.score(X_train, y_train))
print("accuracy on test set: %f" % gbrt.score(X_test, y_test))

accuracy on training set: 0.990610

accuracy on test set: 0.972028

gbrt = GradientBoostingClassifier(random_state=0, learning_rate=0.01)
gbrt.fit(X_train, y_train)

print("accuracy on training set: %f" % gbrt.score(X_train, y_train))
print("accuracy on test set: %f" % gbrt.score(X_test, y_test))

accuracy on training set: 0.988263

accuracy on test set: 0.965035

```

Both methods of decreasing the model complexity decreased the training set accuracy as expected. In this case, lowering the maximum depth of the trees provided a significant improvement of the model, while lowering the learning rate only increased the generalization performance slightly.

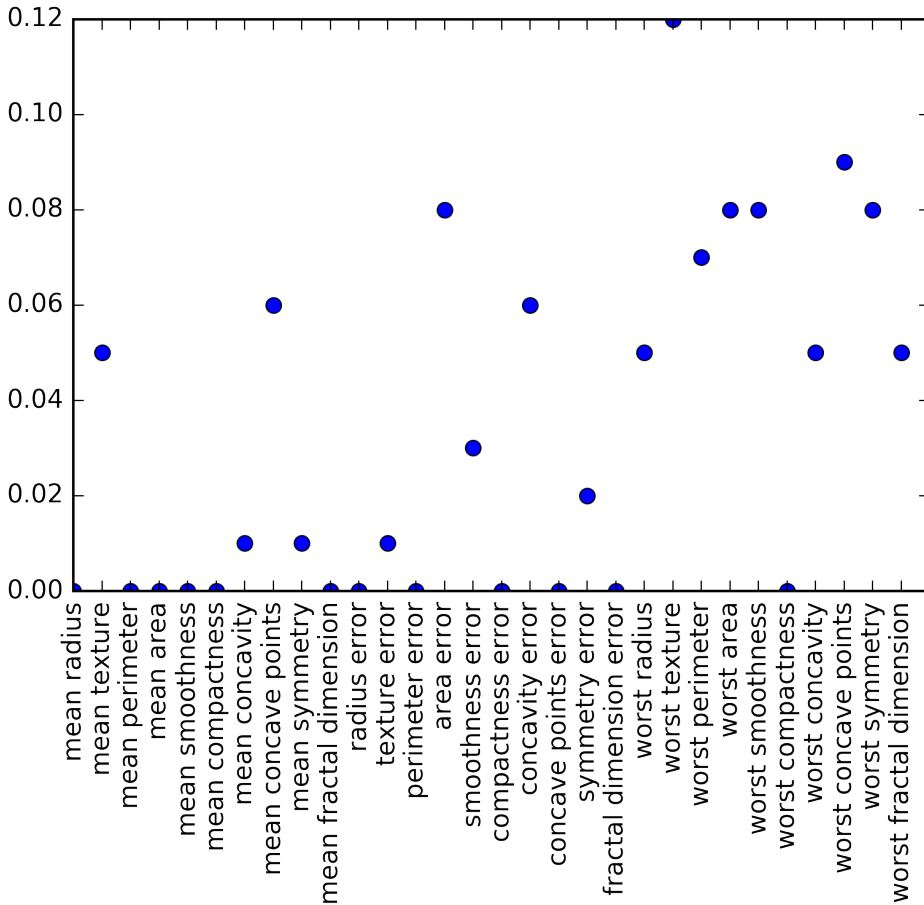
As for the other decision tree based models, we can again visualize the feature importances to get more insight into our model. As we used 100 trees, it is impractical to inspect them all, even if they are all of depth 1.

```

gbrt = GradientBoostingClassifier(random_state=0, max_depth=1)
gbrt.fit(X_train, y_train)

plt.plot(gbrt.feature_importances_, 'o')
plt.xticks(range(cancer.data.shape[1]), cancer.feature_names, rotation=90);

```



We can see that the feature importances of the gradient boosted trees are somewhat similar to the feature importances of the random forests, though the gradient boosting completely ignored some of the features.

As gradient boosting and random forest perform well on similar kinds of data, a common approach is to first try random forests, which work quite robustly. If random forests work well, but prediction time is at a premium, or it is important to squeeze out the last percentage of accuracy from the machine learning model, moving to gradient boosting often helps.

If you want to apply gradient boosting to a large scale problem, it might be worth looking into the `xgboost` package and its python interface, which at the time of writing is faster (and sometimes easier to tune) than the `scikit-learn` implementation of gradient boosting on many datasets.



## Strengths, weaknesses and parameters

Gradient boosted decision trees are among the most powerful and widely used models for supervised learning.

Their main drawback is that they require careful tuning of the parameters, and may take a long time to train.

Similarly to other tree-based models, the algorithm works well without scaling and on a mixture of binary and continuous features. As other tree-based models, it also often does not work well on high-dimensional sparse data.

The main parameters of the gradient boosted tree models are the number of trees `n_estimators`, and the `learning_rate`, which controls how much each tree is allowed to correct the mistakes of the previous trees.

These two parameters are highly interconnected, as a lower `learning_rate` means that more trees are needed to build a model of similar complexity. In contrast to random forests, where higher `n_estimators` is always better, increasing `n_estimators` in gradient boosting leads to a more complex model, which may lead to overfitting.

A common practice is to fit `n_estimators` depending on the time and memory budget, and then search over different `learning_rates`.

Another important parameter is `max_depth`, which is usually very low for gradient boosted models, often not deeper than five splits.

## Kernelized Support Vector Machines

The next type of supervised model we will discuss is kernelized support vector machines (SVMs).

We already saw linear support vector machines for classification in the linear model section. Kernelized support vector machines (often just referred to as SVMs) are an extension that allows for more complex models which are not defined simply by hyperplanes in the input space. While there are support vector machines for classification and regression, we will restrict ourself to the classification case, as implemented in `SVC`. Similar concepts apply to support vector regression, as implemented in `SVR`.

The math behind kernelized support vector machines is a bit involved, and is mostly beyond the scope of this book.

However, we will try to give you some intuitions about the idea behind the method.

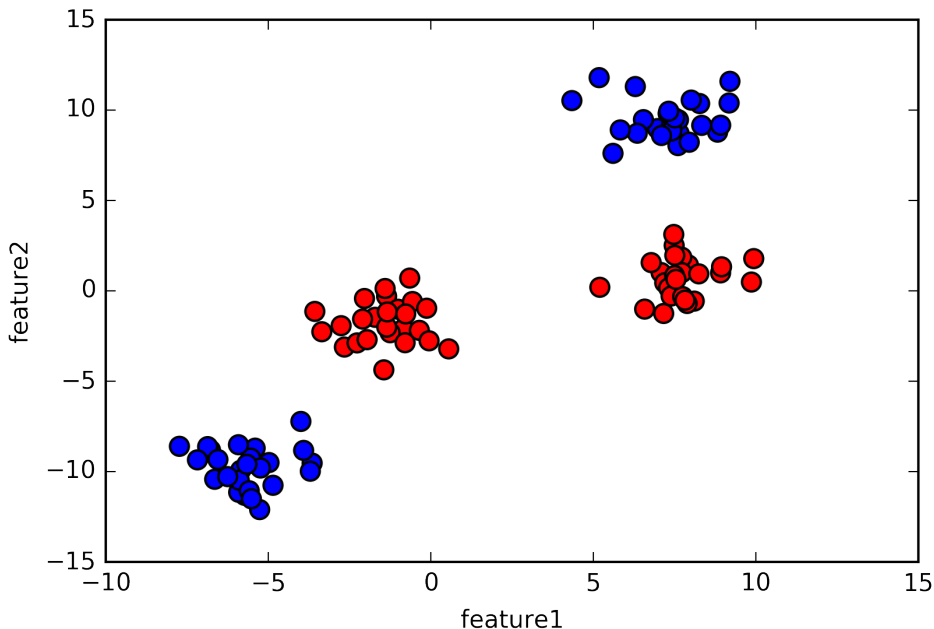
## Linear Models and Non-linear Features

As you saw in Figure `linear_classifiers`, linear models can be quite limiting in low-dimensional spaces, as lines or hyperplanes have limited flexibility. One way to make a linear model more flexible is by adding more features, for example by adding interactions or polynomials of the input features.

Let's look at the synthetic dataset we used in Figure `tree_not_monotone`:

```
X, y = make_blobs(centers=4, random_state=8)
y = y % 2

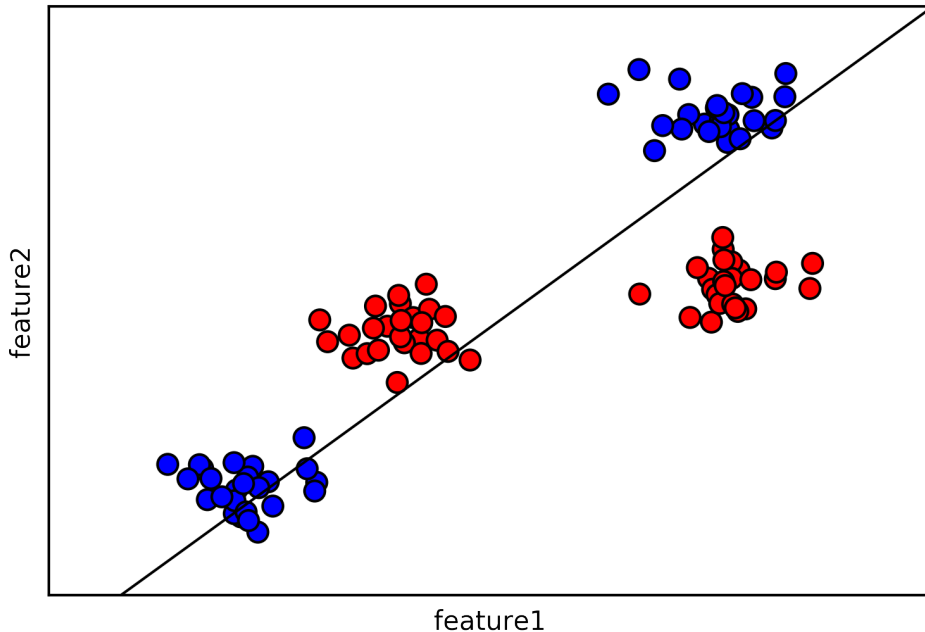
plt.scatter(X[:, 0], X[:, 1], c=y, s=60, cmap=mglearn.cm2)
plt.xlabel("feature1")
plt.ylabel("feature2")
```



A linear model for classification can only separate points using a line, and will not be able to do a very good job on this dataset:

```
from sklearn.svm import LinearSVC
linear_svm = LinearSVC().fit(X, y)

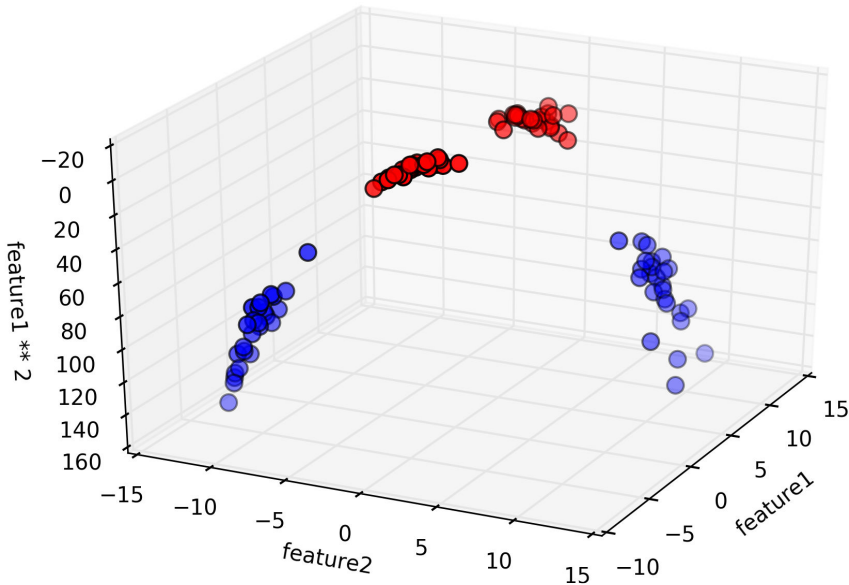
mglearn.plots.plot_2d_separator(linear_svm, X)
plt.scatter(X[:, 0], X[:, 1], c=y, s=60, cmap=mglearn.cm2)
plt.xlabel("feature1")
plt.ylabel("feature2")
```



Now, let's expand the set of input features, say by also adding  $\text{feature2}^2$ , the square of the second feature, as a new feature. Instead of representing each data point as a two-dimensional point ( $\text{feature1}$ ,  $\text{feature2}$ ), we now represent it as a three-dimensional point ( $\text{feature1}$ ,  $\text{feature2}$ ,  $\text{feature2}^2$ ) (Footnote: We picked this particular feature to add for illustration purposes. The choice is not particularly important.). This new representation is illustrated below in a three-dimensional scatter plot:

```
# add the squared first feature
X_new = np.hstack([X, X[:, 1:] ** 2])

from mpl_toolkits.mplot3d import Axes3D, axes3d
figure = plt.figure()
# visualize in 3D
ax = Axes3D(figure, elev=-152, azim=-26)
ax.scatter(X_new[:, 0], X_new[:, 1], X_new[:, 2], c=y, cmap=mglearn.cm2, s=60)
ax.set_xlabel("feature1")
ax.set_ylabel("feature2")
ax.set_zlabel("feature1 ** 2")
```



In the new, three-dimensional representation of the data, it is now indeed possible to separate the red and the blue points

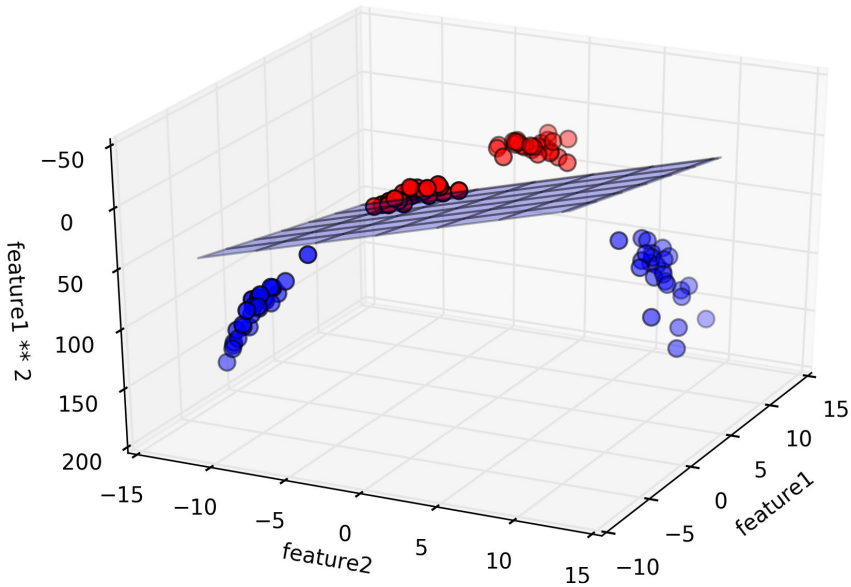
using a linear model, a plane in three dimensions. We can confirm this by fitting a linear model to the augmented data:

```
linear_svm_3d = LinearSVC().fit(X_new, y)
coef, intercept = linear_svm_3d.coef_.ravel(), linear_svm_3d.intercept_

# show linear decision boundary
figure = plt.figure()
ax = Axes3D(figure, elev=-152, azim=-26)
xx = np.linspace(X_new[:, 0].min(), X_new[:, 0].max(), 50)
yy = np.linspace(X_new[:, 1].min(), X_new[:, 1].max(), 50)

XX, YY = np.meshgrid(xx, yy)
ZZ = (coef[0] * XX + coef[1] * YY + intercept) / -coef[2]
ax.scatter(X_new[:, 0], X_new[:, 1], X_new[:, 2], c=y, cmap=mglearn.cm2, s=60)
ax.plot_surface(XX, YY, ZZ, rstride=8, cstride=8, alpha=0.3)

ax.set_xlabel("feature1")
ax.set_ylabel("feature2")
ax.set_zlabel("feature1 ** 2")
```

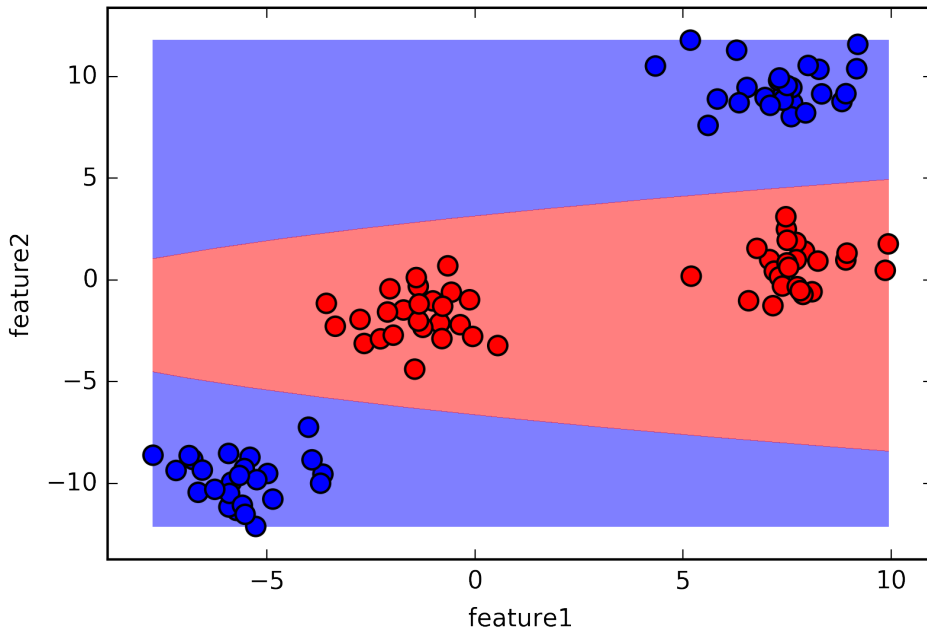


As a function of the original features, the linear SVM model is not actually linear anymore. It is not a line, but more of an ellipse.

```

ZZ = YY ** 2
dec = linear_svm_3d.decision_function(np.c_[XX.ravel(), YY.ravel(), ZZ.ravel()])
plt.contourf(XX, YY, dec.reshape(XX.shape), levels=[dec.min(), 0, dec.max()],
             cmap=mglearn.cm2, alpha=0.5)
plt.scatter(X[:, 0], X[:, 1], c=y, s=60, cmap=mglearn.cm2)
plt.xlabel("feature1")
plt.ylabel("feature2")

```



## The Kernel Trick

The lesson here is that adding non-linear features to the representation of our data can make linear models much more powerful. However, often we don't know which features to add, and adding many features (like all possible interactions in a 100 dimensional feature space) might make computation very expensive.

Luckily, there is a clever mathematical trick that allows us to learn a classifier in a higher dimensional space without actually computing the new, possibly very large representation. This trick is known as the *kernel trick*.

The kernel trick works by directly computing the distance (more precisely, the scalar products) of the data points for the expanded feature representation, without ever actually computing the expansion.

There are two ways to map your data into a higher dimensional space that are commonly used with support vector machines: the polynomial kernel, which computes all possible polynomials up to a certain degree of the original features (like `feature1 ** 2 * feature2 ** 5`), and the radial basis function (rbf) kernel, also known as Gaussian kernel.

The Gaussian kernel is a bit harder to explain, as it corresponds to an infinite dimensional feature space. One way to explain the Gaussian kernel is that it considers all possible polynomials of all degrees, but the importance of the features decreases for

higher degrees. [Footnote: this follows from the Taylor expansion of the exponential map].

If all of this is too much math talk for you, don't worry. You can still use SVMs without trying to imagine infinite dimensional feature spaces. In practice, how a SVM with an rbf kernel makes a decision can be summarized quite easily.

## Understanding SVMs

During training, the SVM learns how important each of the training data points is to represent the decision boundary between the two classes. Typically only a subset of the training points matter for defining the decision boundary: the ones that lie on the border between the classes. These are called *support vectors* and give the support vector machine its name.

To make a prediction for a new point, the distance to the support vectors is measured. A classification decision is made based on the distance to the support vectors, and the importance of the support vectors that was learned during training (stored in the `dual_coef_` attribute of `SVC`).

The way distance between data points is measured by the Gaussian kernel:

```
\begin{align*}
& k_{\text{rbf}}(x_1, x_2) = \exp(-\gamma \|x_1 - x_2\|^2) \quad \text{(4) Gaussian kernel}
\end{align*}
```

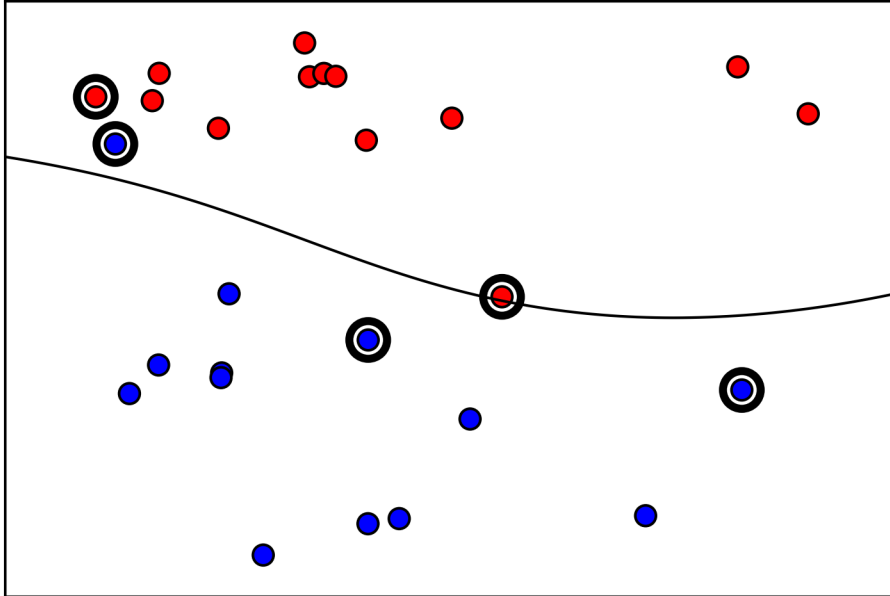
Here,  $x_1$  and  $x_2$  are data points,  $\|x_1 - x_2\|$  denotes Euclidean distance and  $\gamma$  is a parameter that controls the width of the Gaussian kernel.

Below is the result of training an support vector machine on a two-dimensional two-class dataset.

The decision boundary is shown in black, and the support vectors are the points with wide black circles.

```
from sklearn.svm import SVC

X, y = mglearn.tools.make_handcrafted_dataset()
svm = SVC(kernel='rbf', C=10, gamma=0.1).fit(X, y)
mglearn.plots.plot_2d_separator(svm, X, eps=.5)
# plot data
plt.scatter(X[:, 0], X[:, 1], s=60, c=y, cmap=mglearn.cm2)
# plot support vectors
sv = svm.support_vectors_
plt.scatter(sv[:, 0], sv[:, 1], s=200, facecolors='none', zorder=10, linewidth=3)
```



In this case, the SVM yields a very smooth and non-linear (not a straight line) boundary.

There are two parameters we adjusted here: The C parameter and the gamma parameter, which we will now discuss in detail.

## Tuning SVM parameters

The gamma parameter is the one shown in Formula (4), which controls the width of the Gaussian kernel. It determines the scale of what it means for points to be close together.

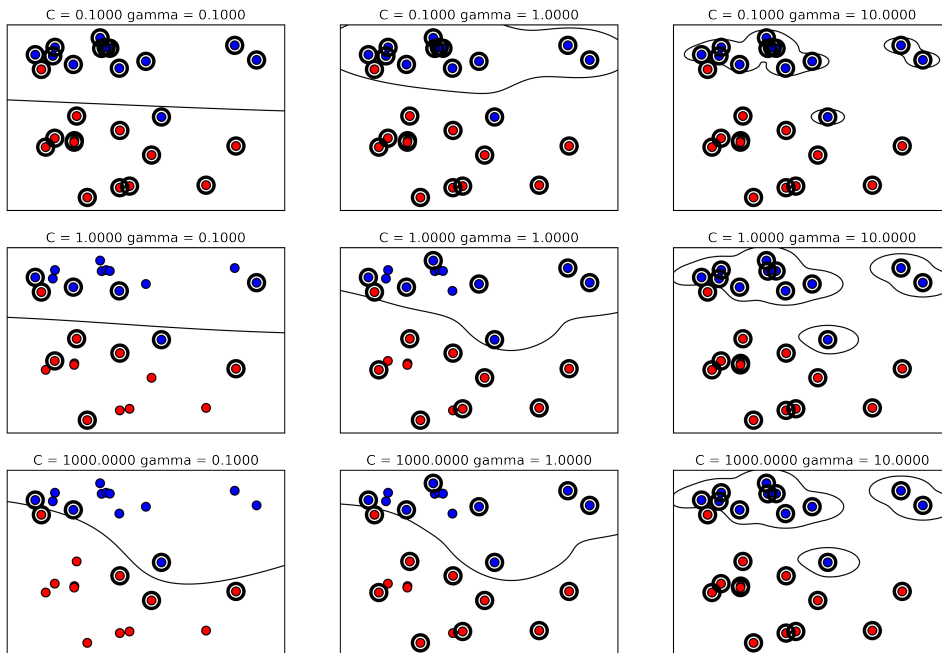
The C parameter is a regularization parameter similar to the linear models. It limits the importance of each point (or more precisely, their `dual_coef_`).

Let's have a look at what happens when we vary these parameters:

```
fig, axes = plt.subplots(3, 3, figsize=(15, 10))

for ax, C in zip(axes, [-1, 0, 3]):
    for a, gamma in zip(ax, range(-1, 2)):
        mglearn.plots.plot_svm(log_C=C, log_gamma=gamma, ax=ax)
```





Going from left to right, we increase the parameter  $\gamma$  from 0.1 to 10. A small  $\gamma$  means a large radius for the Gaussian kernel, which means that many points are considered close-by. This is reflected in very smooth decision boundaries on the left, and boundaries that focus more on single points further to the right. A low value of  $\gamma$  means that the decision boundary will vary slowly, which yields a model of low complexity, while a high value of  $\gamma$  yields a more complex model.

Going from top to bottom, we increase the  $C$  parameter from 0.1 to 1000. As with the linear models, a small  $C$  means a very restricted model, where each data point can only have very limited influence. You can see that in the top left, the decision boundary looks nearly linear, with the red and blue points that are misclassified barely changing the line.

Increasing  $C$ , as shown on the bottom right, allows these points to have a stronger influence on the model, and makes the decision boundary bend to correctly classify them.

Let's apply the rbf kernel SVM to the breast cancer dataset. By default,  $C=1$  and  $\gamma=1./n\_features$ .

```
X_train, X_test, y_train, y_test = train_test_split(
    cancer.data, cancer.target, random_state=0)

svc = SVC()
svc.fit(X_train, y_train)
```

```

print("accuracy on training set: %f" % svc.score(X_train, y_train))
print("accuracy on test set: %f" % svc.score(X_test, y_test))

accuracy on training set: 1.000000

accuracy on test set: 0.629371

```

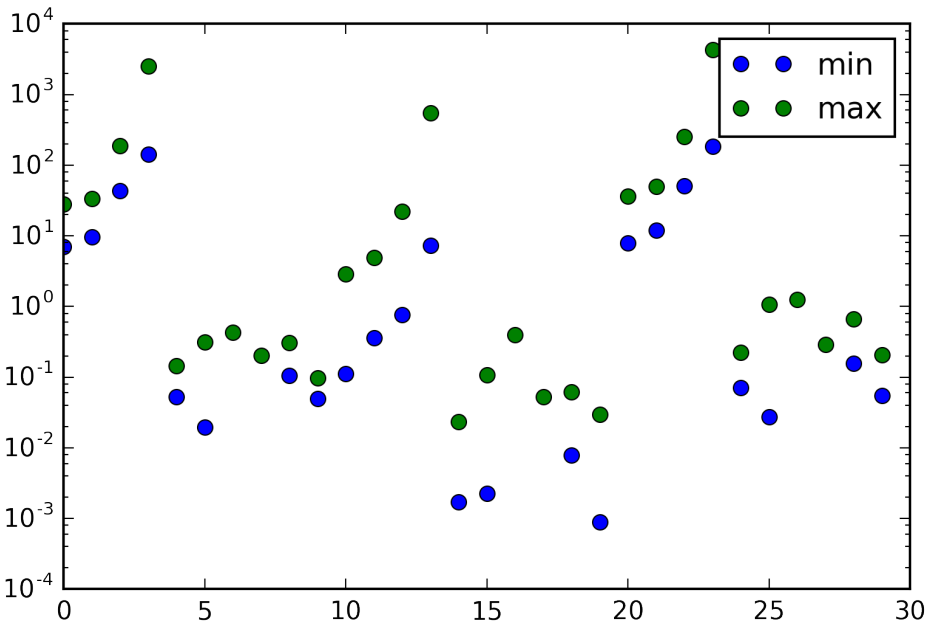
The model overfit quite substantially, with a perfect score on the training set and only 62% accuracy on the test set.

While SVMs often perform quite well, they are very sensitive to the settings of the parameters, and to the scaling of the data. In particular, they require all the features to vary on a similar scale. Let's look at the minimum and maximum values for each feature, plotted in log-space:

```

plt.plot(X_train.min(axis=0), 'o', label="min")
plt.plot(X_train.max(axis=0), 'o', label="max")
plt.legend(loc="best")
plt.yscale("log")

```



From this plot we can determine that features in the breast cancer dataset are of completely different orders of magnitude.

This can be somewhat of a problem for other models (like linear models), but it has devastating effects for the kernel SVM.

## Preprocessing Data for SVMs

One way to resolve this problem is by rescaling each feature, so that they are approximately on the same scale.

A common rescaling methods for kernel SVMs is to scale the data such that all features are between zero and one. We will see how to do this using the `MinMaxScaler` preprocessing method in Chapter 3 (Unsupervised Learning), where we'll give more details.

For now, let's do this "by hand":

```
# Compute the minimum value per feature on the training set
min_on_training = X_train.min(axis=0)
# Compute the range of each feature (max - min) on the training set
range_on_training = (X_train - min_on_training).max(axis=0)

# subtract the min, divide by range
# afterwards min=0 and max=1 for each feature
X_train_scaled = (X_train - min_on_training) / range_on_training
print("Minimum for each feature\n%s" % X_train_scaled.min(axis=0))
print("Maximum for each feature\n %s" % X_train_scaled.max(axis=0))

Minimum for each feature

[ 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.]

Maximum for each feature

[ 1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.

  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.]

# use THE SAME transformation on the test set,
# using min and range of the training set. See Chapter 3 (unsupervised learning) for details.
X_test_scaled = (X_test - min_on_training) / range_on_training

svc = SVC()
svc.fit(X_train_scaled, y_train)

print("accuracy on training set: %f" % svc.score(X_train_scaled, y_train))
print("accuracy on test set: %f" % svc.score(X_test_scaled, y_test))

accuracy on training set: 0.948357

accuracy on test set: 0.951049
```

Scaling the data made a huge difference! Now we are actually in an underfitting regime, where training and test set performance are quite similar. From here, we can try increasing either `C` or `gamma` to fit a more complex model:

```

svc = SVC(C=1000)
svc.fit(X_train_scaled, y_train)

print("accuracy on training set: %f" % svc.score(X_train_scaled, y_train))
print("accuracy on test set: %f" % svc.score(X_test_scaled, y_test))

accuracy on training set: 0.988263

accuracy on test set: 0.972028

```

Here, increasing C allows us to improve the model significantly, resulting in 97.2% accuracy.

## Strengths, weaknesses and parameters

Kernelized support vector machines are very powerful models and perform very well on a variety of datasets.

SVMs allow for very complex decision boundaries, even if the data has only a few features. SVMs work well on low-dimensional and high-dimensional data (i.e. few and many features), but don't scale very well with the number of samples. Running on data with up to 10000 samples might work well, but working with datasets of size 100000 or more can become challenging in terms of runtime and memory usage.

Another downside of SVMs is that they require careful preprocessing of the data and tuning of the parameters.

For this reason, SVMs have been replaced by tree-based models such as random forests (that require little or no preprocessing) in many applications. Furthermore, SVM models are hard to inspect; it can be difficult to understand why a particular prediction was made, and it might be tricky to explain the model to a non-expert.

Still it might be worth trying SVMs, particularly if all of your features represent measurements in similar units (i.e. all are pixel intensities) and are on similar scales.

The important parameters in kernel SVMs are the regularization parameter C, the choice of the kernel, and the kernel-specific parameters. We only talked about the rbf kernel in any depth above, but other choices are available in scikit-learn. The rbf kernel has only one parameter,  $\gamma$ , which is the inverse of the width of the Gaussian kernel.  $\gamma$  and C both control the complexity of the model, with large values in either resulting in a more complex model. Therefore, good settings for the two parameters are usually strongly correlated, and C and  $\gamma$  should be adjusted together.

## Neural Networks (Deep Learning)

A family of algorithms known as neural networks has recently seen a revival under the name “deep learning”.

While deep learning shows great promise in many machine learning applications, many deep learning algorithms are tailored very carefully to a specific use-case. Here, we will only discuss some relatively simple methods, namely *multilayer perceptrons* for classification and regression, that can serve as a starting point for more involved deep learning methods. Multilayer perceptrons (MLPs) are also known as (vanilla) feed-forward neural networks, or sometimes just neural networks.

## The Neural Network Model

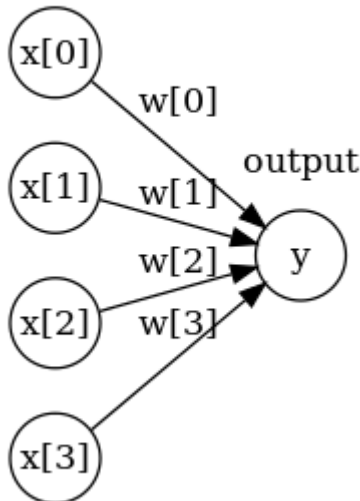
MLPs can be viewed as generalizations of linear models which perform multiple stages of processing to come to a decision.

Remember that the prediction by a linear regressor is given as:

In words,  $y$  is a weighted sum of the input features  $x[0]$  to  $x[p]$ , weighted by the learned coefficients  $w[0]$  to  $w[p]$ . We could visualize this graphically as:

```
mglearn.plots.plot_logistic_regression_graph()
```

inputs



where each node on the left represents an input feature, the connecting lines represent the learned coefficients, and the node on the right represents the output, which is a weighted sum of the inputs.

In an MLP, this process of computing weighted sums is repeated multiple times, first computing *hidden units* that represent an intermediate processing step, which are again combined using weighted sums, to yield the final result:

```
print("Figure single_hidden_layer")
mglearn.plots.plot_single_hidden_layer_graph()
```

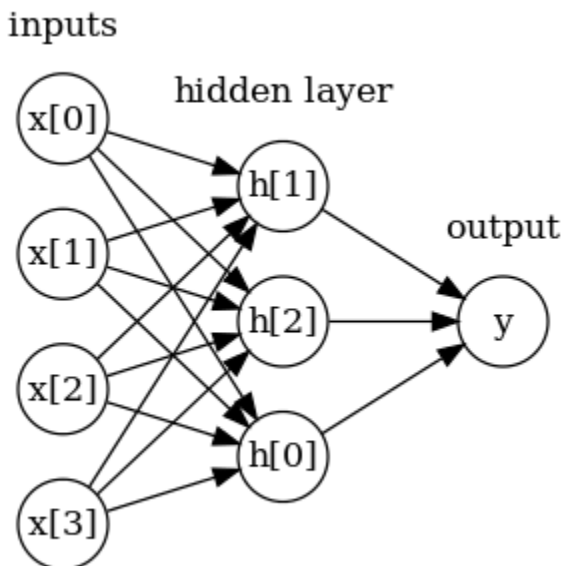


Figure single\_hidden\_layer

This model has a lot more coefficients (also called weights) to learn: there is one between every input and every hidden unit (which make up the *hidden layer*), and one between every unit in the hidden layer and the output.

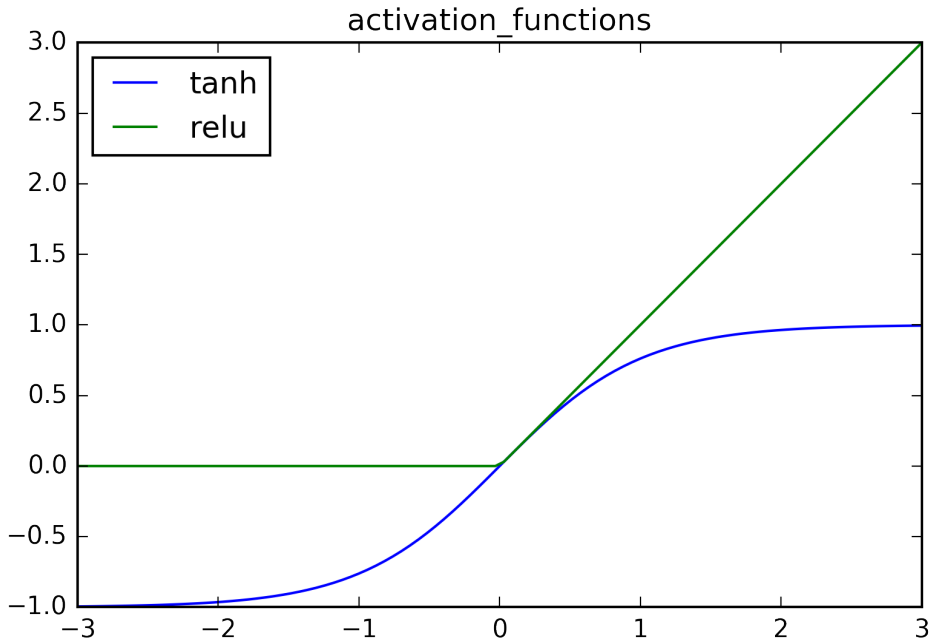
Computing a series of weighted sums is mathematically the same as computing just one weighted sum, so to make this model truly more powerful than a linear model, there is one extra trick we need. After computing a weighted sum for each hidden unit, a non-linear function is applied to the result, usually the *rectifying nonlinearity* (also known as rectified linear unit or relu) or the *tangens hyperbolicus* (tanh). The result of this function is then used in the weighted sum that computes the output  $y$ .

The two functions are visualized in Figure activation\_functions. The relu cuts off values below zero, while tanh saturates to -1 for low input values and +1 for high input values. Either non-linear function allows the neural network to learn much more complicated function than a linear model could.

```

line = np.linspace(-3, 3, 100)
plt.plot(line, np.tanh(line), label="tanh")
plt.plot(line, np.maximum(line, 0), label="relu")
plt.legend(loc="best")
plt.title("activation_functions")

```



For the small neural network pictures in Figure `single_hidden_layer` above, the full formula for computing  $y$  in the case of regression would be (when using a tanh non-linearity):

Here,  $w$  are the weights between the input  $x$  and the hidden layer  $h$ , and  $v$  are the weights between the hidden layer  $h$  and the output  $y$ . The weights  $v$  and  $w$  are learned from data,  $x$  are the input features,  $y$  is the computed output, and  $h$  are intermediate computations.

An important parameter that needs to be set by the user is the number of nodes in the hidden layer, and can be as small as 10 for very small or simple datasets, and can be as big as 10000 for very complex data.

It is also possible add additional hidden layers, as in Figure `two_hidden_layers` below. Having large neural networks made up of many of these layers of computation is what inspired the term “deep learning”.

```

print("Figure two_hidden_layers")
mglearn.plots.plot_two_hidden_layer_graph()

```

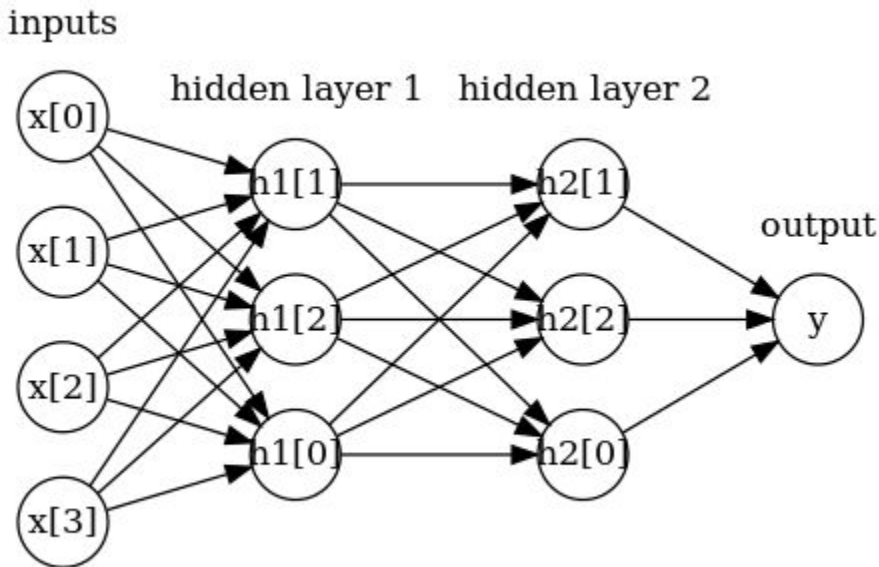


Figure two\_hidden\_layers

## Tuning Neural Networks

Let's look into the workings of the MLP by applying the MLPClassifier to the two\_moons dataset we saw above.

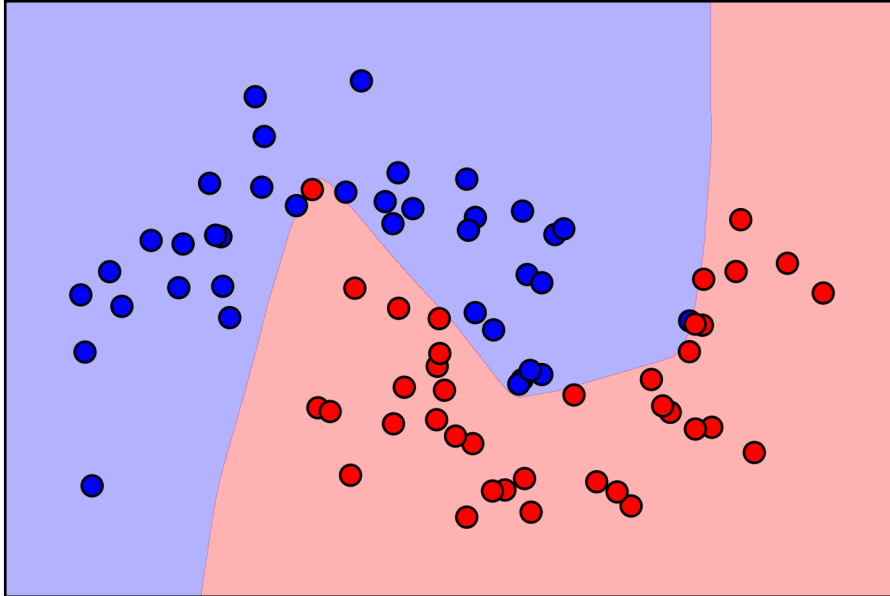
```
from sklearn.neural_network import MLPClassifier
from sklearn.datasets import make_moons

X, y = make_moons(n_samples=100, noise=0.25, random_state=3)

X_train, X_test, y_train, y_test = train_test_split(X, y, stratify=y, random_state=42)

mlp = MLPClassifier(algorithm='l-bfgs', random_state=0).fit(X_train, y_train)
mglearn.plots.plot_2d_separator(mlp, X_train, fill=True, alpha=.3)
plt.scatter(X_train[:, 0], X_train[:, 1], c=y_train, s=60, cmap=mglearn.cm2)
```



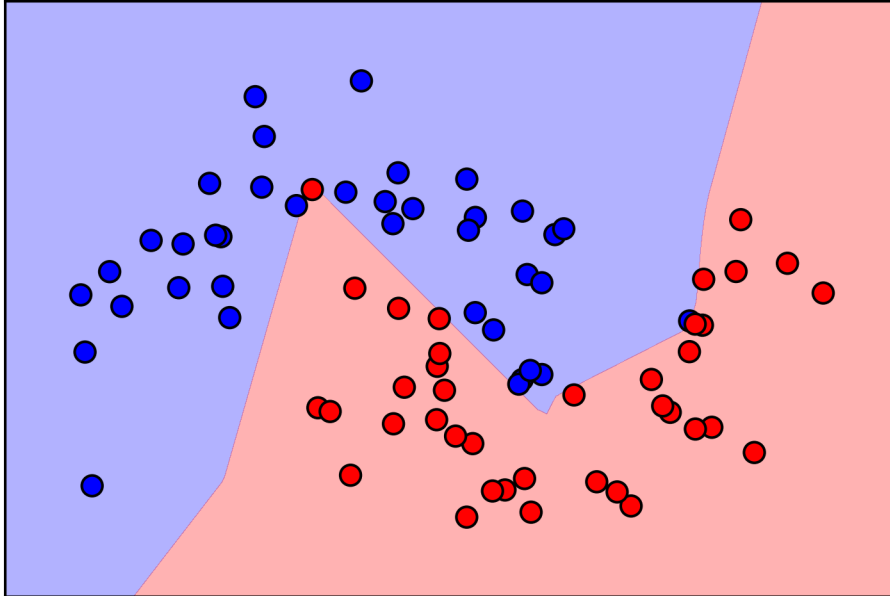


As you can see, the neural network learned a very nonlinear but relatively smooth decision boundary.

We used `algorithm='l-bfgs'` which we will discuss later.

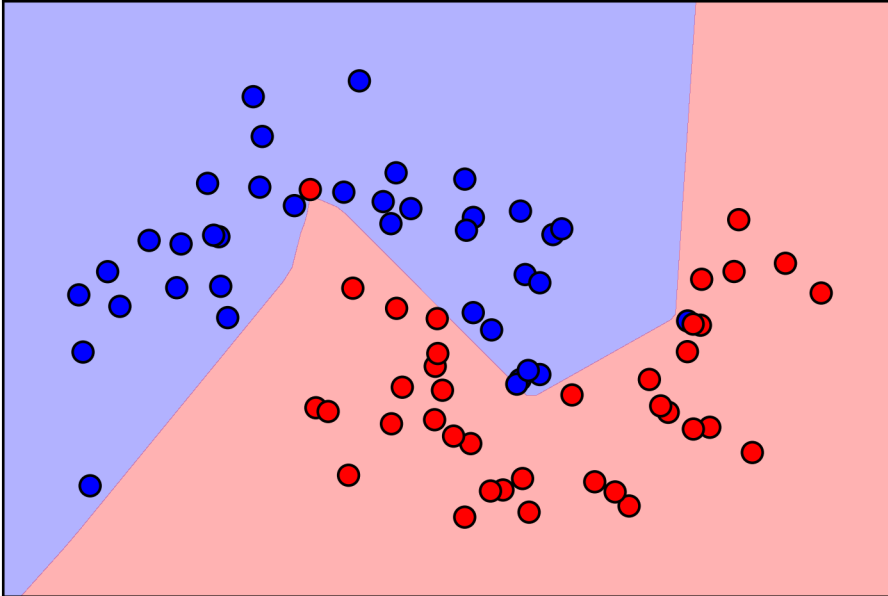
By default, the MLP uses 100 hidden nodes, which is quite a lot for this small dataset. We can reduce the number (which reduces the complexity of the model) and still get a good result:

```
mlp = MLPClassifier(algorithm='l-bfgs', random_state=0, hidden_layer_sizes=[10])
mlp.fit(X_train, y_train)
mglearn.plots.plot_2d_separator(mlp, X_train, fill=True, alpha=.3)
plt.scatter(X_train[:, 0], X_train[:, 1], c=y_train, s=60, cmap=mglearn.cm2)
```

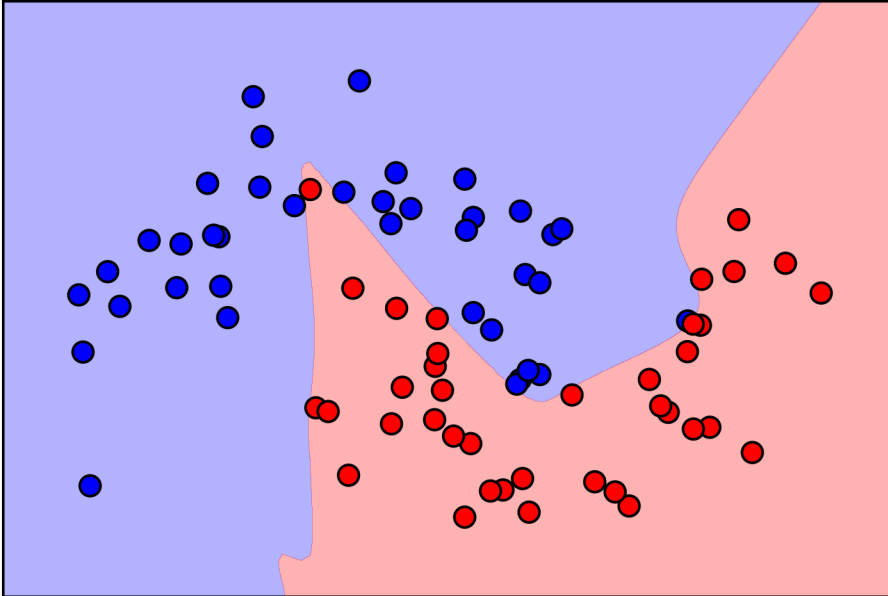


With only 10 hidden units, the decision boundary looks somewhat more ragged. The default nonlinearity is 'relu', shown in Figure activation\_function. With a single hidden layer, this means the decision function will be made up of 10 straight line segments. If we want a smoother decision boundary, we could either add more hidden units (as in the figure above), add second hidden layer, or use the "tanh" nonlinearity:

```
# using two hidden layers, with 10 units each
mlp = MLPClassifier(algorithm='l-bfgs', random_state=0, hidden_layer_sizes=[10, 10])
mlp.fit(X_train, y_train)
mglearn.plots.plot_2d_separator(mlp, X_train, fill=True, alpha=.3)
plt.scatter(X_train[:, 0], X_train[:, 1], c=y_train, s=60, cmap=mglearn.cm2)
```



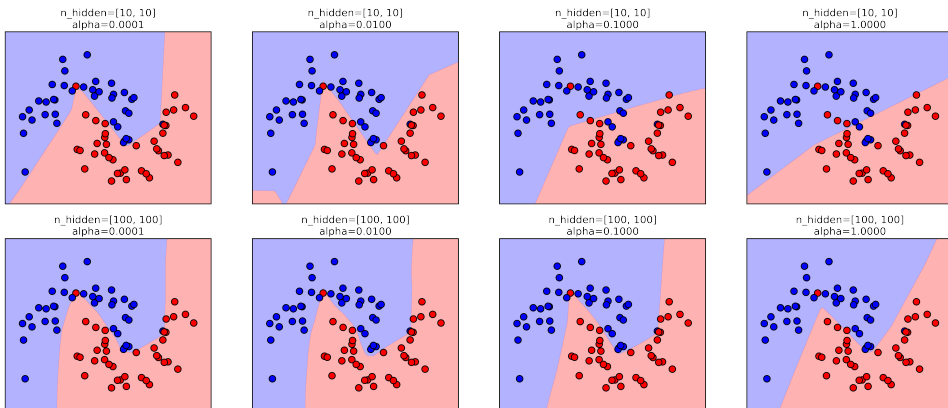
```
# using two hidden layers, with 10 units each, now with tanh nonlinearity.
mlp = MLPClassifier(algorithm='l-bfgs', activation='tanh',
                   random_state=0, hidden_layer_sizes=[10, 10])
mlp.fit(X_train, y_train)
mglearn.plots.plot_2d_separator(mlp, X_train, fill=True, alpha=.3)
plt.scatter(X_train[:, 0], X_train[:, 1], c=y_train, s=60, cmap=mglearn.cm2)
```



Finally, we can also control the complexity of a neural network by using an “l2” penalty to shrink the weights towards zero, as we did in ridge regression and the linear classifiers. The parameter for this in the `MLPClassifier` is `alpha` (as in the linear regression models), and is set to a very low value (little regularization) by default.

Here is the effect of different values of `alpha` on the `two_moons` dataset, using two hidden layers of 10 or 100 units each:

```
fig, axes = plt.subplots(2, 4, figsize=(20, 8))
for ax, n_hidden_nodes in zip(axes, [10, 100]):
    for axx, alpha in zip(ax, [0.0001, 0.01, 0.1, 1]):
        mlp = MLPClassifier(algorithm='l-bfgs', random_state=0,
                           hidden_layer_sizes=[n_hidden_nodes, n_hidden_nodes],
                           alpha=alpha)
        mlp.fit(X_train, y_train)
        mglearn.plots.plot_2d_separator(mlp, X_train, fill=True, alpha=.3, ax=axx)
        axx.scatter(X_train[:, 0], X_train[:, 1], c=y_train, s=60, cmap=mglearn.cm2)
        axx.set_title("n_hidden=[%d, %d]\nalpha=%.4f"
                     % (n_hidden_nodes, n_hidden_nodes, alpha))
```



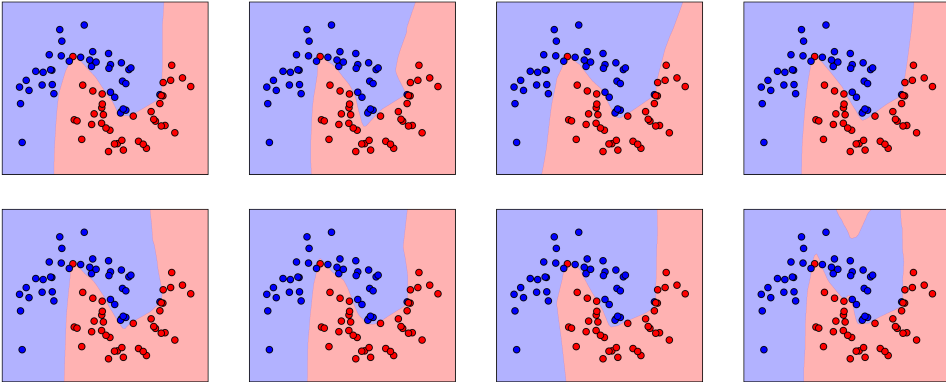
As you probably have realized by now, there are many ways to control the complexity of a neural network: the number of hidden layers, the number of units in each hidden layer, and the regularization (alpha). There are actually even more, which we won't go into here.

An important property of neural networks is that their weights are set randomly before learning is started, and this random initialization affects the model that is learned. That means that even when using exactly the same parameters, we can obtain very different models when using different random seeds.

If the networks are large, and their complexity is chosen properly, this should not affect accuracy too much, but it is worth keeping in mind (particularly for smaller networks).

Here are plots of several models, all learned with the same settings of the parameters:

```
fig, axes = plt.subplots(2, 4, figsize=(20, 8))
for i, ax in enumerate(axes.ravel()):
    mlp = MLPClassifier(algorithm='l-bfgs', random_state=i,
                       hidden_layer_sizes=[100, 100])
    mlp.fit(X_train, y_train)
    mglearn.plots.plot_2d_separator(mlp, X_train, fill=True, alpha=.3, ax=ax)
    ax.scatter(X_train[:, 0], X_train[:, 1], c=y_train, s=60, cmap=mglearn.cm2)
```



To get a better understanding of neural networks on real-world data, let's apply the `MLPClassifier` to the breast cancer dataset. We start with the default parameters:

```
X_train, X_test, y_train, y_test = train_test_split(
    cancer.data, cancer.target, random_state=0)

mlp = MLPClassifier()
mlp.fit(X_train, y_train)

print("accuracy on training set: %f" % mlp.score(X_train, y_train))
print("accuracy on test set: %f" % mlp.score(X_test, y_test))

accuracy on training set: 0.373239

accuracy on test set: 0.370629
```

As you can see, the result on both the training and the test set are devastatingly bad (even worse than random guessing!). As in the SVC example above, this is likely due to scaling of the data. Neural networks also expect all input features to vary in a similar way, and ideally should have a mean of zero, and a variance of one.

We [must] rescale our data so that it fulfills these requirements. Again, we will do this “by hand” here, but introduce the `StandardScaler` to do this automatically in Chapter 3 (Unsupervised Learning).

```
# compute the mean value per feature on the training set
mean_on_train = X_train.mean(axis=0)
# compute the standard deviation of each feature on the training set
std_on_train = X_train.std(axis=0)

# subtract the mean, scale by inverse standard deviation
# afterwards, mean=0 and std=1
X_train_scaled = (X_train - mean_on_train) / std_on_train
# use THE SAME transformation (using training mean and std) on the test set
X_test_scaled = (X_test - mean_on_train) / std_on_train

mlp = MLPClassifier(random_state=0)
```

```

mlp.fit(X_train_scaled, y_train)

print("accuracy on training set: %f" % mlp.score(X_train_scaled, y_train))
print("accuracy on test set: %f" % mlp.score(X_test_scaled, y_test))

/home/andy/checkout/scikit-learn/sklearn/neural_network/multilayer_perceptron.py:560: ConvergenceWarning:

  % (), ConvergenceWarning)

```

The results are much better after scaling, and already quite competitive. We got a warning from the model, though, that tells us that the maximum number of iterations has been reached. This is part of the adam algorithm for learning the model, and tells us that we should increase the number of iterations:

```

mlp = MLPClassifier(max_iter=1000, random_state=0)
mlp.fit(X_train_scaled, y_train)

print("accuracy on training set: %f" % mlp.score(X_train_scaled, y_train))
print("accuracy on test set: %f" % mlp.score(X_test_scaled, y_test))

accuracy on training set: 0.995305

accuracy on test set: 0.965035

```

Increasing the number of iterations only increased the training set performance, but not the generalization performance. Still, the model is performing quite well. As there is some gap between the training

and the test performance, we might try to decrease the model complexity to get better generalization performance. Here, we choose to increase the alpha parameter (quite aggressively, from 0.0001 to 1), to add stronger regularization of the weights.

```

mlp = MLPClassifier(max_iter=1000, alpha=1, random_state=0)
mlp.fit(X_train_scaled, y_train)

print("accuracy on training set: %f" % mlp.score(X_train_scaled, y_train))
print("accuracy on test set: %f" % mlp.score(X_test_scaled, y_test))

accuracy on training set: 0.988263

accuracy on test set: 0.972028

```

This leads to a performance on par with the best models so far. [Footnote: You might have noticed at this point that many of the well-performing models achieved exactly the same accuracy of 0.972. This means that all of the models make exactly the same number of mistakes, which is four. If you comparing the actual predictions, you can even see that they make exactly the same mistakes! This might be either a consequence of data being very small, or may be because these points are really different from the rest.]

While it is possible to analyze what a neural network learned, this is usually much trickier than analyzing a linear model or a tree-based model. One way to introspect

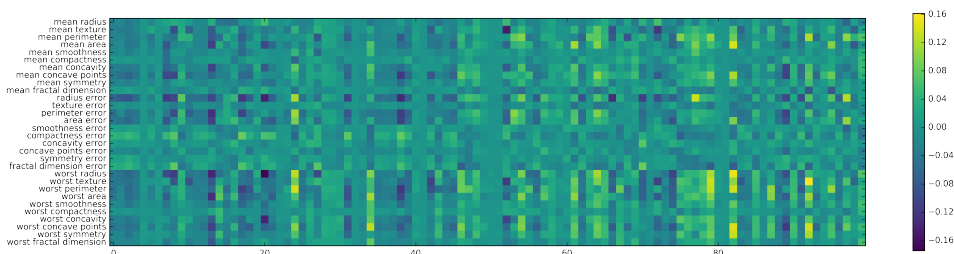
what was learned is to look at the weights in the model. You can see an example of this in the scikit-learn example gallery on the website. For the breast cancer dataset, this might be a bit hard to understand.

The plot below shows the weights that were learned connecting the input to the first hidden layer.

The rows in this plot correspond to the 30 input features, while the columns correspond to the 100 hidden units.

Light green represents large positive values, while dark blue represents negative values.

```
plt.figure(figsize=(20, 5))
plt.imshow(mlp.coefs_[0], interpolation='none', cmap='viridis')
plt.yticks(range(30), cancer.feature_names)
plt.colorbar()
```



One possible inference we can make is that features that have very small weights for all of the hidden units are “less important” to the model. We can see that “mean smoothness” and “mean compactness” in addition to the features found between “smoothness error” and “fractal dimension error” have relatively low weights compared to other features. This could mean that these are less important features, or, possibly, that we didn’t represent them in a way that the neural network could use.

We could also visualize the weights connecting the hidden layer to the output layer, but those are even harder to interpret.

While the `MLPClassifier` and `MLPRegressor` provide easy-to-use interfaces for the most common neural network architectures, they only capture a small subset of what is possible with neural networks. If you are interested in working with more flexible or larger models, we encourage you to look beyond scikit-learn into the fantastic deep learning libraries that are out there. For python users, the most well-established are `keras`, `lasagna` and `tensor-flow`. `Keras` and `lasagna` both build on the  `theano`  library.

These libraries provide a much more flexible interface to build neural networks, and track the rapid process in deep learning research. All of the popular deep learning libraries also allow the use of high-performance graphic processing units (GPUs), which scikit-learn does not support.



Using GPUs allows to accelerate computations by factors of 10x to 100x, and are essential for applying deep learning methods to large-scale datasets.

## Strengths, weaknesses and parameters

Neural networks have re-emerged as state of the art models in many applications of machine learning. One of their main advantages is that they are able to capture information contained in large amounts of data and build incredibly complex models. Given enough computation time, data, and careful tuning of the parameters, neural networks often beat other machine learning algorithms (for classification and regression tasks).

This brings us to the downsides; neural networks, in particular the large and powerful ones, often take a long time to train. They also require careful preprocessing of the data, as we saw above. Similarly to SVMs, they work best with “homogeneous” data, where all the features have similar meanings. For data that has very different kinds of features, tree-based models might work better.

Tuning neural network parameters is also an art onto itself. In our experiments above, we barely scratched the surface of possible ways to adjust neural network models, and how to train them.

### Estimating complexity in neural networks

The most important parameters are the number of layers and the number of hidden units per layer. You should start with one or two hidden layers, and possibly expand from there. The number of nodes per hidden layer is often around the number of the input features, but rarely higher than in the low to mid thousands.

A helpful measure when thinking about model complexity of a neural network is the number of weights or coefficients that are learned. If you have a binary classification dataset with 100 features, and you have 100 hidden units, then there are  $100 * 100 = 10,000$  weights between the input and the first hidden layer. There are also  $100 * 1 = 100$  weights between the hidden layer and the output layer, for a total of around 10,100 weights. If you add a second hidden layer with 100 hidden units, there will be another  $100 * 100 = 10,000$  weights from the first hidden layer to the second hidden layer, resulting in a total of 20,100 weights.

If instead, you use one layer with 1000 hidden units, you are learning  $100 * 1000 = 100,000$  weights from the input to the hidden layer, and  $1000 * 1$  weights from the hidden to the output layer, for a total of 101,000.

If you add a second hidden layer, you add  $1000 * 1000 = 1,000,000$  weights, for a whopping 1,101,000, which is 50 times larger than the model with two hidden layers of size 100.

A common way to adjust parameters in a neural network is to first create a network that is large enough to overfit, making sure that the task can actually be learned by the network. Once you know the training data can be learned, either shrink the network or increase alpha to add regularization, which will improve generalization performance.

During our experiments above, we focused mostly on the definition of the model: the number of layers and nodes per layer, the regularization, and the nonlinearity. These define the model we want to learn. There is also the question of *how* to learn the model, or the algorithm that is used for learning of the parameters, which is set using the `algorithm` parameter.

There are two easy-to-use choices for the `algorithm`. The default is `'adam'`, which works well in most situations but is quite sensitive to the scaling of the data (so it is important to always scale your data to zero mean and unit variance). The other one is `'l-bfgs'`, which is quite robust, but might take a long time on larger models or larger datasets.

There is also the more advanced `'sgd'` option, which is what many deep learning researchers use. The `'sgd'` option comes with many additional parameters that need to be tuned for best results. You can find all of these parameters and their definitions in the user-guide. When starting to work with MLPs, we recommend sticking to `adam` and `l-bfgs`.

## Uncertainty estimates from classifiers

Another useful part of the scikit-learn interface that we haven't talked about yet is the ability of classifiers to provide uncertainty estimates of predictions.

Often, you are not only interested in which class a classifier predicts for a certain test point, but also how certain it is that this is the right class. In practice, different kinds of mistakes lead to very different outcomes in real world applications. Imagine a medical application testing for cancer. Making a false positive prediction might lead to a patient undergoing additional tests, while a false negative prediction might lead to a serious disease not being treated.

We will go into this topic in more detail in Chapter 6 (Model Selection).

There are two different functions in scikit-learn that can be used to obtain uncertainty estimates from classifiers, `decision_function` and `predict_proba`. Most (but not all) classifiers have at least one of them, and many classifiers have both. Let's look at what these two functions do on as synthetic two-dimensional dataset, when building a `GradientBoostingClassifier` classifier. `GradientBoostingClassifier` has both a `decision_function` method and a `predict_proba`.

```

# create and split a synthetic dataset
from sklearn.ensemble import GradientBoostingClassifier
from sklearn.datasets import make_blobs, make_circles
# X, y = make_blobs(centers=2, random_state=59)
X, y = make_circles(noise=0.25, factor=0.5, random_state=1)

# we rename the classes "blue" and "red" for illustration purposes:
y_named = np.array(["blue", "red"])[y]

# we can call train test split with arbitrary many arrays
# all will be split in a consistent manner
X_train, X_test, y_train_named, y_test_named, y_train, y_test = \
    train_test_split(X, y_named, y, random_state=0)

# build the gradient boosting model model
gbrt = GradientBoostingClassifier(random_state=0)
gbrt.fit(X_train, y_train_named)

GradientBoostingClassifier(init=None, learning_rate=0.1, loss='deviance',

                             max_depth=3, max_features=None, max_leaf_nodes=None,

                             min_samples_leaf=1, min_samples_split=2,

                             min_weight_fraction_leaf=0.0, n_estimators=100,

                             presort='auto', random_state=0, subsample=1.0, verbose=0,

                             warm_start=False)

```

## The Decision Function

In the binary classification case, the return value of `decision_function` is of shape `(n_samples,)`, it returns one floating point number for each sample:

```

print(X_test.shape)
print(gbrt.decision_function(X_test).shape)

(25, 2)

(25,)

```

This value encodes how strongly the model believes a data point to belong to the “positive” class, in this case class 1.

Positive values indicate a preference for the positive class, negative values indicate preference for the “negative”, that is the other class:

```

# show the first few entries of decision_function
gbrt.decision_function(X_test)[:6]

```

```
array([ 4.13592629, -1.68343075, -3.95106099, -3.6261613 ,  4.28986668,
        3.66166106])
```

We can recover the prediction by looking only at the sign of the decision function:

```
print(gbrt.decision_function(X_test) > 0)
print(gbrt.predict(X_test))

[ True False False False  True  True False  True  True  True False  True
  True False  True False False False  True  True  True  True  True False
  False]

['red' 'blue' 'blue' 'blue' 'red' 'red' 'blue' 'red' 'red' 'red' 'blue'
 'red' 'red' 'blue' 'red' 'blue' 'blue' 'blue' 'red' 'red' 'red' 'red'
 'red' 'blue' 'blue']
```

For binary classification, the “negative” class is always the first entry of the `classes_` attribute, and the “positive” class is the second entry of `classes_`. So if you want to fully recover the output of `predict`, you need to make use of the `classes_` attribute:

```
# make the boolean True/False into 0 and 1
greater_zero = (gbrt.decision_function(X_test) > 0).astype(int)
# use 0 and 1 as indices into classes_
pred = gbrt.classes_[greater_zero]
# pred is the same as the output of gbrt.predict
np.all(pred == gbrt.predict(X_test))

True
```

The range of `decision_function` can be arbitrary, and depends on the data and the model parameters:

```
decision_function = gbrt.decision_function(X_test)
np.min(decision_function), np.max(decision_function)

(-7.6909717730121798, 4.289866676868515)
```

This arbitrary scaling makes the output of `decision_function` often hard to interpret.

Below we plot the `decision_function` for all points in the 2d plane using a color coding, next to a visualization of the decision boundary, as we saw it in Chapter 2. We show training points as circles and test data as triangles.

Encoding not only the predicted outcome, but also how certain the classifier is provides additional information. However, in this visualization, it is hard to make out the boundary between the two classes.

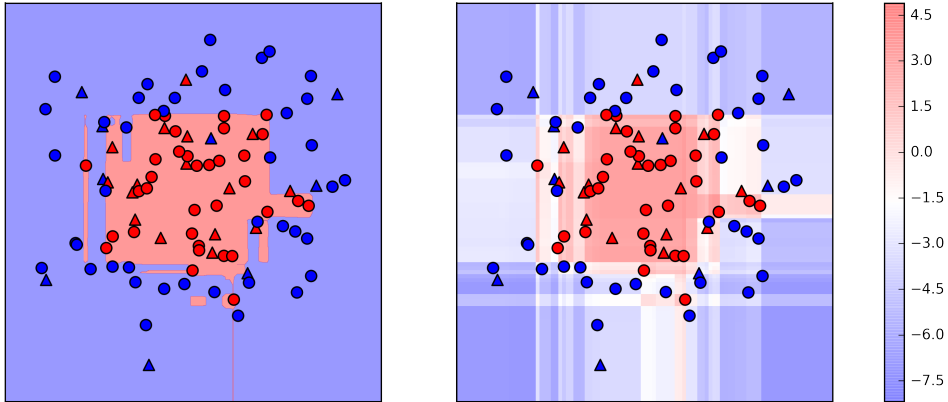
```

fig, axes = plt.subplots(1, 2, figsize=(13, 5))

mglearn.tools.plot_2d_separator(gbrt, X, ax=axes[0], alpha=.4, fill=True, cm=mglearn.cm2)
scores_image = mglearn.tools.plot_2d_scores(gbrt, X, ax=axes[1], alpha=.4, cm='bwr')

for ax in axes:
    # plot training and test points
    ax.scatter(X_test[:, 0], X_test[:, 1], c=y_test, cmap=mglearn.cm2, s=60, marker='^')
    ax.scatter(X_train[:, 0], X_train[:, 1], c=y_train, cmap=mglearn.cm2, s=60)
plt.colorbar(scores_image, ax=axes.tolist())

```



## Predicting probabilities

The output of `predict_proba` however is a probability for each class, and is often more easily understood. It is always of shape  $(n\_samples, 2)$  for binary classification:

```

gbrt.predict_proba(X_test).shape
(25, 2)

```

The first entry in each row is the estimated probability of the first class, the second entry is the estimated probability of the second class. Because it is a probability, the output of `predict_proba` is always between zero and 1, and the sum of the entries for both classes is always 1:

```

np.set_printoptions(suppress=True, precision=3)
# show the first few entries of predict_proba
gbrt.predict_proba(X_test[:6])
array([[ 0.016,  0.984],
       [ 0.843,  0.157],
       [ 0.981,  0.019],

```

```
[ 0.974,  0.026],
 [ 0.014,  0.986],
 [ 0.025,  0.975]])
```

Because the probabilities for the two classes sum to one, exactly one of the classes is above 50% certainty. That class is the one that is predicted.

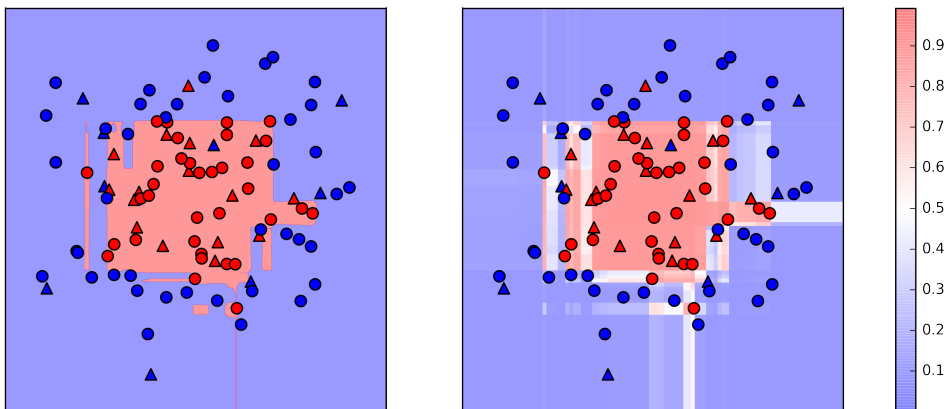
You can see in the output above, that the classifier is relatively certain for most points. How well the uncertainty actually reflects uncertainty in the data depends on the model and parameters. A model that is more overfit tends to make more certain predictions, even if they might be wrong. A model with less complexity usually has more uncertainty in predictions. A model is called *calibrated* if the reported uncertainty actually matches how correct it is - in a calibrated model, a prediction made with 70% certainty would be correct 70% of the time.

Below we show again the decision boundary on the dataset, next to the class probabilities for the blue class:

```
fig, axes = plt.subplots(1, 2, figsize=(13, 5))

mglearn.tools.plot_2d_separator(gbrt, X, ax=axes[0], alpha=.4,
                               fill=True, cm=mglearn.cm2)
scores_image = mglearn.tools.plot_2d_scores(gbrt, X, ax=axes[1], alpha=.4,
                                             cm='bwr', function='predict_proba')

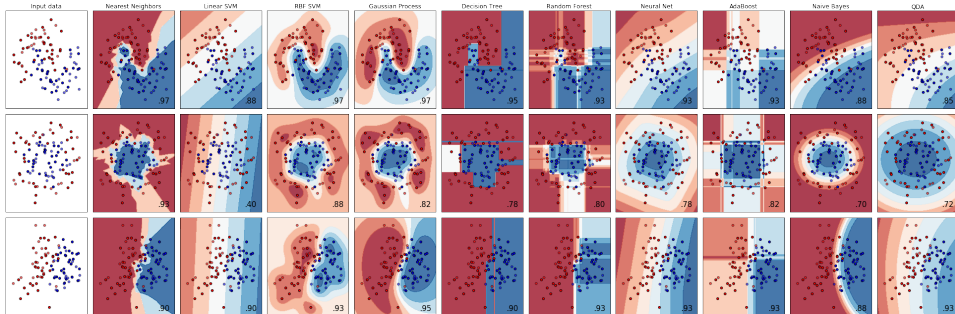
for ax in axes:
    # plot training and test points
    ax.scatter(X_test[:, 0], X_test[:, 1], c=y_test, cmap=mglearn.cm2, s=60, marker='^')
    ax.scatter(X_train[:, 0], X_train[:, 1], c=y_train, cmap=mglearn.cm2, s=60)
plt.colorbar(scores_image, ax=axes.tolist())
```



The boundaries in this this plot are much more well-defined, and the small areas of uncertainty are clearly visible.

The scikit-learn website [Footnote: [http://scikit-learn.org/stable/auto\\_examples/classification/plot\\_classifier\\_comparison.html](http://scikit-learn.org/stable/auto_examples/classification/plot_classifier_comparison.html)] has a great comparison of many models, and how their uncertainty estimates look like.

We reproduced the figure below, and encourage you to go through the example there.



## Uncertainty in multi-class classification

Above we only talked about uncertainty estimates in binary classification. But the `decision_function` and `predict_proba` methods also work in the multi-class setting.

Let's apply them on the `iris` dataset, which is a three-class classification dataset:

```
from sklearn.datasets import load_iris

iris = load_iris()
X_train, X_test, y_train, y_test = train_test_split(
    iris.data, iris.target, random_state=42)

gbdt = GradientBoostingClassifier(learning_rate=0.01, random_state=0)
gbdt.fit(X_train, y_train)

GradientBoostingClassifier(init=None, learning_rate=0.01, loss='deviance',

    max_depth=3, max_features=None, max_leaf_nodes=None,

    min_samples_leaf=1, min_samples_split=2,

    min_weight_fraction_leaf=0.0, n_estimators=100,

    presort='auto', random_state=0, subsample=1.0, verbose=0,

    warm_start=False)

print(gbdt.decision_function(X_test).shape)
# plot the first few entries of the decision function
print(gbdt.decision_function(X_test)[:6, :])

(38, 3)
```

```

[[-0.529  1.466 -0.504]
 [ 1.512 -0.496 -0.503]
 [-0.524 -0.468  1.52 ]
 [-0.529  1.466 -0.504]
 [-0.531  1.282  0.215]
 [ 1.512 -0.496 -0.503]]

```

In the multi-class case, the `decision_function` has the shape  $(n\_samples, n\_classes)$ , and each column provides a “certainty score” for each class, where a large score means that a class is more likely, and a small score means the class is less likely. You can recover the prediction from these scores by finding the maximum entry for each data point:

```

print(np.argmax(gbrt.decision_function(X_test), axis=1))
print(gbrt.predict(X_test))
[1 0 2 1 1 0 1 2 1 1 2 0 0 0 0 1 2 1 1 2 0 2 0 2 2 2 2 2 0 0 0 0 1 0 0 2 1
 0]
[1 0 2 1 1 0 1 2 1 1 2 0 0 0 0 1 2 1 1 2 0 2 0 2 2 2 2 2 0 0 0 0 1 0 0 2 1
 0]

```

The output of `predict_proba` has the same shape,  $(n\_samples, n\_classes)$ . Again, the probabilities for the possible classes for each data point sum to one:

```

# show the first few entries of predict_proba
print(gbrt.predict_proba(X_test)[:6])
# show that sums across rows are one
print("sums: %s" % gbrt.predict_proba(X_test)[:6].sum(axis=1))
[[ 0.107  0.784  0.109]
 [ 0.789  0.106  0.105]
 [ 0.102  0.108  0.789]
 [ 0.107  0.784  0.109]
 [ 0.108  0.663  0.228]
 [ 0.789  0.106  0.105]]

sums: [ 1.  1.  1.  1.  1.  1.]

```

We can again recover the predictions by computing the `argmax` of `predict_proba`:



```

print(np.argmax(gbrt.decision_function(X_test), axis=1))
print(gbrt.predict(X_test))

[1 0 2 1 1 0 1 2 1 1 2 0 0 0 0 1 2 1 1 2 0 2 0 2 2 2 2 2 0 0 0 0 1 0 0 2 1

 0]

[1 0 2 1 1 0 1 2 1 1 2 0 0 0 0 1 2 1 1 2 0 2 0 2 2 2 2 2 0 0 0 0 1 0 0 2 1

 0]

```

To summarize, `predict_proba` and `decision_function` always have shape `(n_samples, n_classes)` -- apart from the special case of `decision_function` in the binary case. In the binary case, `decision_function` only has one column, corresponding to the “positive” class `classes_[1]`. This is mostly for historical reasons.

You can recover the prediction when there are `n_classes` many columns by simply computing the `argmax` across columns.

Be careful, though, if your classes are strings, or you use integers, but they are not consecutive and starting from 0. If you want to compare results obtained with `predict` to results obtained via `decision_function` or `predict_proba` make sure to use the `classes_` attribute of the classifier to get the actual class names.

## Summary and Outlook

We started this chapter with a discussion of model complexity, and discussed *generalization*, or learning a model that is able to perform well on new, unseen data. This led us to the concepts of underfitting, which describe a model that can not capture the variations present in the training data, and overfitting, which describe a model that focuses too much on the training data, and is not able to generalize to new data very well.

We then discussed a wide array of machine learning models for classification and regression, what their advantages and disadvantages are, and how to control model complexity for each of them.

We saw that for many of the algorithms, setting the right parameters is important for good performance. Some of the algorithms are also sensitive to how we represent the input data, in particular to how the features are scaled.

Therefore, blindly applying an algorithm to a dataset without understanding the assumptions the models makes and the meaning of the parameter settings will rarely lead to an accurate model.

This chapter contains a lot of information about the algorithms, and it is not necessary for you to remember all of these details for the following chapters. However, knowing the models described above, and knowing which to use in a specific situa-

tion, is important for successfully applying machine learning in practice. Here is a quick summary of when to use which model:

- Nearest neighbors: for small datasets, good as a baseline, easy to explain.
- Linear models: Go-to as a first algorithm to try, good for very large datasets, good for very high-dimensional data.
- Naive Bayes: Only for classification. Even faster than linear models, good for very large, high-dimensional data. Often less accurate than linear models.
- Decision trees: Very fast, don't need scaling of the data, can be visualized and easily explained.
- Random forests: Nearly always perform better than a single decision tree, very robust and powerful. Don't need scaling of data. Not good for very high-dimensional sparse data.
- Gradient Boosted Decision Trees: Often slightly more accurate than random forest. Slower to train but faster to predict than random forest, and smaller in memory. Need more parameter tuning than random forest.
- Support Vector Machines: Powerful for medium-sized datasets of features with similar meaning. Needs scaling of data, sensitive to parameters.
- Neural Networks: Can build very complex models, in particular for large datasets. Sensitive to scaling of the data, and to the choice of parameters. Large models need a long time to train.

When working with a new dataset, it is in general a good idea to start with a simple model, such as a linear model, naive Bayes or nearest neighbors and see how far you can get. After understanding more about the data, you can consider moving to an algorithm that can build more complex models, such as random forests, gradient boosting, SVMs or neural networks.

You should now be in a position where you have some idea how to apply, tune, and analyze the models we discussed above.

In this chapter, we focused on the binary classification case, as this is usually easiest to understand.

Most of the algorithms presented above have classification and regression variants, however, and all of the classification algorithms support both binary and multi-class classification.

Try to apply any of these algorithms to the build-in datasets in scikit-learn, like the `boston_housing` or `diabetes` datasets for regression, or the `digits` dataset for multi-class classification.

Playing around with the algorithms on different datasets will give you a better feel on how long they need to train, how easy it is to analyze the model, and how sensitive they are to the representation of the data.

While we analyzed the consequences of different parameter settings for the algorithms we investigated, building a model that actually generalizes well to new data in production is a bit trickier than that. We will see how to properly adjust parameters, and how to find good parameters automatically in Chapter 6 Model Selection.

Before we do this, we will dive in more detail into preprocessing and unsupervised learning in the next chapter.



---

# Unsupervised Learning and Preprocessing

The second family of machine learning algorithms that we will discuss is unsupervised learning.

Unsupervised learning subsumes all kinds of machine learning where there is no known output, no teacher to instruct the learning algorithm. In unsupervised learning, the learning algorithm is just shown the input data, and asked to extract knowledge from this data.

## Types of unsupervised learning

We will look into two kinds of unsupervised learning in this chapter: transformations of the dataset, and clustering.

*Unsupervised transformations* of a dataset are algorithms that create a new representation of the data which might be easier for humans or other machine learning algorithms to understand.

A common application of unsupervised transformations is dimensionality reduction, which takes a high-dimensional representation of the data, consisting of many features, and finding a new way to represent this data that summarizes the essential characteristics about the data with fewer features. A common application for dimensionality reduction is reduction to two dimensions for visualization purposes.

Another application for unsupervised transformations is finding the parts or components that “make up” the data. An example of this is topic extraction on collections of text documents. Here, the task is to find the unknown *topics* that are talked about in each document, and to learn what topics appear in each document.

This can be useful for tracking the discussion of themes like elections, gun control or talk about pop-stars on social media.

*Clustering algorithms* on the other hand partition data into distinct groups of similar items.

Consider the example of uploading photos to a social media site. To allow you to organize your pictures, the site might want to group together pictures that show the same person. However, the site doesn't know which pictures show whom, and it doesn't know how many different people appear in your photo collection. A sensible approach would be to extract all faces, and divide them into groups of faces that look similar. Hopefully, these correspond to the same person, and can be grouped together for you.

## Challenges in unsupervised learning

A major challenge in unsupervised learning is evaluating whether the algorithm learned something useful. Unsupervised learning algorithms are usually applied to data that does not contain any label information, so we don't know what the right output should be. Therefore it is very hard to say whether a model “did well”. For example, the clustering algorithm could have grouped all face pictures that are shown in profile together, and all the face pictures that are face-forward together.

This would certainly be a possible way to divide a collection of face pictures, but not the one we were looking for. However, there is no way for us to “tell” the algorithm what we are looking for, and often the only way to evaluate the result of an unsupervised algorithm is to inspect it manually.

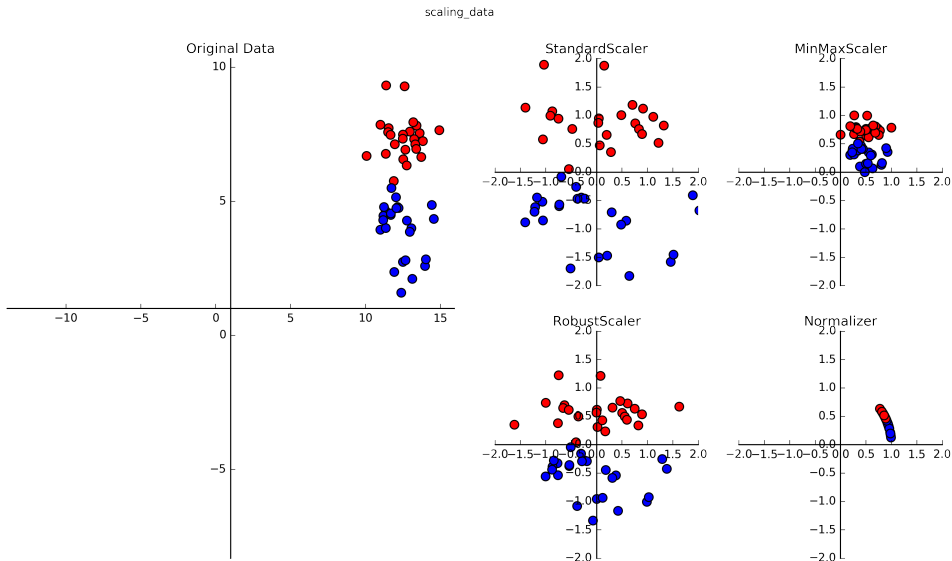
As a consequence, unsupervised algorithms are used often in an exploratory setting, when a data scientist wants to understand the data better, rather than as part of a larger automatic system. Another common application for unsupervised algorithms is as a preprocessing step for supervised algorithms. Learning a new representation of the data can sometimes improve the accuracy of supervised algorithms, or can lead to reduced memory and time consumption.

Before we start with “real” unsupervised algorithms, we will briefly discuss some simple preprocessing methods that often come in handy. Even though preprocessing and scaling are often used in tandem with supervised learning algorithms, scaling methods don't make use of the supervised information, making them unsupervised.

## Preprocessing and Scaling

In the last chapter we saw that some algorithms, like neural networks and SVMs, are very sensitive to the scaling of the data. Therefore a common practice is to adjust the features so that the data representation is more suitable for these algorithms. Often, this is a simple per-feature rescaling and shift of the data. A simple example is shown in Figure `scaling_data`.

```
mglearn.plots.plot_scaling()  
plt.suptitle("scaling_data");
```



## Different kinds of preprocessing

The first plot shows a synthetic two-class classification dataset with two features. The first feature (the x-axis value) is between 10 and 15. The second feature (the y-axis value) is between around 1 and 9.

The following four plots show four different ways to transform the data that yield more standard ranges.

The `StandardScaler` in scikit-learn ensures that for each feature, the mean is zero, and the variance is one, bringing all features to the same magnitude. However, this scaling does not ensure any particular minimum and maximum values for the features.

The `RobustScaler` works similarly to the `StandardScaler` in that it ensures statistical properties for each feature that guarantee that they are on the same scale. However, the `RobustScaler` uses the median and quartiles [Footnote: the median of a set of numbers is the number  $x$  such that half of the numbers are smaller than  $x$  and half of the numbers are larger than  $x$ . The lower quartile is the number  $x$  such that 1/4th of the numbers are smaller than  $x$ , the upper quartile is so that 1/4th of the numbers is larger than  $x$ ], instead of mean and variance. This makes the `RobustScaler` ignore data points that are very different from the rest (like measurement errors). These odd data points are also called *outliers*, and might often lead to trouble for other scaling techniques.

The `MinMaxScaler` on the other hand shifts the data such that all features are exactly between 0 and 1. For the two-dimensional dataset this means all of the data is contained within the rectangle created by the x axis between 0 and 1 and the y axis between zero and one.

Finally, the `Normalizer` does a very different kind of rescaling. It scales each data point such that the feature vector has a euclidean length of one. In other words, it projects a data point on the circle (or sphere in the case of higher dimensions) with a radius of 1. This means every data point is scaled by a different number (by the inverse of it's length).

This normalization is often used when only the direction (or angle) of the data matters, not the length of the feature vector.

## Applying data transformations

After seeing what the different kind of transformations do, let's apply them using `scikit-learn`.

We will use the cancer dataset that we saw in chapter 2. Preprocessing methods like the scalers are usually applied before applying a supervised machine learning algorithm. As an example, say we want to apply the kernel SVM (SVC) to the cancer dataset, and use `MinMaxScaler` for preprocessing the data. We start by loading and splitting our dataset into a training set and a test set. We need a separate training and test set to evaluate the supervised model we will build after the preprocessing:

```
from sklearn.datasets import load_breast_cancer
from sklearn.model_selection import train_test_split
cancer = load_breast_cancer()

X_train, X_test, y_train, y_test = train_test_split(cancer.data, cancer.target,
                                                    random_state=1)

print(X_train.shape)
print(X_test.shape)

(426, 30)

(143, 30)
```

As a reminder, the data contains 150 data points, each represented by four measurements. We split the dataset into 112 samples for the training set and 38 samples for the test set.

As with the supervised models we built earlier, we first import the class implementing the preprocessing, and then instantiate it:

```
from sklearn.preprocessing import MinMaxScaler

scaler = MinMaxScaler()
```



We then fit the scaler using the `fit` method, applied to the training data. For the `MinMaxScaler`, the `fit` method computes the minimum and maximum value of each feature on the training set. In contrast to the classifiers and regressors of chapter 2, the scaler is only provided with the data `X_train` when `fit` is called, and `y_train` is not used:

```
scaler.fit(X_train)

MinMaxScaler(copy=True, feature_range=(0, 1))
```

To apply the transformation that we just learned, that is, to actually *scale* the training data, we use the `transform` method of the scaler. The `transform` method is used in scikit-learn whenever a model returns a new representation of the data:

```
# don't print using scientific notation
np.set_printoptions(suppress=True, precision=2)
# transform data
X_train_scaled = scaler.transform(X_train)
# print data set properties before and after scaling
print("transformed shape: %s" % (X_train_scaled.shape,))
print("per-feature minimum before scaling:\n %s" % X_train.min(axis=0))
print("per-feature maximum before scaling:\n %s" % X_train.max(axis=0))
print("per-feature minimum after scaling:\n %s" % X_train_scaled.min(axis=0))
print("per-feature maximum after scaling:\n %s" % X_train_scaled.max(axis=0))

transformed shape: (426, 30)

per-feature minimum before scaling:

[  6.98   9.71  43.79 143.5   0.05   0.02   0.    0.    0.11
   0.05   0.12   0.36   0.76   6.8    0.    0.    0.    0.
   0.01   0.    7.93  12.02  50.41 185.2   0.07   0.03   0.
   0.    0.16   0.06]

per-feature maximum before scaling:

[ 28.11  39.28 188.5  2501.    0.16   0.29   0.43   0.2
   0.3    0.1    2.87   4.88  21.98 542.2   0.03   0.14
   0.4    0.05   0.06   0.03  36.04  49.54 251.2  4254.
   0.22   0.94   1.17   0.29   0.58   0.15]

per-feature minimum after scaling:

[ 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.]
```

per-feature maximum after scaling:

```
[ 1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.
  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.  1.]
```

The transformed data has the same shape as the original data - the features are simply shifted and scaled.

You can see that all of the feature are now between zero and one, as desired.

To apply the SVM to the scaled data, we also need to transform the test set. This is done by again calling the transform method, this time on `X_test`:

```
# transform test data
X_test_scaled = scaler.transform(X_test)
# print test data properties after scaling
print("per-feature minimum after scaling: %s" % X_test_scaled.min(axis=0))
print("per-feature maximum after scaling: %s" % X_test_scaled.max(axis=0))

per-feature minimum after scaling: [ 0.03  0.02  0.03  0.01  0.14  0.04  0.    0.    0.15 -0.01 -0.0
  0.    0.    0.04  0.01  0.    0.   -0.03  0.01  0.03  0.06  0.02  0.01
  0.11  0.03  0.    0.   -0.   -0.   ]

per-feature maximum after scaling: [ 0.96  0.82  0.96  0.89  0.81  1.22  0.88  0.93  0.93  1.04  0.9
  0.44  0.28  0.49  0.74  0.77  0.63  1.34  0.39  0.9   0.79  0.85  0.74
  0.92  1.13  1.07  0.92  1.21  1.63]
```

Maybe somewhat surprisingly, you can see that for the test set, after scaling, the minimum and maximum are not zero and one. Some of the features are even outside the 0-1 range!

The explanation is that the `MinMaxScaler` (and all the other scalers) always applies exactly the same transformation to the training and the test set. So the transform method always subtracts the training set minimum, and divides by the training set range, which might be different than the minimum and range for the test set.

## Scaling training and test data the same way

It is important that exactly the same transformation is applied to the training set and the test set for the supervised model to make sense on the test set. The following figure illustrates what would happen if we would use the minimum and range of the test set instead:

```
from sklearn.datasets import make_blobs
# make synthetic data
```

```

X, _ = make_blobs(n_samples=50, centers=5, random_state=4, cluster_std=2)
# split it into training and test set
X_train, X_test = train_test_split(X, random_state=5, test_size=.1)

# plot the training and test set
fig, axes = plt.subplots(1, 3, figsize=(13, 4))
axes[0].scatter(X_train[:, 0], X_train[:, 1],
                c='b', label="training set", s=60)
axes[0].scatter(X_test[:, 0], X_test[:, 1], marker='^',
                c='r', label="test set", s=60)
axes[0].legend(loc='upper left')
axes[0].set_title("original data")

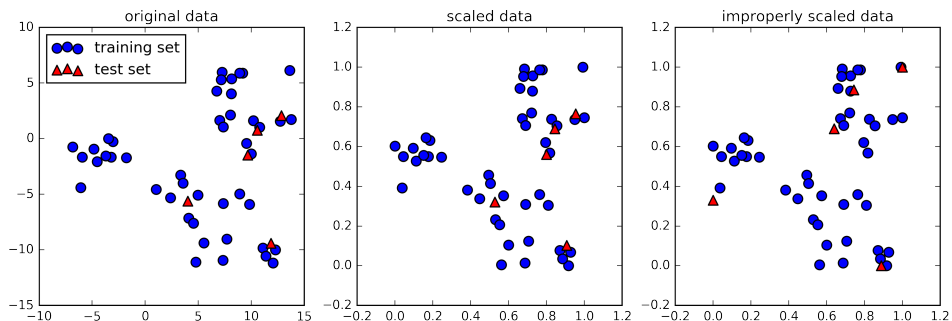
# scale the data using MinMaxScaler
scaler = MinMaxScaler()
scaler.fit(X_train)
X_train_scaled = scaler.transform(X_train)
X_test_scaled = scaler.transform(X_test)

# visualize the properly scaled data
axes[1].scatter(X_train_scaled[:, 0], X_train_scaled[:, 1],
                c='b', label="training set", s=60)
axes[1].scatter(X_test_scaled[:, 0], X_test_scaled[:, 1], marker='^',
                c='r', label="test set", s=60)
axes[1].set_title("scaled data")

# rescale the test set separately, so that test set min is 0 and test set max is 1
# DO NOT DO THIS! For illustration purposes only
test_scaler = MinMaxScaler()
test_scaler.fit(X_test)
X_test_scaled_badly = test_scaler.transform(X_test)

# visualize wrongly scaled data
axes[2].scatter(X_train_scaled[:, 0], X_train_scaled[:, 1],
                c='b', label="training set", s=60)
axes[2].scatter(X_test_scaled_badly[:, 0], X_test_scaled_badly[:, 1], marker='^',
                c='r', label="test set", s=60)
axes[2].set_title("improperly scaled data")

```



The first panel is an unscaled two-dimensional dataset, with the training set shown in blue and the test set shown in red. The second figure is the same data, but scaled using the `MinMaxScaler`. Here, we called `fit` on the training set, and then `transform` on the training and the test set. You can see that the dataset in the second panel looks identical to the first, only the ticks on the axes changed. Now all the features are between 0 and 1.

You can also see that the minimum and maximum feature values for the test data (the red points) are not 0 and 1.

The third panel shows what would happen if we scaled training and test set separately. In this case, the minimum and maximum feature values for both the training and the test set are 0 and 1. But now the dataset looks different. The test points moved incongruously to the training set, as they were scaled differently. We changed the arrangement of the data in an arbitrary way. Clearly this is not what we want to do.

Another way to reason about this is the following: Imagine your test set was a single point. There is no way to scale a single point correctly, to fulfill the minimum and maximum requirements of the `MinMaxScaler`. But the size of your test set should not change your processing.

## The effect of preprocessing on supervised learning

Now let's go back to the cancer dataset and see what the effect of using the `MinMaxScaler` is on learning the SVC (this is a different way of doing the same scaling we did in chapter 2).

First, let's fit the SVC on the original data again for comparison:

```
from sklearn.svm import SVC

X_train, X_test, y_train, y_test = train_test_split(cancer.data, cancer.target,
                                                    random_state=0)

svm = SVC(C=100)
svm.fit(X_train, y_train)
print(svm.score(X_test, y_test))

0.629370629371
```

Now, let's scale the data using `MinMaxScaler` before fitting the SVC:

```
# preprocessing using 0-1 scaling
scaler = MinMaxScaler()
scaler.fit(X_train)
X_train_scaled = scaler.transform(X_train)
X_test_scaled = scaler.transform(X_test)

# learning an SVM on the scaled training data
```

```

svm.fit(X_train_scaled, y_train)
# scoring on the scaled test set

svm.score(X_test_scaled, y_test)

0.965034965034965

```

As we saw before, the effect of scaling the data is quite significant. Even though scaling the data doesn't involve any complicated math, it is good practice to use the scaling mechanisms provided by scikit-learn, instead of reimplementing them yourself, as making mistakes even in these simple computations is easy.

You can also easily replace one preprocessing algorithm by another by changing the class you use, as all of the preprocessing classes have the same interface, consisting of the `fit` and `transform` methods:

```

# preprocessing using zero mean and unit variance scaling
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
scaler.fit(X_train)
X_train_scaled = scaler.transform(X_train)
X_test_scaled = scaler.transform(X_test)

# learning an SVM on the scaled training data
svm.fit(X_train_scaled, y_train)
# scoring on the scaled test set
svm.score(X_test_scaled, y_test)

0.95804195804195802

```

Now that we've seen how simple data transformations for preprocessing work, let's move on to more interesting transformations using unsupervised learning.

## Dimensionality Reduction, Feature Extraction and Manifold Learning

As we discussed above, transforming data using unsupervised learning can have many motivations. The most common motivations are visualization, compressing the data, and finding a representation that is more informative for further processing.

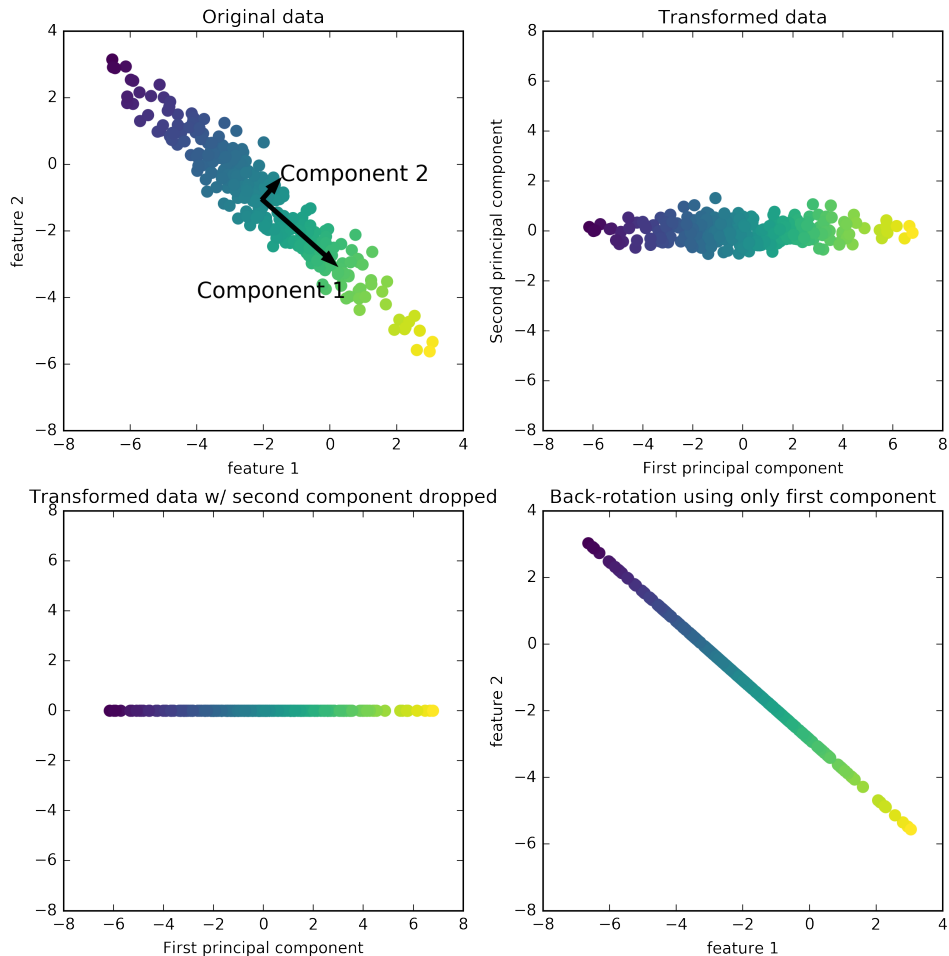
One of the simplest and most widely used algorithms for all of these is Principal Component Analysis.

### Principal Component Analysis (PCA)

Principal component analysis (PCA) is a method that rotates the dataset in a way such that the rotated features are statistically uncorrelated. This rotation is often followed by selecting only a subset of the new features, according to how important they are for explaining the data.

```
mglearn.plots.plot_pca_illustration()
plt.suptitle("pca_illustration");
```

pca\_illustration



The plot above shows a simple example on a synthetic two-dimensional dataset. The first plot shows the original data points, colored to distinguish the points. The algorithm proceeds by first finding the direction of maximum variance, labeled as “Component 1”. This is the direction in the data that contains most of the information, or in other words, the direction along which the features are most correlated with each other.

Then, the algorithm finds the direction that contains the most information while being orthogonal (is at a right angle) to the first direction. In two dimensions, there is

only one possible orientation that is at a right angle, but in higher dimensional spaces there would be (infinitely) many orthogonal directions.

Although the two components are drawn as arrows, it doesn't really matter where the head and the tail is; we could have drawn the first component from the center up to the top left instead of to the bottom right. The directions found using this process are called *principal components*, as they are the main directions of variance in the data. In general, there are as many principal components as original features.

The second plot shows the same data, but now rotated so that the first principal component aligns with the x axis, and the second principal component aligns with the y axis. Before the rotation, the mean was subtracted from the data, so that the transformed data is centered around zero. In the rotated representation found by PCA, the two axes are uncorrelated, meaning that the correlation matrix of the data in this representation is zero except for the diagonal.

We can use PCA for dimensionality reduction by retaining only some of the principal components. In this example, we might keep only the first principal component, as shown in the third panel in Figure X.

This reduced the data from a two-dimensional dataset to a one-dimensional dataset. But instead of keeping only one of the original features, we found the most interesting direction (top left to bottom right in the first panel) and kept this direction, the first principal component.

Finally, we can undo the rotation, and add the mean back to the data. This will result in the data shown in the last panel. These points are in the original feature space, but we kept only the information contained in the first principal component. This transformation is sometimes used to remove noise effects from the data, or visualize what part of the information is kept in the PCA.

### Applying PCA to the cancer dataset for visualization

One of the most common applications of PCA is visualizing high-dimensional datasets. As we already saw in Chapter 1, it is hard to create scatter plots of data that has more than two features. For the iris dataset, we could create a pair plot (Figure `iris_pairplot` in Chapter 1), which gave us us a partial picture of the data by showing us all combinations of two features. If we want to look at the breast cancer dataset, even using a pair-plot is tricky. The breast cancer dataset has 30 features, which would result in  $30 * 14 = 420$  scatter plots! You'd never be able to look at all these plots in detail, let alone try to understand them.

We could go for an even simpler visualization, showing histograms of each of the features for the two classes, benign and malignant cancer:

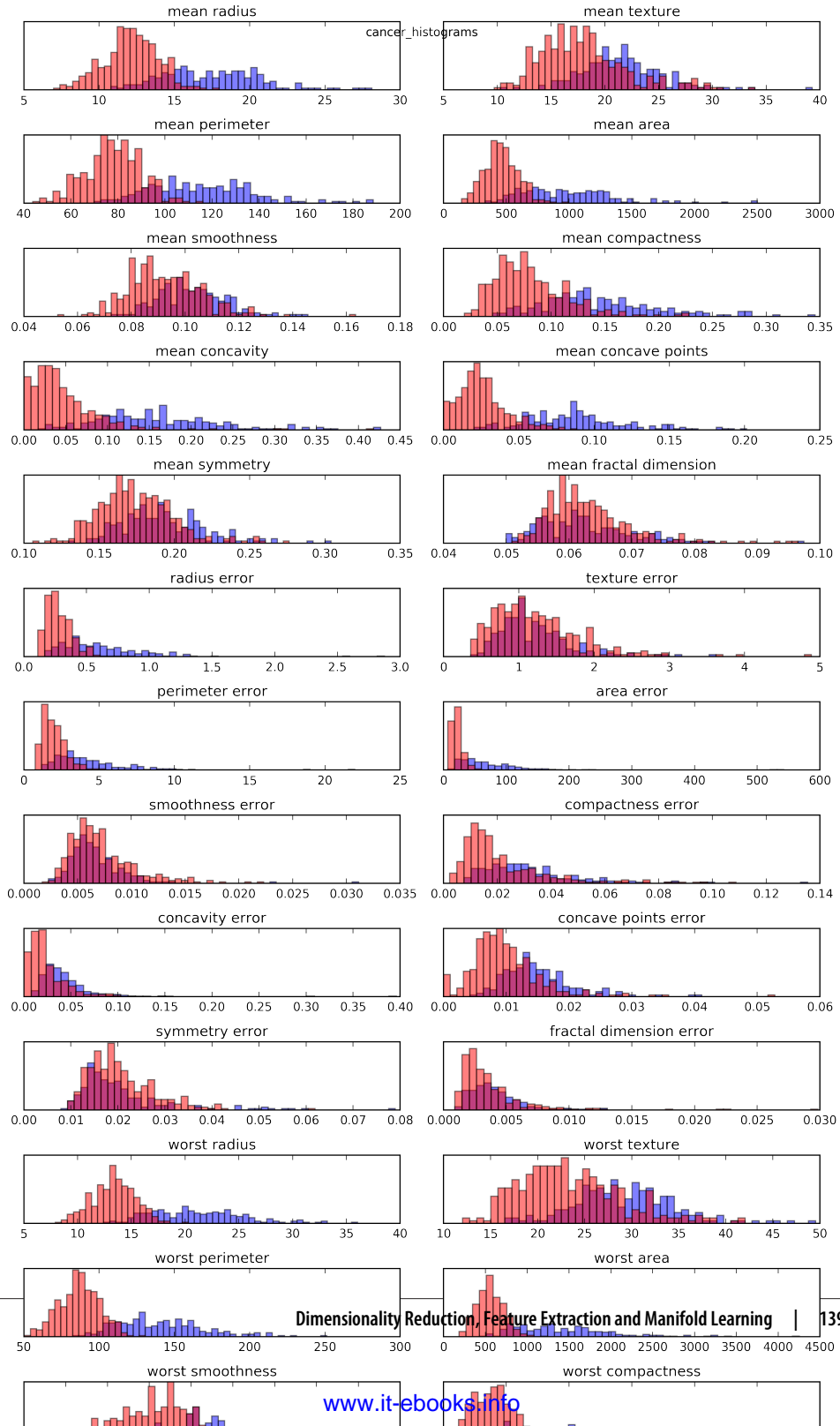
```
fig, axes = plt.subplots(15, 2, figsize=(10, 20))
malignant = cancer.data[cancer.target == 0]
```

```
benign = cancer.data[cancer.target == 1]

ax = axes.ravel()

for i in range(30):
    _, bins = np.histogram(cancer.data[:, i], bins=50)
    ax[i].hist(malignant[:, i], bins=bins, color='b', alpha=.5)
    ax[i].hist(benign[:, i], bins=bins, color='r', alpha=.5)
    ax[i].set_title(cancer.feature_names[i])
    ax[i].set_yticks(())
fig.tight_layout()
plt.suptitle("cancer_histograms")
```





Here we create a histogram for each of the features, counting how often a data point appears with a feature in a certain range (called a bin).

Each plot overlays two histograms, one for all of the points of the benign class (blue) and one for all the points in the malignant class (red). This gives us some idea of how each feature is distributed across the two classes, and allows us to venture a guess as to which features are better at distinguishing malignant and benign samples. For example, the feature “smoothness error” seems quite uninformative, because the two histograms mostly overlap, while the feature “worst concave points” seems quite informative, because the histograms are quite disjoint.

However, this plot doesn’t show us anything about the, which indicate variables that are varying together . We can find the first two principal components, and visualize the data in this new, two-dimensional space, with a single scatter-plot.

Before we apply PCA, we scale our data so that each feature has unit variance using `StandardScaler`:

```
from sklearn.datasets import load_breast_cancer
cancer = load_breast_cancer()

scaler = StandardScaler()
scaler.fit(cancer.data)
X_scaled = scaler.transform(cancer.data)
```

Learning the PCA transformation and applying it is as simple as applying a preprocessing transformation. We instantiate the PCA object, find the principal components by calling the `fit` method, and then apply the rotation and dimensionality reduction by calling `transform`.

By default, PCA only rotates (and shifts) the data, but keeps all principal components. To reduce the dimensionality of the data, we need to specify how many components we want to keep when creating the PCA object:

```
from sklearn.decomposition import PCA
# keep the first two principal components of the data
pca = PCA(n_components=2)
# fit PCA model to breast cancer data
pca.fit(X_scaled)

# transform data onto the first two principal components
X_pca = pca.transform(X_scaled)
print("Original shape: %s" % str(X_scaled.shape))
print("Reduced shape: %s" % str(X_pca.shape))

Original shape: (569, 30)

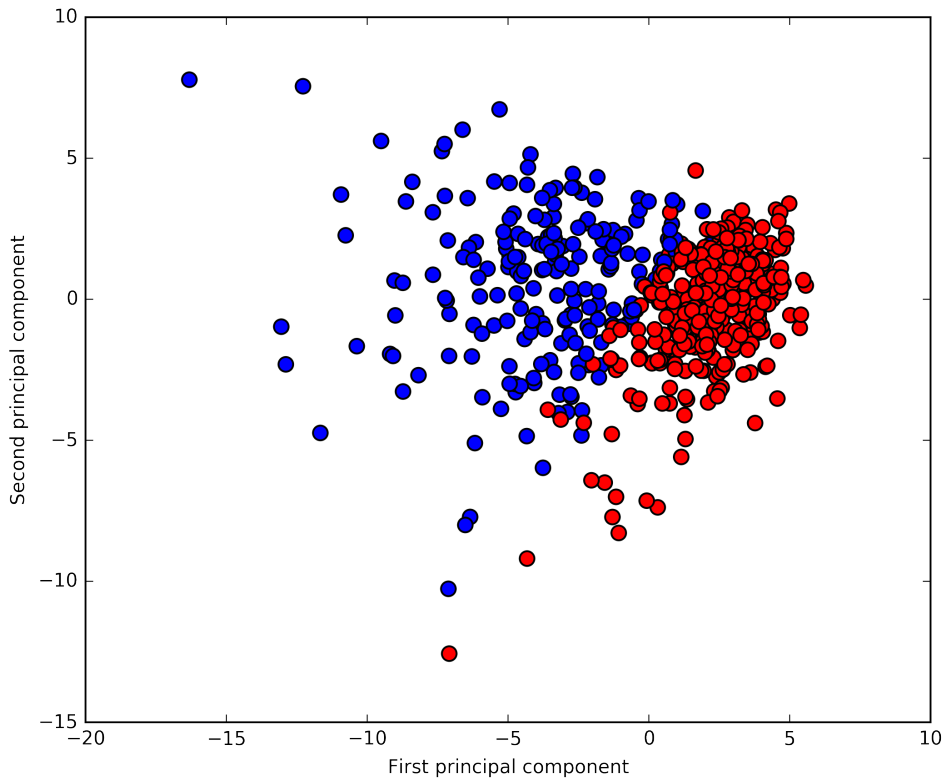
Reduced shape: (569, 2)
```

We can now plot the first two principal components:

```

# plot fist vs second principal component, color by class
plt.figure(figsize=(8, 8))
plt.scatter(X_pca[:, 0], X_pca[:, 1], c=cancer.target, cmap=mglearn.tools.cm, s=60)
plt.gca().set_aspect("equal")
plt.xlabel("First principal component")
plt.ylabel("Second principal component")

```



It is important to note is that PCA is an unsupervised method, and does not use any class information when finding the rotation. It simply looks at the correlations in the data. For the scatter plot above, we plotted the first principal component against the second principal component, and then used the class information to color the points.

You can see that the two classes separate quite well in this two-dimensional space. This can lead us to believe that even a linear classifier (that would learn a line in this space) could do a reasonably good job at distinguishing the two classes. We can also see that the malignant (red) points are more spread-out than the benign (blue) points, something that we could already see a bit from the histograms in Figure cancer\_histograms.

A downside of PCA is that the two axes in the plot above are often not very easy to interpret. The principal components correspond to directions in the original data, so they are combinations of the original features. However, these combinations are usually very complex, as we'll see below.

The principal components themselves are stored in the `components_` attribute of the PCA during fitting:

```
pca.components_.shape
(2, 30)
```

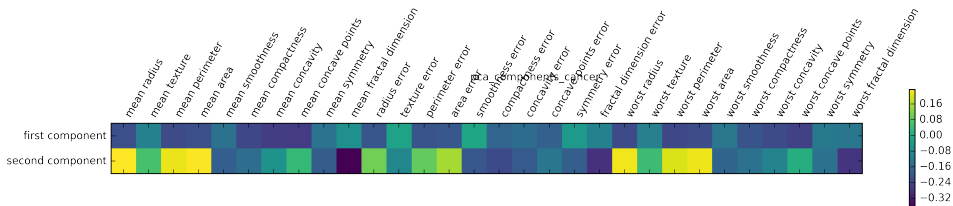
Each row in `components_` corresponds to one principal component, sorted by their importance (the first principal component comes first, etc). The columns correspond to the original features, in this example “mean radius”, “mean texture” and so on.

Let's have a look at the content of `components_`:

```
print(pca.components_)
[[-0.22 -0.1 -0.23 -0.22 -0.14 -0.24 -0.26 -0.26 -0.14 -0.06 -0.21 -0.02
 -0.21 -0.2 -0.01 -0.17 -0.15 -0.18 -0.04 -0.1 -0.23 -0.1 -0.24 -0.22
 -0.13 -0.21 -0.23 -0.25 -0.12 -0.13]
 [ 0.23  0.06  0.22  0.23 -0.19 -0.15 -0.06  0.03 -0.19 -0.37  0.11 -0.09
  0.09  0.15 -0.2 -0.23 -0.2 -0.13 -0.18 -0.28  0.22  0.05  0.2  0.22
 -0.17 -0.14 -0.1  0.01 -0.14 -0.28]]
```

We can also visualize the coefficients using a heatmap, which might be easier to understand:

```
plt.matshow(pca.components_, cmap='viridis')
plt.yticks([0, 1], ["first component", "second component"])
plt.colorbar()
plt.xticks(range(len(cancer.feature_names)),
           cancer.feature_names, rotation=60, ha='left');
plt.suptitle("pca_components_cancer")
```



You can see that in the first component, all feature have the same sign (it's negative, but as we mentioned above, it doesn't matter in which direction you point the arrow).

That means that there is a general correlation between all features. As one measurement is high, the others are likely to be high as well.

The second component has mixed signs, and both of the components involve all of the 30 features. This mixing of all features is what makes explaining the axes in Figure `pca_components_cancer` above so tricky.

### Eigenfaces for feature extraction

Another application of PCA that we mentioned above is feature extraction. The idea behind feature extraction is that it is possible to find a representation of your data that is better suited to analysis than the raw representation you were given. A great example of an application when feature extraction is helpful is with images. Images are usually stored as red, green and blue intensities for each pixel. But images are made up of many pixels, and only together are they meaningful; objects in images are usually made up of thousands of pixels.

We will give a very simple application of feature extraction on images using PCA, using face images from the “labeled faces in the wild” dataset. This dataset contains face images of celebrities downloaded from the internet, and it includes faces of politicians, singers, actors and athletes from the early 2000s. We use gray-scale versions of these images, and scale them down for faster processing. You can see some of the images below:

```
from sklearn.datasets import fetch_lfw_people
people = fetch_lfw_people(min_faces_per_person=20, resize=0.7)
image_shape = people.images[0].shape

fig, axes = plt.subplots(2, 5, figsize=(15, 8), subplot_kw={'xticks': (), 'yticks': ()})
for target, image, ax in zip(people.target, people.images, axes.ravel()):
    ax.imshow(image)
    ax.set_title(people.target_names[target])
plt.suptitle("some_faces")
```

some\_faces



There are 3023 images, each 87 x 65 pixels large, belonging to 62 different people:

```
print(people.images.shape)
print(len(people.target_names))

(3023, 87, 65)

62
```

The dataset is a bit skewed, however, containing a lot of images of George W. Bush and Colin Powell, as you can see here:

```
# count how often each target appears
counts = np.bincount(people.target)
# print counts next to target names:
for i, (count, name) in enumerate(zip(counts, people.target_names)):
    print("{0:25} {1:3}".format(name, count), end='  ')
    if (i + 1) % 3 == 0:
        print()
```

Alejandro Toledo	39	Alvaro Uribe	35	Amelie Mauresmo	21
Andre Agassi	36	Angelina Jolie	20	Ariel Sharon	77
Arnold Schwarzenegger	42	Atal Bihari Vajpayee	24	Bill Clinton	29
Carlos Menem	21	Colin Powell	236	David Beckham	31
Donald Rumsfeld	121	George Robertson	22	George W Bush	530
Gerhard Schroeder	109	Gloria Macapagal Arroyo	44	Gray Davis	26

Guillermo Coria	30	Hamid Karzai	22	Hans Blix	39
Hugo Chavez	71	Igor Ivanov	20	Jack Straw	28
Jacques Chirac	52	Jean Chretien	55	Jennifer Aniston	21
Jennifer Capriati	42	Jennifer Lopez	21	Jeremy Greenstock	24
Jiang Zemin	20	John Ashcroft	53	John Negroponte	31
Jose Maria Aznar	23	Juan Carlos Ferrero	28	Junichiro Koizumi	60
Kofi Annan	32	Laura Bush	41	Lindsay Davenport	22
Lleyton Hewitt	41	Luiz Inacio Lula da Silva	48	Mahmoud Abbas	29
Megawati Sukarnoputri	33	Michael Bloomberg	20	Naomi Watts	22
Nestor Kirchner	37	Paul Bremer	20	Pete Sampras	22
Recep Tayyip Erdogan	30	Ricardo Lagos	27	Roh Moo-hyun	32
Rudolph Giuliani	26	Saddam Hussein	23	Serena Williams	52
Silvio Berlusconi	33	Tiger Woods	23	Tom Daschle	25
Tom Ridge	33	Tony Blair	144	Vicente Fox	32
Vladimir Putin	49	Winona Ryder	24		

To make the data less skewed, we will only take up to 50 images of each person. Otherwise the feature extraction would be overwhelmed by the likelihood of George W Bush.

```

mask = np.zeros(people.target.shape, dtype=np.bool)
for target in np.unique(people.target):
    mask[np.where(people.target == target)[0][:50]] = 1

X_people = people.data[mask]
y_people = people.target[mask]

# scale the grey-scale values to be between 0 and 1
# instead of 0 and 255 for better numeric stability:
X_people = X_people / 255.

```

A common task in face recognition is to ask if a previously unseen face belongs to a known person from a database. This has applications in photo collection, social media and security. One way to solve this problem would be to build a classifier where each person is a separate class. However, there are usually many different people in face databases, and very few images of the same person (i.e. very few training

examples per class). That makes it hard to train most classifiers. Additionally, you often want to easily add new people, without retraining a large model.

A simple solution is to use a one-nearest-neighbor classifier which looks for the most similar face image to the face you are classifying. A one-nearest-neighbor could in principle work with only a single training example per class. Let's see how well `KNeighborsClassifier` does here:

```
from sklearn.neighbors import KNeighborsClassifier
# split the data in training and test set
X_train, X_test, y_train, y_test = train_test_split(
    X_people, y_people, stratify=y_people, random_state=0)
# build a KNeighborsClassifier with using one neighbor:
knn = KNeighborsClassifier(n_neighbors=1)
knn.fit(X_train, y_train)
knn.score(X_test, y_test)

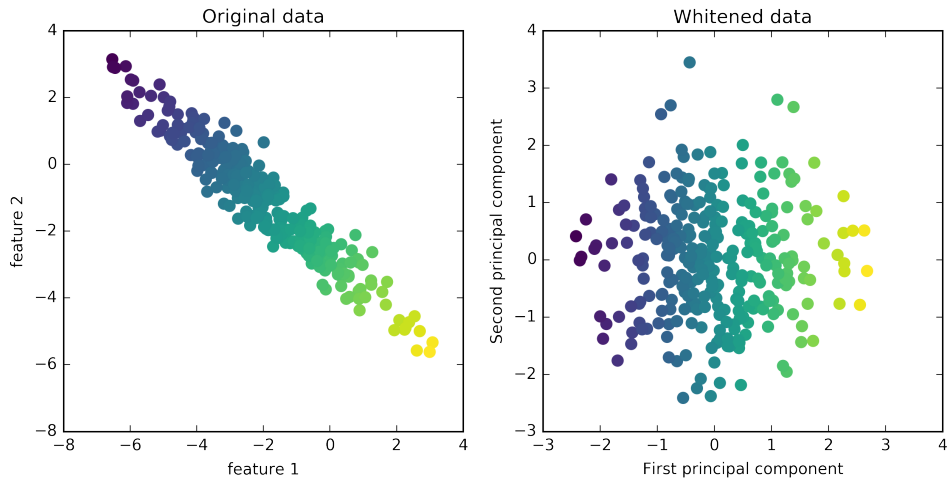
0.26615969581749049
```

We obtain an accuracy of 26.6%, which is not actually that bad for a 62 class classification problem (random guessing would give you around  $1/62 = 1.5\%$  accuracy), but is also not great. We only correctly identify a person a every fourth time.

This is where PCA comes in. Computing distances in the original pixel space is quite a bad way to measure similarity between faces [add a sentence saying why]. We hope that using distances along principal components can improve our accuracy. Here we enable the *whitening* option of PCA, which rescales the principal components to have the same scale. This is the same as using `StandardScaler` after the transformation. Reusing the data from Figure `pca_illustration` again, whitening corresponds to not only rotating the data, but also rescaling it so that the center panel is a circle instead of an ellipse:

```
mglearn.plots.plot_pca_whitening()
```





We fit the PCA object to the training data and extract the first 100 principal components. Then we transform the training and test data:

```
pca = PCA(n_components=100, whiten=True).fit(X_train)
X_train_pca = pca.transform(X_train)
X_test_pca = pca.transform(X_test)

print(X_train_pca.shape)

(1537, 100)
```

The new data has 100 features, the first 100 principal components. Now, we can use the new representation to classify our images using one-nearest-neighbors:

```
knn = KNeighborsClassifier(n_neighbors=1)
knn.fit(X_train_pca, y_train)
knn.score(X_test_pca, y_test)

0.36882129277566539
```

Our accuracy improved quite significantly, from 26.6% to 36.8%, confirming our intuition that the principal components might provide a better representation of the data.

For image data, we can also easily visualize the principal components that are found. Remember that components correspond to directions in the input space. The input space here is 50x37 gray-scale images, and so directions within this space are also 50x37 gray-scale images. Let's look at the first couple of principal components:

```
pca.components_.shape

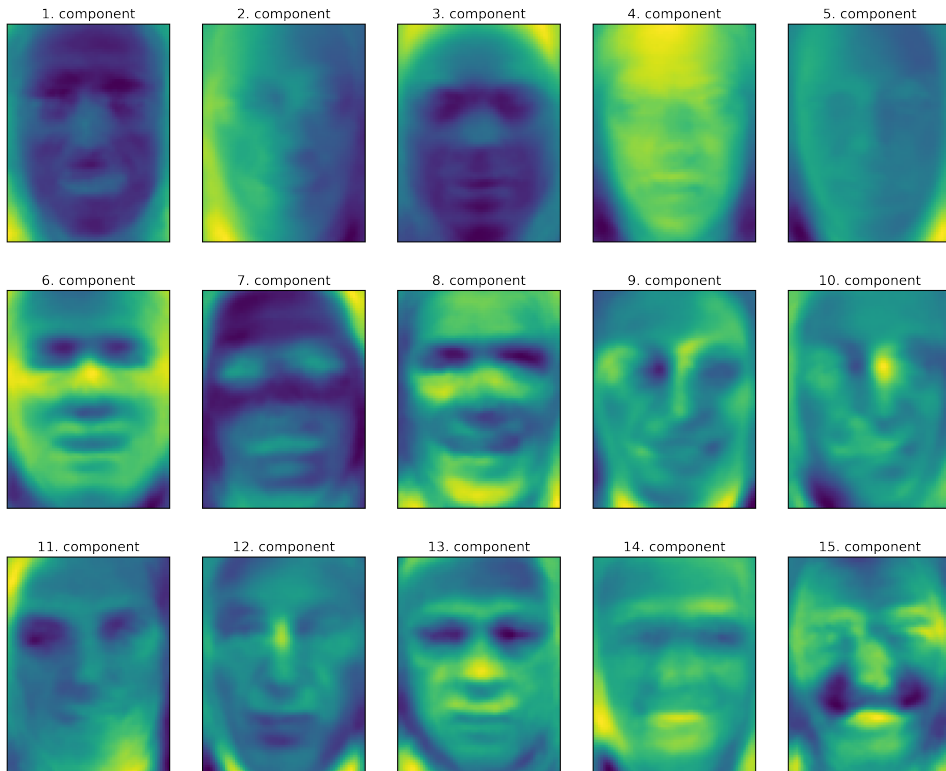
(100, 5655)

fig, axes = plt.subplots(3, 5, figsize=(15, 12),
                          subplot_kw={'xticks': (), 'yticks': ()})
```

```

fig.suptitle("pca_face_components")
for i, (component, ax) in enumerate(zip(pca.components_, axes.ravel())):
    ax.imshow(component.reshape(image_shape),
               cmap='viridis')
    ax.set_title("%d. component" % (i + 1))

```



While we certainly can not understand all aspects of these components, we can guess which aspects of the face images some of the components are capturing. The first component seems to mostly encode the contrast between the face and the background, the second component encodes differences in lighting between the right and the left half of the face, and so on. While this representation is slightly more semantic than the raw pixel values, it is still quite far from how a human might perceive a face. As the PCA is based on pixels, the alignment of the face (the position of eyes, chin and nose), as well as the lighting, both have a strong influence on how similar to images are in their pixel representation. Alignment and lighting are probably not what a human would perceive first. When asking a person to rate similarity of faces, they are more likely to use attributes like age, gender, facial expression and hair style, which are attributes that are hard to infer from the pixel intensities.

It's important to keep in mind that algorithms often interpret data, in particular data that humans are used to understand, like images, quite differently from how a human would.

Let's come back to the specific case of PCA, though.

Above we introduced the PCA transformation as rotating the data, and then dropping the components with low variance.

Another useful interpretation is that we try to find some numbers (the new feature values after the PCA rotation), so that we can express the test points as a weighted sum of the principal components:

```
from matplotlib.offsetbox import OffsetImage, AnnotationBbox

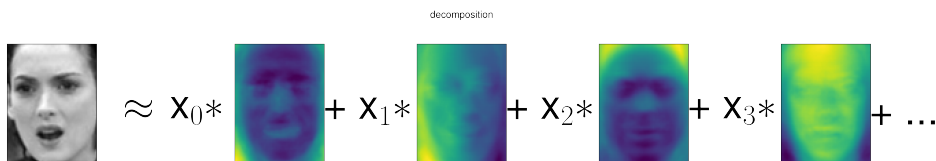
image_shape = people.images[0].shape
plt.figure(figsize=(20, 3))
ax = plt.gca()

imagebox = OffsetImage(people.images[0], zoom=7, cmap="gray")
ab = AnnotationBbox(imagebox, (.05, 0.4), pad=0.0, xycoords='data')
ax.add_artist(ab)

for i in range(4):
    imagebox = OffsetImage(pca.components_[i].reshape(image_shape), zoom=7, cmap="viridis")
    ab = AnnotationBbox(imagebox, (.3 + .2 * i, 0.4),
                        pad=0.0,
                        xycoords='data'
                        )
    ax.add_artist(ab)
    if i == 0:
        plt.text(.18, .25, 'x_%d *' % i, fontdict={'fontsize': 50})
    else:
        plt.text(.15 + .2 * i, .25, '+ x_%d *' % i, fontdict={'fontsize': 50})

plt.text(.95, .25, '+ ...', fontdict={'fontsize': 50})

plt.rc('text', usetex=True)
plt.text(.13, .3, r'\approx', fontdict={'fontsize': 50})
plt.axis("off")
plt.title("decomposition")
```



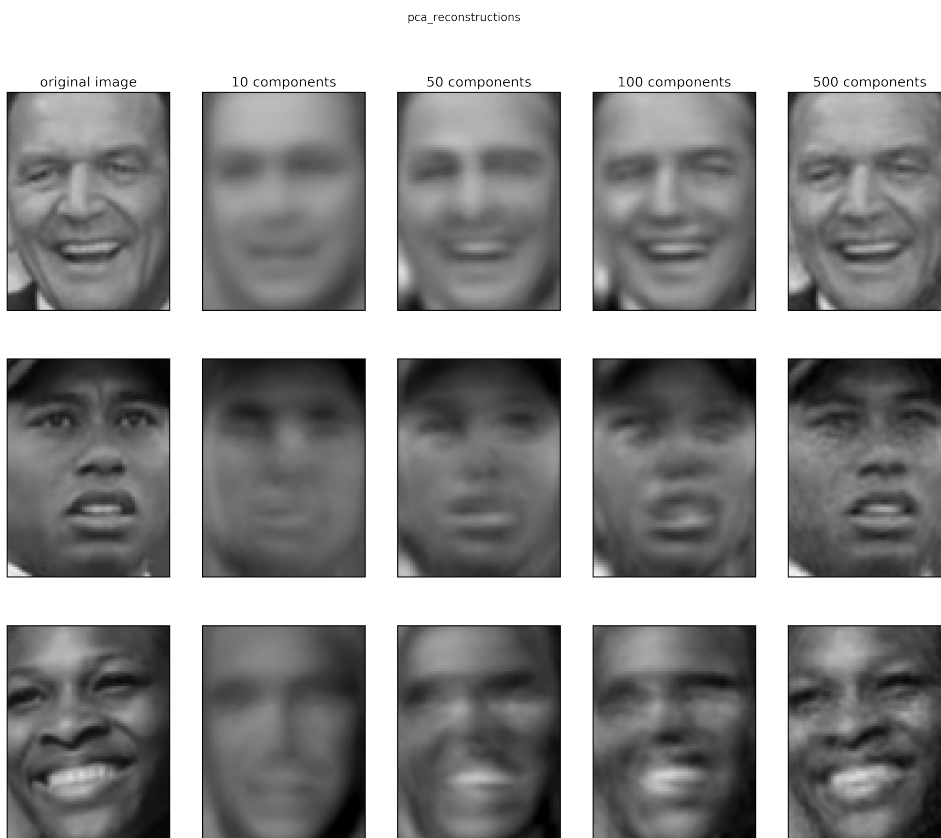
```
plt.rc('text', usetex=False) # THIS SHOULD NOT SHOW IN THE BOOK! it's needed for the figure above
```

Here,  $x_0$ ,  $x_1$  and so on are the coefficients of the principal components for this data point; in other words, they are the representation [of what? of the image? this is not clear] in the rotated space.

Another way we can try to understand what a PCA model is doing is by looking at the reconstructions of the original data using only some components. In Figure `pca_illustration`, after dropping the second component and arriving at the third panel, we undid the rotation and added the mean back to obtain new points in the original space with the second component removed, as shown in the last panel.

We can do a similar transformation for the faces by reducing the data to only some principal components and then rotating back into the original space. This return to the original feature space can be done using the `inverse_transform` method. Here we visualize the reconstruction of some faces using 10, 50, 100, 500 or 2000 components:

```
mglearn.plots.plot_pca_faces(X_train, X_test, image_shape)
plt.suptitle("pca_reconstructions");
```



```
/home/andy/checkout/scikit-learn/sklearn/externals/joblib/logger.py:77: DeprecationWarning: The 'w
logging.warn("[%s]: %s" % (self, msg))
```

---

```
[Memory] Calling mglearn.plot_pca.pca_faces...
```

```
pca_faces(array([[ 0.036601, ...,  0.742484],
...,
[ 0.105882, ...,  0.393464]], dtype=float32),
array([[ 0.162091, ...,  0.677124],
...,
[ 0.109804, ...,  0.07451 ]], dtype=float32))
```

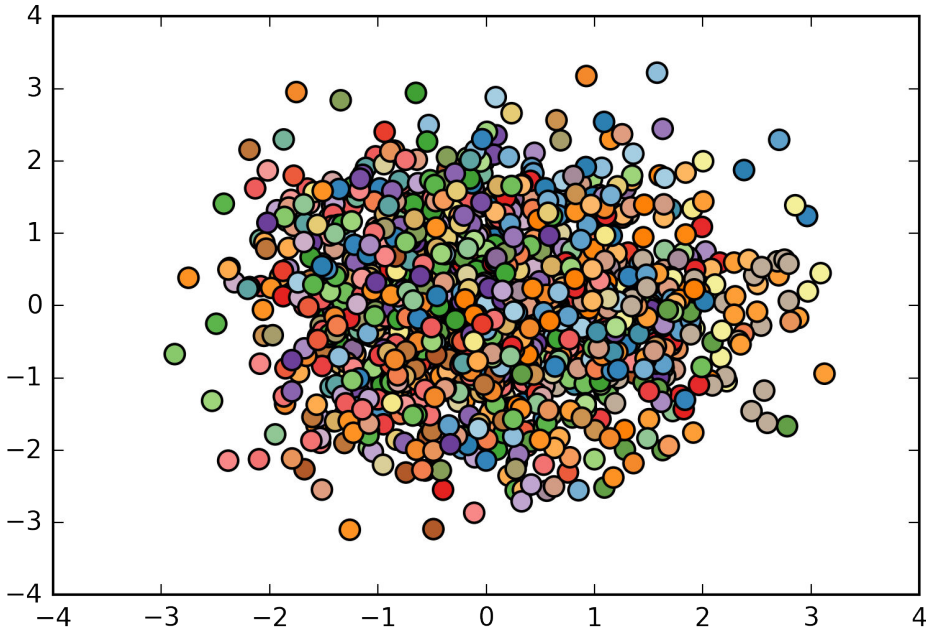
---

```
pca_faces - 12.9s, 0.2min
```

You can see that with using only the first 10 principal components, only the essence of the picture, like the face orientation and lighting, is captured. Using more and more principal components, more and more details in the image are preserved. This corresponds to extending the sum in Figure decomposition to include more and more terms. Using as many components as there are pixels would mean that we would not discard any information after the rotation, and we would reconstruct the image perfectly.

We can also try to use PCA to visualize all the faces in the dataset in a scatter plot using the first two principal components, with classes given by who is shown in the image, similarly to what we did for the cancer dataset:

```
plt.scatter(X_train_pca[:, 0], X_train_pca[:, 1], c=y_train, cmap='Paired', s=60)
```



As you can see, when using just the first two principal components, the whole data is just a big blob, with no separation of classes visible. This is not very surprising, given that even with 10 components, as shown in Figure `faces_pca_reconstruction` above, PCA only captures very rough characteristics of the faces.

## Non-Negative Matrix Factorization (NMF)

Non-negative matrix factorization is another unsupervised learning algorithm that aims to extract useful features. It works similarly to PCA and can also be used for dimensionality reduction. As in PCA we are trying to write each data point as a weighted sum of some components as illustrated in Figure `decomposition`. In PCA, we wanted components that are orthogonal, and that explain as much variance of the data as possible. In NMF, we want the components and the coefficients to be non-negative; that is, we want both the components and the coefficients to be greater or equal than zero.

Consequently, this method can only be applied to data where each feature is non-negative, as a non-negative sum of non-negative components can not become negative. The process of decomposing data into a non-negative weighted sum is particularly helpful for data that is created as the addition of several independent sources, such as an audio track of multiple speakers, or music with many instruments. In these situations, NMF can identify the original components that make up the combined data. Overall, NMF leads to more interpretable components than PCA, as neg-

ative components and coefficients can lead to hard-interpret cancellation effects. The eigenfaces in Figure `pca_face_components` for example contain both positive and negative parts, and as we mentioned in the description of PCA, the sign is actually arbitrary.

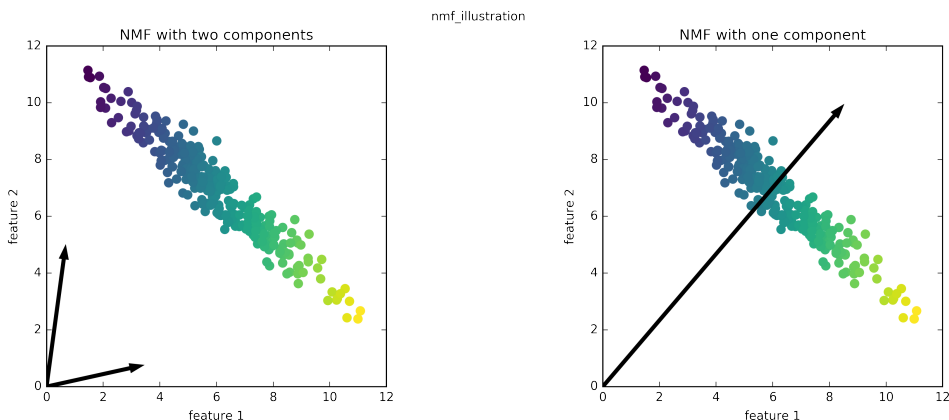
Before we apply NMF to the face dataset, let's briefly revisit the synthetic data.

### Applying NMF to synthetic data

In contrast to PCA, we need to ensure that our data is positive for NMF to be able to operate on the data.

This means where the data lies relative to the origin (0, 0) actually matters for NMF. Therefore, you can think of the non-negative components that are extracted as directions from (0, 0) towards the data.

```
mglearn.plots.plot_nmf_illustration()  
plt.suptitle("nmf_illustration")
```



The figure above shows the results of NMF on the two-dimensional toy data. For NMF with two components, as shown on the left, it is clear that all points in the data can be written as a positive combination of the two components. If there are enough components to perfectly reconstruct the data (as many components are there are features), the algorithm will choose directions that point towards the extremes of the data.

If we only use a single component, NMF creates a component that points towards the mean, as pointing there best explains the data. You see that in contrast to PCA, reducing the number of components not only removes directions, it actually changes all directions! Components in NMF are also not ordered in any specific way, so there is no “first non-negative component”: all components play an equal part.

NMF uses a random initialization, which might lead to different results depending on the random seed. In relatively easy cases as the synthetic data with two components, where all the data can be explained perfectly, the randomness has little effect (though it might change the order or scale of the components). In more complex situations, there might be more drastic changes.

### Applying NMF to face images

Now, let's apply NMF to the "labeled faces in the wild" dataset we used above.

The main parameter of NMF is how many components we want to extract. Usually this is lower than the number of input features (otherwise the data could be explained by making each pixel a separate component).

First, let's inspect how the number of components impacts how well the data can be reconstructed using NMF:

```
mglearn.plots.plot_nmf_faces(X_train, X_test, image_shape)
```



---

[Memory] Calling mglearn.plot\_nmf.nmf\_faces...



```
nmf_faces(array([[ 0.036601, ...,  0.742484],
...,
[ 0.105882, ...,  0.393464]], dtype=float32),
array([[ 0.162091, ...,  0.677124],
...,
[ 0.109804, ...,  0.07451 ]], dtype=float32))

_____nmf_faces - 763.1s, 12.7min
```

The quality of the back-transformed data is similar to PCA, but slightly worse. This is expected, as PCA finds the optimum directions in terms of reconstruction. NMF is usually not used for the ability to reconstruct or encode data, but rather for finding interesting patterns within the data.

As a first look into the data, let's try extracting only a few components, say 15, on the faced data:

```
from sklearn.decomposition import NMF
nmf = NMF(n_components=15, random_state=0)
nmf.fit(X_train)
X_train_nmf = nmf.transform(X_train)
X_test_nmf = nmf.transform(X_test)

fig, axes = plt.subplots(3, 5, figsize=(15, 12),
                          subplot_kw={'xticks': (), 'yticks': ()})
for i, (component, ax) in enumerate(zip(nmf.components_, axes.ravel())):
    ax.imshow(component.reshape(image_shape))
    ax.set_title("%d. component" % i)
```



These components are all positive, and so resemble prototypes of faces much more so than the components shown for PCA in Figure Eigenfaces. For example, one can clearly see that component 3 shows a face rotated somewhat to the right, while component 7 shows a face somewhat rotated to the left. Let's look at the images for which these components are particularly strong:

```

compn = 3
# sort by 3rd component, plot first 10 images
inds = np.argsort(X_train_nmf[:, compn])[:, :-1]
fig, axes = plt.subplots(2, 5, figsize=(15, 8),
                        subplot_kw={'xticks': (), 'yticks': ()})
fig.suptitle("Large component 3")
for i, (ind, ax) in enumerate(zip(inds, axes.ravel())):
    ax.imshow(X_train[ind].reshape(image_shape))

compn = 7
# sort by 7th component, plot first 10 images
inds = np.argsort(X_train_nmf[:, compn])[:, :-1]
fig.suptitle("Large component 7")
fig, axes = plt.subplots(2, 5, figsize=(15, 8),
                        subplot_kw={'xticks': (), 'yticks': ()})

```

```
for i, (ind, ax) in enumerate(zip(inds, axes.ravel())):
    ax.imshow(X_train[ind].reshape(image_shape))
```



As expected, faces that have a high coefficient for component 3 are faces looking to the right, while faces with a high component 7 are looking to the left. As mentioned above, extracting patterns like these works best for data with additive structure, including audio, gene expression data, and text data. We will see applications of NMF to text data in Chapter 7 (Text Data).

There are many other algorithms that can be used to decompose each data point into a weighted sum of a fixed set of components, as PCA and NMF do. Discussing all of them is beyond the scope of this book, and describing the constraints made on the components and coefficients often involves probability theory. If you are interested in these kinds of pattern extraction, we recommend to study the user guide of Independent Component Analysis (ICA), Factor Analysis (FA) and Sparse Coding (dictionary learning), which are widely used decomposition methods.

## Manifold learning with t-SNE

While PCA is often a good first approach for transforming your data so that you might be able to visualize it using a scatter plot, the nature of the method (applying a rotation and then dropping directions) limits its usefulness, as we saw with the scatter plot of the labeled faces in the wild. There is a class of algorithms for visualization called *manifold learning* algorithms which allows for much more complex mappings, and often provides better visualizations. A particular useful one is the t-SNE algorithm.

Manifold learning algorithms are mainly aimed at visualization, and so are rarely used to generate more than two new features. Some of them, including t-SNE,

compute a new representation of the training data, but don't allow transformations of new data. This means these algorithms can not be applied to a test set: rather, they can only transform the data they were trained for. Manifold learning can be useful for exploratory data analysis, but is rarely used if the final goal is supervised learning.

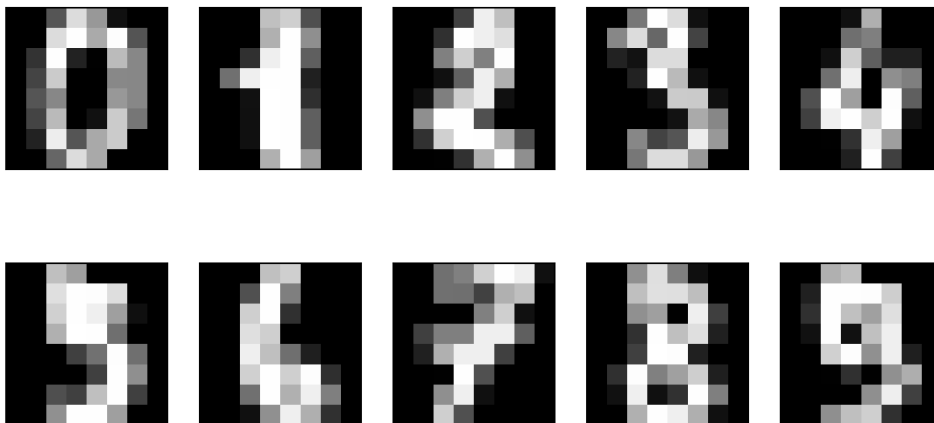
The idea behind t-SNE is to find a two-dimensional representation of the data that preserve the distances between points as best as possible. t-SNE starts with a random two-dimensional representation for each data point, and then tries to make points closer that are close in the original feature space, and points far apart that are far apart in the original feature space. t-SNE puts more emphasis on points that are close by, rather than preserving distances between far apart points. In other words, it tries to preserve the information of which points are neighbors to each other.

We will apply the t-SNE manifold learning algorithm on a dataset of handwritten digits that is included in scikit-learn [Footnote: not to be confused with the much larger MNIST dataset].

Each data point in this dataset is a 8x8 grey-scale image of a handwritten digit between 0 and 1. Here is an example image for each class:

```
from sklearn.datasets import load_digits
digits = load_digits()

fig, axes = plt.subplots(2, 5, figsize=(10, 5),
                        subplot_kw={'xticks':(), 'yticks': ()})
for ax, img in zip(axes.ravel(), digits.images):
    ax.imshow(img)
```



Let's use PCA to visualize the data reduced to two dimensions. We plot the first two principal components, and color each dot by its class:

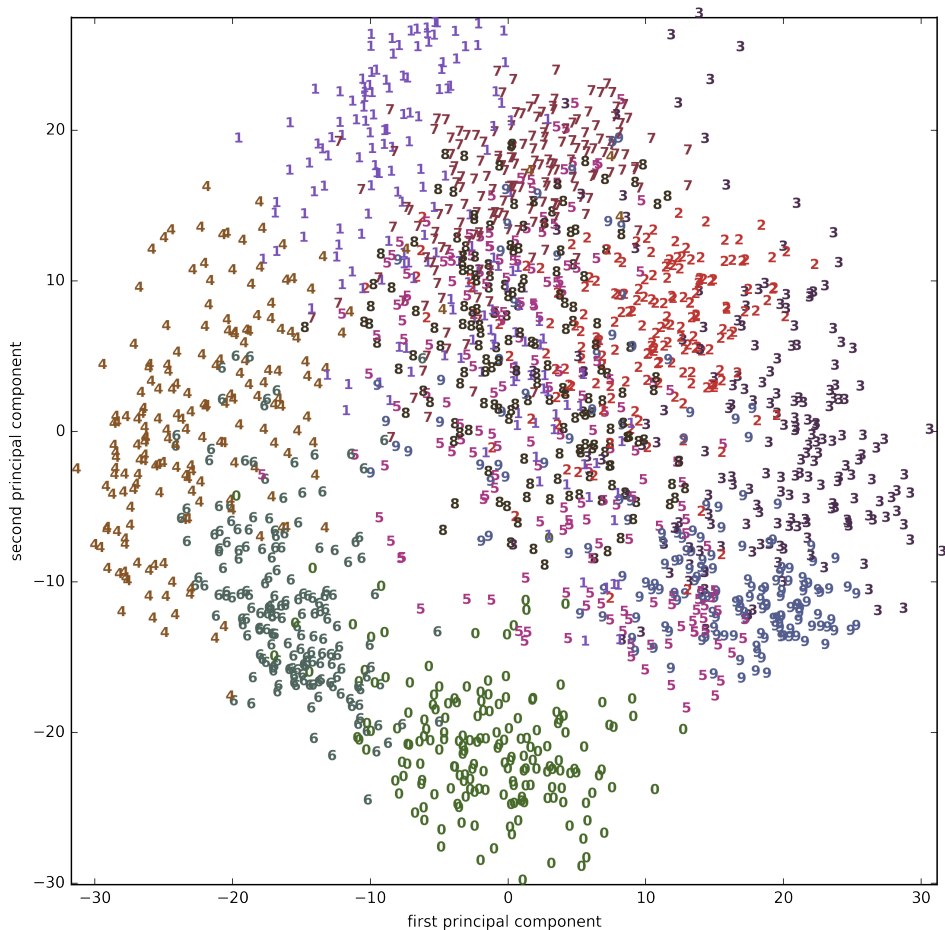
```
# build a PCA model
pca = PCA(n_components=2)
```

```

pca.fit(digits.data)
# transform the digits data onto the first two principal components
digits_pca = pca.transform(digits.data)
colors = ["#476A2A", "#7851B8", "#BD3430", "#4A2D4E", "#875525",
          "#A83683", "#4E655E", "#853541", "#3A3120", "#535D8E"]

plt.figure(figsize=(10, 10))
plt.xlim(digits_pca[:, 0].min(), digits_pca[:, 0].max())
plt.ylim(digits_pca[:, 1].min(), digits_pca[:, 1].max())
for i in range(len(digits.data)):
    # actually plot the digits as text instead of using scatter
    plt.text(digits_pca[i, 0], digits_pca[i, 1], str(digits.target[i]),
            color = colors[digits.target[i]],
            fontdict={'weight': 'bold', 'size': 9})
plt.xlabel("first principal component")
plt.ylabel("second principal component")

```

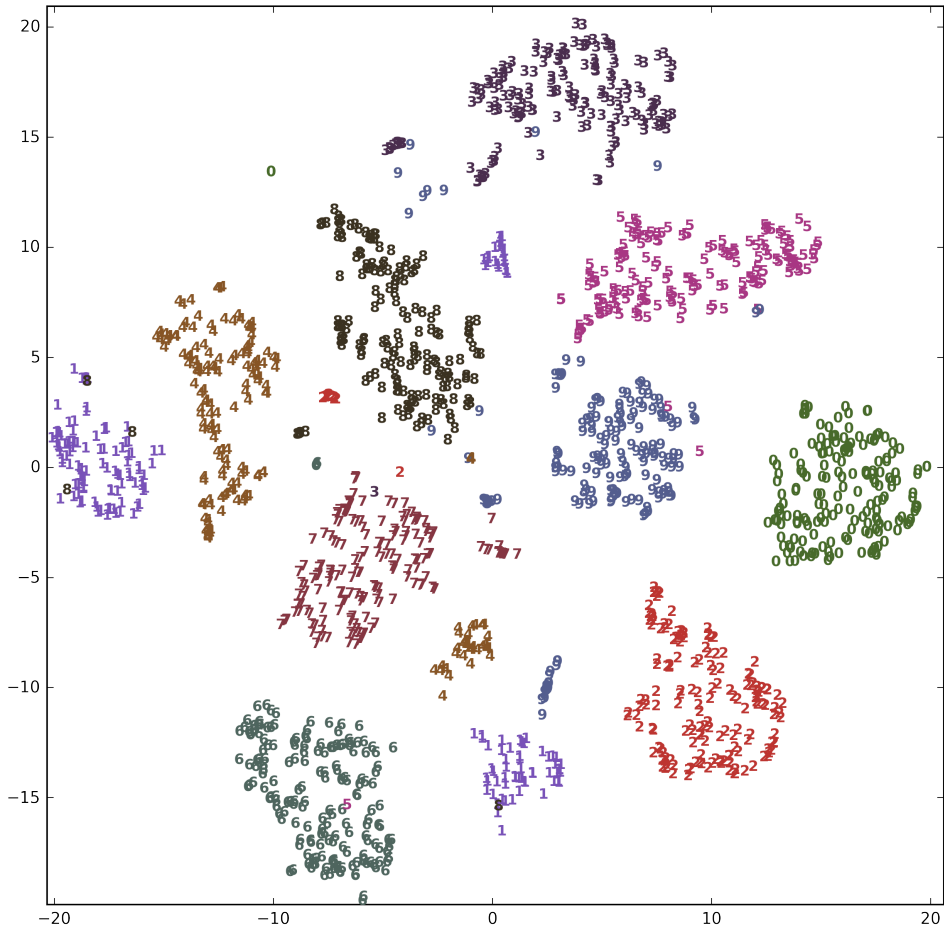


Here, we actually used the true digit classes as glyphs, to show which class is where. The digits zero, six and four are relatively well-separated using the first two principal components, though they still overlap. Most of the other digits overlap significantly.

Let's apply t-SNE to the same dataset, and compare results. As t-SNE does not support transforming new data, the TSNE class has no transform method. Instead, we can call the fit\_transform method, which will build the model, and immediately return the transformed data:

```
from sklearn.manifold import TSNE
tsne = TSNE(random_state=42)
# use fit_transform instead of fit, as TSNE has no transform method:
digits_tsne = tsne.fit_transform(digits.data)

plt.figure(figsize=(10, 10))
plt.xlim(digits_tsne[:, 0].min(), digits_tsne[:, 0].max() + 1)
plt.ylim(digits_tsne[:, 1].min(), digits_tsne[:, 1].max() + 1)
for i in range(len(digits.data)):
    # actually plot the digits as text instead of using scatter
    plt.text(digits_tsne[i, 0], digits_tsne[i, 1], str(digits.target[i]),
            color = colors[digits.target[i]],
            fontdict={'weight': 'bold', 'size': 9})
```



The result of t-SNE is quite remarkable. All the classes are quite clearly separated. The ones and nines are somewhat split up, but most of the classes form a single dense group. Keep in mind that this method has no knowledge of the class labels: it is completely unsupervised. Still, it can find a representation of the data in two dimensions that clearly separates the classes, based solely on how close points are in the original space.

t-SNE has some tuning parameters, though it often works well with the default settings. You can try playing with perplexity and early\_exaggeration, though the effects are usually minor.

# Clustering

As we described above, clustering is the task of partitioning the dataset into groups, called clusters. The goal is to split up the data in such a way that points within a single cluster are very similar and points in different clusters are different. Similarly to classification algorithms, clustering algorithms assign (or predict) a number to each data point, indicating which cluster a particular point belongs to.

## k-Means clustering

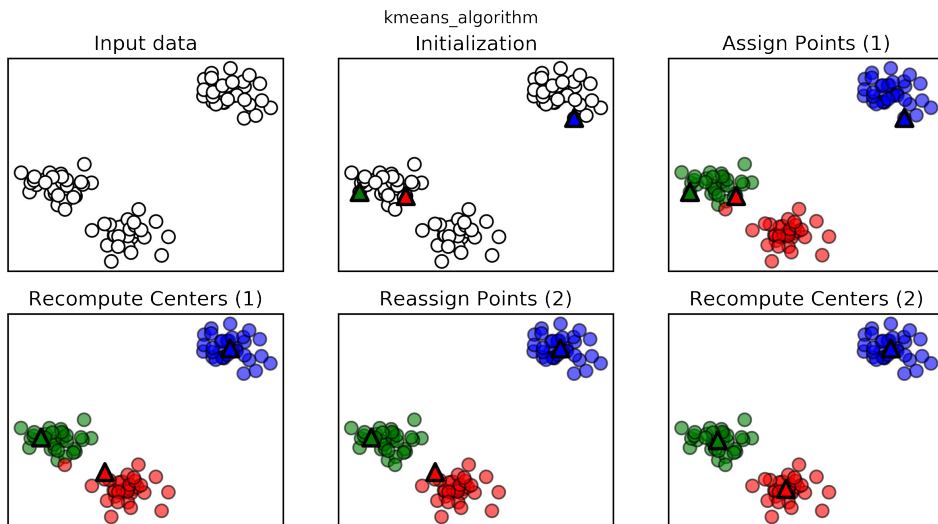
k-Means clustering is one of the simplest and most commonly used clustering algorithms. It tries to find *cluster centers* that are representative of certain regions of the data.

The algorithm alternates between two steps: assigning each data point to the closest cluster center, and then setting each cluster center as the mean of the data points that are assigned to it.

The algorithm is finished when the assignment of instances to clusters no longer changes.

Figure `kmeans_algorithm` illustrates the algorithm on a synthetic dataset:

```
mglearn.plots.plot_kmeans_algorithm()  
plt.suptitle("kmeans_algorithm");
```



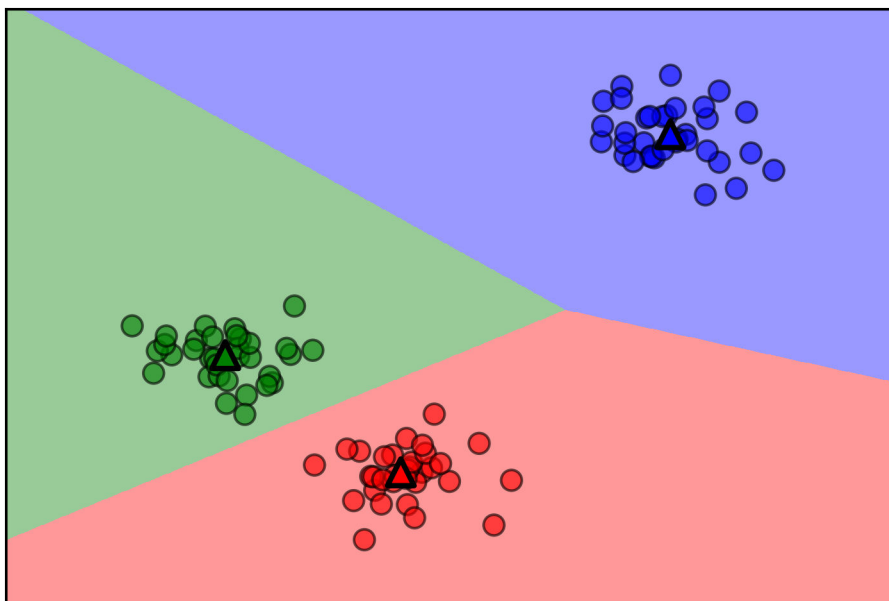
We specified that we are looking for three clusters, so the algorithm was initialized by declaring three data points as cluster centers (see “Initialization”). Then the iterative algorithm starts: Each data point is assigned to the cluster center it is closest to (see



“Assign Points (1)”). Next, the cluster centers are updated to be the mean of the assigned points (see “Recompute Centers (1)”). Then the process is repeated. After the second iteration, the assignment of points to cluster centers remained unchanged, so the algorithm stops.

Given new data points, k-Means will assign them to the closest cluster center. Here are the boundaries of the cluster centers that were learned in the diagram above:

```
mglearn.plots.plot_kmeans_boundaries()
```



Applying k-Means with scikit-learn is quite straight-forward. Here we apply it to the synthetic data that we used for the plots above. We instantiate the `KMeans` class, and set the number of clusters we are looking for [footnote: If you don't provide `n_clusters` it is set to eight by default. There is no particular reason why you should use eight.]. Then we call the `fit` method with the data:

```
from sklearn.datasets import make_blobs
from sklearn.cluster import KMeans

# generate synthetic two-dimensional data
X, y = make_blobs(random_state=1)

# build the clustering model:
kmeans = KMeans(n_clusters=3)
kmeans.fit(X)
```

```
KMeans(copy_x=True, init='k-means++', max_iter=300, n_clusters=3, n_init=10,
       n_jobs=1, precompute_distances='auto', random_state=None, tol=0.0001,
       verbose=0)
```

During the algorithm, each training data point in *X* is assigned a cluster label. You can find these labels in the `kmeans.labels_` attribute:

```
print(kmeans.labels_)
[1 9 3 6 9 4 1 2 1 2 7 8 9 2 0 1 5 8 5 0 4 2 5 2 7 3 9 4 3 5 1 7 2 3 1 4 8
 1 0 3 8 7 5 3 9 7 1 0 3 2 0 8 4 6 2 1 5 2 5 7 8 6 9 1 2 6 7 9 7 6 8 6 8 3
 2 6 3 1 5 8 4 7 8 4 3 7 1 7 8 4 5 1 4 0 4 9 9 8 6 3 2 4 7 1 6 3 6 7 9 5 0
 7 7 6 1 9 5 4 8 1 1 0 3 7 3 0 1 3 2 4 1 0 6 8 2 9 2 6 4 1 3 3 5 7 7 1 3 2
 5 3 8 9 1 5 8 7 2 8 5 5 3 2 5 9 8 9 5 8 9 2 5 6 6 0 3 2 4 0 0 5 9 6 4 9 4
 5 7 2 6 0 6 5 1 1 3 0 4 3 5 9]
```

As we asked for three clusters, the clusters are numbered 0 to 2.

You can also assign cluster labels to new points, using the `predict` method. Each new point is assigned to the closest cluster center when predicting, but the existing model is not changed. Running `predict` on the training set returns the same as `labels_`:

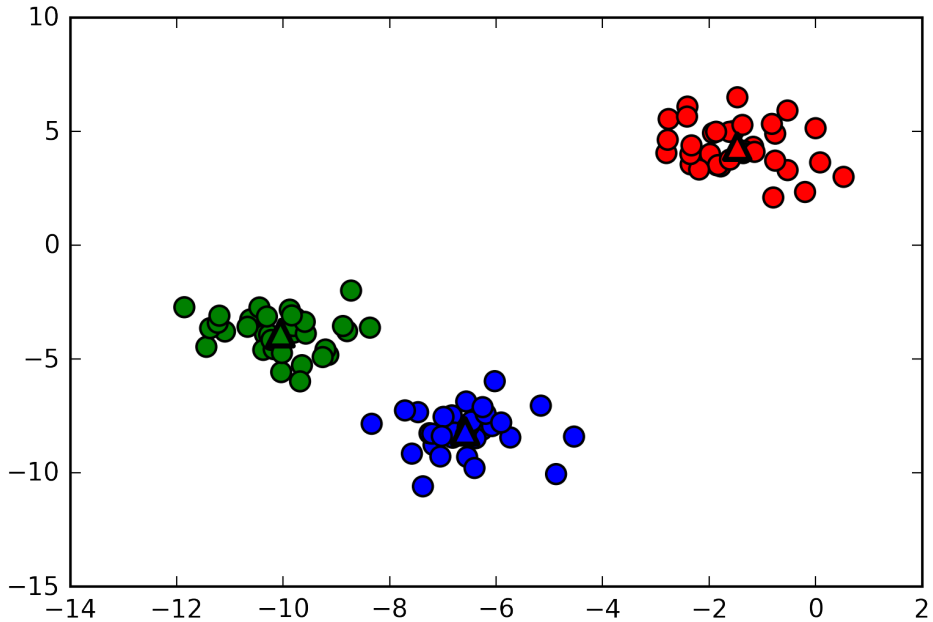
```
print(kmeans.predict(X))
[1 2 2 2 0 0 0 2 1 1 2 2 0 1 0 0 0 1 2 2 0 2 0 1 2 0 0 1 1 0 1 1 0 1 2 0 2
 2 2 0 0 2 1 2 2 0 1 1 1 1 2 0 0 0 1 0 2 2 1 1 2 0 0 2 2 0 1 0 1 2 2 2 0 1
 1 2 0 0 1 2 1 2 2 0 1 1 1 1 2 1 0 1 1 2 2 0 0 1 0 1]
```

You can see that clustering is somewhat similar to classification, in that each item gets a label. However, there is no ground truth, and consequently the labels themselves have no *a priori* meaning. Let's go back to the example of clustering face images that we discussed before. It might be that the cluster 3 found by the algorithm contains only faces of your friend Bela. You can only know that after you looked at the pictures, though, and the number 3 is arbitrary. The only information the algorithm gives you is that all faces labeled as 3 are similar.

For the clustering we just computed on the two dimensional toy dataset, that means that

Here is a plot of this data again. The cluster centers are stored in the `cluster_centers_` attribute, and we plot them as triangles:

```
plt.scatter(X[:, 0], X[:, 1], c=kmeans.labels_, cmap=mglearn.cm3, s=60)
plt.scatter(kmeans.cluster_centers_[0], kmeans.cluster_centers_[1],
            marker='^', s=100, linewidth=2, c=[0, 1, 2], cmap=mglearn.cm3)
```



We can also use more or less cluster centers:

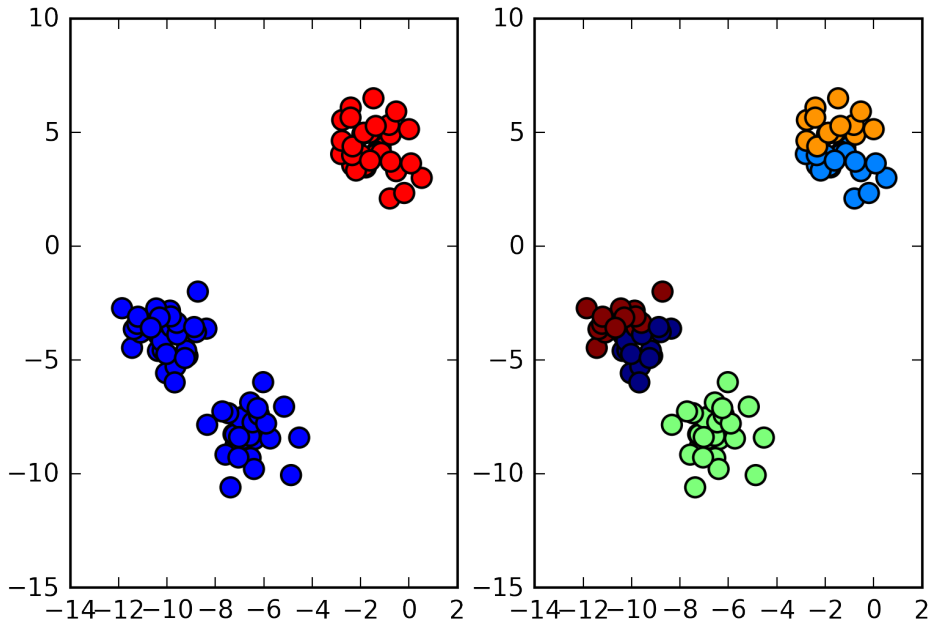
```
fig, axes = plt.subplots(1, 2)

# using two cluster centers:
kmeans = KMeans(n_clusters=2)
kmeans.fit(X)
assignments = kmeans.labels_

axes[0].scatter(X[:, 0], X[:, 1], c=assignments, cmap=mglearn.cm2, s=60)

# using five cluster centers:
kmeans = KMeans(n_clusters=5)
kmeans.fit(X)
assignments = kmeans.labels_

axes[1].scatter(X[:, 0], X[:, 1], c=assignments, cmap='jet', s=60);
```

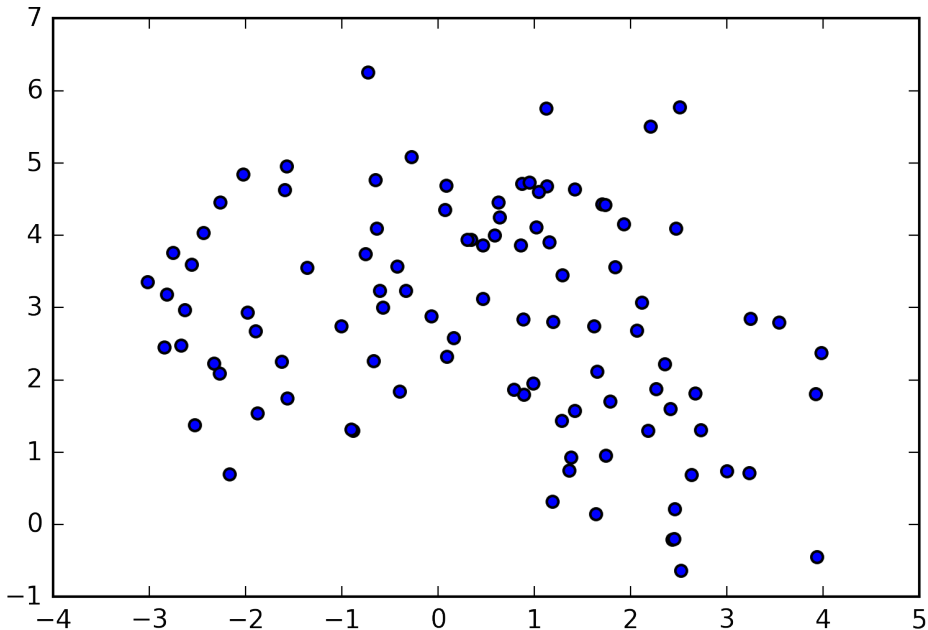


### Failure cases of k-Means

Even if you know the “right” number of clusters for a given dataset, k-Means might not always be able to recover them. Each cluster is defined solely by its center, which means that each cluster is a convex shape. As a result of this is that k-Means can only capture relatively simple shapes.

k-Means also assumes that all clusters have the same “diameter” in some sense; it always draws the boundary between clusters to be exactly in the middle between the cluster centers. That can sometimes lead to surprising results, as shown below:

```
X, y = make_blobs(random_state=0)
plt.scatter(X[:, 0], X[:, 1]);
```



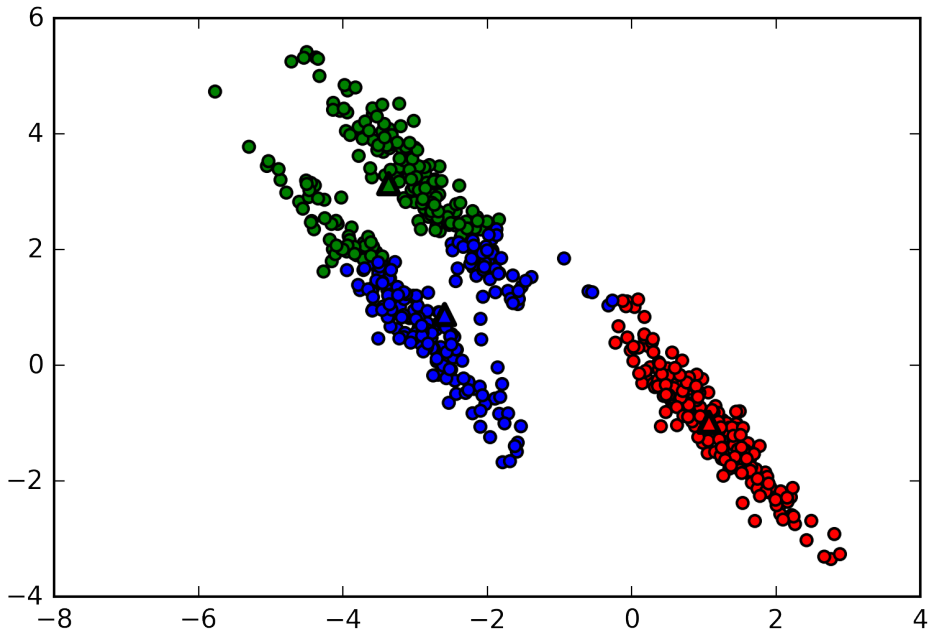
k-Means also assumes that all directions are equally important for each cluster. The plot below shows a two-dimensional dataset where there are three clearly separated parts in the data. However, these groups are stretched towards the diagonal. As k-Means only considers the distance to the nearest cluster center, it can't handle this kind of data.

```
# generate some random cluster data
X, y = make_blobs(random_state=170, n_samples=600)
rng = np.random.RandomState(74)

# transform the data to be stretched
transformation = rng.normal(size=(2, 2))
X = np.dot(X, transformation)

# cluster the data into three clusters
kmeans = KMeans(n_clusters=3)
kmeans.fit(X)
y_pred = kmeans.predict(X)

# plot the cluster assignments and cluster centers
plt.scatter(X[:, 0], X[:, 1], c=y_pred, cmap=mglearn.cm3)
plt.scatter(kmeans.cluster_centers_[0], kmeans.cluster_centers_[1],
            marker='^', c=['b', 'r', 'g'], s=60, linewidth=2);
```

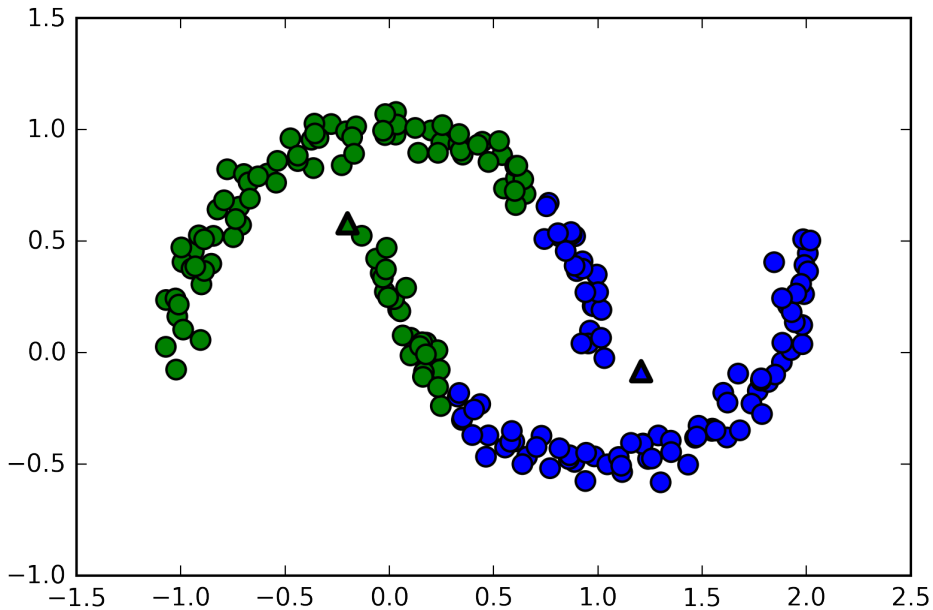


k-Means also performs poorly if the clusters have more complex shapes, like the `two_moons` data we encountered in Chapter 2:

```
# generate synthetic two_moons data (with less noise this time)
from sklearn.datasets import make_moons
X, y = make_moons(n_samples=200, noise=0.05, random_state=0)

# cluster the data into two clusters
kmeans = KMeans(n_clusters=2)
kmeans.fit(X)
y_pred = kmeans.predict(X)

# plot the cluster assignments and cluster centers
plt.scatter(X[:, 0], X[:, 1], c=y_pred, cmap=mpl.cm3, s=60)
plt.scatter(kmeans.cluster_centers_[0], kmeans.cluster_centers_[1],
            marker='^', c=['b', 'g'], s=60, linewidth=2);
```



Here, we would hope that the clustering algorithm can discover the two half-moon shapes. However, this is not possible using the k-Means algorithm.

### Vector Quantization - Or Seeing k-Means as Decomposition

Even though k-Means is a clustering algorithm, there are interesting parallels between k-Means and decomposition methods like PCA and NMF that we discussed above. You might remember that PCA tries to find directions of maximum variance in the data, while NMF tries to find additive components, which often correspond to “extremes” or “parts” of the data (see Figure *nmf\_illustration*). Both methods tried to express data points as a sum over some components.

k-Means on the other hand tries to represent each data point using a cluster center. You can think of that as each point being represented using only a single component, which is given by the cluster center. This view of k-Means as a decomposition method, where each point is represented using a single component, is called *vector quantization*.

Here is a side-by-side comparison of PCA, NMF and k-Means, showing the components extracted, as well as reconstructions of faces from the test set using 100 components. For k-Means, the reconstruction is the closest cluster center found on the training set:

```
X_train, X_test, y_train, y_test = train_test_split(X_people, y_people, stratify=y_people, random_
nmf = NMF(n_components=100)
```

```

nmf.fit(X_train)
pca = PCA(n_components=100)
pca.fit(X_train)
kmeans = KMeans(n_clusters=100)
kmeans.fit(X_train)

X_reconstructed_pca = pca.inverse_transform(pca.transform(X_test))
X_reconstructed_kmeans = kmeans.cluster_centers_[kmeans.predict(X_test)]
X_reconstructed_nmf = np.dot(nmf.transform(X_test), nmf.components_)

fig, axes = plt.subplots(3, 5, figsize=(8, 8)) #, subplot_kw={'xticks': (), 'yticks': ()}
fig.suptitle("Extracted Components")
for ax, comp_kmeans, comp_pca, comp_nmf in zip(axes.T, kmeans.cluster_centers_, pca.components_, nmf.components_):
    ax[0].imshow(comp_kmeans.reshape(image_shape))
    ax[1].imshow(comp_pca.reshape(image_shape), cmap='viridis')
    ax[2].imshow(comp_nmf.reshape(image_shape))

axes[0, 0].set_ylabel("kmeans")
axes[1, 0].set_ylabel("pca")
axes[2, 0].set_ylabel("nmf")

fig, axes = plt.subplots(4, 5, subplot_kw={'xticks': (), 'yticks': ()}, figsize=(8, 8))
fig.suptitle("Reconstructions")
for ax, orig, rec_kmeans, rec_pca, rec_nmf in zip(axes.T, X_test, X_reconstructed_kmeans, X_reconstructed_pca, X_reconstructed_nmf):
    ax[0].imshow(orig.reshape(image_shape))
    ax[1].imshow(rec_kmeans.reshape(image_shape))
    ax[2].imshow(rec_pca.reshape(image_shape))
    ax[3].imshow(rec_nmf.reshape(image_shape))

axes[0, 0].set_ylabel("original")
axes[1, 0].set_ylabel("kmeans")
axes[2, 0].set_ylabel("pca")
axes[3, 0].set_ylabel("nmf")

```



## Reconstructions

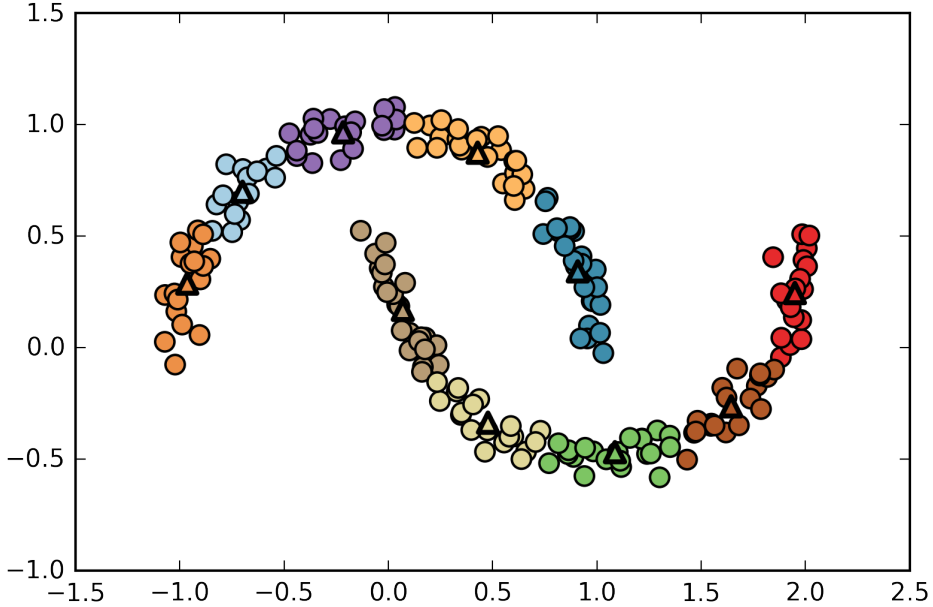


An interesting aspect of vector quantization using k-Means is that we can use many more clusters than input dimensions to encode our data. Let's go back to the `two_moons` data. Using PCA or NMF, there is nothing much we can do to this data, as it lives in only two dimensions. Reducing it to one dimension with PCA or NMF would completely destroy the structure of the data. But we can find a more expressive representation using k-Means, by using more cluster centers:

```
X, y = make_moons(n_samples=200, noise=0.05, random_state=0)

kmeans = KMeans(n_clusters=10)
kmeans.fit(X)
y_pred = kmeans.predict(X)
```

```
plt.scatter(X[:, 0], X[:, 1], c=y_pred, s=60, cmap='Paired')
plt.scatter(kmeans.cluster_centers[:, 0], kmeans.cluster_centers[:, 1],
            marker='^', c=range(kmeans.n_clusters), s=60, linewidth=2, cmap='Paired')
print(y_pred)
```



```
[1 9 3 6 9 4 1 2 1 2 7 8 9 2 0 1 5 8 5 0 4 2 5 2 7 3 9 4 3 5 1 7 2 3 1 4 8
 1 0 3 8 7 5 3 9 7 1 0 3 2 0 8 4 6 2 1 5 2 5 7 8 6 9 1 2 6 7 9 7 6 8 6 8 3
 2 6 3 1 5 8 4 7 8 4 3 7 1 7 8 4 5 1 4 0 4 9 9 8 6 3 2 4 7 1 6 3 6 7 9 5 0
 7 7 6 1 9 5 4 8 1 1 0 3 7 3 0 1 3 2 4 1 0 6 8 2 9 2 6 4 1 3 3 5 7 7 1 3 2
 5 3 8 9 1 5 8 7 2 8 5 5 3 2 5 9 8 9 5 8 9 2 5 6 6 0 3 2 4 0 0 5 9 6 4 9 4
 5 7 2 6 0 6 5 1 1 3 0 4 3 5 9]
```

We used 10 cluster centers, which means each point is now assigned a number between 0 and 9. We can see this as the data being represented using 10 components (that is, we have ten new features), with all features being zero, apart from the one that represents the cluster center the point is assigned to. Using this 10-dimensional representation, it would now be possible to separate the two half-moon shapes using a linear model, which would not have been possible using the original two features. [really? can you show what that would look like, maybe?]

It is also possible to get an even more expressive representation of the data by using the distances to each of the cluster centers as features. This can be done using the transform method of kmeans:

```
distance_features = kmeans.transform(X)
print(distance_features.shape)
print(distance_features)

(200, 10)

[[ 1.53  0.2   1.03 ...,  1.12  0.92  1.14]
 [ 2.56  1.01  0.54 ...,  2.28  1.14  0.12]
 [ 0.8   0.93  1.33 ...,  0.72  0.79  1.75]
 ...,
 [ 1.12  0.81  1.02 ...,  1.05  0.45  1.49]
 [ 0.88  1.03  1.76 ...,  0.34  1.39  1.98]
 [ 2.5   0.91  0.59 ...,  2.19  1.15  0.05]]
```

k-Means is a very popular algorithm for clustering, not only because it is relatively easy to understand and implement, but also because it runs relatively quickly. k-Means scales easily to large datasets, and scikit-learn even includes a more scalable variant in the `MiniBatchKMeans` class, which can handle very large datasets.

One of the drawbacks of k-Means is that it relies on a random initialization, which means the outcome of the algorithm depends on a random seed. By default, scikit-learn runs the algorithm 10 times with 10 different random initializations, and returns the best result [Footnote: best here meaning that the sum of variances of the clusters is small].

Further downsides of k-Means are the relatively restrictive assumptions made on the shape of clusters, and the requirement to specify the number of clusters you are looking for (which might not be known in a real-world application).

Next, we will look at two more clustering algorithms that improve upon these properties in some ways.

## Agglomerative Clustering

Agglomerative clustering refers to a collection of clustering algorithms that all build upon the same principles: The algorithm starts by declaring each point its own cluster, and then merges the two most similar clusters until some stopping criterion is satisfied.

The stopping criterion implemented in scikit-learn is the number of clusters, so similar clusters are merged until only the specified number of clusters is left.

There are several *linkage* criteria that specify how exactly “most similar cluster” is measured. [this sentence looks a lot like the next sentence - combine into one]

The following three choices are implemented in scikit-learn:

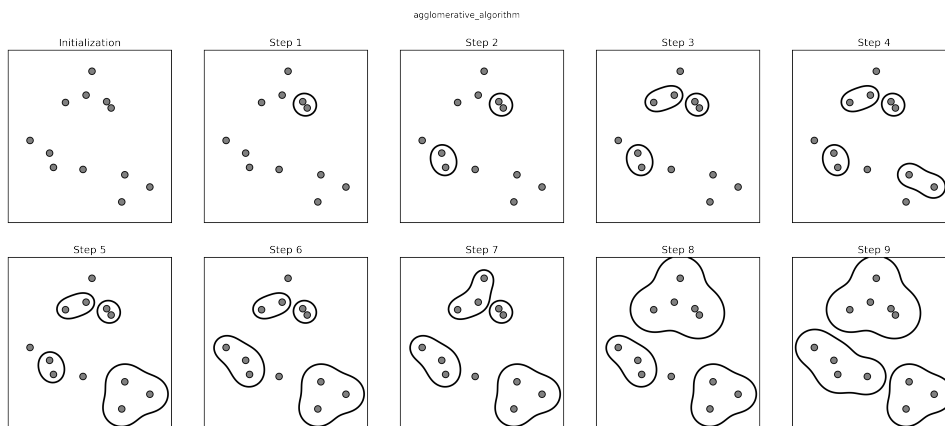
- “ward”, which is the default choice. Ward picks the two clusters to merge such that the variance within all clusters increases the least. This often leads to clusters that are relatively equally sized.
- “average” linkage merges the two clusters that have the smallest average distance between all their points.
- “complete” linkage (also known as maximum linkage) merges the two clusters that have the smallest maximum distance between their points.

[you keep writing ‘the two clusters’, but you did not specify that there would be two clusters - rather said that there are a ‘number of clusters’]

Ward is generally a good default; all our examples below will use ward.

The plot below illustrates the progression of agglomerative clustering on a two-dimensional dataset, looking for three clusters.

```
mglearn.plots.plot_agglomerative_algorithm()  
plt.suptitle("agglomerative_algorithm");
```



In the beginning, each point is its own cluster. Then, in each step, the two clusters that are closest are merged. In the first four steps, two single point clusters are picked and these are joined into two-point clusters. In step four, one of the two-point clusters is extended to a third point, and so on. In step 9, there are only three clusters

remaining. As we specified that we are looking for three clusters, the algorithm then stops.

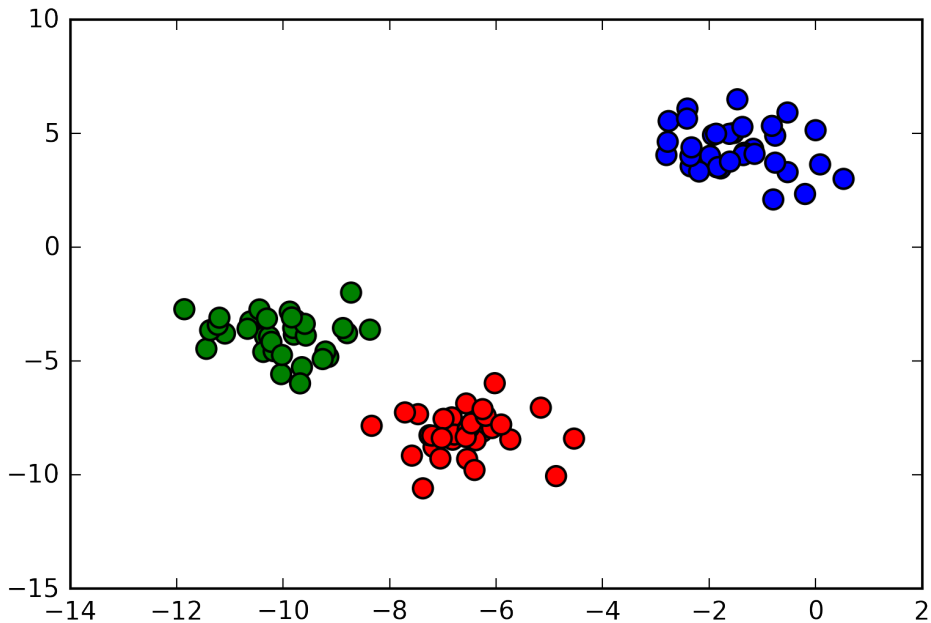
Let's have a look at how agglomerative clustering performs on the simple three-cluster data we used above.

Because of the way the algorithm works, agglomerative clustering can not make predictions for new data points. Therefore, agglomerative clustering has no `predict` method. To build the model, and get the cluster memberships on the training set, use the `fit_predict` method instead. [footnote: we could also use the `labels_` attribute as we did for k-Means]

```
from sklearn.cluster import AgglomerativeClustering
X, y = make_blobs(random_state=1)

agg = AgglomerativeClustering(n_clusters=3)
assignment = agg.fit_predict(X)

plt.scatter(X[:, 0], X[:, 1], c=assignment, cmap=mglearn.cm3, s=60)
```



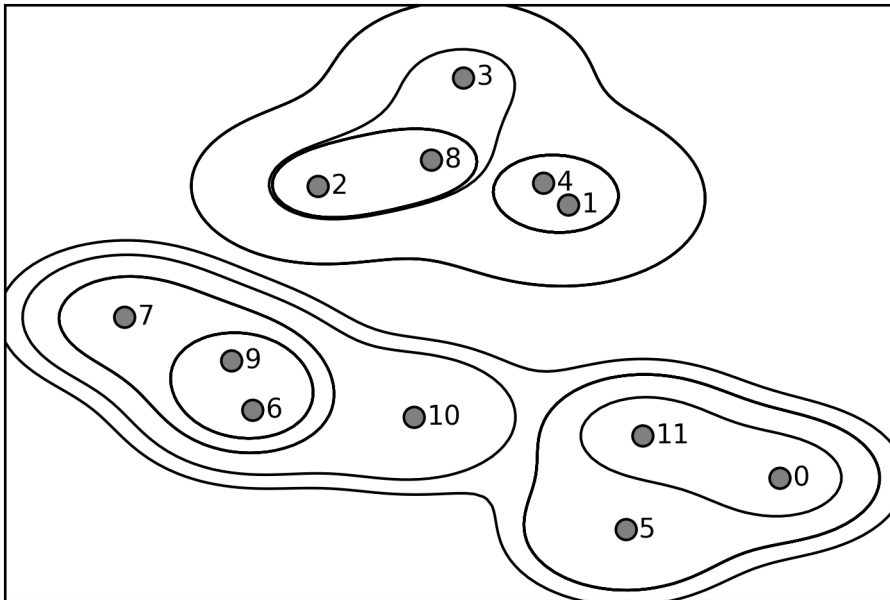
As expected, the algorithm recovers the clustering perfectly. While the scikit-learn implementation of agglomerative clustering requires you to specify a number of clusters you want the algorithm to find, agglomerative clustering methods provide some help with choosing the right number, which we will now discuss next.

## Hierarchical Clustering and Dendrograms

Agglomerative clustering produces what is known as a *hierarchical clustering*. The clustering proceeds iteratively, and every point makes a journey from being a single point cluster to belonging to some final cluster. Each intermediate step provides a clustering of the data (with a different number of clusters). It is sometimes helpful to look at all possible clusterings jointly.

The figure below shows an overlay of all possible clusterings shown in Figure `agglomerative_algorithm`, providing some insight into how each cluster breaks up into smaller clusters.

```
mglearn.plots.plot_agglomerative()
```



While this visualization provides a very detailed view of the hierarchical clustering, it relies on the two-dimensional nature of the data, and can therefore not be used on datasets that have more than two features. There is, however, another tool to visualize hierarchical clustering, called a *dendrogram* (as shown in Figure `dendrogram` below).

Unfortunately, scikit-learn currently does not have the functionality to draw dendrograms. However, you can generate them easily using `scipy`.

The `scipy` clustering algorithms have a slightly different interface from the scikit-learn clustering algorithms.

`scipy` provides function that take data arrays X *linkage array* encoding cluster similarities.

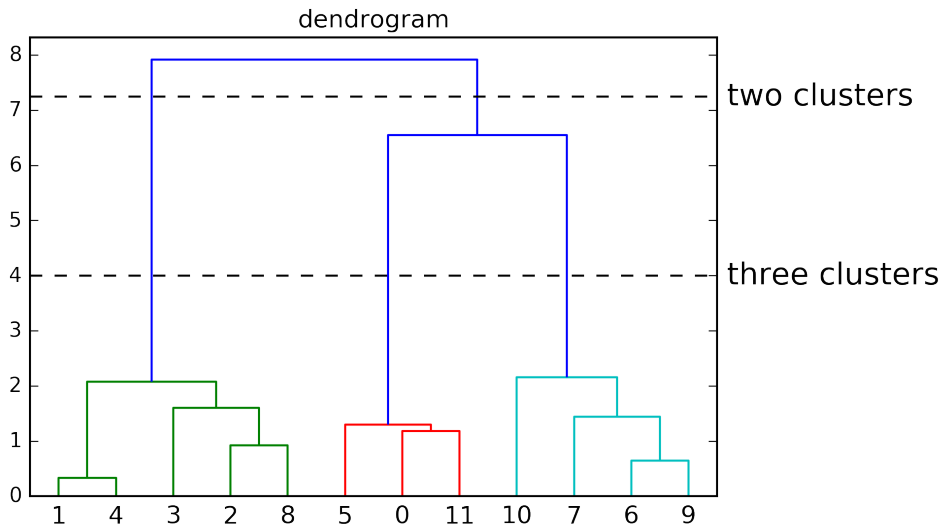
We can then feed this linkage array into the `scipy dendrogram` function to plot the dendrogram:

```
# import the dendrogram function and the ward clustering function from scipy
from scipy.cluster.hierarchy import dendrogram, ward

X, y = make_blobs(random_state=0, n_samples=12)
# apply the ward clustering to the data array X
# The scipy ward function returns an array that specifies the distances bridged when performing ag
linkage_array = ward(X)
# now we plot the dendrogram for the linkage_array containing the distances between clusters
dendrogram(linkage_array);

# mark the cuts in the tree that signify two or three clusters
ax = plt.gca()
bounds = ax.get_xbound()
ax.plot(bounds, [7.25, 7.25], '--', c='k')
ax.plot(bounds, [4, 4], '--', c='k')

ax.text(bounds[1], 7.25, ' two clusters', verticalalignment='center', fontdict={'size': 15})
ax.text(bounds[1], 4, ' three clusters', verticalalignment='center', fontdict={'size': 15})
plt.title("dendrogram")
```



The dendrogram shows data points as points on the bottom (numbered from zero to eleven). Then, a tree is plotted with these points (representing single-point clusters) as the leaves, and a new node parent is added for each two clusters that are joined.

Reading from bottom to top, the data points 1 and 4 are joined first (as you could see in Figure `agglomerative_algorithm`). Next, points 6 and 9 are joined into a cluster, and so on. The top level, there are two branches, one consisting of point 11, 0, 5, 10,

7, 6 and 9, and the other one consisting of points 1, 4, 3, 2 and 8. These correspond to the two largest clusters in in the left hand side of the plot.

The y axis in the dendrogram not only specifies when in the agglomerative algorithm two clusters get merged. The length of each branch also shows how far apart the merged clusters are. The longest branches in this dendrogram are the three lines that are around the “10” mark on the y-axis. That these are the longest branches indicates that going from three to two clusters meant merging some very far-apart points. We see this again at the top of the chart, where merging the two remaining clusters into a single cluster again bridges a large distance.

Unfortunately, agglomerative clustering still fails at separating complex shapes like the `two_moons` dataset. The same is not true for the next algorithm we will look at, DBSCAN.

## DBSCAN

Another very useful clustering algorithm is DBSCAN (which stands for “Density-based spatial clustering of applications with noise”). The main benefits of DBSCAN are that a) it does not require the user to set the number of clusters *a priori*, b) it can capture clusters of complex shapes, and c) it can identify point that are not part of any cluster.

DBSCAN is somewhat slower than agglomerative clustering and k-Means, but still scales to relatively large datasets.

The way DBSCAN works is by identifying points that are in “crowded” regions of the feature space, where many data points are close together. These regions are referred to as *dense* regions in feature space. The idea behind DBSCAN is that clusters form dense regions of data, separated by regions that are relatively empty.

Points that are within a dense region are called *core samples*, and they are defined as follows.

There are two parameters in DBSCAN, `min_samples` and `eps`. If there are at least `min_samples` many data points within a distance of `eps` to a given data point, it’s called a *core sample*. Core samples that are closer than the distance `eps` are put into the same cluster by DBSCAN.

The algorithm works by picking a point to start with.

It then finds all points with distance `eps` or less. If there are less than `min_samples` points within distance `eps` or less, this point is labeled as *noise*, meaning that this point doesn’t belong to any cluster.

If there are more than `min_samples` points within a distance of `eps`, the point is labeled a core sample and assigned a new cluster label. Then, all neighbors (withing



eps) of the point are visited. If they have not been assigned a cluster yet, they are assigned the new cluster label we just created. If they are core samples, their neighbors are visited in turn, and so on.

The cluster grows, until there are no more core-samples within distance eps of the cluster.

Then another point, which hasn't yet been visited, is picked, and the same procedure is repeated.

In the end, there are three kinds of points: core points, points that are within distance eps of core points (called boundary points), and noise. When running the DBSCAN algorithm on a particular dataset multiple times, the clustering of the core points is always the same, and the same points will always be labeled as noise. However, a boundary point might be neighbor to core samples of more than one cluster. Therefore, the cluster membership of boundary points depends on the order in which points are visited. Usually there are only few boundary points, and this slight dependence on the order of points is not important.

Let's apply DBSCAN on the synthetic data from above. As in agglomerative clustering, DBSCAN does not allow predictions on new test data, so we will use the `fit_predict` method to perform clustering and return the cluster labels in one step:

```
from sklearn.cluster import DBSCAN
X, y = make_blobs(random_state=0, n_samples=12)

dbscan = DBSCAN()
clusters = dbscan.fit_predict(X)
clusters

array([-1, -1, -1, -1, -1, -1, -1, -1, -1, -1, -1, -1])
```

As you can see, all data points were assigned the label -1, which stands for noise. This is a consequence of the default parameter settings for `eps` and `min_samples`, which are not attuned to small toy datasets.

Let's investigate the effect of changing `eps` and `min_samples`.

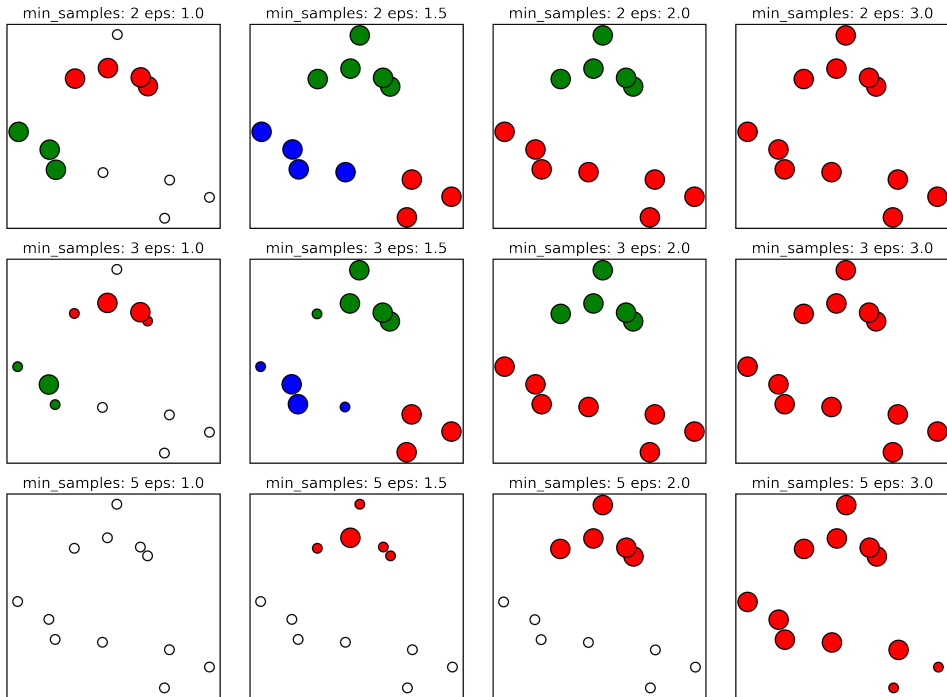
```
fig, axes = plt.subplots(3, 4, figsize=(11, 8), subplot_kw={'xticks': (), 'yticks': ()})
# Plot clusters as red, green and blue, and outliers (-1) as white
colors = np.array(['r', 'g', 'b', 'w'])

# iterate over settings of min_samples and eps
for i, min_samples in enumerate([2, 3, 5]):
    for j, eps in enumerate([1, 1.5, 2, 3]):
        # instantiate DBSCAN with a particular setting
        dbscan = DBSCAN(min_samples=min_samples, eps=eps)
        # get cluster assignments
        clusters = dbscan.fit_predict(X)
        print("min_samples: %d eps: %f cluster: %s" % (min_samples, eps, clusters))
```

```

# visualize core samples and clusters.
sizes = 60 * np.ones(X.shape[0])
# size is given by whether something is a core sample
sizes[dbscan.core_sample_indices_] *= 4
axes[i, j].scatter(X[:, 0], X[:, 1], c=colors[clusters], s=sizes)
axes[i, j].set_title("min_samples: %d eps: %.1f" % (min_samples, eps))
fig.tight_layout()

```



```

min_samples: 2 eps: 1.000000 cluster: [-1  0  0 -1  0 -1  1  1  0  1 -1 -1]
min_samples: 2 eps: 1.500000 cluster: [0  1  1  1  1  0  2  2  1  2  2  0]
min_samples: 2 eps: 2.000000 cluster: [0  1  1  1  1  0  0  0  1  0  0  0]
min_samples: 2 eps: 3.000000 cluster: [0  0  0  0  0  0  0  0  0  0  0  0]
min_samples: 3 eps: 1.000000 cluster: [-1  0  0 -1  0 -1  1  1  0  1 -1 -1]
min_samples: 3 eps: 1.500000 cluster: [0  1  1  1  1  0  2  2  1  2  2  0]
min_samples: 3 eps: 2.000000 cluster: [0  1  1  1  1  0  0  0  1  0  0  0]
min_samples: 3 eps: 3.000000 cluster: [0  0  0  0  0  0  0  0  0  0  0  0]
min_samples: 5 eps: 1.000000 cluster: [-1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1]

```

```

min_samples: 5 eps: 1.500000 cluster: [-1 0 0 0 0 -1 -1 -1 0 -1 -1 -1]
min_samples: 5 eps: 2.000000 cluster: [-1 0 0 0 0 -1 -1 -1 0 -1 -1 -1]
min_samples: 5 eps: 3.000000 cluster: [0 0 0 0 0 0 0 0 0 0 0 0]

```

In this plot, points that belong to clusters are colored, while the noise points are shown in white.

Core samples are shown as large points, while border points are displayed as smaller points.

Increasing `eps` (going from left to left to right in the figure) means that more points will be included in a cluster. This makes clusters grow, but might also lead to multiple clusters joining into one. Increasing `min_samples` (going from top to bottom in the figure) means that fewer points will be core points, and more points will be labeled as noise.

The parameter `eps` is somewhat more important, as it determines what it means for points to be “close”.

Setting `eps` to be very small will mean that no points are core samples, and may lead to all points being labeled as noise. Setting `eps` to be very large will result in all points forming a single cluster.

The setting of `min_samples` mostly determines whether points in less dense regions will be labeled as outliers, or as their own cluster. If you decrease `min_samples`, anything that would have been a cluster with less than `min_samples` many samples will now be labeled as noise. The `min_samples` therefore determines the minimum cluster size. You can see this very clearly in the plot above, when going from `min_samples=3` to `min_samples=5` with `eps=1.5`. With `min_samples=3`, there are three clusters: one of four points, one of five points and one of three points. Using `min_samples=5`, the two smaller clusters (with three or four points) are now labeled as noise, and only the cluster with 5 samples remains.

While DBSCAN doesn’t require setting the number of clusters explicitly, setting `eps` implicitly controls how many clusters will be found.

Finding a good setting for `eps` is sometimes easier after scaling the data using `StandardScaler` or `MinMaxScaler`, as using these scaling techniques will ensure that all features have similar ranges.

Below is the result of DBSCAN running on the `two_moons` dataset. The algorithm actually finds the two half-circles and separates them using the default settings.

```

X, y = make_moons(n_samples=200, noise=0.05, random_state=0)

# Rescale the data to zero mean and unit variance

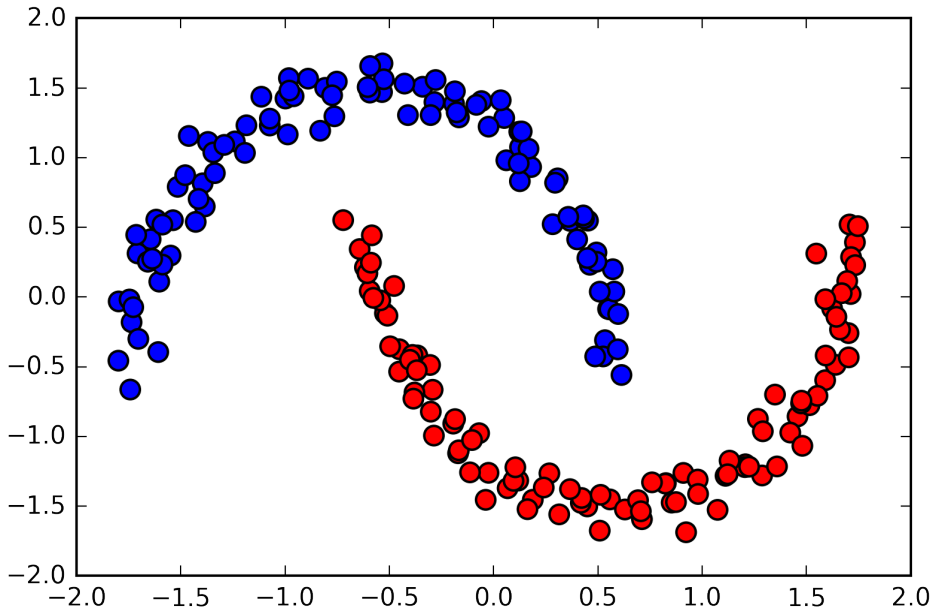
```

```

scaler = StandardScaler()
scaler.fit(X)
X_scaled = scaler.transform(X)

dbscan = DBSCAN()
clusters = dbscan.fit_predict(X_scaled)
# plot the cluster assignments
plt.scatter(X_scaled[:, 0], X_scaled[:, 1], c=clusters, cmap=mglearn.cm2, s=60)

```



As the algorithm produced the desired number of clusters (two), the parameter settings seem to work well.

If we decrease `eps` to 0.2 (from the default of 0.5), we will get 8 clusters, which are clearly too many. Increasing `eps` to 0.7 results in a single cluster.

When using DBSCAN, you need to be careful about handling the returned cluster assignments. The use of -1 to indicate noise might result in unexpected effects when using the cluster labels to index another array. [an example here could be useful - sort of know what you're talking about, but sort of not]

### Comparing and evaluating clustering algorithms

After talking about the algorithms behind k-Means, agglomerative clustering and DBSCAN, we will now compare them on some real world datasets. One of the challenges in applying clustering algorithms is that it is very hard to access how well a clustering algorithm worked, and to compare outcomes between different algorithms.

## Evaluating clustering with ground truth

There are metrics that can be used to assess the outcome of a clustering algorithm relative to a ground truth clustering, the most important ones being the *adjusted rand index* (ARI) and *normalized mutual information* (NMI), which both provide a quantitative measure between 0 and 1.

Below we compare the k-Means, agglomerative clustering and DBSCAN algorithms using ARI. We also include what it looks like when we randomly assign points to two clusters for comparison.

```
from sklearn.metrics.cluster import adjusted_rand_score
X, y = make_moons(n_samples=200, noise=0.05, random_state=0)

# Rescale the data to zero mean and unit variance
scaler = StandardScaler()
scaler.fit(X)
X_scaled = scaler.transform(X)

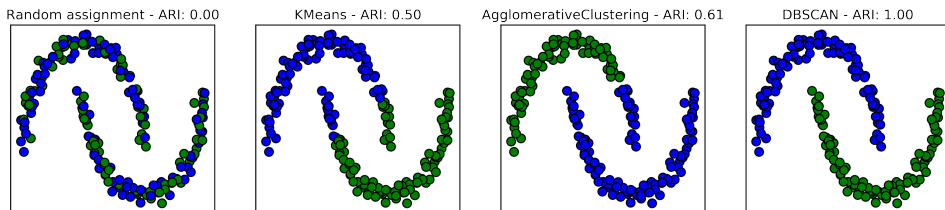
fig, axes = plt.subplots(1, 4, figsize=(15, 3), subplot_kw={'xticks': (), 'yticks': ()})

# make a list of algorithms to use
algorithms = [KMeans(n_clusters=2), AgglomerativeClustering(n_clusters=2), DBSCAN()]

# create a random cluster assignment for reference:
random_state = np.random.RandomState(seed=0)
random_clusters = random_state.randint(low=0, high=2, size=len(X))

# plot random assignment:
axes[0].scatter(X_scaled[:, 0], X_scaled[:, 1], c=random_clusters, cmap=mpl.cm3, s=60)
axes[0].set_title("Random assignment - ARI: %.2f" % adjusted_rand_score(y, random_clusters))

for ax, algorithm in zip(axes[1:], algorithms):
    # plot the cluster assignments and cluster centers
    clusters = algorithm.fit_predict(X_scaled)
    ax.scatter(X_scaled[:, 0], X_scaled[:, 1], c=clusters, cmap=mpl.cm3, s=60)
    ax.set_title("%s - ARI: %.2f" % (algorithm.__class__.__name__, adjusted_rand_score(y, clusters)))
```



The adjusted rand index provides intuitive results, with a random cluster assignment having a score of 0, and DBSCAN (which recovers the desired clustering perfectly) having a score of 1. A common mistake when evaluating clustering in this way is to

use `accuracy_score` instead of a clustering metric like `adjusted_rand_score` and `normalized_mutual_info_score`.

The problem in using accuracy is that it requires the assigned cluster labels to exactly match the ground truth. However, the cluster labels themselves are meaningless, and only which points are in the same cluster matters:

```
from sklearn.metrics import accuracy_score

# These two labelings of points correspond to the same clustering:
clusters1 = [0, 0, 1, 1, 0]
clusters2 = [1, 1, 0, 0, 1]
# accuracy is zero, as none of the labels are the same:
print("Accuracy: %.2f" % accuracy_score(clusters1, clusters2))
# adjusted rand score is 1, as the clustering is exactly the same:
print("ARI: %.2f" % adjusted_rand_score(clusters1, clusters2))

Accuracy: 0.00

ARI: 1.00
```

## Evaluating clustering without ground truth

Although we have just shown how to evaluate on clustering algorithms, in practice, there is a big problem with the evaluation using measures like ARI.

When applying clustering algorithms, there is usually no ground truth to which to compare. If we knew the right clustering of the data, we could use this information to build a supervised model like a classifier.

Therefore, using metric like ARI and NMI usually only really helps in developing algorithms, not in assessing success in an application.

There are scoring metrics for clustering that don't require ground truth, like the *silhouette coefficient*. However, these often don't work well in practice. The silhouette score computes the compactness of a cluster, where higher is better, with a perfect score of 1. While compact clusters are good, compactness doesn't allow for complex shapes.

Here is an example comparing the outcome of k-Means, agglomerative clustering and DBSCAN on the two moons using the silhouette score:

```
from sklearn.metrics.cluster import silhouette_score

X, y = make_moons(n_samples=200, noise=0.05, random_state=0)

# Rescale the data to zero mean and unit variance
scaler = StandardScaler()
scaler.fit(X)
X_scaled = scaler.transform(X)
```

```

fig, axes = plt.subplots(1, 4, figsize=(15, 3), subplot_kw={'xticks': (), 'yticks': ()})

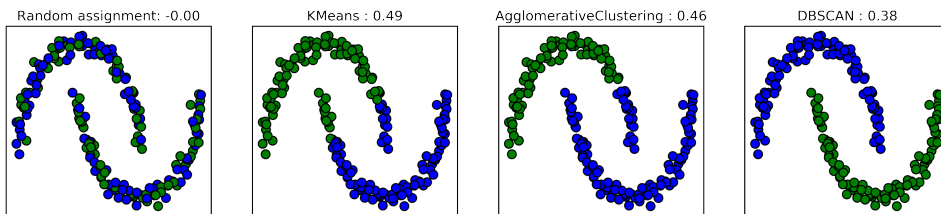
# create a random cluster assignment for reference:
random_state = np.random.RandomState(seed=0)
random_clusters = random_state.randint(low=0, high=2, size=len(X))

# plot random assignment:
axes[0].scatter(X_scaled[:, 0], X_scaled[:, 1], c=random_clusters, cmap=mglern.cm3, s=60)
axes[0].set_title("Random assignment: %.2f" % silhouette_score(X_scaled, random_clusters))

algorithms = [KMeans(n_clusters=2), AgglomerativeClustering(n_clusters=2), DBSCAN()]

for ax, algorithm in zip(axes[1:], algorithms):
    clusters = algorithm.fit_predict(X_scaled)
    # plot the cluster assignments and cluster centers
    ax.scatter(X_scaled[:, 0], X_scaled[:, 1], c=clusters, cmap=mglern.cm3, s=60)
    ax.set_title("%s : %.2f" % (algorithm.__class__.__name__, silhouette_score(X_scaled, clusters)))

```



As you can see, k-Means gets the highest silhouette score, even though we might prefer the result produced by DBSCAN.

A slightly better strategy for evaluating clusters are *robustness-based* clustering metrics. These run an algorithm after adding some noise to the data, or using different parameter settings, and compare the outcomes. The idea is that if many algorithm parameters and many perturbations of the data return the same result, it is likely to be trustworthy.

Unfortunately, this strategy is not implemented in scikit-learn at the time of writing.

Even if we get a very robust clustering, or a very high silhouette score, we still don't know if there is any semantic meaning in the clustering, or whether the clustering reflects an aspect of the data that we are interested in.

Let's go back to the example of face images. We hope to find groups of similar faces, say men and women, or old people and young people, or people with beards and without. Let's say we cluster the data into two clusters, and all algorithms agree about which points should be clustered together. We still don't know if the clusters that are found correspond in any way to the concepts we are interested in. It could be that they found side-views versus front-views. Or pictures taken at night versus pictures taken during the day. Or pictures taken with iPhones versus pictures taken with Android phones.

Only if we actually analyze the clusters can we know whether the clustering corresponds to anything we are interested in.

## Comparing algorithms on the faces dataset

Let's apply the k-Means, DBSCAN and agglomerative clustering algorithms to the labeled faces in the wild dataset, and see if any of them find interesting structure.

We will use the eigenface representation of the data, as produced by `PCA(whiten=True)`, with 100 components. We saw above that this is a more semantic representation of the face images than the raw pixels. It will also make computation faster.

It's a good exercise for you to run the experiments below on the original data and compare results.

```
# extract eigenfaces from lfw data and transform data
from sklearn.decomposition import PCA
pca = PCA(n_components=100, whiten=True)
pca.fit_transform(X_people)
X_pca = pca.transform(X_people)
```

We will start by applying DBSCAN, which we just discussed.

## Analyzing the faces dataset with DBSCAN

```
# apply DBSCAN with default parameters
dbscan = DBSCAN()
labels = dbscan.fit_predict(X_pca)
np.unique(labels)

array([-1])
```

We see that all returned labels are -1, so all of the data was labeled as “noise” by DBSCAN. There are two things we can change to help this: we can make `eps` higher, to expand the neighborhood of each point, and `min_samples` lower, to consider smaller groups of points as clusters. Let's try changing `min_samples` first:

```
dbscan = DBSCAN(min_samples=3)
labels = dbscan.fit_predict(X_pca)
np.unique(labels)

array([-1])
```

Even when considering groups of three points, everything is labeled as noise. So we need to increase `eps`.

```
dbscan = DBSCAN(min_samples=3, eps=15)
labels = dbscan.fit_predict(X_pca)
np.unique(labels)

array([-1,  0])
```



Using a much larger `eps=15` we get only a single clusters and noise points. We can use this result and find out what the “noise” looks like compared to the rest of the data. To understand better what’s happening, let’s look at how many points are noise, and how many points are inside the cluster:

```
# count number of points in all clusters and noise.
# bincount doesn't allow negative numbers, so we need to add 1.
# the first number in the result corresponds to noise points
np.bincount(labels + 1)

array([ 27, 2036])
```

There are only very few noise points, 27, so we can look at all of them:

```
noise = X_people[labels==-1]

fig, axes = plt.subplots(3, 9, subplot_kw={'xticks': (), 'yticks': ()}, figsize=(12, 4))
for image, ax in zip(noise, axes.ravel()):
    ax.imshow(image.reshape(image_shape), vmin=0, vmax=1)
```



Comparing these images to the random sample of face images from Figure `some_faces`, we can guess why they were labeled as noise: the image in the sixth image in the first row one has a person drinking from a glass, there are images with hats, and the second to last image has a hand in front of the face. The other images contain odd angles or crops that are too close (see the first image in the first row) or too wide (see the last image in the first row).

This kind of analysis, trying to find “the odd one out”, is called *outlier detection*. If this was a real application, we might try to do a better job in cropping images, to get more homogeneous data. There is little we can do about people sometimes wearing hats or drinking from a glass, but it’s good to know that these are issues in the data that any algorithm we might apply needs to handle.

If we want to find more interesting clusters than just one large one, we need to set `eps` smaller, somewhere between 15 and 0.5 (the default). Let’s have a look at what different values of `eps` result in:

```

for eps in [1, 3, 5, 7, 9, 11, 13]:
    print("\neps=%d" % eps)
    dbscan = DBSCAN(eps=eps, min_samples=3)
    labels = dbscan.fit_predict(X_pca)
    print("Number of clusters: %s" % np.unique(labels))
    print("Clusters: %s" % np.bincount(labels + 1))

eps=1
Number of clusters: [-1]
Clusters: [2063]

eps=3
Number of clusters: [-1]
Clusters: [2063]

eps=5
Number of clusters: [-1]
Clusters: [2063]

eps=7
Number of clusters: [-1  0  1  2  3  4  5  6  7  8  9 10 11 12]
Clusters: [2008  4  6  3  6  9  5  3  3  4  3  3  3  3]

eps=9
Number of clusters: [-1  0  1  2]
Clusters: [1273  784  3  3]

eps=11
Number of clusters: [-1  0]

```

```
Clusters: [ 429 1634]
```

```
eps=13
```

```
Number of clusters: [-1  0]
```

```
Clusters: [ 115 1948]
```

For small numbers of `eps`, again all points are labeled as noise. For `eps=7`, we get many noise points, and many smaller clusters. For `eps=9` we still get many noise points, one big cluster and some smaller clusters. Starting from `eps=11` we get only one large cluster and noise.

What is interesting to note is that there are never more than one large cluster. There is at most one large cluster containing most of the points, and some smaller clusters. This indicates that there are not two or three different kinds of face images in the data that are very distinct, but that all images are more or less equally similar (or dissimilar) from the rest.

The results for `eps=7` look most interesting, with many small clusters. We investigate this clustering in more detail, by visualizing all of the points in each of the 13 small clusters:

```
# dbscan = DBSCAN(min_samples=3, eps=7)
labels = dbscan.fit_predict(X_pca)

for cluster in range(max(labels)):
    mask = labels == cluster
    n_images = np.sum(mask)
    fig, axes = plt.subplots(1, n_images, subplot_kw={'xticks': (), 'yticks': ()}, figsize=(n_images, 1))
    for image, label, ax in zip(X_people[mask], y_people[mask], axes):

        ax.imshow(image.reshape(image_shape), vmin=0, vmax=1)
        ax.set_title(people.target_names[label].split()[-1])
```

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Some of the clusters correspond to people with very distinct faces (within this dataset), such as Tayyip or Koizumi. Within each cluster, the orientation of the face is also quite fixed, as well as the facial expression. Some of the clusters contain faces of multiple people, but they share a similar orientation of the face and expression.

This concludes our analysis of the DBSCAN algorithm applied to the faces dataset.

As you can see, we are doing a very manual analysis here, different from the much more automatic search approach we could use for supervised learning, based on  $R^2$  or accuracy.

Let's move on to applying k-Means and Agglomerative Clustering.

### Analyzing the faces dataset with k-Means

We saw that it was not possible to create more than one big cluster using DBSCAN. Agglomerative clustering and k-Means are much more likely to create clusters of even size, but we do need to set a number of clusters.

We could set the number of clusters to the known number of people in the dataset, though it is very unlikely that an unsupervised clustering algorithm will recover them.

Instead, we can start with a low number of clusters, like 10, which might allow us to analyze each of the clusters.

```
n_clusters = 10
# extract clusters with k-Means
km = KMeans(n_clusters=n_clusters, random_state=0)
labels_km = km.fit_predict(X_pca)
print("cluster sizes k-Means: %s" % np.bincount(labels_km))

cluster sizes k-Means: [185 146 168 190 153 284 263 133 223 318]
```

As you can see, k-Means clustering partitioned the data into relatively similarly sized clusters from 133 to 318. This is quite different from the result of DBSCAN.

We can further analyze the outcome of k-Means by visualizing the cluster centers. As we clustered in the representation produced by PCA, we need to rotate the cluster centers back into the original space to visualize them, using `pca.inverse_transform`.

```
fig, axes = plt.subplots(2, 5, subplot_kw={'xticks': (), 'yticks': ()}, figsize=(12, 4))
for center, ax in zip(km.cluster_centers_, axes.ravel()):
    ax.imshow(pca.inverse_transform(center).reshape(image_shape), vmin=0, vmax=1)
```



The cluster centers found by k-Means are very smooth version of faces. This is not very surprising, given that each center is an average of 133 to 318 face images. Working with a reduced PCA representation adds to the smoothness of the images (compared to faces reconstructed using 100 PCA dimensions in Figure `pca_reconstructions`).

The clustering seems to pick up on different orientations of the face, different expression (the third cluster center seems to show a smiling face), and presence of collars (see the second to last cluster center).

For a more detailed view, we show for each cluster center the five most typical images in the cluster (the images that are assigned to the cluster and closest to the cluster center) and the five most atypical images in the cluster (the images that are assigned to the cluster and furthest to the cluster center):

```

n_clusters = 10
for cluster in range(n_clusters):
    center = km.cluster_centers_[cluster]
    mask = km.labels_ == cluster
    dists = np.sum((X_pca - center) ** 2, axis=1)
    dists[~mask] = np.inf
    inds = np.argsort(dists)[:5]
    dists[~mask] = -np.inf
    inds = np.r_[inds, np.argsort(dists)[-5:]]
    fig, axes = plt.subplots(1, 11, subplot_kw={'xticks': (), 'yticks': ()}, figsize=(10, 8))
    axes[0].imshow(pca.inverse_transform(center).reshape(image_shape), vmin=0, vmax=1)
    for image, label, asdf, ax in zip(X_people[inds], y_people[inds], labels_km[inds], axes[1:]):
        ax.imshow(image.reshape(image_shape), vmin=0, vmax=1)
        ax.set_title("%s" % (people.target_names[label].split()[-1]), fontdict={'fontsize': 9})
print("kmeans_face_clusters")

```



```
kmeans_face_clusters
```

Figure `kmeans_face_clusters` confirms our intuition about smiling faces for the third cluster, and also the importance of orientation for the other clusters. The “atypical” points are not very similar to the cluster center, though, and the assignment seems somewhat arbitrary. This can be attributed to the fact that k-Means partitions all the data points, and doesn’t have a concept of “noise” points, as DBSCAN does.

Using a larger number of clusters, the algorithm could find finer distinctions. However, adding more clusters makes manual inspection even harder.

## Analyzing the faces dataset with agglomerative clustering

Now, let’s look at the results of agglomerative clustering:

```
# extract clusters with ward agglomerative clustering
agglomerative = AgglomerativeClustering(n_clusters=10)
labels_agg = agglomerative.fit_predict(X_pca)
print("cluster sizes agglomerative clustering: %s" % np.bincount(labels_agg))

cluster sizes agglomerative clustering: [167  50 252 367 160  80  50  67 521 349]
```

Agglomerative clustering produces relatively equally sized clusters, with cluster sizes between 50 and 521. These are more uneven than k-Means, but much more even than the ones produced by DBSCAN.

We can compute the ARI to measure if the two partitions of the data given by agglomerative clustering and k-Means are similar:

```
adjusted_rand_score(labels_agg, labels_km)

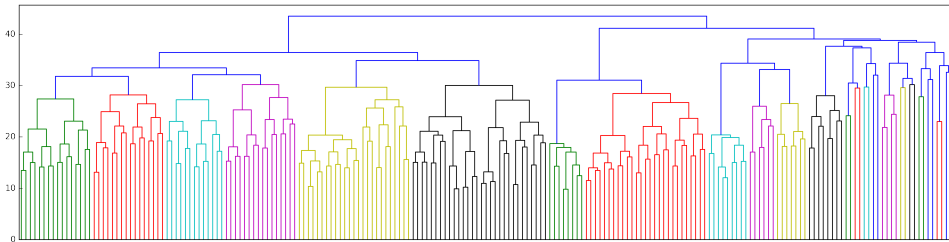
0.09733057984938646
```

An ARI of only 0.1 means that the two clusterings `labels_agg` and `labels_km` have quite little in common. This is not very surprising, given the fact that points further away from the cluster centers seem to have little in common for k-Means.

Next, we might want to plot the dendrogram. We limit the depth of the tree in the plot, as branching down to the individual 2063 data points would result in an unreadably dense plot.

```
# import the dendrogram function and the ward clustering function from scipy
from scipy.cluster.hierarchy import dendrogram, ward

# apply the ward clustering to the data array X
# The scipy ward function returns an array that specifies the distances bridged
# when performing agglomerative clustering
linkage_array = ward(X_pca)
# now we plot the dendrogram for the linkage_array containing the distances between clusters
plt.figure(figsize=(20, 5))
dendrogram(linkage_array, p=7, truncate_mode='level', no_labels=True);
```



Creating ten clusters, we cut across the tree at the very top, where there are 10 vertical lines. In the dendrogram for the toy data shown in Figure dendrogram, you could see by the length of the branches that two or three clusters might capture the data appropriately. For the faces data, there doesn't seem to be a very natural cut-off point. There are some branches that represent more distinct groups, but there doesn't seem to be a particular number of clusters that is a good fit. This is not particularly surprising, given the results of DBSCAN, which tried to cluster all points together.

Here is a visualization of the ten clusters, similarly to k-Means above.

Note that there is no notion of cluster center in agglomerative clustering (though we could compute the mean), and we simply show the first couple of points in each cluster. We show the number of points in each cluster to the left of the first image.

```
n_clusters = 10
for cluster in range(n_clusters):
    mask = labels_agg == cluster
    fig, axes = plt.subplots(1, 10, subplot_kw={'xticks': (), 'yticks': ()}, figsize=(15, 8))
    axes[0].set_ylabel(np.sum(mask))
    for image, label, asdf, ax in zip(X_people[mask], y_people[mask], labels_agg[mask], axes):
        ax.imshow(image.reshape(image_shape), vmin=0, vmax=1)
        ax.set_title("%s" % people.target_names[label].split()[-1], fontdict={'fontsize': 9})
```



While some of the clusters seem to have a semantic theme, many of them are too large to be actually homogeneous. To get more homogeneous cluster, we run the algorithm again, this time with 40 clusters, and pick out some of the clusters that are particularly interesting:

```
# extract clusters with ward agglomerative clustering
agglomerative = AgglomerativeClustering(n_clusters=40)
labels_agg = agglomerative.fit_predict(X_pca)
print("cluster sizes agglomerative clustering: %s" % np.bincount(labels_agg))

n_clusters = 40
for cluster in [15, 7, 17, 20, 25, 29]: # hand-picked "interesting" clusters
```

```

mask = labels_agg == cluster
fig, axes = plt.subplots(1, 15, subplot_kw={'xticks': (), 'yticks': ()}, figsize=(15, 8))
cluster_size = np.sum(mask)
axes[0].set_ylabel(cluster_size)
for image, label, asdf, ax in zip(X_people[mask], y_people[mask], labels_agg[mask], axes):
    ax.imshow(image.reshape(image_shape), vmin=0, vmax=1)
    ax.set_title("%s" % (people.target_names[label].split()[-1]), fontdict={'fontsize': 9})
for i in range(cluster_size, 15):
    axes[i].set_visible(False)

```



```

cluster sizes agglomerative clustering: [ 50 111 103 120 60 169 50 53 10 33 187 30 50 85
111 18 3 78 81 36 10 16 22 5 57 27 75 26 92 5 13 35
8 23 20 69]

```

Here, the clustering seems to have picked up on “dark skinned and smiling”, “serious eyebrows”, “collared shirt”, “white hat and showing front teeth”, “high forehead” and “Asian”.

We could also find these highly similar clusters using the dendrogram, if we did more a detailed analysis.

## Summary of Clustering Methods

We saw above that applying and evaluating clustering is a highly qualitative procedure, and often most helpful in the exploratory phase of data analysis. We looked at three clustering algorithms, k-Means, DBSCAN and Agglomerative Clustering. All three have a way of controlling the granularity of clustering. k-Means and Agglomerative Clustering allow you to directly specify the number of desired clusters, while DBSCAN lets you define proximity using the eps parameter, which indirectly influences cluster size.

All three methods can be used on large, real-world datasets, are relatively easy to understand, and allow for clustering into many clusters.

Each of the algorithms has somewhat different strengths. k-Means allows for a characterization of the clusters using the cluster means. It can also be viewed as a decomposition method, where each data point is represented by its cluster center.

DBSCAN allows for the detection of “noise points” that are not assigned any cluster, and it can help automatically determine the number of clusters. In contrast to the other two methods, it allow for complex cluster shapes, as we saw in the two\_moons example. DBSCAN sometimes produces clusters of very differing size, which can be a



strength or a weakness. Agglomerative clustering can provide a whole hierarchy of possible partitions of the data, which can be easily inspected via dendrograms.

## Summary and Outlook

This chapter introduced a range of unsupervised learning algorithms that can be applied for exploratory data analysis and preprocessing. Having the right representation of the data is often crucial for supervised or unsupervised learning to succeed, and preprocessing and decomposition methods play an important part in data preparation.

Decomposition, manifold learning and clustering are essential tools to further your understanding of your data, and can be the only way to make sense of your data in the absence of supervision information. Even in the supervised setting, exploratory tools are important for a better understanding of the properties of the data.

Often it is hard to quantify the usefulness of an unsupervised algorithm, though this shouldn't deter you from using them to create insights from your data.

With these methods under your belt, you are now equipped with all the essential learning algorithms that machine learning practitioners use every day.

We encourage you to try clustering and decomposition methods both on two-dimensional toy data, as well as real world datasets included in scikit-learn, like the `digits`, `iris` and `cancer` data sets.



---

# Summary of scikit-learn methods and usage

In this chapter, we briefly recapitulate the main parts of the scikit-learn API that we have seen so far, as well as show some ways to simplify your code.

## The Estimator Interface

All algorithms in scikit-learn, whether preprocessing, supervised learning or unsupervised learning algorithms are all implemented as classes. These classes are called *estimators* in scikit-learn. To apply an algorithm, you first have to instantiate an object of the particular class:

```
from sklearn.linear_model import LogisticRegression
logreg = LogisticRegression()
```

The estimator class contains the algorithm, and also stores the model that is learned from data using the algorithm.

When constructing the model object, this is also the time when you should set any parameters of the model. These parameters include regularization, complexity control, number of clusters to find, etc, as we discussed in detail in Chapter 2 and Chapter 3.

All estimators have a `fit` method, which is used to build the model. The `fit` method always requires as first argument the data  $X$ , represented as a numpy array or a scipy sparse matrix, where each row represents a single data point. The data  $X$  is always assumed to be a numpy array or scipy sparse matrix that has continuous (floating point) entries.

Supervised algorithms also require a `y` argument, which is a one-dimensional numpy array, containing target values for regression or classification, i.e. the known output labels or responses.

There are two main ways to apply a learned model in scikit-learn. To create a prediction in the form of a new output like `y`, you use the `predict` method. To create a new representation of the input data `X`, you use the `transform` method. Table `api_summary` summarizes the use-cases of the `predict` and `transform` methods.

<b>estimator.fit(X_train, [y_train])</b>	
<b>estimator.predict(X_test)</b>	<b>estimator.transform(X_test)</b>
Classification	Preprocessing
Regression	Dimensionality Reduction
Clustering	Feature Extraction
	Feature selection

Table `api_summary`

Additionally, all supervised models have a `score(X_test, y_test)` method, that allows an evaluation of the model.

Here `X_train` and `y_train` refer to the training data and training labels, while `X_test` and `y_test` refer to the test data and test labels (if applicable).

## Fit resets a model

An important property of scikit-learn models is that calling `fit` will always reset everything a model previously learned. So if you build a model on one dataset, and then call `fit` again on a different dataset, the model will “forget” everything it learned from the first data. You can call `fit` as often as you like on a model, and the outcome will be the same as calling `fit` on a “new” model:

```
# get some data
from sklearn.datasets import make_blobs, load_iris
from sklearn.model_selection import train_test_split

# load iris
iris = load_iris()

# create some blobs
X, y = make_blobs(random_state=0, centers=4)
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)

# build a model on the iris dataset
logreg = LogisticRegression()
```

```

logreg.fit(iris.data, iris.target)
# fit the model again on the blob dataset
logreg.fit(X_train, y_train)
# the outcome is the same as training a "fresh" model:
new_logreg = LogisticRegression()
new_logreg.fit(X_train, y_train)

# predictions made by the two models are the same
pred_new_logreg = new_logreg.predict(X_test)
pred_logreg = logreg.predict(X_test)

pred_logreg == pred_new_logreg
array([ True,  True,  True,  True,  True,  True,  True,  True,  True,
        True,  True,  True,  True,  True,  True,  True,  True,  True,
        True,  True,  True,  True,  True,  True,  True], dtype=bool)

```

As you can see, fitting the `logreg` model first on the `iris` dataset has no effect. The `iris` dataset has a different number of features and classes than the `blobs` dataset, but all about the first fit is erased when `fit` is called again.

Next, we will go into several shortcuts that allow you to write less code for common tasks, and speed up some computations. The first way to write more compact code is to make use *method chaining*.

## Method chaining

The `fit` method of all scikit-learn models returns `self`. This allows you to write code like this:

```

# instantiate model and fit it in one line
logreg = LogisticRegression().fit(X_train, y_train)

```

Here, we used the return value of `fit` (which is `self`) to assign the trained model to the variable `logreg`. This concatenation of method calls (here `__init__` and then `fit`) is known as *method chaining*. Another common application of method chaining in scikit-learn is to `fit` and `predict` in one line:

```

logreg = LogisticRegression()
y_pred = logreg.fit(X_train, y_train).predict(X_test)

```

Finally, you can even do model instantiation, fitting and predicting in one line:

```

y_pred = LogisticRegression().fit(X_train, y_train).predict(X_test)

```

This very short variant is not ideal, though. A lot is happening in a single line, which might make the code hard to read. Additionally, the fitted logistic regression model isn't stored in any variable. So we can't inspect it, or use it to predict on any other data.

## Shortcuts and efficient alternatives

Often, you want to fit a model on some dataset, and then immediately predict on the same data, or transform it. These are very common tasks, which can often be computed more efficiently than simply calling `fit` and then `predict` or `fit` and then `transform`. For this use-case, all models that have a `predict` method also have a `fit_predict` method, and all model that have a `transform` method also have a `fit_transform` method. Here is an example using PCA:

```
from sklearn.decomposition import PCA
pca = PCA()
# calling fit and transform in sequence (using method chaining)
X_pca = pca.fit(X).transform(X)
# same result, but more efficient computation
X_pca_2 = pca.fit_transform(X)
```

While `fit_transform` and `fit_predict` are not more efficient for all algorithms, it is still good practice to use them when trying to predict on, or transform the training set.

For some unsupervised methods that we saw in Chapter 3, like some clustering and manifold learning methods, using `fit_transform` and `fit_predict` are the only options. For example DBSCAN does not have a `predict` method, only `fit_predict`, and t-SNE does not have a `transform` method, only `fit_transform`. T-SNE and DBSCAN are algorithms that can not be applied to new data, they can only be applied to the training data.

## Important Attributes

scikit-learn has some standard attributes that allow you to inspect what a model learned. All these attributes are available after the call to `fit`, and, as we mentioned before, all attributes learned from the data are marked with a trailing underscore.

We already discussed the following common attributes:

- For clustering algorithms, the `labels_` attribute stores the cluster membership for the training data.
- For manifold learning algorithms, the `embedding_` attribute stores the embedding (transformation) of the training data in the lower-dimensional space.
- For linear models, the `coef_` attribute stores the weight or coefficient vector.

- For linear decomposition and dimensionality reduction methods, `components_` stores the array of components (the prototypes in the additive decomposition in Figure decomposition in Chapter 3).

Additionally, for classifiers, `classes_` contains the names of the classes the classifier was trained on, that is the unique entries of the training labels `y_train`:

```
import numpy as np
logreg = LogisticRegression()
# fit model using original data
logreg.fit(iris.data, iris.target)
print("unique entries of iris.target: %s" % np.unique(iris.target))
print("classes using iris.target: %s" % logreg.classes_)

# represent each target by its class name
named_target = iris.target_names[iris.target]
logreg.fit(iris.data, named_target)
print("unique entries of named_target: %s" % np.unique(named_target))
print("classes using named_target: %s" % logreg.classes_)

unique entries of iris.target: [0 1 2]

classes using iris.target: [0 1 2]

unique entries of named_target: ['setosa' 'versicolor' 'virginica']

classes using named_target: ['setosa' 'versicolor' 'virginica']
```

## Summary and outlook

You should now be intimately familiar with the interfaces of supervised and unsupervised models in scikit-learn, and how to use them. With a good grasp on how to use the different models, we will continue with more complex topics, such as evaluating and selecting models.





---

# Representing Data and Engineering Features

So far, we assumed that our data comes in as a two-dimensional array of floating point numbers, where each column is a *continuous feature* that describes the data points. For many applications, this is not how the data is collected. A particular common type of feature is *categorical features*, also known as *discrete features*, which are usually not numeric. The distinction between categorical feature and continuous feature is analogous to the distinction between classification and regression - only on the input side, not the output side.

Examples for continuous features that we saw are pixel brightnesses and size measurements of plant flowers. Examples for categorical features are the brand of a product, the color of a product, or the department (books, clothing, hardware) it is sold in. These are all properties that can describe a product, but they don't vary in a continuous way. A product belongs either in the clothing department or in the books department. There is no middle ground between books and clothing, and no natural order for the different categories (books is not greater or smaller than clothing, hardware is not between books and clothing, etc).

Regardless of the type of features your data consists of, how you represent them can have an enormous effect on the performance of machine learning models. We saw in Chapter 2 and Chapter 3 that scaling of the data is important. In other words, if you don't rescale your data (say, to unit variance), then it makes a difference whether you represent a measurement in centimeters or inches. We also saw in Chapter 2 that it can be helpful to *augment* your data with additional features, like adding interactions (products) of features or more general polynomials.

The question of how to represent your data best for a particular application is known as *feature engineering*, and it is one of the main tasks of data scientists and machine

learning practitioners trying to solve real-world problems. Representing your data in the right way can have a bigger influence on the performance of a supervised model than the exact parameters you choose.

We will first go over the important and very common case of categorical features, and then give some examples of helpful transformations for specific combinations of features and models.

## Categorical Variables

As an example, we will use the dataset of adult incomes in the United States, derived from the 1994 census database.

The task of the `adult` dataset is to predict whether a worker has an income of over 50.000\$ or under 50.000\$.

The features in this dataset include the workers age, how they are employed (self employed, private industry employee, government employee, ...), their education, their gender, their working hours per week, occupation and more.

Below is a table showing the first few entries in the data set:

	age	workclass	education	gender	hours-per-week	occupation	income
0	39	State-gov	Bachelors	Male	40	Adm-clerical	<=50K
1	50	Self-emp-not-inc	Bachelors	Male	13	Exec-managerial	<=50K
2	38	Private	HS-grad	Male	40	Handlers-cleaners	<=50K
3	53	Private	11th	Male	40	Handlers-cleaners	<=50K
4	28	Private	Bachelors	Female	40	Prof-specialty	<=50K
5	37	Private	Masters	Female	40	Exec-managerial	<=50K
6	49	Private	9th	Female	16	Other-service	<=50K
7	52	Self-emp-not-inc	HS-grad	Male	45	Exec-managerial	>50K
8	31	Private	Masters	Female	50	Prof-specialty	>50K
9	42	Private	Bachelors	Male	40	Exec-managerial	>50K
10	37	Private	Some-college	Male	80	Exec-managerial	>50K

The task is phrased as a classification task with the two classes being income  $\leq 50k$  and  $> 50k$ . It would also be possible to predict the exact income, and make this a regression task. However, that would be much more difficult, and the 50K division is interesting to understand on its own.

In this dataset, `age` and `hours-per-week` are continuous features, which we know how to treat. The `workclass`, `education`, `sex` and `occupation` features are categorical, however. All of them come from a fixed list of possible values, as opposed to a range, and denote a qualitative property, as opposed to a quantity.

As a starting point, let's say we want to learn a logistic regression classifier on this data. We know from Chapter 2 that a logistic regression makes predictions  $\hat{y}$  using the formula

$$\hat{y} = w[0] x[0] + w[1] x[1] + \dots + w[p] x[p] + b > 0 \quad \text{(1) linear binary classification}$$

where  $w[i]$  and  $b$  are coefficients learned from the training set and  $x[i]$  are the input features.

This formula makes sense when  $x[i]$  are numbers, but not when  $x[2]$  is "Masters" or "Bachelors".

So clearly we need to represent our data in some different way when applying logistic regression.

## One-Hot-Encoding (Dummy variables)

By far the most common way to represent categorical variables is using the *one-hot-encoding* or *one-out-of-N* encoding, also known as *dummy variables*.

The idea behind dummy variables is to replace a categorical variable with one or more new features that can have the values 0 and 1. The values 0 and 1 make sense in Formula (1) (and for all other models in scikit-learn), and we can represent any number of categories by introducing one new feature per category as follows.

Let's say for the `workclass` feature we have possible values of "Government Employee", "Private Employee", "Self Employed" and "Self Employed Incorporated". To encode this four possible values, we create four new features, called "Government Employee", "Private Employee", "Self Employed" and "Self Employed Incorporated". The feature is 1 if `workclass` for this person has the corresponding value, and 0 otherwise.

So exactly one of the four new features will be 1 for each data point. This is why this is called one-hot or one-out-of-N encoding.

The principle is illustrated here. A single feature is encoded using four new features. When using this data in a machine learning algorithm, we would drop the original `workclass` feature and only keep the 0-1 features.

```
| workclass | Government Employee | Private Employee | Self Employed | Self  
Employed Incorporated |
```

```
|-----|-----|-----|-----|-----|
```

```
| Government Employee | 1 | 0 | 0 | 0 |
```

```
| Private Employee | 0 | 1 | 0 | 0 |
```

```
| Self Employed | 0 | 0 | 1 | 0 |
```

```
| Self Employed Incorporated | 0 | 0 | 0 | 1 |
```

There are two ways to convert your data to a one-hot encoding of categorical variables, either using pandas or using scikit-learn. At the time of writing, using pandas for this setting is slightly easier, so let's go this route. First we load the data using pandas from a comma separated values (CSV) file:

```
import pandas as pd
# The file has no headers naming the columns, so we pass header=None and provide the column names
data = pd.read_csv("/home/andy/datasets/adult.data", header=None, index_col=False,
                  names=['age', 'workclass', 'fnlwgt', 'education', 'education-num',
                        'marital-status', 'occupation', 'relationship', 'race', 'gender',
                        'capital-gain', 'capital-loss', 'hours-per-week', 'native-country', 'income'])
# For illustration purposes, we only select some of the columns:
data = data[['age', 'workclass', 'education', 'gender', 'hours-per-week', 'occupation', 'income']]
# print the first 5 rows
data.head()
```

	age	workclass	education	gender	hours-per-week	occupation	income
0	39	State-gov	Bachelors	Male	40	Adm-clerical	<=50K
1	50	Self-emp-not-inc	Bachelors	Male	13	Exec-managerial	<=50K
2	38	Private	HS-grad	Male	40	Handlers-cleaners	<=50K
3	53	Private	11th	Male	40	Handlers-cleaners	<=50K
4	28	Private	Bachelors	Female	40	Prof-specialty	<=50K

## Checking string-encoded categorical data

After reading a dataset like this, it is often good to first check if a column actually contains meaningful categorical data. When working with data that was input by humans (say users on a website), there might not be a fixed set of categories, and differences in spelling and capitalization might require preprocessing. For example, it might be that some people specified gender as “male” and some as “man”, and we might want to represent these two inputs using the same category.

A good way to check the contents of a column is using the `value_counts` function of a pandas series (the type of a single column in a dataframe), to show us what the unique values are, and how often they appear:

```
data.gender.value_counts()
Male      21790
Female    10771
```

```
Name: gender, dtype: int64
```

We can see that there are exactly two values for gender in this datasets, Male and Female, meaning the data is already in a good format to be represented using one-hot-encoding. In a real application, you should look at all columns, and check their values. We will skip this here for brevity's sake.

There is a very simple way to encode the data in pandas, using the `get_dummies` function:

```
print("Original features:\n", list(data.columns), "\n")
data_dummies = pd.get_dummies(data)
print("Features after get_dummies:\n", list(data_dummies.columns))
```

```
Original features:
```

```
['age', 'workclass', 'education', 'gender', 'hours-per-week', 'occupation', 'income']
```

```
Features after get_dummies:
```

```
['age', 'hours-per-week', 'workclass_?', 'workclass_Federal-gov', 'workclass_Local-gov', 'workclass_Never-worked', 'workclass_Private', 'workclass_Self-emp-inc', 'workclass_Self-emp-not-inc', 'workclass_State-gov', 'workclass_Union-gov']
```

You can see that the continuous features age and hours-per-week were not touched, while the categorical features were expanded into one new feature for each possible value:

```
data_dummies.head()
```

	age	hours-per-week	workclass_?	workclass_Federal-gov	workclass_Local-gov	workclass_Never-worked	workclass_Private	workclass_Self-emp-inc	workclass_Self-emp-not-inc	workclass_State-gov	workclass_Union-gov	...	occupation_Machine-op-inspct
0	39	40	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	...	0.0
1	50	13	0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	0.0	...	0.0
2	38	40	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	...	0.0
3	53	40	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	...	0.0
4	28	40	0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	...	0.0

5 rows × 46 columns

We can use the `values` attribute to convert the `data_dummies` dataframe into a numpy array, and then train a machine learning model on it. Be careful to separate the

target variable (which is now encoded in two `income` columns) from the data before training a model. Including the output variable, or some derived property of the output variable, into the feature representation is a very common mistake in building supervised machine learning models. [Warning box] Careful: column indexing in pandas includes the end of the range, so `age:occupation_Transport-moving` is inclusive of `occupation_Transport-moving`. This is in contrast to slicing a numpy array, where the end of a range is not included: `np.arange(11)[0:10]` does not include the entry with index 10. [Warning box] `age` to `occupation_Transport-moving` # This range contains all the features but not the target features = `data_dummies.ix[:, 'age':occupation_Transport-moving]` # extract numpy arrays `X = features.values` `y = data_dummies['income_ >50K'].values` `print(X.shape, y.shape)` `(32561, 44)` `(32561,)` Now the data is represented in a way that scikit-learn can work with, and we can proceed as usual: `from sklearn.linear_model import LogisticRegression` `from sklearn.model_selection import train_test_split` `X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)` `logreg = LogisticRegression()` `logreg.fit(X_train, y_train)` `print(logreg.score(X_test, y_test))` `0.808745854318` [FIXME Warning callout] Above, we called `get_dummies` on a dataframe containing both the training and the test data. This is important to ensure categorical values are represented in the same way in the training set and the test set. Imagine we had the training and the test set in two different dataframes. If the “Private Employee” value for the `workclass` feature does not appear in the test set, pandas would assume there are only three possible values for this feature, and would create only three new dummy features. Now our training and test set have different numbers of features, and we can’t apply the model we learned on the training set to the test set any more. Even worse, imagine the `workclass` feature had the values “Government Employee” and “Private Employee” in the training set, and “Self Employed” and “Self Employed Incorporated” in the test set. In both cases, pandas would create two new dummy features, so the encoded dataframes would have the same number of features. However, the two dummy features have entirely different meanings on the training and the test set. The column that means “Government Employee” for the training set would encode “Self Employed” for the test set. If we build a machine learning model on this data, it would work very badly, because it assumes the columns mean the same (because they are in the same position), when they mean very different things. To fix this, either call `get_dummies` on a dataframe that contains the training and the test data points, or make sure that the column names are the same for training and test set after calling `get_dummies`, to ensure they have the same semantics. ### Numbers can encode categorical In the example of the `adult` dataset, the categorical variables were encoded as strings. On the one hand, that opens up the possibility of spelling errors, but on the other hand, it clearly marks a variable as categorical. Often, whether for ease of storage or because of the way the data is collected, categorical variables are actually encoded as integers. For example, imagine the census data in the `adult` dataset was collected using a questionnaire, and the answers for `workclass` were recorded as 0 (first box ticked), 1 (second box ticked), 2 (third box ticked) and so on. Now the column contains number from 0 to eight, instead of strings like `Private`, and looking at the table representing

the dataset, it is not clear from the numbers whether we should treat this variable as continuous or categorical. Knowing that the numbers indicate employment status, it is clear that these are very distinct states, and should not be modelled by a single continuous variable. [Warning box] Categorical features are often encoded using integers. That they are numbers doesn't mean that they should be treated as continuous features, as we mentioned above. It is not always clear whether an integer feature should be treated as continuous or discrete (and [one-hot-encoded]). If there is no ordering between the semantics that are encoded (like the ``workclass`` example above), the feature must be treated as discrete. For other cases like 5-star ratings, the better encoding depends on the the particular task and data and which machine learning algorithm is used.[/warning box] The ``get\_dummies`` function in pandas treats all numbers as continuous and will not create dummy variables for them. To get around this, you can either use ``scikit-learn``'s ``OneHotEncoder``, for which you can specify which variables are continuous and which are discrete, or convert numeric columns in the dataframe to strings. To illustrate, we create a dataframe object with two columns, one containing strings and one containing integers. `` # create a dataframe with an integer feature and a categorical string feature demo\_df = pd.DataFrame({'Integer Feature': [0, 1, 2, 1], 'Categorical Feature': ['socks', 'fox', 'socks', 'box']}) demo\_df ``

	Categorical Feature	Integer Feature
<b>0</b>	socks	0
<b>1</b>	fox	1
<b>2</b>	socks	2
<b>3</b>	box	1

Using get\_dummies will only encode the string feature, and not change “Integer Feature”:  
 `` pd.get\_dummies(demo\_df) ``

	Integer Feature	Categorical Feature_box	Categorical Feature_fox	Categorical Feature_socks
<b>0</b>	0	0.0	0.0	1.0
<b>1</b>	1	0.0	1.0	0.0
<b>2</b>	2	0.0	0.0	1.0
<b>3</b>	1	1.0	0.0	0.0

If you want dummy variables to be created for the “Integer Feature” column, one solution is to convert it to a string. Then, both features will be treated as categorical: `` demo\_df['Integer Feature'] = demo\_df['Integer Feature'].astype(str) pd.get\_dummies(demo\_df) ``

	Categorical Feature_box	Categorical Feature_fox	Categorical Feature_socks	Integer Feature_0	Integer Feature_1	Integer Feature_2
0	0.0	0.0	1.0	1.0	0.0	0.0
1	0.0	1.0	0.0	0.0	1.0	0.0
2	0.0	0.0	1.0	0.0	0.0	1.0
3	1.0	0.0	0.0	0.0	1.0	0.0

## Binning, Discretization, Linear Models and Trees

The best way to represent data not only depends on the semantics of the data, but also on the kind of model you are using. Two large and very commonly used families of models are linear models and tree-based models (such as decision trees, gradient boosted trees and random forests). Linear models and tree-based models have very different properties when it comes to how they work with different feature representations.

Let's go back to the wave regression dataset that we used in chapter 2. It only has a single input feature. Here is a comparison of a linear regression model and a decision tree regressor on this dataset:

```

from sklearn.linear_model import LinearRegression
from sklearn.tree import DecisionTreeRegressor

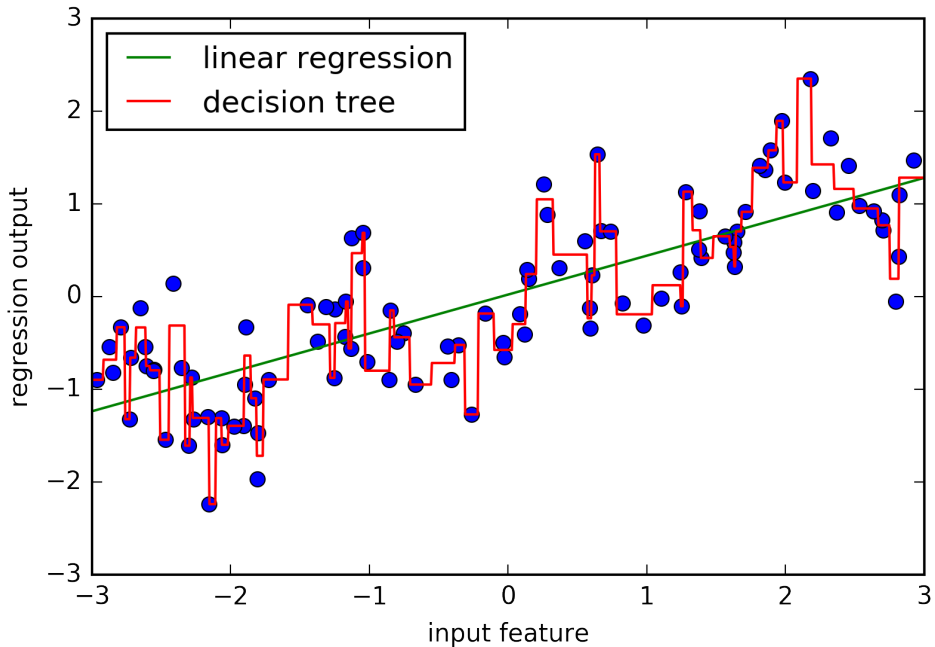
X, y = mglearn.datasets.make_wave(n_samples=100)
plt.plot(X[:, 0], y, 'o')
line = np.linspace(-3, 3, 1000)[:1].reshape(-1, 1)

reg = LinearRegression().fit(X, y)
plt.plot(line, reg.predict(line), label="linear regression")

reg = DecisionTreeRegressor(min_samples_split=3).fit(X, y)
plt.plot(line, reg.predict(line), label="decision tree")
plt.ylabel("regression output")
plt.xlabel("input feature")
plt.legend(loc="best")

```





As you know, linear models can only model linear relationships, which are lines in the case of a single feature. The decision tree can build a much more complex model of the data.

However, this is strongly dependent on our representation of the data. One way to make linear models more powerful on continuous data is to use *binning* (also known as *discretization*) of the feature to split it up into multiple features as follows:

We imagine a partition of the input range of -3 to 3 of this feature into a fixed number of *bins*. Here, we pass bin boundaries from -3 to 3 with 11 equally sized steps. An array of 11 bin boundaries will create 10 bins - they are the space in between two consecutive boundaries.

```
np.set_printoptions(precision=2)
bins = np.linspace(-3, 3, 11)
bins

array([-3. , -2.4, -1.8, -1.2, -0.6,  0. ,  0.6,  1.2,  1.8,  2.4,  3. ])
```

Here, the first bin contains all data points with feature values -3 to -2.68, the second bin contains all points feature values from -2.68 to -2.37 and so on.

Next, we record for each data point which bin it falls into. This can be easily computed using the `np.digitize` function:

```
which_bin = np.digitize(X, bins=bins)
print("\nData points:\n", X[:5])
print("\nBin membership for data points:\n", which_bin[:5])
```

Data points:

```
[[ -0.75]
 [  2.7 ]
 [  1.39]
 [  0.59]
 [-2.06]]
```

Bin membership for data points:

```
[[ 4]
 [10]
 [ 8]
 [ 6]
 [ 2]]
```

What we did here is transform the single continuous input feature in the wave dataset into a categorical feature which encodes which bin a data point is in. To use a scikit-learn model on this data, we transform this discrete feature to a one-hot encoding using the `OneHotEncoder` from the preprocessing module. The `OneHotEncoder` does the same encoding as `pandas.get_dummies`, though it currently only works on categorical variables that are integers.

```
from sklearn.preprocessing import OneHotEncoder
# transform using the OneHotEncoder.
encoder = OneHotEncoder(sparse=False)
# encoder.fit finds the unique values that appear in which_bin
encoder.fit(which_bin)
# transform creates the one-hot encoding
X_binned = encoder.transform(which_bin)
print(X_binned[:5])

[[ 0.  0.  0.  1.  0.  0.  0.  0.  0.  0.]
 [ 0.  0.  0.  0.  0.  0.  0.  0.  0.  1.]
```

```
[ 0.  0.  0.  0.  0.  0.  0.  1.  0.  0.]
[ 0.  0.  0.  0.  0.  1.  0.  0.  0.  0.]
[ 0.  1.  0.  0.  0.  0.  0.  0.  0.  0.]]
```

Because we specified 10 bins, the transformed dataset `X_binned` now is made up of 10 features:

```
X_binned.shape
(100, 10)
```

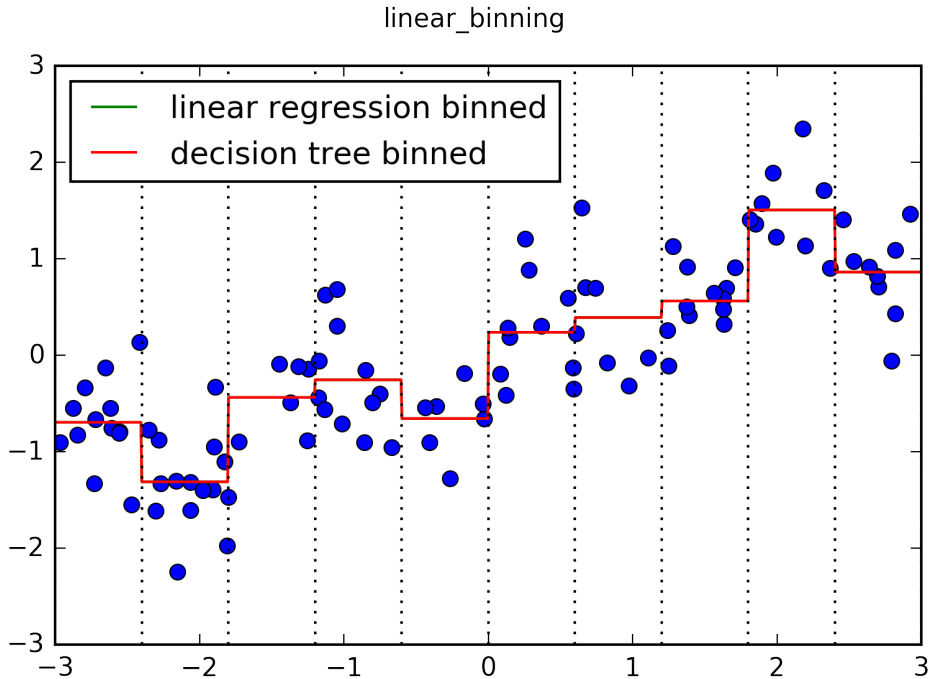
Now we build a new linear regression model and a new decision tree model on the one-hot encoded data.

The result is visualized below, together with the bin boundaries, shown as dotted black lines:

```
line_binned = encoder.transform(np.digitize(line, bins=bins))

plt.plot(X[:, 0], y, 'o')
reg = LinearRegression().fit(X_binned, y)
plt.plot(line, reg.predict(line_binned), label='linear regression binned')

reg = DecisionTreeRegressor(min_samples_split=3).fit(X_binned, y)
plt.plot(line, reg.predict(line_binned), label='decision tree binned')
for bin in bins:
    plt.plot([bin, bin], [-3, 3], ':', c='k')
plt.legend(loc="best")
plt.suptitle("linear_binning")
```



The green line and red line are exactly on top of each other, meaning the linear regression model and the decision tree make exactly the same predictions. For each bin, they predict a constant value. As features are constant within each bin, any model must predict the same value for all points within a bin. Comparing what the models learned before binning the features and after, we see that the linear model became much more flexible, because it now has a different value for each bin, while the decision tree model got much less flexible.

Binning features generally has no beneficial effect for tree-based models, as the model can learn to split up the data anywhere. In a sense, that means the decision trees can learn a binning that is particularly beneficial for predicting on this data. Additionally, decision trees look at multiple features at once, while binning is usually done on a per-feature basis.

However, the linear model benefited greatly in expressiveness from the transformation of the data.

If there are good reasons to use a linear model for a particular data set, say because it is very large and high-dimensional, but some features have non-linear relations with the output, binning can be a great way to increase modelling power.

# Interactions and Polynomials

Another way to enrich a feature representation, in particular for linear models, is adding *interaction features* and *polynomial features* of the original data. This kind of feature engineering is often used in statistical modelling, but also common in many practical machine learning applications.

As a first example, look again at Figure `linear_binning` above. The linear model learned a constant value for each bin on the `wave` dataset. We know, however, that linear models can not only learn offsets, but also slopes. One way to add a slope to the linear model on the binned data, is to add the original feature (the x axis in the plot) back in.

This leads to a 11 dimensional dataset:

```
X_combined = np.hstack([X, X_binned])
print(X_combined.shape)

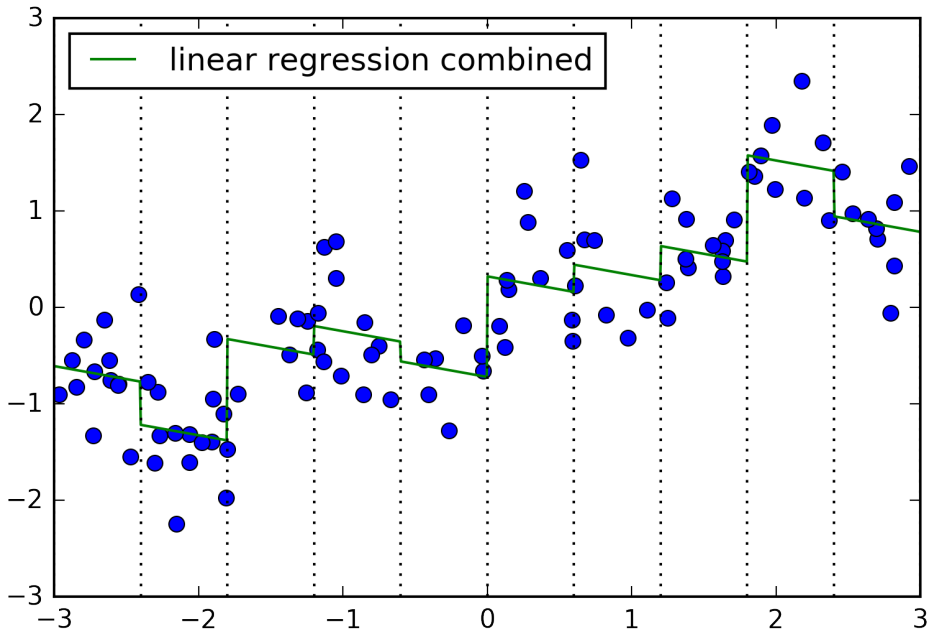
(100, 11)

plt.plot(X[:, 0], y, 'o')

reg = LinearRegression().fit(X_combined, y)

line_combined = np.hstack([line, line_binned])
plt.plot(line, reg.predict(line_combined), label='linear regression combined')

for bin in bins:
    plt.plot([bin, bin], [-3, 3], ':', c='k')
plt.legend(loc="best")
```



Now, the model learned an offset for each bin, together with a slope. The learned slope is downward, and shared across all the bins - there is the single x-axis feature which has a single slope. Because the slope is shared across all bins, it doesn't seem to be very helpful. We would rather have a separate slope for each bin! We can achieve this by adding an interaction or product feature that indicates in which bin a data-point is *and* where it lies on the x-axis.

This feature is a product of the bin-indicator and the original feature. Let's create this dataset:

```
X_product = np.hstack([X_binned, X * X_binned])
print(X_product.shape)

(100, 20)
```

This dataset not has 20 features: the indicator for which bin a data point is in, and a product of the original feature and the bin indicator. You can think of the product feature as a separate copy of the x-axis feature for each bin. It is the original feature within the bin, and zero everywhere else.

Here is the linear model on this new representation:

```
plt.plot(X[:, 0], y, 'o')

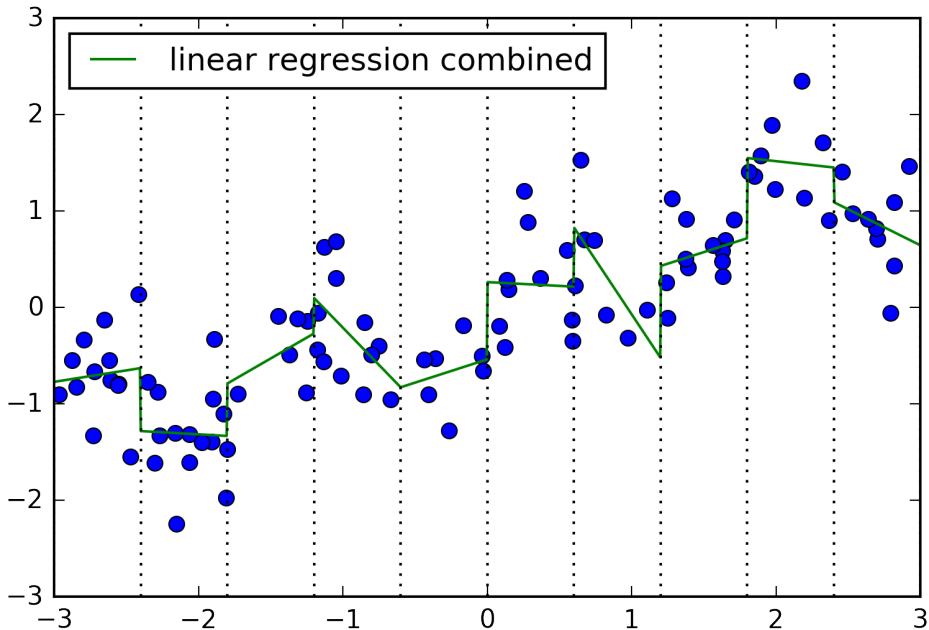
reg = LinearRegression().fit(X_product, y)
```

```

line_product = np.hstack([line_binned, line * line_binned])
plt.plot(line, reg.predict(line_product), label='linear regression combined')

for bin in bins:
    plt.plot([bin, bin], [-3, 3], ':', c='k')
plt.legend(loc="best")

```



As you can see, now each bin has its own offset and slope in this model.

Using binning is one way to expand a continuous feature. Another one is to use *polynomials* of the original features.

For a given feature  $x$ , we might want to consider  $x ** 2$ ,  $x ** 3$ ,  $x ** 4$  and so on.

This is implemented in `PolynomialFeatures` in the preprocessing module:

```

from sklearn.preprocessing import PolynomialFeatures

# include polynomials up to x ** 10:
poly = PolynomialFeatures(degree=10)
poly.fit(X)
X_poly = poly.transform(X)

```

Using a degree of 10 yields 11 features, as by default, a constant feature ( $x ** 0$ ) is added, too:

```
X_poly.shape
```

```
(100, 11)
```

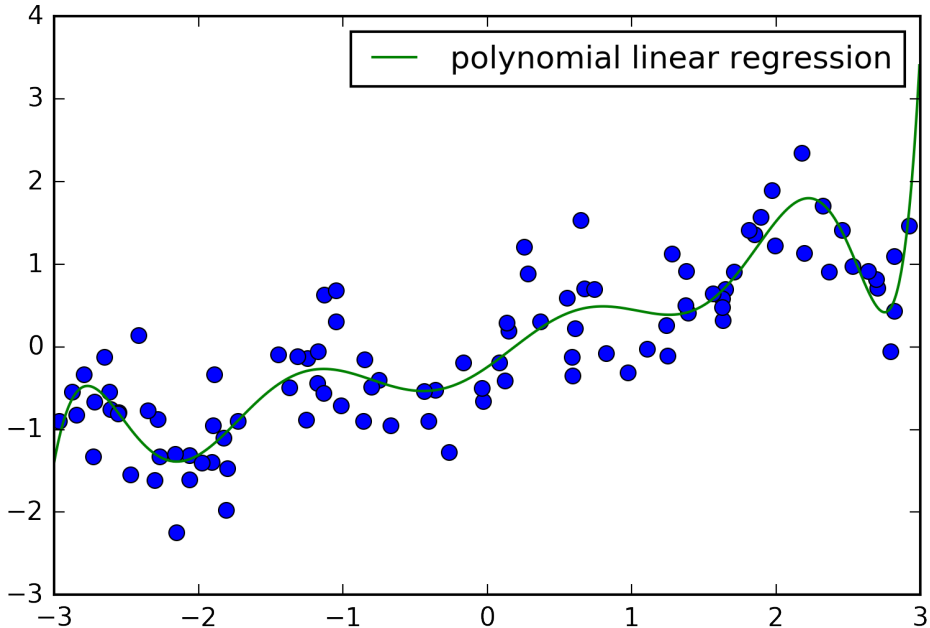
You can obtain the semantics of the features by looking at the `powers_` attribute, which gives the exponents for each feature:

```
poly.powers_  
array([[ 0],  
       [ 1],  
       [ 2],  
       [ 3],  
       [ 4],  
       [ 5],  
       [ 6],  
       [ 7],  
       [ 8],  
       [ 9],  
       [10]])
```

Using polynomial features together with a linear regression model yields the classical model of *polynomial regression*:

```
plt.plot(X[:, 0], y, 'o')  
  
reg = LinearRegression().fit(X_poly, y)  
  
line_poly = poly.transform(line)  
plt.plot(line, reg.predict(line_poly), label='polynomial linear regression')  
plt.legend(loc="best")
```





As you can see, polynomial feature yield a very smooth fit on this one-dimensional data. However, polynomials of high degree tend to behave in extreme ways on the boundaries or in regions of little data.

As a comparison, here is a kernel SVM model learned on the original data, without any transformation:

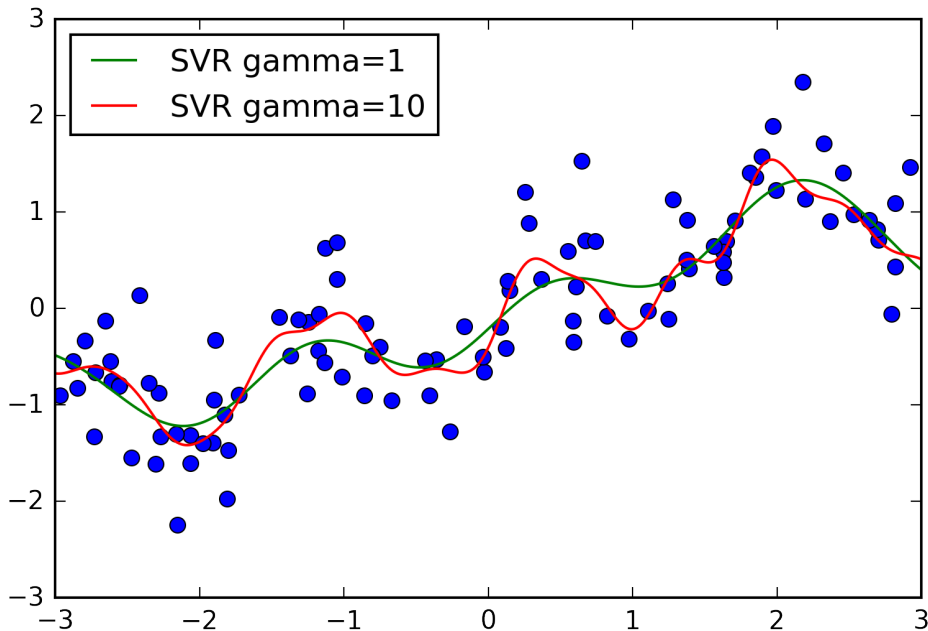
```

from sklearn.svm import SVR
plt.plot(X[:, 0], y, 'o')

for gamma in [1, 10]:
    svr = SVR(gamma=gamma).fit(X, y)
    plt.plot(line, svr.predict(line), label='SVR gamma=%d' % gamma)

plt.legend(loc="best")

```



Using a more complex model, a kernel SVM, we are able to learn a similarly complex prediction to the polynomial regression without using any transformations of the features.

As a more realistic application of interactions and polynomials, let's look again at the Boston Housing data set. We already used polynomial features on this dataset in Chapter 2. Now let us have a look at how these features were constructed, and at how much the polynomial features help. First we load the data, and rescale it to be between 0 and 1 using `MinMaxScaler`:

```

from sklearn.datasets import load_boston
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import MinMaxScaler

boston = load_boston()
X_train, X_test, y_train, y_test = train_test_split(boston.data, boston.target, random_state=0)

# rescale data:
scaler = MinMaxScaler()
X_train_scaled = scaler.fit_transform(X_train)
X_test_scaled = scaler.transform(X_test)

```

Now, we extract polynomial features and interactions up to a degree of 2:

```

poly = PolynomialFeatures(degree=2).fit(X_train_scaled)
X_train_poly = poly.transform(X_train_scaled)

```

```
X_test_poly = poly.transform(X_test_scaled)
print(X_train.shape)
print(X_train_poly.shape)
```

```
(379, 13)
```

```
(379, 105)
```

The data originally had 13 features, which were expanded into 105 interaction features. These new features represent all possible interactions between two different original features, as well as the square of each original feature. `degree=2` here means that we look at all features that are the product of up to two original features. The exact correspondence between input and output features can be found using the `get_feature_names` method:

```
print(poly.get_feature_names())
```

```
['1', 'x0', 'x1', 'x2', 'x3', 'x4', 'x5', 'x6', 'x7', 'x8', 'x9', 'x10', 'x11', 'x12', 'x0^2', 'x0
```

The first new feature is a constant feature, called “1” here. The next 13 features are the original features (called “x0” to “x12”). Then follows the first feature squared (“x0<sup>2</sup>”) and combinations of the first and the other features.

Let’s compare the performance using Ridge on the data with and without interactions:

```
from sklearn.linear_model import Ridge
ridge = Ridge().fit(X_train_scaled, y_train)
print("score without interactions: %f" % ridge.score(X_test_scaled, y_test))
ridge = Ridge().fit(X_train_poly, y_train)
print("score with interactions: %f" % ridge.score(X_test_poly, y_test))
```

```
score without interactions: 0.621370
```

```
score with interactions: 0.753423
```

Clearly the interactions and polynomial features gave us a good boost in performance when using Ridge. When using a more complex model like a random forest, the story is a bit different, though:

```
from sklearn.ensemble import RandomForestRegressor
rf = RandomForestRegressor(n_estimators=100).fit(X_train_scaled, y_train)
print("score without interactions: %f" % rf.score(X_test_scaled, y_test))
rf = RandomForestRegressor(n_estimators=100).fit(X_train_poly, y_train)
print("score with interactions: %f" % rf.score(X_test_poly, y_test))
```

```
score without interactions: 0.794226
```

```
score with interactions: 0.775016
```

You can see that even without additional features, the random forest beats the performance of Ridge. Adding interactions and polynomials actually decreases performance slightly.

# Univariate Non-linear transformations

We just saw that adding squared or cubed features can help linear models for regression. There are other transformations that often prove useful for transforming certain features, in particular applying mathematical functions like `log`, `exp` or `sin`. While tree-based models only care about the ordering of the features, linear models and neural networks are very tied to the scale and distribution of each feature, and if there is a non-linear relation between the feature and the target, that becomes hard to model---in particular in regression. The functions `log` and `exp` can help adjusting the relative scales in the data so that they can be captured better by a linear model or neural network.

The `sin` or `cos` functions can come in handy when dealing with data that encodes periodic patterns.

Most models work best when each feature (and in regression also the target) are loosely Gaussian distributed, that is a histogram of each feature should have something resembling the familiar bell-curve shape. Using transformations like `log` and `exp` are a hacky, but simple and efficient way to achieve this. A particular common case when such a transformation can be helpful is when dealing with integer count data. By count data, we mean features like “how often did user A log in”. Counts are never negative, and often follow particular statistical patterns. We are using a synthetic dataset of counts here, that has properties similar to those you can find in the wild. The features are all integer, while the response is continuous:

```
rnd = np.random.RandomState(0)
X_org = rnd.normal(size=(1000, 3))
w = rnd.normal(size=3)

X = np.random.poisson(10 * np.exp(X_org))
y = np.dot(X_org, w)
```

Let’s look at the first ten entries of the first feature. All are integer and positive, but apart from that it’s hard to make out a particular pattern:

If we count the appearance of each value, the distribution of values becomes more clear:

```
np.bincount(X[:, 0])
array([17, 44, 65, 42, 62, 57, 51, 46, 59, 42, 39, 35, 28, 28, 25, 20, 32,
       22, 16, 14, 20, 12,  7, 21, 12,  9, 18,  8, 11, 10,  8, 10,  4,  6,
       6,  0,  4,  4,  4,  2,  2,  4,  1,  3, 10,  2,  1,  4,  2,  3,  2,
       1,  2,  1,  3,  2,  1,  1,  3,  1,  0,  2,  1,  1,  4,  2,  0,  0,
       0,  0,  1,  0,  0,  0,  0,  1,  0,  1,  0,  2,  1,  1,  1,  1,  1,  1,
```

```

0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 0, 0,
0, 2, 1, 2, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 0, 0, 0, 0, 1, 1])

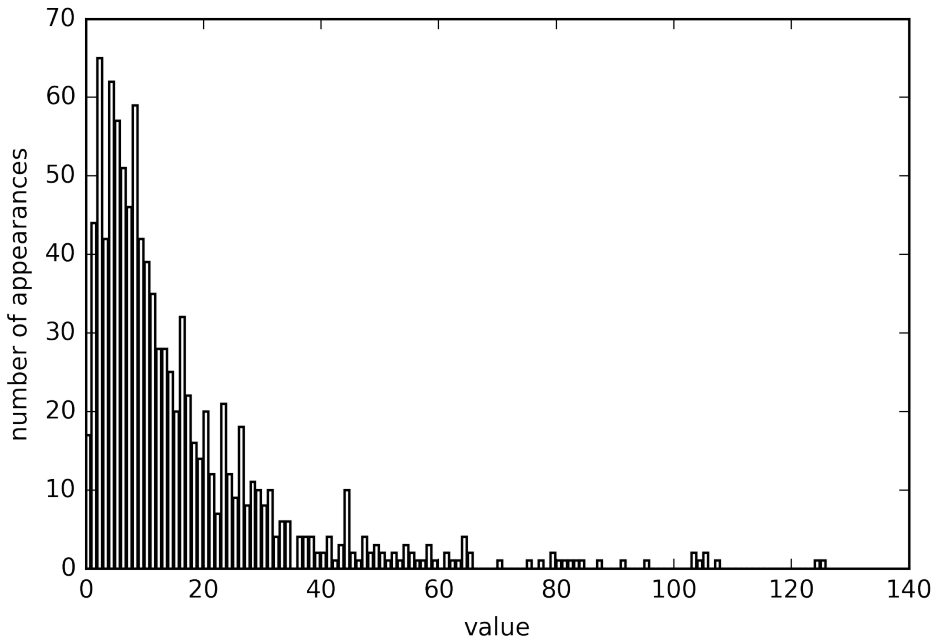
```

The value 2 seems to be the most common with 62 appearances (bincount always starts at 0), and the counts for higher values fall quickly. However, there are some very high values, like 134 appearing twice. We visualized the counts below:

```

bins = np.bincount(X[:, 0])
plt.bar(range(len(bins)), bins, color='w')
plt.ylabel("number of appearances")
plt.xlabel("value")

```



Features  $X[:, 1]$  and  $X[:, 2]$  have similar properties. This kind of distribution of values (many small ones, and a few very large ones) is very common in practice [foot-note: This is a Poisson distribution, which is quite fundamental to count data]. However, it is something most linear models can't handle very well. Let's try to fit a Ridge regression to this model:

```

from sklearn.linear_model import Ridge
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
Ridge().fit(X_train, y_train).score(X_test, y_test)

0.61099786602482975

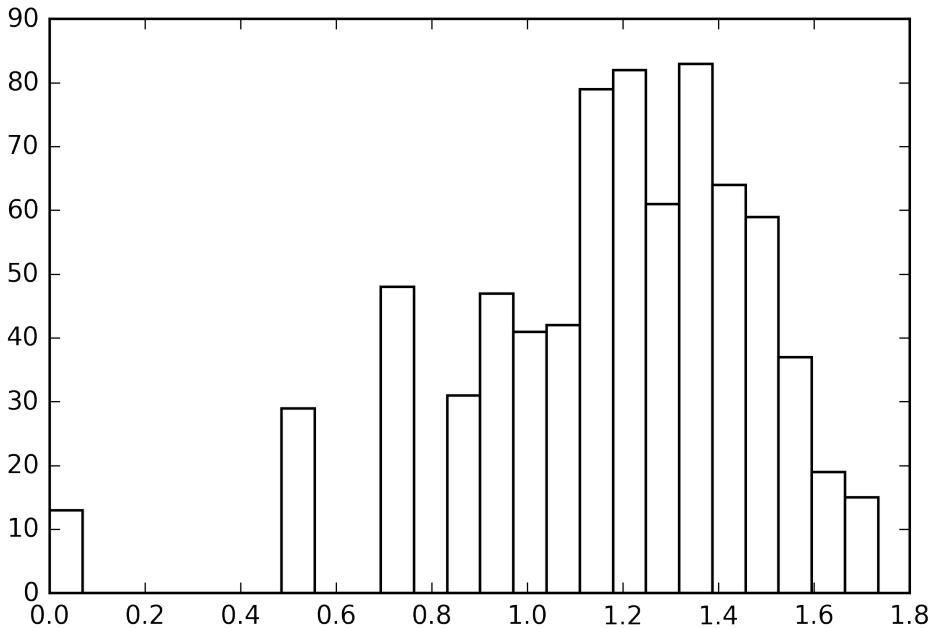
```

Applying a logarithmic transformation can help, though. Because the value 0 appears in the data (and the logarithm is not defined at 0), we can not actually just apply `log`, but we have to compute `log(X + 1)`:

```
X_train_log = np.log(X_train + 1)
X_test_log = np.log(X_test + 1)
```

After the transformation, the distribution of the data is less asymmetrical and doesn't have very large outliers any more:

```
plt.hist(np.log(X_train_log[:, 0] + 1), bins=25, color='w');
```



Building a ridge model on the new data provides a much better fit:

```
Ridge().fit(X_train_log, y_train).score(X_test_log, y_test)
0.85919272057341256
```

Finding the transformation that works best for each combination of dataset and model is somewhat of an art. In this example, all the features had the same properties. This is rarely the case in practice, and usually only a subset of the features should be transformed, or sometimes each feature needs to be transformed in a different way. As we mentioned above, these kind of transformations are irrelevant for tree-based models, but might be essential for linear models.

Sometimes it is also a good idea to transform the target variable `y` in regression. Trying to predict counts (say, number of orders) is a fairly common task, and using the

$\log(y + 1)$  transformation often helps [footnote: this is a very crude approximation of using Poisson regression, which would be the proper solution from a probabilistic standpoint.]

As you saw in the examples above, binning, polynomials and interactions can have a huge influence on how models perform on a given dataset. This is in particular true for less complex models like linear models and naive Bayes.

Tree-based models on the other hand are often able to discover important interactions themselves, and don't require transforming the data explicitly most of the time.

Other models like SVMs, nearest neighbors and neural networks might sometimes benefit from using binning, interactions or polynomials, but the implications there are usually much less clear than in the case of linear models.

## Automatic Feature Selection

With so many ways to create new features, you might get tempted to increase the dimensionality of the data way beyond the number of original features. However, adding more features makes all models more complex, and so increases the chance of overfitting. When adding new features, or with high-dimensional datasets in general, it can be a good idea to reduce the number of features to only the most useful ones, and discard the rest. This can lead to simpler models that generalize better.

But how can you know how good each feature is?

There are three basic strategies: *Univariate statistics*, *model-based selection* and *iterative selection*. We will discuss all three of them in detail. All three of these methods are supervised methods, meaning they need the target for fitting the model. This means we do need to split the data into training and test set

and fit the feature selection only on the training part of the data.

### Univariate statistics

In univariate statistics, we compute whether there is a statistically significant relationship between each feature and the target. Then the features that are related with the highest confidence are selected. In the case of classification, this is also known as analysis of variance (ANOVA).

A key property of these tests are that they are *univariate* meaning that they only consider each feature individually. Consequently a feature will be discarded if it is only informative when combined with another feature. Univariate tests are often very fast to compute, and don't require building a model. On the other hand, they are completely independent of the model that you might want to apply after the feature selection.

To use univariate feature selection in scikit-learn, you need to choose a test, usually either `f_classif` (the default) for classification or `f_regression` for regression, and a method to discard features based on the p-values determined in the test. All methods for discarding parameters use a threshold to discard all features with too high a p-values (which means they are unlikely to be related to the target). The methods differ in how they compute this threshold, with the simplest ones being `SelectKBest` which selects a fixed number `k` of features, and `SelectPercentile`, which selects a fixed percentage of features.

Let's apply the feature selection for classification on the cancer dataset. To make the task a bit harder, we add some non-informative noise features to the data. We expect the feature selection to be able to identify the features that are non-informative and remove them.

```
from sklearn.datasets import load_breast_cancer
from sklearn.feature_selection import SelectPercentile
from sklearn.model_selection import train_test_split

cancer = load_breast_cancer()

# get deterministic random numbers
rng = np.random.RandomState(42)
noise = rng.normal(size=(len(cancer.data), 50))
# add noise features to the data
# the first 30 features are from the dataset, the next 50 are noise
X_w_noise = np.hstack([cancer.data, noise])

X_train, X_test, y_train, y_test = train_test_split(
    X_w_noise, cancer.target, random_state=0, test_size=.5)
# use f_classif (the default) and SelectPercentile to select 10% of features:
select = SelectPercentile(percentile=50)
select.fit(X_train, y_train)
# transform training set:
X_train_selected = select.transform(X_train)

print(X_train.shape)
print(X_train_selected.shape)

(284, 80)

(284, 40)
```

As you can see, the number of features was reduced from 80 to 40 (50 percent of the original number of features). We can find out which features have been selected using the `get_support` method, which returns a boolean mask of the selected features:

```
mask = select.get_support()
print(mask)
# visualize the mask. black is True, white is False
plt.matshow(mask.reshape(1, -1), cmap='gray_r')
```





```
[ True True True True True True True True True False True False
  True True True True True True False False True True True True
  True True True True True True False False False True False True
  False False True False False False False True False False True False
  False True False True False False False False False False True False
  True False False False False True False True False False False False
  True True False True False False False False]
```

As you can see from the visualization of the mask above, most of the selected features are the original features, and most of the noise features were removed. However, the recovery of the original features is not perfect.

Let's compare the performance of logistic regression on all features against the performance using only the selected features:

```
from sklearn.linear_model import LogisticRegression

# transform test data:
X_test_selected = select.transform(X_test)

lr = LogisticRegression()
lr.fit(X_train, y_train)
print("Score with all features: %f" % lr.score(X_test, y_test))
lr.fit(X_train_selected, y_train)
print("Score with only selected features: %f" % lr.score(X_test_selected, y_test))

Score with all features: 0.929825

Score with only selected features: 0.940351
```

In this case, removing the noise features improved performance, even though some of the original features were lost. This was a very simple synthetic example, though, and outcomes on real data is usually mixed. Univariate feature selection can still be very helpful if there is such a large number of features that building a model on them is infeasible, or if you suspect that many features are completely uninformative.

## Model-based Feature Selection

Model based feature selection uses a supervised machine learning model to judge the importance of each feature, and keeps only the most important ones. The supervised model that is used for feature selection doesn't need to be the same model that is used for the final supervised modeling.

The model that is used for feature selection needs to provide some measure of importance for each feature, so that they can be ranked by this measure. Decision trees and decision tree based models provide feature importances, which can be used; Linear models have coefficients which can be used by considering the absolute value. As we saw in Chapter 2, linear models with L1 penalty learn sparse coefficients, which only use a small subset of features. This can be viewed as a form of feature selection for the model itself, but can also be used as a preprocessing step to select features for another model.

In contrast to univariate selection, model-based selection considers all features at once, and so can capture interactions (if the model can capture them).

To use model based feature selection, we need to use the `SelectFromModel` transformer:

```
from sklearn.feature_selection import SelectFromModel
from sklearn.ensemble import RandomForestClassifier
select = SelectFromModel(RandomForestClassifier(n_estimators=100, random_state=42), threshold="median")
```

The `SelectFromModel` class selects all features that have an importance measure of the feature (as provided by the supervised model) greater than the provided threshold. To get a comparable result to what we got with univariate feature selection, we used the median as a threshold, so that half of the features will be selected. We use a random forest classifier with 100 trees to compute the feature importances. This is a quite complex model and much more powerful than using univariate tests. Now let's actually fit the model:


```
select.fit(X_train, y_train)
X_train_l1 = select.transform(X_train)
print(X_train.shape)
print(X_train_l1.shape)

(284, 80)

(284, 40)
```

Again, we can have a look at the features that were selected:

```
mask = select.get_support()
# visualize the mask. black is True, white is False
plt.matshow(mask.reshape(1, -1), cmap='gray_r')
```



This time, all but two of the original features were selected. Because we specified to select 40 features, some of the noise features are also selected.

```
X_test_l1 = select.transform(X_test)
LogisticRegression().fit(X_train_l1, y_train).score(X_test_l1, y_test)

0.9508771929824561
```

With the better feature selection, we also gained some improvements in performance.

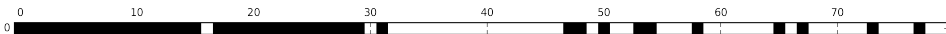
## Iterative feature selection

In univariate testing, we build used no model, while in model based selection we used a single model to select features. In iterative feature selection, a series of models is built, with varying numbers of features. There are two basic methods: starting with no features and adding features one by one, until some stopping criterion is reached, or starting with all features and removing features one by one, until some stopping criterion is reached. Because a series of models is built, these methods are much more computationally expensive then the methods we discussed above. One particular method of this kind is *recursive feature elimination* (RFE) which starts with all features, builds a model, and discards the least important feature according to the model. Then, a new model is built, using all but the discarded feature, and so on, until only a pre-specified number of features is left. For this to work, the model used for selection needs to provide some way to determine feature importance, as was the case for the model based selction.

We use the same random forest model that we used above:

```
from sklearn.feature_selection import RFE
select = RFE(RandomForestClassifier(n_estimators=100, random_state=42), n_features_to_select=40)
#select = RFE(LogisticRegression(penalty="l1"), n_features_to_select=40)

select.fit(X_train, y_train)
# visualize the selected features:
mask = select.get_support()
plt.matshow(mask.reshape(1, -1), cmap='gray_r')
```



The feature selection got better compared to the univariate and model based selection, but one feature was still missed. Running the above code takes significantly longer than the model based selection, because a random forest model is trained 40 times, once for each feature that is dropped.

```
X_train_rfe= select.transform(X_train)
X_test_rfe= select.transform(X_test)

LogisticRegression().fit(X_train_rfe, y_train).score(X_test_rfe, y_test)

0.9508771929824561
```

We can also use the model used inside the RFE to make predictions. This uses only the feature set that was selected:

```
select.score(X_test, y_test)

0.9508771929824561
```

If you are unsure when selecting what to use as input to your machine learning algorithms, automatic feature selection can be quite helpful. It is also great to reduce the amount of features needed, for example to speed up prediction, or allow for more interpretable models. In most real-world cases, applying feature selection is unlikely to provide large gains in performance. However, it is still a valuable tool in the toolbox of the feature engineer.

## Utilizing Expert Knowledge

Feature engineering is often an important place to use *expert knowledge* for a particular application. While the purpose of machine learning often is to avoid having to create a set of expert-designed rules, that doesn't mean that prior knowledge of the application or domain should be discarded. Often, domain experts can help in identifying useful features that are much more informative than the initial representation of the data.

Imagine you are a travel agency and want to predict flight prices. Let's say we have a record of prices together with date, airline, start location and destination. A machine learning model might be able to build a decent model from that. Some important factors in flight prices, however can not be learned. For example, flights are usually more expensive during school holidays or around public holidays. While some holidays can potentially be learned from the dates, like Christmas, others might depend on the phases of the moon (like Hannukah and Easter), or be set by authorities like school holidays. These events can not be learned from the data if each flight is only recorded using the (Gregorian) date. It is easy to add a feature that encodes whether a flight was on, preceding, or following a public or school holiday. In this way, prior knowledge about the nature of the task can be encoded in the features to aid a machine learning algorithm. Adding a feature does not force a machine learning algorithm to use it, and even if the holiday information turns out to be non-informative for flight prices, augmenting the data with this information doesn't hurt.

We'll now go through one particular case of using expert knowledge - though in this case it might be more rightfully called "common sense". The task is predicting citibike rentals in front of Andreas' house.

In New York, there is a network of bicycle rental stations, with a subscription system. The stations are all over the city and provide a convenient way to get around. Bike rental data is made public in an anonymized form [Footnote: at <https://www.citibike-nyc.com/system-data>] and has been analyzed in various ways.

The task we want to solve is to predict for a given time and day how many people will rent a bike in front of Andreas' house - so he knows if any bikes will be left for him.

We first load the data for August 2015 of this particular station as a pandas dataframe. We resampled the data into 3 hour intervals to obtain the main trends for each day.

```

from importlib import reload
reload(mglearn.datasets)
citibike = mglearn.datasets.load_citibike()

/home/andy/checkout/book/notebooks/mglearn/datasets.py:40: FutureWarning: how in .resample() is de

the new syntax is .resample(...).sum()

    data_resampled = data_starttime.resample("3h", how="sum").fillna(0)
citibike.head()
starttime

2015-08-01 00:00:00    3.0
2015-08-01 03:00:00    0.0
2015-08-01 06:00:00    9.0
2015-08-01 09:00:00   41.0
2015-08-01 12:00:00   39.0

Freq: 3H, Name: one, dtype: float64

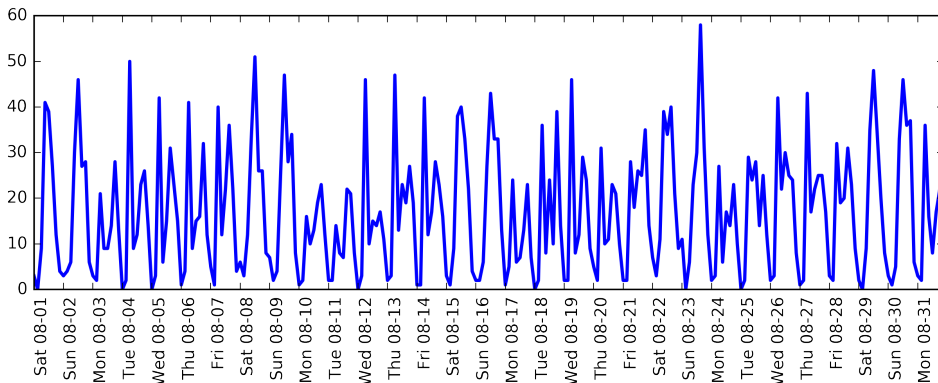
```

Below is a visualization of the rental frequencies for the whole month:

```

plt.figure(figsize=(10, 3))
xticks = pd.date_range(start=citibike.index.min(), end=citibike.index.max(), freq='D')
plt.xticks(xticks, xticks.strftime("%a %m-%d"), rotation=90, ha="left")
plt.plot(citibike, linewidth=2)

```



Looking at the data, we can clearly distinguish day and night for each day. The patterns for week days and weekends also seem to be quite different.

When evaluating a prediction task on a time series like this, we usually want to learn *from the past* and predict *for the future*. This means when doing a split into a training

and a test set, we want to use all the data up to a certain date as training set, and all the data past that date as a test set. This is how we would usually use time series prediction: given everything that we know about rentals in the past, what do we think will happen tomorrow?

We will use the first 184 data points, corresponding to the first 23 days, as our training set, and the remaining 64 data points corresponding to the remaining 8 days as our test set.

The only feature that we are using in our prediction task is the date and time when a particular number of rentals occurred. So the input feature is the time, say 2015-08-01 00:00:00, and the output is the number of rentals in the following three hours, 3 in this case (according to the dataframe above).

A (surprisingly) common way that dates are stored on computers is using POSIX time, which is the number of seconds since January 1970 00:00:00 (aka the beginning of time). As a first try, we can use this single integer feature as our data representation:

```
# extract the target values (number of rentals)
y = citibike.values
# convert the time to posixtime using "%s"
X = citibike.index.strftime("%s").astype("int").reshape(-1, 1)

from sklearn.linear_model import LinearRegression
from sklearn.ensemble import RandomForestRegressor
```

We first define a function to split the data into training and test set, build the model, and visualize the result:

```
# use the first 184 data points for training, the rest for testing
n_train = 184

# function to evaluate and plot a regressor on a given feature set
def eval_on_features(features, target, regressor):
    # split the given features into a training and test set
    X_train, X_test = features[:n_train], features[n_train:]
    # split also the
    y_train, y_test = target[:n_train], target[n_train:]
    regressor.fit(X_train, y_train)
    print("Test-set R^2: ", regressor.score(X_test, y_test))
    y_pred = regressor.predict(X_test)
    y_pred_train = regressor.predict(X_train)
    plt.figure(figsize=(10, 3))

    plt.xticks(range(0, len(X), 8), xticks.strftime("%a %m-%d"), rotation=90, ha="left");

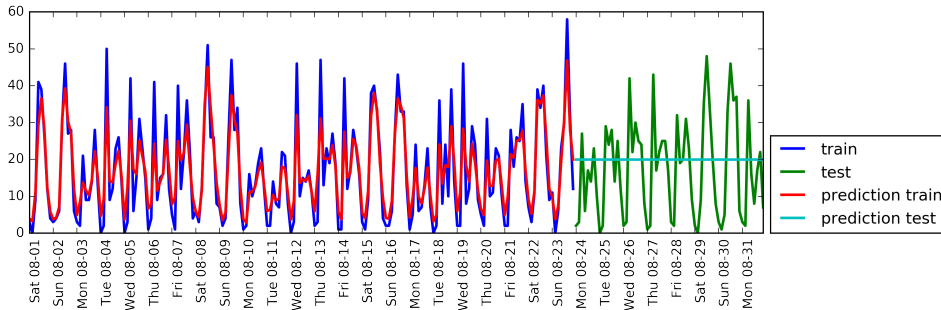
    plt.plot(range(n_train), y_train, label="train", linewidth=2)
    plt.plot(range(n_train, len(y_test) + n_train), y_test, label="test", linewidth=2)
    plt.plot(range(n_train), y_pred_train, label="prediction train", linewidth=2)
```

```
plt.plot(range(n_train, len(y_test) + n_train), y_pred, label="prediction test", linewidth=2)
plt.legend(loc=(1.01, 0))
```

We saw above that random forests need very little preprocessing of the data, which makes it seem like a good model to start with.

We use the POSIX time feature  $X$  and pass a random forest regressor to our `eval_on_features` function:

```
regressor = RandomForestRegressor(n_estimators=100, random_state=0)
plt.figure()
eval_on_features(X, y, regressor);
```



Test-set  $R^2$ : `-0.035486463626`

The predictions on the training set are quite good, as is usual for random forests. However, for the test set, a constant line is predicted. The  $R^2$  is `-0.03`, which means that we learned nothing. What happened?

The problem lies in the combination of our feature and the random forest. The value of the POSIX time feature for the test set is outside of the range of the feature values on the training set: the points in the test set have time stamps that are later than all the points in the training set.

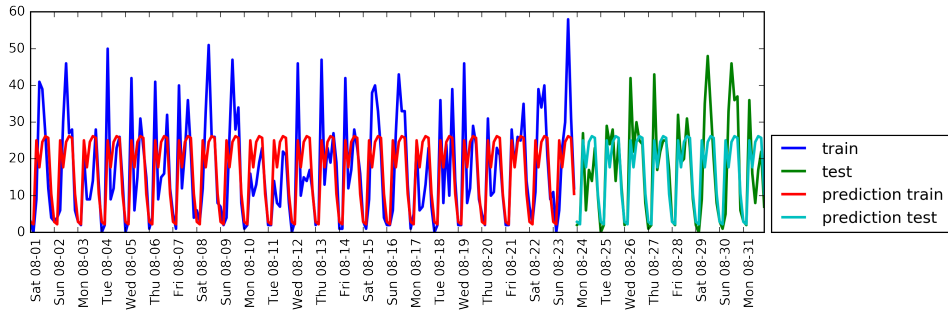
Trees, and therefore random forests, can not *extrapolate* to feature ranges outside the training set.

The result is that the model simply predicts the same as for the closest point in the training set - which is the last time it observed any data.

Clearly we can do better than this. This is where our “expert knowledge” comes in. From looking at the rental figures on the training data, two factors seem to be very important: the time of day, and the day of the week. So let’s add these two features. We can’t really learn anything from the POSIX time, so we drop that feature.

First, let’s use only the hour of the day:

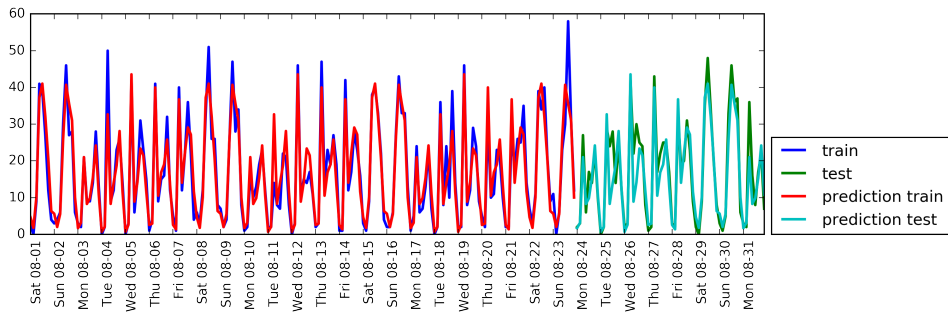
```
X_hour = citibike.index.hour.reshape(-1, 1)
eval_on_features(X_hour, y, regressor)
```



Test-set  $R^2$ : 0.599577599331

Now the predictions have the same pattern for each day of the week. The  $R^2$  is already much better, but the predictions clearly miss the weekly pattern. Now let's also add the day of the week:

```
X_hour_week = np.hstack([citibike.index.dayofweek.reshape(-1, 1), citibike.index.hour.reshape(-1, 1),
eval_on_features(X_hour_week, y, regressor)
```



Test-set  $R^2$ : 0.841948858797

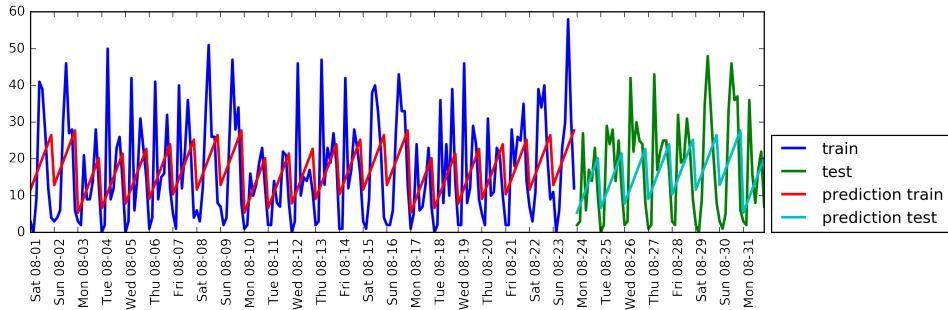
Now, we have a model that models the periodic behavior considering day of week and time of day. It has an  $R^2$  of 0.84, and show pretty good predictive performance.

What this model likely is learning is the mean number of rentals for each combination of weekday and time of day from the first 23 days of August. This would actually not require a complex model like a random forest.

So let's try with a simpler model, LinearRegression:

```
eval_on_features(X_hour_week, y, LinearRegression())
```

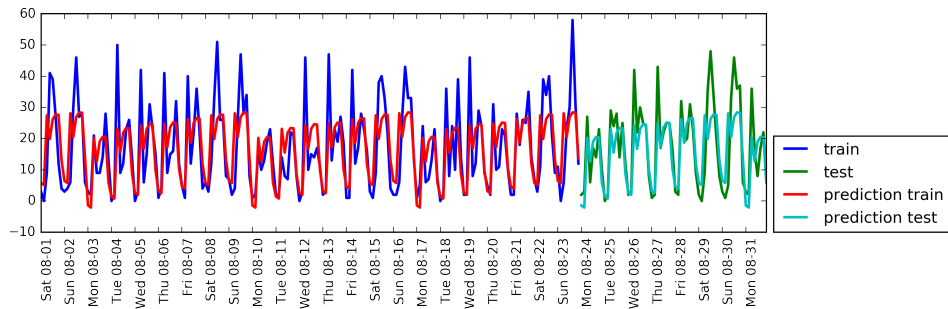




Test-set  $R^2$ : 0.132041572622

Linear Regression works much worse, and the periodic pattern looks odd. The reason for this is that we encoded day of the week and time of the day using integers, which are interpreted as categorical variables. Therefore, the linear model can only learn a linear function of the time of day - and it learned that later in the day, there are more rentals. However, the patterns are much more complex than that, which we can capture by interpreting the integers as categorical variables, by transforming them using OneHotEncoder:

```
enc = OneHotEncoder()
X_hour_week_onehot = enc.fit_transform(X_hour_week).toarray()
eval_on_features(X_hour_week_onehot, y, Ridge())
```



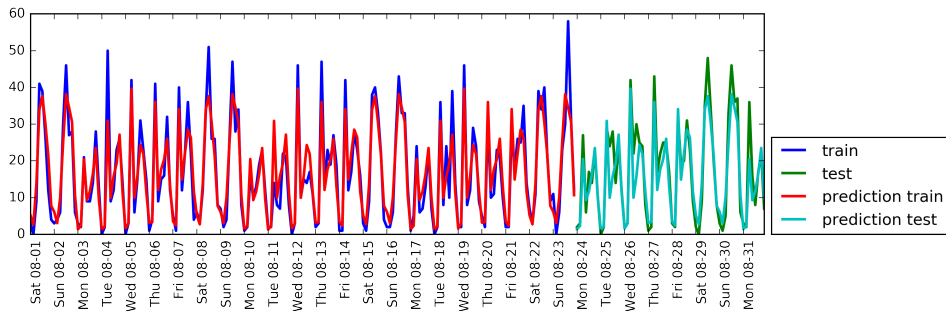
Test-set  $R^2$ : 0.619113916866

This gave us a much better match than the continuous feature encoding. Now, the linear model learns one coefficient for each day of the week, and one coefficient for each time of the day. That means that the “time of day” pattern is shared over all days of the week, though.

Using interaction features, we can allow the model to learn one coefficient for each combination of day and time of day:

```
poly_transformer = PolynomialFeatures(degree=2, interaction_only=True, include_bias=False)
X_hour_week_onehot_poly = poly_transformer.fit_transform(X_hour_week_onehot)
```

```
lr = Ridge()
eval_on_features(X_hour_week_onehot_poly, y, lr)
```



Test-set  $R^2$ : 0.845170635797

This transformation finally yields a model that performs similarly well to the random forest.

A big benefit of this model is that it is very clear what is learned: one coefficient for each day and time.

We can simply plot the coefficients learned by the model, something that would not be possible for the random forest.

First, we create feature names for the hour and day features:

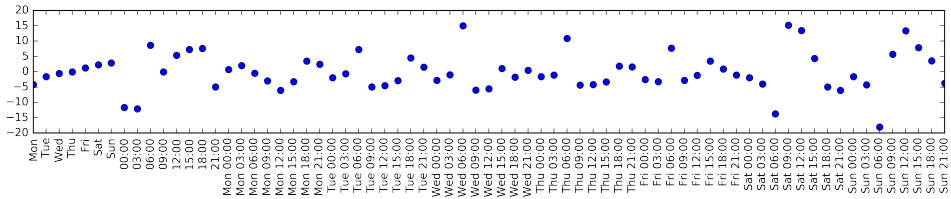
```
hour = ["%02d:00" % i for i in range(0, 24, 3)]
day = ["Mon", "Tue", "Wed", "Thu", "Fri", "Sat", "Sun"]
features = day + hour
```

Then we name all the interaction feature extracted by the PolynomialFeatures, using the `get_feature_names` method, and keep only the feature with non-zero coefficients:

```
features_poly = poly_transformer.get_feature_names(features)
features_nonzero = np.array(features_poly)[lr.coef_ != 0]
coef_nonzero = lr.coef_[lr.coef_ != 0]
```

Now we can visualize the coefficients learned by the linear model:

```
plt.figure(figsize=(15, 2))
plt.plot(coef_nonzero, 'o')
plt.xticks(np.arange(len(coef_nonzero)), features_nonzero, rotation=90);
```



## Summary and outlook

In this chapter, we discussed how to deal with different data types, in particular with categorical variables.

We emphasized the importance of representing your data in a way that is suitable for the machine learning algorithm, for example by one-hot-encoding categorical variables.

We also discussed the importance of engineering new features, and the possibility of utilizing expert knowledge in creating derived features from your data.

In particular linear models might benefit greatly from generating new features via binning and adding polynomials and interactions, while more complex, nonlinear models like random forests and SVMs might be able to learn more complex tasks without explicitly expanding the feature space.

In practice, the features that are used, and the match between features and method is often the most important piece in making a machine learning approach work well.

Having our data represented in an appropriate way, and knowing which algorithm to use for which task, the next chapter will focus on evaluating performance of machine learning models and selecting the right parameter settings.



---

# Model evaluation and improvement

Having discussed the fundamentals of supervised and unsupervised learning, and having explored a variety of machine learning algorithms, we will now dive more deeply into evaluating models and selecting parameters.

We will focus on the supervised methods, regression and classification, as evaluating and selecting models in unsupervised learning is often a very qualitative process (as we have seen in Chapter 3).

To evaluate our supervised models, so far we have split our data set in to a training set and a test set using the `train_test_split` function, built a model on the training set calling the `fit` method, and evaluated it on the test set using the `score` method, which, for classification, computes the fraction of correctly classified samples:

```
from sklearn.datasets import make_blobs
from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import train_test_split

# create a synthetic dataset
X, y = make_blobs(random_state=0)
# split data and labels into a training and a test set
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
# Instantiate a model and fit it to the training set
logreg = LogisticRegression().fit(X_train, y_train)
# evaluate the model on the test set
logreg.score(X_test, y_test)
# we predicted the correct class on 88% of the samples in X_test

0.88
```

As a reminder, the reason we split our data into training and test sets is that we are interested in measuring how well our model *generalizes* to new, unseen data. We are

not interested in how well our model fit the training set, but rather, how well it can make predictions for data that was not observed during training.

In this chapter, we will expand on two aspects of this evaluation. We will a) introduce *cross-validation*, a more robust way to assess generalization performance than a single split of the data into a training and a test set and b) discuss methods to evaluate classification and regression performance that go beyond the default measures of accuracy and  $R^2$  provided by the score method.

We will also discuss *grid search*, an effective method for adjusting the parameters in supervised models for the best generalization performance.

## Cross-validation

*Cross-validation* is a statistical method to evaluate generalization performance in a more stable and thorough way than using a split into training and test set.

In cross-validation, instead of splitting the data set in to a training set and a test set, the data is split repeatedly and multiple models are trained.

The most commonly used version of cross-validation is *k-fold cross-validation*, where  $k$  is a user specified number, usually five or ten. When performing five-fold cross-validation, the data is first partitioned into five parts of (approximately) equal size, called *folds*.

Next, a sequence of models is trained. The first model is trained using the first fold as the test set, and the remaining folds 2-5 as the training set. The model is build using the data in the folds 2-5, and then the accuracy is evaluated on fold 1.

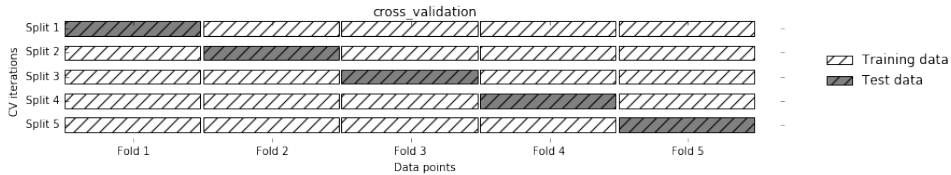
Then another model is build, this time using fold 2 as the test set, and the data in folds 1, 3, 4 and 5 as the training set.

This process is repeated using the folds 3, 4 and 5 as test sets. For each of these five *splits* of the data into training and test set, we computed the accuracy. In the end, we have collected five accuracy values.

The process is illustrated in Figure `cross_validation`.

Usually, the first fifth of the data is the first fold, the second fifth of the data is the second fold, and so on.

```
mglern.plots.plot_cross_validation()
```



## Cross-validation in scikit-learn

Cross-validation is implemented in scikit-learn using the `cross_val_score` function from the `model_selection` module.

The parameters of the `cross_val_score` function are the model we want to evaluate, the training data and the ground-truth labels. Let's evaluate `LogisticRegression` on the `iris` dataset:

```
from sklearn.model_selection import cross_val_score
from sklearn.datasets import load_iris
from sklearn.linear_model import LogisticRegression

iris = load_iris()
logreg = LogisticRegression()

scores = cross_val_score(logreg, iris.data, iris.target)
print("cross-validation scores: ", scores)

cross-validation scores: [ 0.961  0.922  0.958]
```

By default, `cross_val_score` performs three-fold cross-validation, returning three accuracy values.

We can change the number of folds used by changing the `cv` parameter:

```
scores = cross_val_score(logreg, iris.data, iris.target, cv=5)
scores
array([ 1.    ,  0.967,  0.933,  0.9    ,  1.    ])
```

A common way to summarize the cross-validation accuracy is to compute the mean:

```
scores.mean()
0.96000000000000019
```

## Benefits of cross-validation

There are several benefits of using cross-validation instead of a single split into a training and test set.

First, remember that `train_test_split` performs a random split of the data. Imagine that we are “lucky” when randomly splitting the data, and all examples that are hard

to classify are in the training set. Then, the test set will only contain “easy” examples, and our test set accuracy will be unrealistically high. Conversely, if we are “unlucky”, we might have randomly put all the hard to classify examples in the test set, and obtain an unrealistically low score.

However, when using cross-validation, each example will be in the training set exactly once: each example is in one of the folds, and each fold is the test set once. Therefore the model needs to generalize well to all of the samples in the data set for all of the cross-validation scores (and their mean) to be high.

Having multiple splits of the data also provides some information about how sensitive our model is to the selection of the training dataset. Looking at the scores for the iris dataset above, we see accuracies between 90% and 100%. This is quite a range, and provides us with an idea about how the model might perform in the worst case and the best case scenarios when applied to new data.

Another benefit of cross-validation as compared to using a single split of the data is that we use our data more effectively. When using `train_test_split`, we usually use 75% of the data for training and 25% of the data for evaluation, which is a good rule of thumb. When using five-fold cross-validation, in each iteration we can use 4/5 of the data (or 80% of our data) to fit the model. When using ten-fold cross-validation, we can use 9/10 of the data (90%) to fit the model. More data will usually result in more accurate models.

The main disadvantage of cross-validation is increased computational cost. As we are now training  $k$  models, instead of a single model, cross-validation will be roughly  $k$  times slower than doing a single split of the data.

[info box] It is important to keep in mind that cross-validation is not a way to build a model that can be applied to new data. Cross-validation does not return a model. When calling `cross_val_score`, multiple models are build internally, but the purpose of cross-validation is only to evaluate how well a given algorithm will generalize when trained on a specific dataset. [/end infobox]

## Stratified K-Fold cross-validation and other strategies

Splitting the dataset into  $k$ -folds by starting with the first  $1/k$ -th part of the data as described above might not always be a good idea. Let’s have a look at the iris dataset for example:

```
from sklearn.datasets import load_iris
iris = load_iris()
print(iris.target)

[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 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```



```
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
2 2]
```

As you can see above, the first third of the data is the class 0, the second third is the class 1, and the last third is class 2. Imagine doing three-fold cross-validation on this dataset. The first fold would be only class 0, so in the first split of the data, the test set would be only class zero, and the training set would be only class 1 and 2.

As the classes in training and test set would be different for all three splits, the three-fold cross-validation accuracy would be zero on this dataset. That is not very helpful, as we can do much better than 0% accuracy on `iris`.

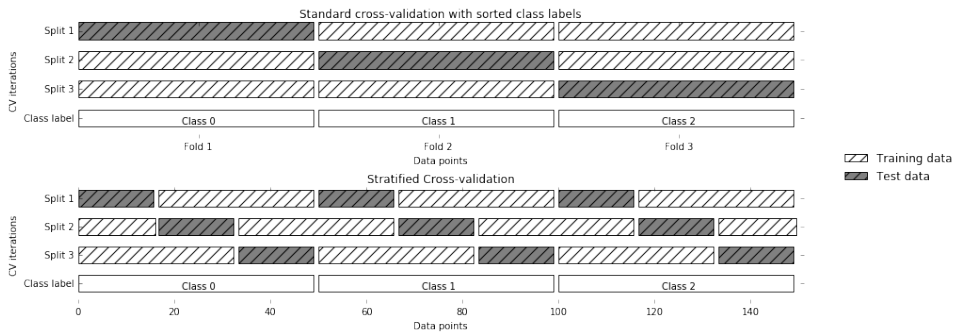
As the simple k-fold strategy fails here, scikit-learn does not use k-fold for classification, but rather *stratified k-fold cross-validation*. In stratified cross-validation, we split the data such that the proportions between classes are the same in each fold as they are in the whole dataset, as illustrated in Figure `stratified_kfold`.

For example, if 90% of your samples belong to class A, and 10% of your samples belong to class B, then stratified cross-validation ensures that in each fold, 90% of samples belong to class A and 10% of samples belong to class B.

It is always a good idea to use stratified k-fold cross-validation instead of k-fold cross-validation to evaluate a classifier, because it results in more reliable estimates of generalization performance. In the case of only 10% of samples belonging to class B, using standard k-fold cross-validation, it might easily happen that one fold only contains samples of class A. Using this fold as a test-set would not be very informative of the overall performance of the classifier.

For regression, scikit-learn uses the standard k-fold cross-validation by default. It would be possibly to also try to make each fold representative of the different values the regression target has, but this is not a commonly used strategy and would be surprising to most users.

```
mglearn.plots.plot_stratified_cross_validation()
```



## More control over cross-validation

We saw above that we can adjust the number of folds that are used in `cross_val_score` using the `cv` parameter. However, scikit-learn allows for much finer control over what happens during the splitting of the data, by providing a *cross-validation splitter* as the `cv` parameter.

For most use cases, the default of k-fold cross validation for regression and stratified k-fold for classification work well, but there are some cases when you might want to use a different strategy.

Say for example we want to use the standard k-fold cross-validation on a classification dataset, to reproduce someone else's results. To do this, we first have to import the `KFold` splitter class from the `model_selection` module, and instantiate it with the number of folds you want to use:

```
from sklearn.model_selection import KFold
kfold = KFold(n_folds=5)
```

Then, we can pass the `kfold` splitter object as the `cv` parameter to `cross_val_score`:

```
cross_val_score(logreg, iris.data, iris.target, cv=kfold)
array([ 1.    ,  0.933,  0.433,  0.967,  0.433])
```

This way, we can verify that it is indeed a really bad idea to use 3-fold (non-stratified) cross-validation on the iris dataset:

```
kfold = KFold(n_folds=3)
cross_val_score(logreg, iris.data, iris.target, cv=kfold)
array([ 0.,  0.,  0.]
```

Remember: each fold corresponds to one of the classes, and so nothing can be learned. [specify again that this is on the iris dataset, it's a little unclear]

Another way to resolve this problem instead of stratifying the folds is to shuffle the data, to remove the ordering of the samples by label. We can do that setting the `shuf`

file parameter of `KFold` to `True`. If we shuffle the data, we also need to fix the `random_state` to get a reproducible shuffling. Otherwise, each run of `cross_val_score` would yield a different result, as each time a different split would be used (this might not be a problem, but can be surprising).

```
kfold = KFold(n_folds=3, shuffle=True, random_state=0)
cross_val_score(logreg, iris.data, iris.target, cv=kfold)

array([ 0.9 ,  0.96,  0.96])
```

## Leave-One-Out cross-validation

Another frequently used cross-validation method is *leave-one-out*. You can think of leave-one-out cross-validation as k-fold cross-validation where each fold is a single sample. For each split, you pick a single data point to be the test set. This can be very time-consuming, in particular for large datasets, but sometimes provides better estimates on small datasets:

```
from sklearn.model_selection import LeaveOneOut
loo = LeaveOneOut()
scores = cross_val_score(logreg, iris.data, iris.target, cv=loo)
print("number of cv iterations: ", len(scores))
print("mean accuracy: ", scores.mean())

number of cv iterations:  150

mean accuracy:  0.953333333333
```

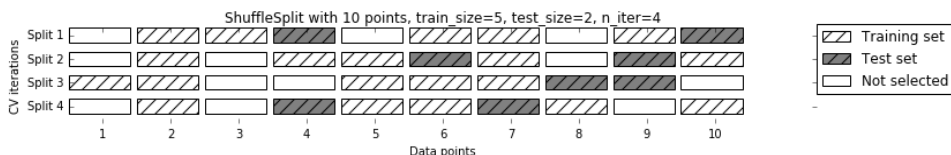
## Shuffle-Split cross-validation

Another, very flexible strategy for cross validation is *shuffle-split cross-validation*. In shuffle-split cross-validation, each split samples `train_size` many points for the training set, and `test_size` many (disjoint) point for the test set. This splitting is repeated `n_iter` many times. Figure `shuffle_split` illustrates running four iterations of splitting a dataset consisting of 10 points, with a training set of 5 points and a test set of 2 points each.

You can use integers for `train_size` and `test_size` to use absolute sizes of these sets, or floating points numbers, to use fractions of the whole dataset.

```
mglearn.plots.plot_shuffle_split()
```

`shuffle_split`



The following code splits the dataset into 50% training set and 50% test set for ten iterations:

```
from sklearn.model_selection import ShuffleSplit
shuffle_split = ShuffleSplit(test_size=.5, train_size=.5, n_iter=10)
cross_val_score(logreg, iris.data, iris.target, cv=shuffle_split)

array([ 1.    ,  0.933,  0.88  ,  0.933,  0.853,  0.973,  0.787,  0.947,

        0.92  ,  0.973])
```

Shuffle-split cross-validation allows for control over the the number of iterations independently of the training and test sizes, which can sometimes be helpful. It also allows for using only part of the data in each iteration, by providing `train_size` and `test_size` settings that don't add up to one. Subsampling the data in this way can be useful for experimenting with large datasets.

There is also a stratified variant of `ShuffleSplit`, aptly named `StratifiedShuffleSplit`, which can provide more reliable results for classification tasks.

## Cross-validation with groups

Another very common setting for cross-validation is when there are groups in the data that are highly related.

Say you want to build a system to recognize emotions from pictures of faces, and you collect a dataset of pictures of 100 people where each person is captured multiple times, showing various emotions. The goal is to build a classifier that can correctly identify emotions of people not in the dataset.

You could use the default stratified cross-validation to measure the performance of a classifier here. However, it is likely that pictures of the same person will be in the training and the test set. It will be much easier for a classifier to detect emotions in a face that is part of the training set, compared to a completely new face.

To accurately evaluate the generalization to new faces, we must therefore ensure that the training and test set contain images of different people.

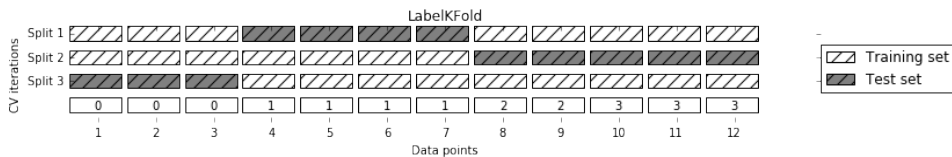
To achieve this, we can use `LabelKFold`, which takes a `label` argument, which we can use to indicate which person is in the image. So `label` here indicates groups in the data that should not be split when creating training and test set, and should not be confused with the class label.

This example of groups in the data is common in medical applications, where you might have multiple samples from the same patient, but are interested in generalizing to new patients. Similarly, in speech recognition, you might have multiple recordings of the same speaker in you dataset, but are interested in recognizing speech of new speakers.

Below is an example of using a synthetic dataset with a grouping given by the labels list. The dataset consists of 12 data points, and for each of the data points, labels specifies which group (think patient) the point belongs to. The labels specify there are four groups, and the first three samples belong to the first group, the next four samples belong to the second group, and so on. The samples don't need to be ordered by group, we just did this for illustration purposes. The splits that are calculated based on these labels are visualized in Figure label\_kfold.

As you can see, for each split, each group is either entirely in the training set, or entirely in the test set.

```
print("label_kfold")
mglearn.plots.plot_label_kfold()
```



label\_kfold

```
from sklearn.model_selection import LabelKFold
# create synthetic dataset
X, y = make_blobs(n_samples=12, random_state=0)
# assume the first three samples belong to the same group, then the next four etc.
labels = [0, 0, 0, 1, 1, 1, 1, 2, 2, 3, 3, 3]
cross_val_score(logreg, X, y, labels, cv=LabelKFold(n_folds=3))

array([ 0.75 ,  0.8  ,  0.667])
```

There are more splitting strategies for cross-validation in scikit-learn, which you can find in the scikit-learn user guide, which allow for even more different use-cases. However, the standard KFold, StratifiedKFold and LabelKFold are by far the most commonly used ones.

## Grid Search

Now that we know how to evaluate how well a model generalizes, we can do the next step and improve the model's generalization performance by tuning its parameters. We discussed the parameter settings of many of the algorithms in scikit-learn in chapters 2 and 3, and it is important to understand what the parameters mean before trying to adjust them.

Finding the values of the important parameters of a model (the ones that provide the best generalization performance) is a tricky task, but necessary for almost all models and datasets.

Because it is such a common task, there are standard methods in scikit-learn to help you with it.

The most commonly used method is *grid search*, which basically means trying all possible combinations of the parameters of interest.

Consider the case of a kernel SVM with an RBF (radial basis function) kernel, as implemented in the SVC class. As we discussed in chapter 2, there are two important parameters: the kernel bandwidth `gamma` and the regularization parameter `C`. Say we want to try values `0.001`, `0.01`, `0.1`, `1` and `10` for the parameter `C`, and the same for `gamma`. Because we have six different settings for `C` and `gamma` that we want to try, we have 36 combinations of parameters in total.

Looking at all possible combinations creates a table (or grid) of parameter settings for the SVM as shown below:

```
| |C = 0.001 | C = 0.01 | C = 0.1 | C = 1 | C = 10 |
|-----|-----|-----|-----|-----|-----|
|gamma=0.001|SVC(C=0.001, gamma=0.001)|SVC(C=0.01, gamma=0.001)|
SVC(C=0.1, gamma=0.001)|SVC(C=1, gamma=0.001)|SVC(C=10, gamma=0.001)|
|gamma=0.01|SVC(C=0.001, gamma=0.01)|SVC(C=0.01, gamma=0.01)|SVC(C=0.1,
gamma=0.01)|SVC(C=1, gamma=0.01)|SVC(C=10, gamma=0.01)|
|gamma=0.1|SVC(C=0.001, gamma=0.1)|SVC(C=0.01, gamma=0.1)|SVC(C=0.1,
gamma=0.1)|SVC(C=1, gamma=0.1)|SVC(C=10, gamma=0.1)|
|gamma=1|SVC(C=0.001, gamma=1)|SVC(C=0.01, gamma=1)|SVC(C=0.1,
gamma=1)|SVC(C=1, gamma=1)|SVC(C=10, gamma=1)|
|gamma=10|SVC(C=0.001, gamma=10)|SVC(C=0.01, gamma=10)|SVC(C=0.1,
gamma=10)|SVC(C=1, gamma=10)|SVC(C=10, gamma=10)|
```

## Simple Grid-Search

We can implement a simple grid-search just as for-loops over the two parameters, training and evaluating a classifier for each combination:

```
# naive grid search implementation
from sklearn.svm import SVC
X_train, X_test, y_train, y_test = train_test_split(iris.data, iris.target, random_state=0)
print("Size of training set: %d size of test set: %d" % (X_train.shape[0], X_test.shape[0]))

best_score = 0

for gamma in [0.001, 0.01, 0.1, 1, 10, 100]:
    for C in [0.001, 0.01, 0.1, 1, 10, 100]:
        # for each combination of parameters
```

```

# train an SVC
svm = SVC(gamma=gamma, C=C)
svm.fit(X_train, y_train)
# evaluate the SVC on the test set
score = svm.score(X_test, y_test)
# if we got a better score, store the score and parameters
if score > best_score:
    best_score = score
    best_parameters = {'C': C, 'gamma': gamma}

print("best score: ", best_score)
print("best parameters: ", best_parameters)

Size of training set: 112   size of test set: 38

best score:  0.973684210526

best parameters:  {'C': 100, 'gamma': 0.001}

best_score
0.97368421052631582

```

## The danger of overfitting the parameters and the validation set

Given this result, we might be tempted to report that we found a model that performs 97.3% accurate on our dataset. However, this claim could be overly optimistic (or just wrong) for the following reason: we tried many different parameters, and selected the one with best accuracy on the test set. However, that doesn't mean that this accuracy carries over to new data.

Because we used the test data to adjust the parameters, we can no longer use it to assess how good the model is. This is the same reason we needed to split the data into training and test set in the first place; we need an independent data set to evaluate, one that was not used to create the model.

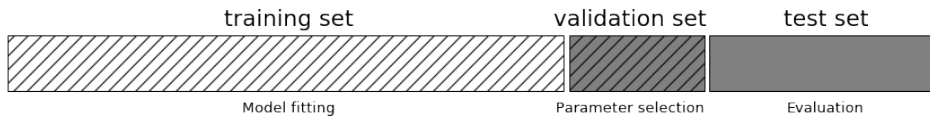
One way to resolve this problem is to split the data again, so we have three sets: the training set to build the model, the validation (or development) set to select the parameters of the model, and the test set, to evaluate the performance of the selected parameters, as shown in Figure `threefold_split` below.

After selecting the best parameters using the validation set, we can rebuild a model using the parameters settings we found, but now training on both the training data and the validation data. This way, we can use as much data as possible to build our model.

```

print("threefold_split")
mglearn.plots.plot_threefold_split()

```



threefold\_split

This leads to the following implementation:

```

from sklearn.svm import SVC
# split data into train+validation set and test set
X_trainval, X_test, y_trainval, y_test = train_test_split(iris.data, iris.target, random_state=0)
# split train+validation set into training and validation set
X_train, X_valid, y_train, y_valid = train_test_split(X_trainval, y_trainval, random_state=1)

print("Size of training set: %d   size of validation set: %d   size of test set: %d" % (X_train.shape[0],
best_score = 0

for gamma in [0.001, 0.01, 0.1, 1, 10, 100]:
    for C in [0.001, 0.01, 0.1, 1, 10, 100]:
        # for each combination of parameters
        # train an SVC
        svm = SVC(gamma=gamma, C=C)
        svm.fit(X_train, y_train)
        # evaluate the SVC on the test set
        score = svm.score(X_valid, y_valid)
        # if we got a better score, store the score and parameters
        if score > best_score:
            best_score = score
            best_parameters = {'C': C, 'gamma': gamma}

# rebuild a model on the combined training and validation set, and evaluate it on the test set
svm = SVC(**best_parameters)
svm.fit(X_trainval, y_trainval)
test_score = svm.score(X_test, y_test)
print("best score on validation set: ", best_score)
print("best parameters: ", best_parameters)
print("test set score with best parameters: ", test_score)

Size of training set: 84   size of validation set: 28   size of test set: 38

best score on validation set:  0.964285714286

best parameters:  {'C': 10, 'gamma': 0.001}

test set score with best parameters:  0.921052631579

```

The best score on the validation set is 96.4%: slightly lower than before, probably because we used less data to train the model ( $X_{\text{train}}$  is smaller now because we split our dataset twice).



However, the score on the test set - the score that actually tells us how well we generalize - is even lower, at 92%.

So we can only claim to classify new data 92% correctly, not 97% correctly as we thought before!

The distinction between the training set, validation set and test set is fundamentally important to apply machine learning methods in practice. Any choices made based on the test set accuracy “leak” information from the test set into the model.

Therefore, it is important to keep a separate test set, which is only used for the final evaluation. It is good practice to do all exploratory analysis and model selection using the combination of a training and a validation set, and reserve the test set for a final evaluation---this is even true for exploratory visualization. Strictly speaking, evaluating more than one model on the test set and choosing the better of the two will result in an overly optimistic estimate of how accurate the model is.

## Grid-search with cross-validation

While the above method of splitting the data into a training, a validation and a test set is workable, and relatively commonly used, it is quite sensitive to how exactly the data is split. From the output of the code [FIXME Reference code above] we can see that GridSearchCV selects 'C': 10, 'gamma': 0.01 as the best parameters, while the output of the code in [FIXME Reference code two up] selects 'C': 10, 'gamma': 0.001 as the best parameters. For a better estimate of the generalization performance, instead of using a single split into a training and a validation set, we can use cross-validation to evaluate the performance of each parameter combination.

This method can be coded up as follows:

```
# reference: manual_grid_search_cv
for gamma in [0.001, 0.01, 0.1, 1, 10, 100]:
    for C in [0.001, 0.01, 0.1, 1, 10, 100]:
        # for each combination of parameters
        # train an SVC
        svm = SVC(gamma=gamma, C=C)
        # perform cross-validation
        scores = cross_val_score(svm, X_trainval, y_trainval, cv=5)
        # compute mean cross-validation accuracy
        score = np.mean(scores)
        # if we got a better score, store the score and parameters
        if score > best_score:
            best_score = score
            best_parameters = {'C': C, 'gamma': gamma}
# rebuild a model on the combined training and validation set
svm = SVC(**best_parameters)
svm.fit(X_trainval, y_trainval)
```

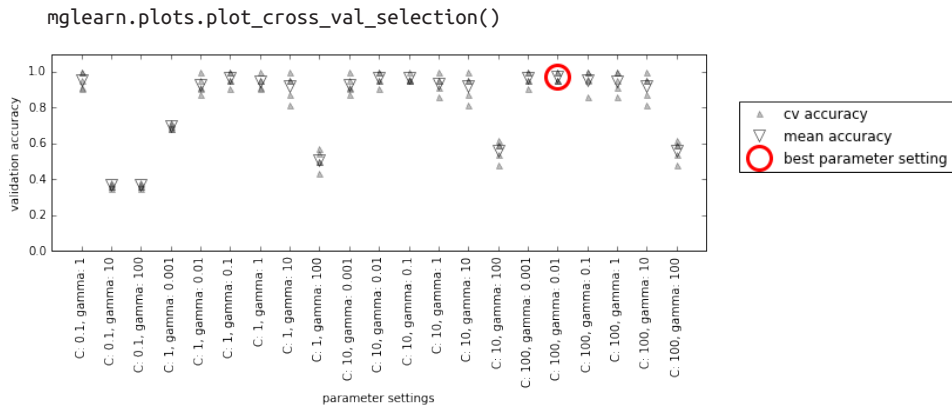
```
SVC(C=100, cache_size=200, class_weight=None, coef0=0.0,
    decision_function_shape=None, degree=3, gamma=0.01, kernel='rbf',
    max_iter=-1, probability=False, random_state=None, shrinking=True,
    tol=0.001, verbose=False)
```

To evaluate the accuracy of the SVM using a particular setting of C and gamma using five-fold cross-validation we need to train  $36 * 5 = 180$  models. As you can imagine, the main down-side of the use of cross-validation is the time it takes to train all these models.

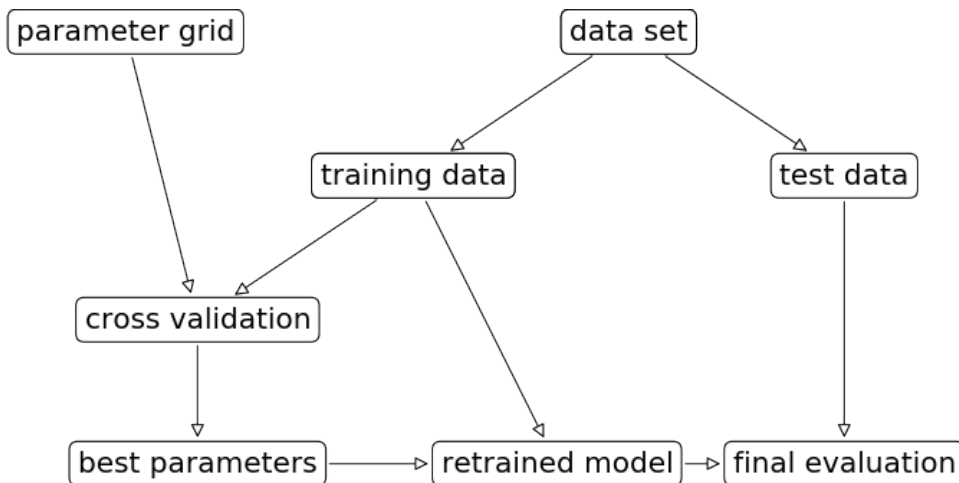
Figure `cross_val_selection` illustrates how the best parameter setting is selected in the code above. For each parameter setting (only a subset is shown), five accuracy values are computed, one for each split in the cross validation. Then the mean validation accuracy is computed for each parameter setting. The parameters with the highest mean validation accuracy are chosen, marked by the circle.

[warning / note box] As we said above, cross-validation is a way to evaluate a given algorithm on a specific dataset.

However, it is often used in conjunction with parameter search methods like grid search. For this reason, many people colloquially use the term `cross-validation` to refer to grid-search with cross-validation. [/end warning box]



`mglearn.plots.plot_grid_search_overview()`



Because grid-search with cross-validation is such a commonly used method to adjust parameters scikit-learn provides the `GridSearchCV` class that implements it in the form of an estimator. To use the `GridSearchCV` class, you first need to specify the parameters you want to search over using a dictionary. `GridSearchCV` will then perform all the necessary model fits. The keys of the dictionary are the names of parameters we want to adjust (as given when constructing the model), in this case `C` and `gamma`, and the values are the parameter settings we want to try out. Trying the values `0.001`, `0.01`, `0.1`, `1`, `10` and `100` for `C` and `gamma` translates to the following dictionary:

```

param_grid = {'C': [0.001, 0.01, 0.1, 1, 10, 100],
              'gamma': [0.001, 0.01, 0.1, 1, 10, 100]}
param_grid
{'C': [0.001, 0.01, 0.1, 1, 10, 100], 'gamma': [0.001, 0.01, 0.1, 1, 10, 100]}

```

We can now instantiate the `GridSearchCV` class with the model `SVC`, the parameter grid to search `param_grid`, and the cross-validation strategy we want to use, say 5 fold (stratified) cross-validation:

```

from sklearn.model_selection import GridSearchCV
from sklearn.svm import SVC
grid_search = GridSearchCV(SVC(), param_grid, cv=5)

```

`GridSearchCV` will use cross-validation in place of the split into a training and validation set that we used before. However, we still need to split the data into a training and a test set, to avoid overfitting the parameters:

```
X_train, X_test, y_train, y_test = train_test_split(iris.data, iris.target, random_state=0)
```

The `grid_search` object that we created behaves just like a classifier; we can call the standard methods `fit`, `predict` and `score` on it [footnote: A scikit-learn estimator that is created using another estimator is called a meta-estimator in scikit-learn. `GridSearchCV` is the most commonly used meta-estimator, but we will see more later.]. However, when we call `fit`, it will run cross-validation for each combination of parameters we specified in `param_grid`.

```
grid_search.fit(X_train, y_train)

GridSearchCV(cv=5, error_score='raise',

             estimator=SVC(C=1.0, cache_size=200, class_weight=None, coef0=0.0,
                           decision_function_shape=None, degree=3, gamma='auto', kernel='rbf',
                           max_iter=-1, probability=False, random_state=None, shrinking=True,
                           tol=0.001, verbose=False),

             fit_params={}, iid=True, n_jobs=1,

             param_grid={'C': [0.001, 0.01, 0.1, 1, 10, 100], 'gamma': [0.001, 0.01, 0.1, 1, 10, 100]},

             pre_dispatch='2*n_jobs', refit=True, scoring=None, verbose=0)
```

Fitting the `GridSearchCV` object not only searches for the best parameters, it also automatically fits a new model on the whole training dataset with the parameters that yielded the best cross-validation performance. What happens in `fit` is therefore equivalent with FIXME reference `manual_grid_search_cv`. The `GridSearchCV` class provides a very convenient interface to access the retrained model using the `predict` and `score` methods. To evaluate how well the best found parameters generalize, we can call `score` on the test set:

```
grid_search.score(X_test, y_test)

0.97368421052631582
```

Choosing the parameters using cross-validation, we actually found a model that achieves 97.3% accuracy on the test set. The important part here is that we *did not use the test set* to choose the parameters.

The parameters that were found are scored in the `best_params_` attribute, and the best cross-validation accuracy (the mean accuracy over the different splits for this parameter setting) is stored in `best_score_`:

```
print(grid_search.best_params_)
print(grid_search.best_score_)
```

```
{'C': 100, 'gamma': 0.01}
```

```
0.973214285714
```

[warning box]

Again, be careful not to confuse `best_score_` with the generalization performance of the model as computed by the `score` method on the test set. Using the `score` method (or evaluating the output of the `predict` method) employs a model *trained on the whole training set*. The `best_score_` attribute stores the mean validation cross-validation accuracy, with *cross-validation performed on the training set*.

[/end warning box]

Sometimes it is helpful to have access to the actual model that was found, for example to look at coefficients or feature importances. You can access the model with the best parameters trained on the whole training set using the `best_estimator_` attribute:

```
grid_search.best_estimator_  
SVC(C=100, cache_size=200, class_weight=None, coef0=0.0,  
    decision_function_shape=None, degree=3, gamma=0.01, kernel='rbf',  
    max_iter=-1, probability=False, random_state=None, shrinking=True,  
    tol=0.001, verbose=False)
```

Because `grid_search` itself has `predict` and `score` methods, using `best_estimator_` is not needed to make predictions or evaluate the model.

## Analyzing the result of cross-validation

It is often helpful to visualize the results of cross-validation, to understand how the model generalization depends on the parameters we are searching. As grid-searches are quite computationally expensive to run, often it is a good idea to start with a relatively coarse and small grid.

We can then inspect the results of the cross-validated grid-search, and possibly expand our search.

The results of a grid search can be found in the `grid_scores_` attribute:

```
grid_search.grid_scores_  
[mean: 0.36607, std: 0.01137, params: {'C': 0.001, 'gamma': 0.001},  
 mean: 0.36607, std: 0.01137, params: {'C': 0.001, 'gamma': 0.01},  
 mean: 0.36607, std: 0.01137, params: {'C': 0.001, 'gamma': 0.1},  
 mean: 0.36607, std: 0.01137, params: {'C': 0.001, 'gamma': 1},
```

mean: 0.36607, std: 0.01137, params: {'C': 0.001, 'gamma': 10},  
mean: 0.36607, std: 0.01137, params: {'C': 0.001, 'gamma': 100},  
mean: 0.36607, std: 0.01137, params: {'C': 0.01, 'gamma': 0.001},  
mean: 0.36607, std: 0.01137, params: {'C': 0.01, 'gamma': 0.01},  
mean: 0.36607, std: 0.01137, params: {'C': 0.01, 'gamma': 0.1},  
mean: 0.36607, std: 0.01137, params: {'C': 0.01, 'gamma': 1},  
mean: 0.36607, std: 0.01137, params: {'C': 0.01, 'gamma': 10},  
mean: 0.36607, std: 0.01137, params: {'C': 0.01, 'gamma': 100},  
mean: 0.36607, std: 0.01137, params: {'C': 0.1, 'gamma': 0.001},  
mean: 0.69643, std: 0.01333, params: {'C': 0.1, 'gamma': 0.01},  
mean: 0.91964, std: 0.04442, params: {'C': 0.1, 'gamma': 0.1},  
mean: 0.95536, std: 0.03981, params: {'C': 0.1, 'gamma': 1},  
mean: 0.36607, std: 0.01137, params: {'C': 0.1, 'gamma': 10},  
mean: 0.36607, std: 0.01137, params: {'C': 0.1, 'gamma': 100},  
mean: 0.69643, std: 0.01333, params: {'C': 1, 'gamma': 0.001},  
mean: 0.92857, std: 0.04278, params: {'C': 1, 'gamma': 0.01},  
mean: 0.96429, std: 0.03405, params: {'C': 1, 'gamma': 0.1},  
mean: 0.94643, std: 0.03251, params: {'C': 1, 'gamma': 1},  
mean: 0.91964, std: 0.06507, params: {'C': 1, 'gamma': 10},  
mean: 0.50893, std: 0.04666, params: {'C': 1, 'gamma': 100},  
mean: 0.92857, std: 0.04278, params: {'C': 10, 'gamma': 0.001},  
mean: 0.96429, std: 0.03405, params: {'C': 10, 'gamma': 0.01},  
mean: 0.96429, std: 0.01793, params: {'C': 10, 'gamma': 0.1},  
mean: 0.93750, std: 0.04556, params: {'C': 10, 'gamma': 1},  
mean: 0.91964, std: 0.06507, params: {'C': 10, 'gamma': 10},  
mean: 0.56250, std: 0.04966, params: {'C': 10, 'gamma': 100},

```

mean: 0.96429, std: 0.03405, params: {'C': 100, 'gamma': 0.001},
mean: 0.97321, std: 0.02234, params: {'C': 100, 'gamma': 0.01},
mean: 0.95536, std: 0.04983, params: {'C': 100, 'gamma': 0.1},
mean: 0.94643, std: 0.05199, params: {'C': 100, 'gamma': 1},
mean: 0.91964, std: 0.06507, params: {'C': 100, 'gamma': 10},
mean: 0.56250, std: 0.04966, params: {'C': 100, 'gamma': 100}]

```

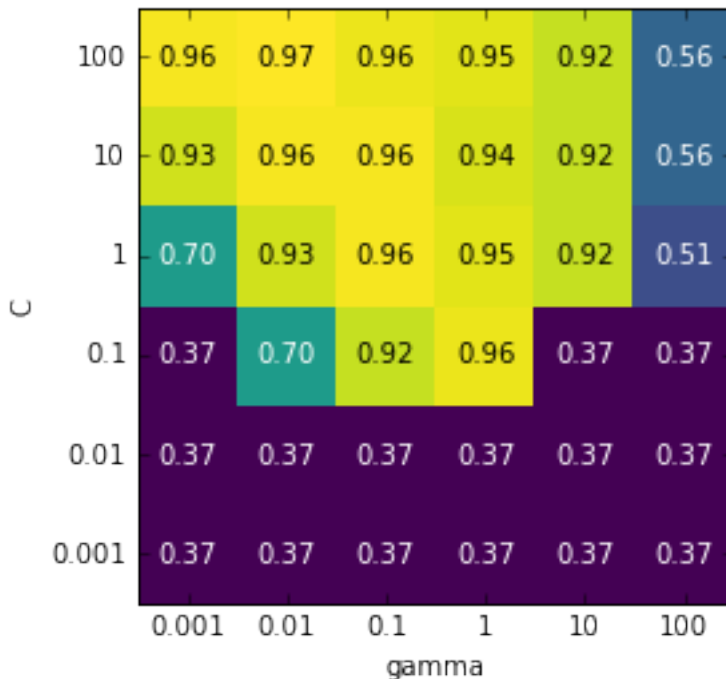
This attribute contains the mean cross-validation accuracy (and its standard deviation) for all parameter settings that we tried. As we were searching a two-dimensional grid of parameters ('C' and 'gamma'), this is best visualized as a heat map. First, we extract the mean validation scores, then we reshape the scores so that the axes correspond to C and gamma:

```

scores = [score.mean_validation_score for score in grid_search.grid_scores_]
scores = np.array(scores).reshape(6, 6)

# plot the mean cross-validation scores
mglearn.tools.heatmap(scores, xlabel='gamma', ylabel='C', xticklabels=param_grid['gamma'],
                      yticklabels=param_grid['C'], cmap="viridis")

```



Each point in the heat map corresponds to one run of cross-validation, with a particular parameter setting. The color encodes the cross-validation accuracy, with light colors meaning high accuracy, and dark colors meaning low accuracy.

You can see that SVC is very sensitive to the setting of the parameters. For many of the parameter settings, the accuracy is around 40%, which is quite bad; for other settings the accuracy is around 96%.

We can take away from this plot several things. First, the parameters we adjusted are *very important* for obtaining good performance. Both parameters `C` and `gamma` matter a lot, as adjusting them can change the accuracy from 40% to 96%. Also, the ranges we picked for the parameters are ranges in which we see significant changes in the outcome. It's also important to note that the ranges for the parameters are large enough: the optimum values for each parameter is not on the edge of the plot.

Figure `gridsearch_failures` shows some plots where the result is less ideal, because the search ranges were not chosen properly.

```
fig, axes = plt.subplots(1, 3, figsize=(13, 5))

param_grid_linear = {'C': np.linspace(1, 2, 6),
                    'gamma': np.linspace(1, 2, 6)}

param_grid_one_log = {'C': np.linspace(1, 2, 6),
                    'gamma': np.logspace(-3, 2, 6)}

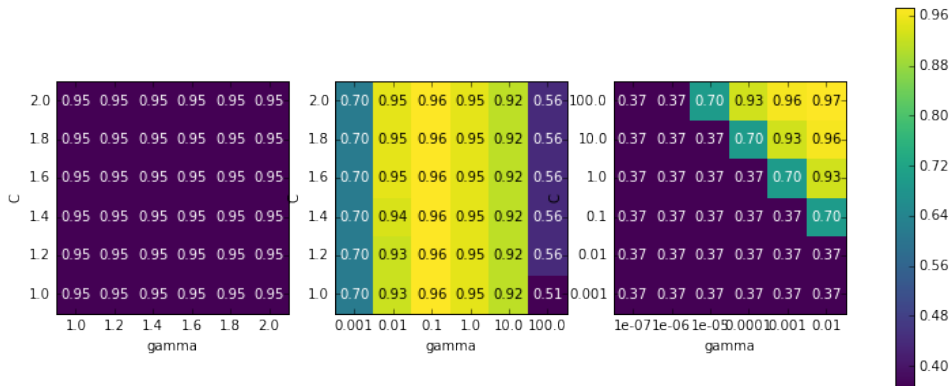
param_grid_range = {'C': np.logspace(-3, 2, 6),
                   'gamma': np.logspace(-7, -2, 6)}

for param_grid, ax in zip([param_grid_linear, param_grid_one_log,
                          param_grid_range], axes):
    grid_search = GridSearchCV(SVC(), param_grid, cv=5)
    grid_search.fit(X_train, y_train)
    scores = [score.mean_validation_score for score in grid_search.grid_scores_]
    scores = np.array(scores).reshape(6, 6)

    # plot the mean cross-validation scores
    scores_image = mglearn.tools.heatmap(scores, xlabel='gamma', ylabel='C',
                                       xticklabels=param_grid['gamma'],
                                       yticklabels=param_grid['C'], cmap="viridis", ax=ax)

plt.colorbar(scores_image, ax=axes.tolist())
print("gridsearch_failures")
```





### gridsearch\_failures

The first panel shows no changes at all, with a constant color over the whole parameter grid. This is caused by improper scaling and range of the parameters `C` and `gamma`. However, if no change in accuracy is visible over the different parameter settings, it could also be that a parameter is just not important at all. It is usually good to try very extreme values first, to see if there are any changes in the accuracy as a result of changing a parameter.

The second panel shows a vertical stripe pattern. This indicates that only the setting of the `gamma` parameter makes any difference. This could mean that the `gamma` parameter is searching over interesting values, but the `C` parameter is not -- or it could mean the `C` parameter is not important at all.

The third panel shows changes in both `C` and `gamma`. However, we can see that in the top right of the plot, nothing interesting is happening. We can probably exclude the very small values from future grid-searches. The optimum parameter setting is on the bottom right. As the optimum is in the border of the plot, we can expect that there might be even better values beyond this border, and we might want to change our search range to include more parameters in this region.

Tuning the parameter grid based on the cross-validation scores is perfectly fine, and a good way to explore the importance of different parameters. However, you should not test different parameter ranges on the the final test set--as we discussed above, evaluation of the test set should happen only once we know exactly what model we want to use.

## Using different cross-validation strategies with grid-search

Similarly to `cross_val_score`, `GridSearchCV` uses stratified k-fold cross-validation by default for classification, and k-fold cross-validation for regression. However, you

can also pass any cross-validation splitter, as described in section XX as the `cv` parameter in `GridSearchCV`.

In particular, to get only a single split into a training and validation set, you can use `ShuffleSplit` or `StratifiedShuffleSplit` with `n_iter=1`. This might be helpful for very large datasets, or very slow models.

## Nested cross-validation

In the above examples, we went from using single split of the data into a training, validation and test set to spitting the data into training and test sets, and then performing cross-validation on the training set. When using `GridSearchCV` as above, we still have a single split of the data in training and test set however, which might still make our results unstable, and may make us depend too much on this single split of the data.

We can go a step further, and instead of splitting the original data into training and test set once, we use multiple splits of cross-validation. This will result in what is called *nested cross-validation*. In nested cross-validation, there is an outer loop over splits of the data into training and test set. For each of them, a grid-search is run (which might result in different best parameters for each split in the outer loop). Then, for each outer split, the test set score using the best settings is reported.

The result of this procedure is a list of scores, not a model, and not a parameter setting. The scores tell us how well a model generalizes, given the best parameters found by grid-search. As it doesn't provide a model that can be used on new data, nested cross-validation is rarely used when looking for a predictive model to apply to future data.

It can be good to evaluate how good a given model works on a particular dataset, though.

Implementing nested cross-validation in scikit-learn is straightforward; we call `cross_val_score` with an instance of `GridSearchCV` as the model:

```
scores = cross_val_score(GridSearchCV(SVC(), param_grid, cv=5), iris.data, iris.target, cv=5)
print("Cross-validation scores: ", scores)
print("Mean cross-validation score: ", scores.mean())

Cross-validation scores: [ 0.967  1.      0.967  0.967  1.    ]

Mean cross-validation score: 0.98
```

The result of our nested cross-validation can be summarized as “SVC can achieve 98% mean cross-validation accuracy on the iris dataset” - nothing more and nothing less.

Here, we used stratified five-fold cross validation in both the inner and the outer loop. As our `param_grid` contains 36 combinations of parameters, this results in a whopping  $36 * 5 * 5 = 900$  models being build, making nested cross-validation a very expensive procedure. Here, we used the same cross-validation splitter in the inner and outer loop; however, this is not necessary and you can use any combination of cross-validation strategies in the inner and outer loop. It can be a bit tricky to understand what is happening in the single line given above, and it can be helpful to visualize it as for loops, as done in simplified implementation given below:

```
def nested_cv(X, y, inner_cv, outer_cv, Classifier, parameter_grid):
    outer_scores = []
    # for each split of the data in the outer cross-validation
    # (split method returns indices)
    for training_samples, test_samples in outer_cv.split(X, y):
        # find best parameter using inner cross-validation:
        best_parms = {}
        best_score = -np.inf
        # iterate over parameters
        for parameters in parameter_grid:
            # accumulate score over inner splits
            cv_scores = []
            # iterate over inner cross-validation
            for inner_train, inner_test in inner_cv.split(X[training_samples], y[training_samples]):
                # build classifier given parameters and training data
                clf = Classifier(**parameters)
                clf.fit(X[inner_train], y[inner_train])
                # evaluate on inner test set
                score = clf.score(X[inner_test], y[inner_test])
                cv_scores.append(score)
            # compute mean score over inner folds
            mean_score = np.mean(cv_scores)
            if mean_score > best_score:
                # if better than so far, remember parameters
                best_score = mean_score
                best_parms = parameters
        # build classifier on best parameters using outer training set
        clf = Classifier(**best_parms)
        clf.fit(X[training_samples], y[training_samples])
        # evaluate
        outer_scores.append(clf.score(X[test_samples], y[test_samples]))
    return outer_scores

from sklearn.model_selection import ParameterGrid, StratifiedKFold
nested_cv(iris.data, iris.target, StratifiedKFold(5), StratifiedKFold(5), SVC, ParameterGrid(parameters=[0.9666666666666667, 1.0, 0.9666666666666667, 0.9666666666666667, 1.0])
```

## Parallelizing cross-validation and grid-search

While running grid-search over many parameters and on large datasets can be computationally challenging, it is also *embarrassingly parallel*. This means that building a

model using a particular parameter setting on a particular cross-validation split can be done completely independently from the other parameter settings and models.

This makes grid-search and cross-validation ideal candidates for parallelization over multiple CPU cores or over a cluster. You can make use of multiple cores in `GridSearchCV` and `cross_val_score` by setting the `n_jobs` parameter to the number of CPU cores you want to use. You can set `n_jobs=-1` to use all available cores.

You should be aware that scikit-learn *does not allow nesting of parallel operations*. So if you are using the `n_jobs` option on your model (for example a random forest), you cannot use it in `GridSearchCV` to search over this model.

If your dataset and model are very large, it might be that using many cores uses up too much memory, and you should monitor your memory usage when building large models in parallel.

It is also possible to parallelize grid-search and cross-validation over multiple machines in a cluster. However, at the time of writing, this is not supported within scikit-learn. It is, however, possible to use the IPython parallel framework for parallel grid-searches, if you don't mind writing the for-loop over parameters as in [reference "naive implementation"] yourself.

For spark users, there is also the recently developed `spark-sklearn` package [footnote <https://github.com/databricks/spark-sklearn>] which allows running grid-search over an already established spark cluster.

## Evaluation Metrics and scoring

So far, we always evaluated classification performance using accuracy (the fraction of correctly classified samples) and regression performance using  $R^2$ . However, these are only two of the many possible ways to summarize how well a supervised model performs on a given dataset.

In practice, these evaluation metrics might not be appropriate for your application, and it is important to choose the right metric when selecting between models and adjusting hyper-parameters.

### Keep the end-goal in mind

When selecting a metric, you should always have the end-goal of the machine learning application in mind. In practice, we are usually not interested in just making accurate predictions, but in using these predictions as part of a larger decision making process. Before picking a machine learning metric, you should think about what the high-level goal of the application is, often called *business metric*. The consequences of choosing a particular algorithm for a machine learning application has is called the *business impact*. [Footnote: We ask scientific minded readers to excuse the

commercial language in this section. Not losing track of the end-goal is equally important in science, though the authors are not aware of a similar phrase as “business impact” being used in the sciences.] Maybe this is avoiding traffic accidents, or decreasing the number of hospital admissions. It could also be getting more users for your website, or having users spend more money in your shop. When choosing models or adjusting parameters, you should then pick the model that has the most positive influence on the business metric.

Often this is hard, as assessing the business impact of a particular model might require putting it in production in a real-life system. In the early stages of development, and for adjusting parameters, it is often infeasible to put models into production just for testing purposes, because of high business risk or personal risks that can be involved. Imagine evaluating the pedestrian avoidance capabilities of a self-driving car by just letting it drive around, without verifying it first; if your model is bad, pedestrians will be in trouble!

Therefore we often need to find some surrogate evaluation procedure, using an evaluation metric that is easier to compute. For example, we could test classifying images of pedestrians against non-pedestrians and measure accuracy. Keep in mind that this is only a surrogate, and it pays off to find the closest metric to the original business goal that is feasible to evaluate. This closest metric should be used whenever possible for model evaluations and selection. This evaluation might not be a single number---the consequence of your algorithm could be that you have 10% more customers, but each customer will spend 15% less---but it should capture the expected business impact of choosing one model over another.

We will first discuss metrics for the important special case of binary classification, then multi-class classification, and finally regression.

## Metrics for binary classification

Binary classification is arguably the most common and conceptually simple application of machine learning in practice. However, there are still a number of caveats in evaluating even this simple task.

Before we dive into alternative metrics, let’s have a look into the ways in which measuring accuracy might be misleading.

Remember that for binary classification, we often speak of a *positive* class and a *negative* class, with the understanding that the positive class is the one we are “looking for”.

### Kinds of Errors

Often, accuracy is not a good measure of predictive performance, as the number of mistakes we make does not contain all the information we are interested in.

Imagine an application to screen for the early detection of cancer using an automated test. If the test is negative, the patient will be assumed healthy, while if the test is positive, the patient will undergo additional screening.

Here, we would call a positive test (indication of cancer) the positive class, and a negative test the negative class.

We can't assume that our model will always work perfectly, and it will make mistakes. For any application, we need to ask ourselves what the consequence of these mistakes are in the real world.

One possible mistake is that a healthy patient will be classified as positive, leading to additional testing. This leads to some costs and a slight inconvenience for the patient. Making an incorrect positive prediction is called a *false positive*.

The other possible mistake is that a sick patient will be classified as negative, and will not receive further tests and treatment. The undiagnosed cancer might lead to serious health issues, and could even be fatal. Making a mistake of this kind, an incorrect negative prediction is called a *false negative*.

In this particular example, it is clear that we want to avoid false negatives as much as possible, while false positives just create a minor nuisance.

While this is a particularly drastic example, the consequence of false positives and false negatives are rarely the same. In commercial applications, it might be possible to assign dollar values to both kinds of mistakes, which would allow measuring the error of a particular prediction in dollars, instead of accuracy - which might be much more meaningful for making business decisions on which model to use.

## Imbalanced datasets

Types of errors in particular play an important role when one of two classes is much more frequent than the other one. This is very common in practice; a good example for this is click-through prediction, where each data point represents an “impression”, an item that was shown to a user. This item might be an ad, or a related story, or a related person to follow on a social media site. The goal is to predict whether, if shown a particular item, a user will click on it (indicating they are interested).

Most things users are shown on the internet (in particular, ads) will not result in a click. You might need to show a user 100 ads or articles before they find something interesting enough to click on.

This results in a dataset where for each 99 “no click” data points, there is 1 “clicked” data point; in other words, 99% of the samples belong to the “no click” class. Datasets in which one class is much more frequent than the other are often called *imbalanced dataset*, or *datasets with imbalanced classes*.

In reality, imbalanced data is the norm, and it is rare that the events of interest have equal or even similar frequency in the data.

Now let's say you build a classifier that is 99% accurate on the click prediction task. What does that tell you? 99% accuracy sounds impressive, but this doesn't take the class imbalance into account. You can achieve 99% accuracy without building a machine learning model, by always predicting "no click". On the other hand, even with imbalanced data, a 99% accurate model could in fact be quite good. However, accuracy doesn't allow us to distinguish the constant "no click" model and a potentially good model.

To illustrate, we create a 9:1 imbalanced dataset from the digits dataset, by classifying the digit four against the nine other classes:

```
from sklearn.datasets import load_digits

digits = load_digits()
y = digits.target == 9

X_train, X_test, y_train, y_test = train_test_split(
    digits.data, y, random_state=0)
```

We can use the `DummyClassifier` to always predict the majority class (here "not four") to see how uninformative accuracy can be:

```
from sklearn.dummy import DummyClassifier
dummy_majority = DummyClassifier(strategy='most_frequent').fit(X_train, y_train)
pred_most_frequent = dummy_majority.predict(X_test)
print("predicted labels: %s" % np.unique(pred_most_frequent))
print("score: %f" % dummy_majority.score(X_test, y_test))

predicted labels: [False]

score: 0.895556
```

We obtained close to 90% accuracy without learning anything. This might seem striking. Imagine someone telling you their model is 90% accurate. You might think they did a very good job. But depending on the problem, that might be possible by just predicting one class! Let's compare this against using an actual classifier:

```
from sklearn.tree import DecisionTreeClassifier
tree = DecisionTreeClassifier(max_depth=2).fit(X_train, y_train)
pred_tree = tree.predict(X_test)
tree.score(X_test, y_test)

0.9177777777777778
```

According to accuracy, the `GaussianNB` model is clearly worse than the constant predictor! This could either indicate that something is wrong with how we use `GaussianNB` or that accuracy is in fact not a good measure here.

For comparison purposes, we evaluate two more classifiers: SVC and the default Dummy Classifier which makes random predictions, but producing classes with the same proportions as in the training set:

```
from sklearn.linear_model import LogisticRegression

dummy = DummyClassifier().fit(X_train, y_train)
pred_dummy = dummy.predict(X_test)
print("dummy score: %f" % dummy.score(X_test, y_test))

logreg = LogisticRegression(C=0.1).fit(X_train, y_train)
pred_logreg = logreg.predict(X_test)
print("logreg score: %f" % logreg.score(X_test, y_test))

dummy score: 0.808889

logreg score: 0.977778
```

The dummy that produces random output is still better than the GaussianNB, while LogisticRegression produces very good results.

Clearly accuracy is an inadequate measure to quantify predictive performance in this imbalanced setting. For the rest of this chapter, we will explore alternative metrics that provide better guidance in selecting models. In particular, we would like to have metrics that tell us how much better a model is than making “most frequent” predictions or random predictions, as they are computed in `pred_most_frequent` and `pred_dummy`. If we use a metric to assess our models, it should definitely be able to weed out these nonsense predictions.

## Confusion matrices

One of the most comprehensive ways to represent the result of evaluating binary classification is using confusion matrices. Let’s inspect the predictions of LogisticRegression above using the `confusion_matrix` function. We already stored the predictions on the test set in `pred_logreg`.

```
from sklearn.metrics import confusion_matrix

confusion = confusion_matrix(y_test, pred_logreg)
print(confusion)

[[401  2]

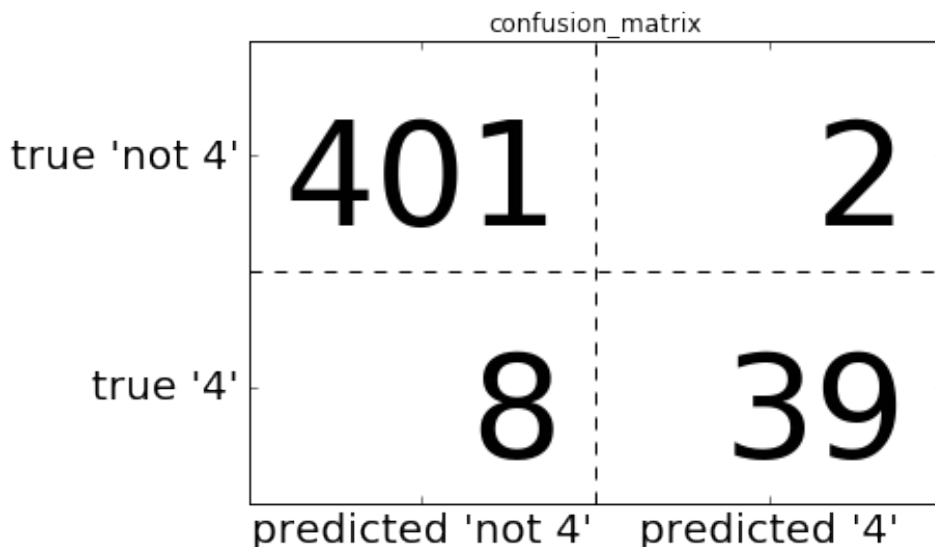
 [ 8 39]]
```

The output of `confusion_matrix` is a two by two array, where the rows correspond to the true classes, and the columns corresponds to the predicted classes. Each entry counts for how many data points in the class given by the row the prediction was the class given by the column.



Figure `confusion_matrix` below illustrates this meaning:

```
mglearn.plots.plot_confusion_matrix_illustration()
```

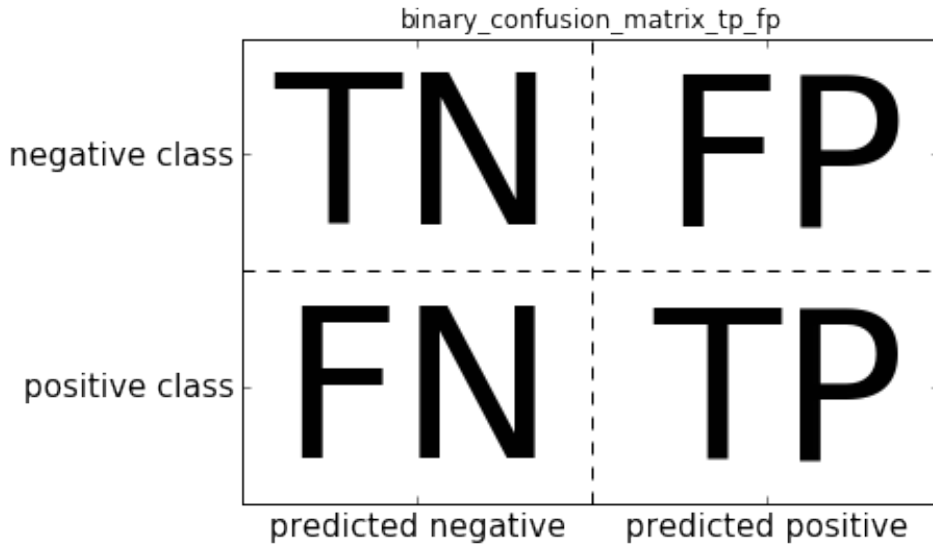


This means of the 403 data points (sum of the first row) that are not a four, 401 got predicted correctly as such, and two of which were incorrectly predicted as a four. Similarly there are 47 data points that are fours, 39 of which got correctly classified, and 8 of which were predicted incorrectly as not a four.

Entries on the main diagonal [footnote: The main diagonal of a two-dimensional array or matrix  $A$  are  $A[i, i]$ ] of the confusion matrix correspond to correct classifications, while other entries tell us how many samples of one class got mistakenly classified as another class.

If we declare “being a four” the positive class, we can relate the entries of the confusion matrix with the terms *false positives* and *false negatives* that we introduced earlier. To complete the picture, we call correctly classified samples belonging to the positive class *true positives* and correctly classified samples of the negative class *true negatives*. These terms are usually abbreviated FP, FN, TP and TN and lead to the following interpretation for the confusion matrix:

```
mglearn.plots.plot_binary_confusion_matrix()
```



Now let's use the confusion matrix to compare the models we fitted above, the two dummy models, the decision tree and the logistic regression:

```
print("Most frequent class:")
print(confusion_matrix(y_test, pred_most_frequent))
print("\nDummy model:")
print(confusion_matrix(y_test, pred_dummy))
print("\nDecision tree:")
print(confusion_matrix(y_test, pred_tree))
print("\nLogistic Regression")
print(confusion_matrix(y_test, pred_logreg))
```

Most frequent class:

```
[[403  0]
 [ 47  0]]
```

Dummy model:

```
[[377 26]
 [ 42  5]]
```

Decision tree:

```
[[390 13]
```

[ 24 23]]

Logistic Regression

[[401 2]

[ 8 39]]

Looking at the confusion matrix, it is quite clear that something is wrong with `pred_most_frequent`, because it always predicts the same class. `pred_dummy` on the other hand has a very small number of true positives (3) in particular compared to the number of false negatives and false positives - there are many more false positives than true positives!

The predictions made by the tree make much more sense than the dummy predictions, even though the accuracy was nearly the same. Finally, we can see that logistic regression does better than tree in all aspects: it has more true positives and true negatives while having fewer false positives and false negatives.

From this comparison, it is clear that only the tree and the logistic regression give reasonable results, and that the logistic regression works better than the tree on all accounts.

However, inspecting the full confusion matrix is a bit cumbersome, and while we gained a lot of insight from looking at all aspects of the matrix, the process was very manual and qualitative.

There are several ways to summarize the information in the confusion matrix, which we will discuss next.

**Relation to accuracy.** We already saw one way to summarize the result in the confusion matrix, by computing accuracy, which can be expressed as

$$\begin{equation} \text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}} \end{equation}$$

In other words: accuracy is the number of correct prediction (TP and TN) divided by the number of all samples (all entries of the confusion matrix summed up).

### Precision, recall and f-score

There are several other ways to summaries the confusion matrix, with the most common one being *precision* and *recall*.

Precision measures how many of the samples predicted as positive are actually positive:

```
\begin{equation}
```

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

```
\end{equation}
```

Precision is used as a performance metric when the goal is to limit the number of false positives. As an example, imagine a model to predict whether a new drug will be effective in treating a disease in clinical trials. Clinical trials are notoriously expensive, and a pharmaceutical company will only want to run an experiment if it is very sure that the predicted drugs will actually work. Therefore, it is important that the model does not produce many false positives, in other words, it has a high precision. Precision is also known as *positive predictive value* (PPV).

Recall on the other hand measures how many of the positive samples are captured by the positive predictions:

```
\begin{equation}
```

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

```
\end{equation}
```

Recall is used as a performance metric when we need to identify all positive samples, that is when it is important to avoid false negatives. The cancer diagnosis example from the Section “Kinds of Errors” is a good example for this: it is important to find all people that are sick, possibly including healthy patients in the prediction. Other names for recall are *sensitivity*, *hit rate* or *true positive rate* (TPR).

There is a trade-off between optimizing recall and optimizing precision. You can trivially obtain a perfect recall if you predict all samples to belong to the positive class - there will be no false negatives, and no true negatives either. However, predicting all samples as positive will result in many false positives, therefore the precision will be

very low. On the other hand, if you find a model that predicts only the single data point it is most sure about as positive, and the rest as negative, then precision will be perfect (assuming this data point is in fact positive), but recall will be very bad.

[info box] Precision and recall are only two of many classification measures derived from TP, FP, TN and FN. You can find a great summary of all the measures on wikipedia: [https://en.wikipedia.org/wiki/Sensitivity\\_and\\_specificity](https://en.wikipedia.org/wiki/Sensitivity_and_specificity) In the machine learning community, precision and recall are arguably the most commonly used measures for binary classification, but other communities might use other, related metrics. [/info box]

So while precision and recall are very important measures, looking at only one of them will not provide you with the full picture. One way to summarize them is the *f-score* or *f-measure*, which is the harmonic mean of precision and recall:

$$F = 2 \cdot \frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}}$$

This particular variant is also known as the  $f_1$ -score. As it takes precision and recall into account, it can be a better measure than accuracy on imbalanced binary classification datasets. Let's run it on the predictions on the "nine vs rest" dataset that we computed above. Here, we will assume that the "nine" class is the positive class (it is labeled as `True` while the rest is labeled as `False`, so the positive class is the minority class).

```
from sklearn.metrics import f1_score
print("f1 score most frequent: %.2f" % f1_score(y_test, pred_most_frequent))
print("f1 score dummy: %.2f" % f1_score(y_test, pred_dummy))
print("f1 score tree: %.2f" % f1_score(y_test, pred_tree))
print("f1 score: %.2f" % f1_score(y_test, pred_logreg))

/home/andy/checkout/scikit-learn/sklearn/metrics/classification.py:1117: UndefinedMetricWarning: F
'precision', 'predicted', average, warn_for)
```

We can note two things: we get an error message for the `most_frequent` prediction, as there was no predictions of the positive class (which makes the denominator in the  $F$  score zero).

Also, we can see a pretty strong distinction between the dummy predictions and the tree predictions, which wasn't clear when looking at accuracy alone.

Using the  $f$ -score for evaluation we summarized the predictive performance again in one number, which reflect our intuition about how well a model predicts much better than accuracy in the imbalanced class setting. A disadvantage of the  $f$ -score however is that it is harder to interpret and explain than accuracy.

If we want a more comprehensive summary of precision, recall and  $f1$  score, we can use the `classification_report` convenience function to compute all three at once, and print them in a nice format:

```
from sklearn.metrics import classification_report
print(classification_report(y_test, pred_most_frequent,
                           target_names=["not nine", "nine"]))

/home/andy/checkout/scikit-learn/sklearn/metrics/classification.py:1117: UndefinedMetricWarning: F
'precision', 'predicted', average, warn_for)
```

The `classification_report` function produces one line per class, here True and False and reports precision, recall and f-score with this class as the positive class.

Before, we assumed the minority “nine” class is the positive class. If we change the positive class to “not nine”, we can see from the output of `classification_report` that we obtain an f-score of .94 with the `most_frequent` model.

Furthermore, for the `not_nine` class we have a recall of 1, as we classified all samples as “not nine”.

The last column next to the f-score provides the *support* of each class, which simply means the number of samples in this class according to the ground truth.

The last row in the classification report shows a weighted (by support) average of the numbers for each class.

Here are two more reports, one for the dummy classifier and one for the logistic regression:

```
print(classification_report(y_test, pred_dummy,
                           target_names=["not nine", "nine"]))
```

	precision	recall	f1-score	support
not nine	0.90	0.94	0.92	403
nine	0.16	0.11	0.13	47
avg / total	0.82	0.85	0.83	450

```
print(classification_report(y_test, pred_logreg,
                           target_names=["not nine", "nine"]))
```

	precision	recall	f1-score	support
not nine	0.98	1.00	0.99	403
nine	0.95	0.83	0.89	47
avg / total	0.98	0.98	0.98	450

As you may notice, when looking at the reports, the differences between the dummy models and a very good model is not as clear any more.

Picking which class is declared the positive class has a big impact on the metrics. While the f-score for the dummy classification vs the logistic regression was 0.13 vs 0.89 on the “nine” class, it is 0.90 vs 0.99 on the “not nine” class, which both seem like reasonable results.

Looking at all numbers together paints a pretty accurate picture, though, and we can clearly see the superiority of the logistic regression model.

### Taking uncertainty into account

The confusion matrix and the classification report provide a very detailed analysis of a particular set of predictions. However, the predictions themselves already threw away a lot of information that is contained in the model. As we discuss in Chapter 2, most classifiers provide a `decision_function` or a `predict_proba` method to assess degrees of certainty about predictions.

Making predictions can be seen as thresholding the output of `decision_function` or `predict_proba` at a certain fixed point - in binary classification zero for the decision function and 0.5 for `predict_proba`.

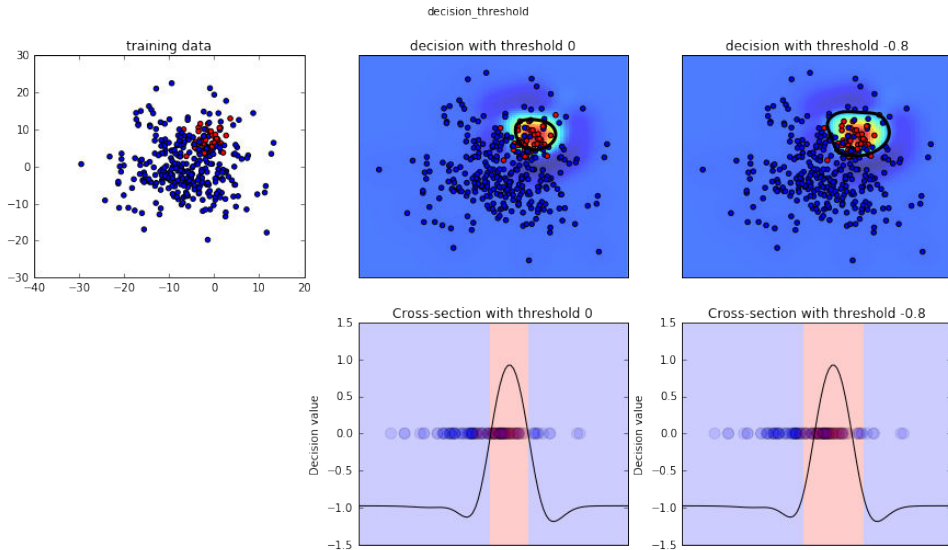
Below is an example of an imbalanced binary classification task, with 400 blue points classified against 50 red points.

The training data is shown on the right of Figure `decision_threshold`. We train a kernel SVM model on this data, and the left of Figure `decision_threshold` illustrates the values of the decision function as a heat-map. A red background means points there will be classified as red, blue background means that points there will be classified as blue.

You can see a black circle, which denotes the threshold of the `decision_function` being exactly zero. Points inside this circle will be classified as red, and outside as blue.

```
from mglearn.datasets import make_blobs
X, y = make_blobs(n_samples=(400, 50), centers=2, cluster_std=[7.0, 2],
                 random_state=22)
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)
svc = SVC(gamma=.05).fit(X_train, y_train)

mglearn.plots.plot_decision_threshold()
```



We can use the `classification_report` to evaluate precision and recall for both classes:

```
print(classification_report(y_test, svc.predict(X_test)))
```

	precision	recall	f1-score	support
0	0.97	0.89	0.93	104
1	0.35	0.67	0.46	9
avg / total	0.92	0.88	0.89	113

In Figure `decision_threshold`, blue is the negative class and red is the positive class.

For class 1, we get a fairly small recall, and precision is mixed. Because class 0 is so much larger, the classifier focuses on getting class 0 right, and not the smaller class 1.

Let's assume in our application it is more important to have a high recall for class 1, as in the cancer screening example above. This means we are willing to risk more false positives (false class 1) in exchange for true positives (which will increase the recall).

The predictions generated by `svc.predict` above really do not fulfill this requirement. But we can adjust the predictions to focus on a higher recall of class 1, by changing the decision threshold away from 0.



By default, points with a `decision_function` value greater than 0 will be classified as class 1. We want *more* points to be classified as class 1, so we need to *decrease* the threshold:

```
y_pred_lower_threshold = svc.decision_function(X_test) > -.8
```

Let's look at the classification report for this prediction:

```
print(classification_report(y_test, y_pred_lower_threshold))
```

	precision	recall	f1-score	support
0	1.00	0.82	0.90	104
1	0.32	1.00	0.49	9
avg / total	0.95	0.83	0.87	113

As expected, the recall of class 1 went up, and the precision went down. We are now classifying a larger region of space as class 1, as illustrated in the right panel of Figure `decision_threshold`.

If you value precision over recall or the other way around, or your data is heavily imbalanced, changing the decision threshold is the easiest way to obtain better results. As the `decision_function` can have arbitrary ranges, how to pick the right threshold is hard to say. If you do set a threshold, you need to be careful not to do this on the test set. As with any other parameter, setting a decision threshold on the test set is likely to give you too optimistic results. Use a validation set or cross-validation instead.

Picking a threshold for models that implement the `predict_proba` method can be easier, as the output of `predict_proba` is on a fixed zero to one scale, and models provide probabilities. By default, the threshold of 0.5 means that if the model is more than 50% “sure” that a point is of the positive class, it will be classified as such. Increasing the threshold means that the model needs to be more confident to make a positive decision (and less confident to make a negative decision). While working with probabilities may be more intuitive than working with arbitrary thresholds, not all models provide realistic models of uncertainty (a `DecisionTree` that is grown to its full depth is always 100% sure on its decisions - even though it might be often wrong). This relates to the concept of *calibration*: A calibrated model is a model that provides an accurate measure of its uncertainty. Discussing calibration in detail is beyond the scope of this book, unfortunately.

## Precision-Recall curves and ROC curves

As we just discussed, changing the threshold that is used to make a classification decision in a model is a way to adjust the trade-off of precision and recall for a given classifier. Maybe you want miss less than 10% of positive samples - meaning a desired recall of 90%. This decision is a decision that depends on the application, and is (or should be) driven by business goals. Once a particular goal is set, say a particular recall or precision value for a class, a threshold can be set appropriately. It is always possible to set a threshold to fulfill a particular target like 90% recall. The hard part is to develop a model that still has reasonable precision with this threshold - if you classify everything as positive, you will have 100% recall, but your model is useless.

Setting a requirement on a classifier like 90% recall is often called the *operating point*. Fixing an operating point is often helpful in business settings to make performance guarantees to customer or other groups inside your organization.

Often, when developing a new model, it is not entirely clear what the operating point will be. For this reason, and to understand a modeling problem better, it is instructive to look at all possible thresholds, or all possible trade-offs of precision and recall *at once*. This is possible using a tool called the *precision-recall curve*.

You can find the function to compute the precision-recall curve in the `sklearn.metrics` module. It needs the ground truth labeling and predicted uncertainties, created via `decision_function` or `predict_proba`:

```
from sklearn.metrics import precision_recall_curve
precision, recall, thresholds = precision_recall_curve(y_test,
                                                    svc.decision_function(X_test))
```

The `precision_recall_curve` function returns a list of precision and recall values for all possible thresholds (all values that appear in the decision function) in sorted order, so we can plot a curve:

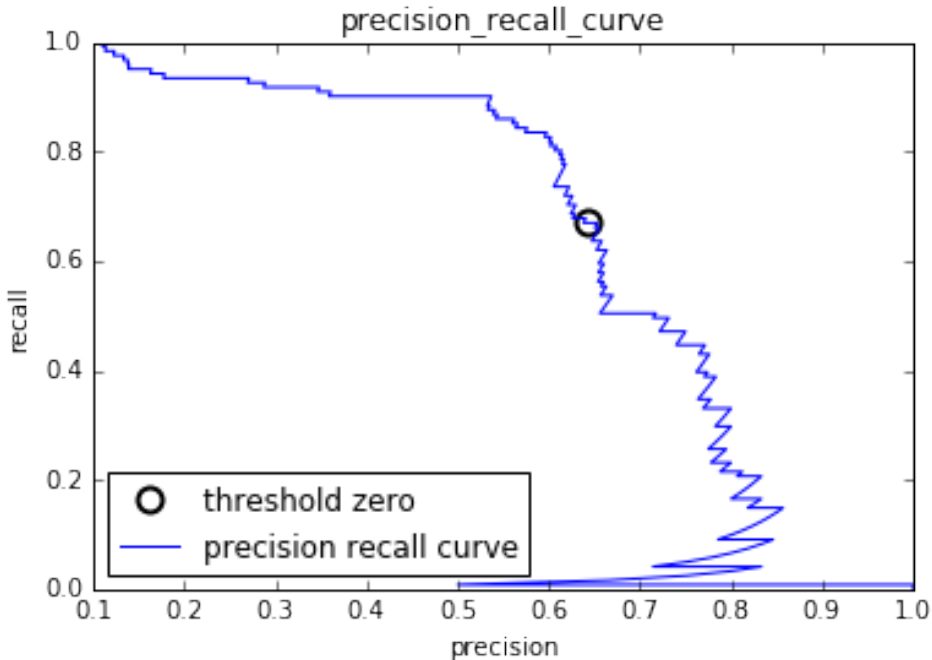
```
# create a similar dataset as before, but with more samples to get a smoother curve
X, y = make_blobs(n_samples=(4000, 500), centers=2, cluster_std=[7.0, 2], random_state=22)
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=0)

svc = SVC(gamma=.05).fit(X_train, y_train)

precision, recall, thresholds = precision_recall_curve(
    y_test, svc.decision_function(X_test))
# find threshold closest to zero:
close_zero = np.argmin(np.abs(thresholds))
plt.plot(precision[close_zero], recall[close_zero], 'o', markersize=10,
         label="threshold zero", fillstyle="none", c='k', mew=2)

plt.plot(precision, recall, label="precision recall curve")
plt.xlabel("precision")
plt.ylabel("recall")
```

```
plt.title("precision_recall_curve");  
plt.legend(loc="best")
```



Each point along the curve in “precision\_recall\_curve” corresponds to a possible threshold on the decision\_function. We can see for example that we can achieve a recall of 0.4 at a precision of about 0.75. The black circle marks the point that corresponds to a threshold of zero, the default threshold for decision\_function. This point is the trade-off that is chosen when calling the predict method.

The closer a curve stays to the upper right corner, the better the classifier. A point at the upper right means high precision *and* high recall for the same threshold. The curve starts at the top left corner, corresponding to a very low threshold, classifying everything as the positive class. Raising the threshold moves the curve towards higher precision, but also lower recall. Raising the threshold more and more, we get to a situation where most of the points classified as being positive are true positives, leading to a very high precision at lower recall. The more the model keeps recall high as precision goes up, the better.

Looking at this particular curve a bit more, we can see that with this model it is possible to get a precision up to around 0.5 with very high recall. If we want a much higher precision, we have to sacrifice a lot of precision. In other words: on the left, the curve is relatively flat, meaning that recall does not go down a lot when we require

increased precision. For precision greater than 0.5, each gain in precision costs us a lot of recall.

Different classifiers can work well in different parts of the curve, that is at different operating points. Below we compare the SVC we trained to a random forest trained on the same dataset.

The `RandomForestClassifier` doesn't have a `decision_function`, only `predict_proba`. The `precision_recall_curve` function expects as second argument a certainty measure for the positive class (class 1), so we pass the probability of a sample being class one, that is `rf.predict_proba(X_test)[:, 1]`. The default threshold for `predict_proba` in binary classification is 0.5, so this is the point we marked on the curve.

```
from sklearn.ensemble import RandomForestClassifier

rf = RandomForestClassifier(n_estimators=100, random_state=0, max_features=2)
rf.fit(X_train, y_train)

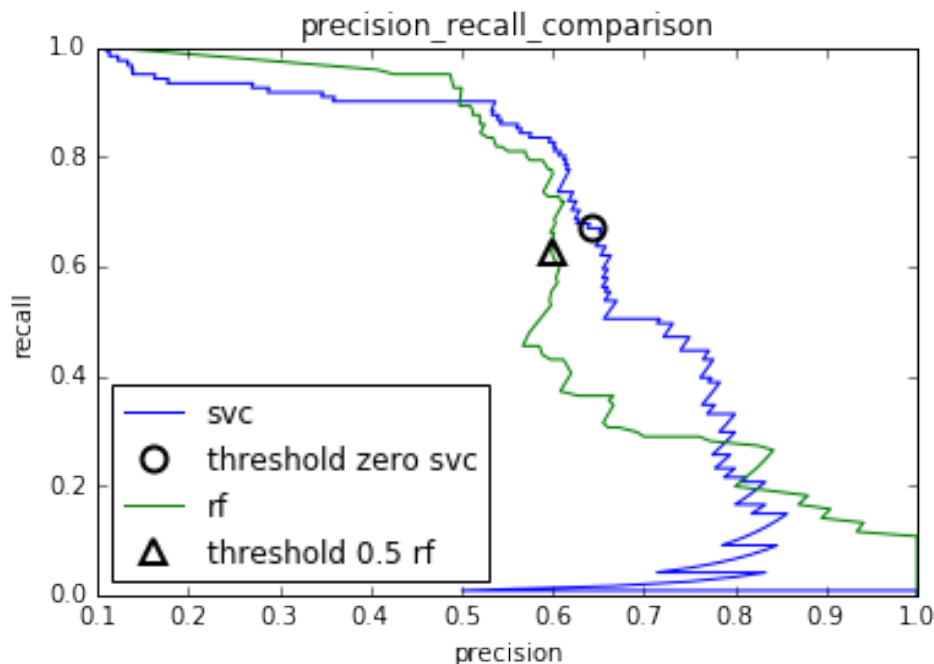
# RandomForestClassifier has predict_proba, but not decision_function
precision_rf, recall_rf, thresholds_rf = precision_recall_curve(
    y_test, rf.predict_proba(X_test)[:, 1])

plt.plot(precision, recall, label="svc")

plt.plot(precision[close_zero], recall[close_zero], 'o', markersize=10,
         label="threshold zero svc", fillstyle="none", c='k', mew=2)

plt.plot(precision_rf, recall_rf, label="rf")

close_default_rf = np.argmin(np.abs(thresholds_rf - 0.5))
plt.plot(precision_rf[close_default_rf], recall_rf[close_default_rf], '^', markersize=10,
         label="threshold 0.5 rf", fillstyle="none", c='k', mew=2)
plt.xlabel("precision")
plt.ylabel("recall")
plt.legend(loc="best")
plt.title("precision_recall_comparison");
```



From the comparison plot we can see that the random forest performs better at the extremes, for very high recall or very high precision requirements. Around the middle (around precision=0.7), the SVM performance better. If we only looked at the f1-score to compare overall performance, we would have missed these subtleties. The f1-score only captures one point on the precision-recall curve, the one given by the default threshold:

```
print("f1_score of random forest: %f" % f1_score(y_test, rf.predict(X_test)))
print("f1_score of svc: %f" % f1_score(y_test, svc.predict(X_test)))

f1_score of random forest: 0.609756

f1_score of svc: 0.655870
```

Comparing two precision-recall curves provides a lot of detailed insight, but is a fairly manual process. For automatic model comparison, we might want to summarize the information contained in the curve, without limiting ourselves to a particular threshold or operating point.

One particular way to summarize the precision-recall curve by computing the integral or area under the curve of the precision-recall curve, also known as *average precision*.

You can compute the average precision using the `average_precision_score`. Because we need to compute the ROC curve, and consider multiple thresholds, we

need to pass the result of `decision_function` or `predict_proba` to `average_precision_score`, not the result of `predict`:

```
from sklearn.metrics import average_precision_score
ap_rf = average_precision_score(y_test, rf.predict_proba(X_test)[: , 1])
ap_svc = average_precision_score(y_test, svc.decision_function(X_test))
print("average precision of random forest: %f" % ap_rf)
print("average precision of svc: %f" % ap_svc)

average precision of random forest: 0.665737

average precision of svc: 0.662636
```

When averaging over all possible thresholds, we see that random forest and SVC perform similarly well, with the random forest even slightly ahead. This is quite different than the result we got from `f1_score` above.

Because average precision is the area under a curve that goes from 0 to 1, average precision always returns a value between 0 (worst) and 1 (best). The average precision of a classifier that assigns `decision_function` at random is the fraction of positive samples in the dataset.

## Receiver Operating Characteristics (ROC) and AUC

There is another tool commonly used to analyze the behavior of classifiers at different thresholds: the *receiver operating characteristics curve*, or *ROC curve* for short. The ROC curve similarly considers all possible thresholds for a given classifier, but instead of reporting precision and recall, it shows the *false positive rate* FPR against the *true positive rate* TPR. Recall that the true positive rate is simply another name for recall, while the false positive rate is the fraction of false positives out of all negative samples:

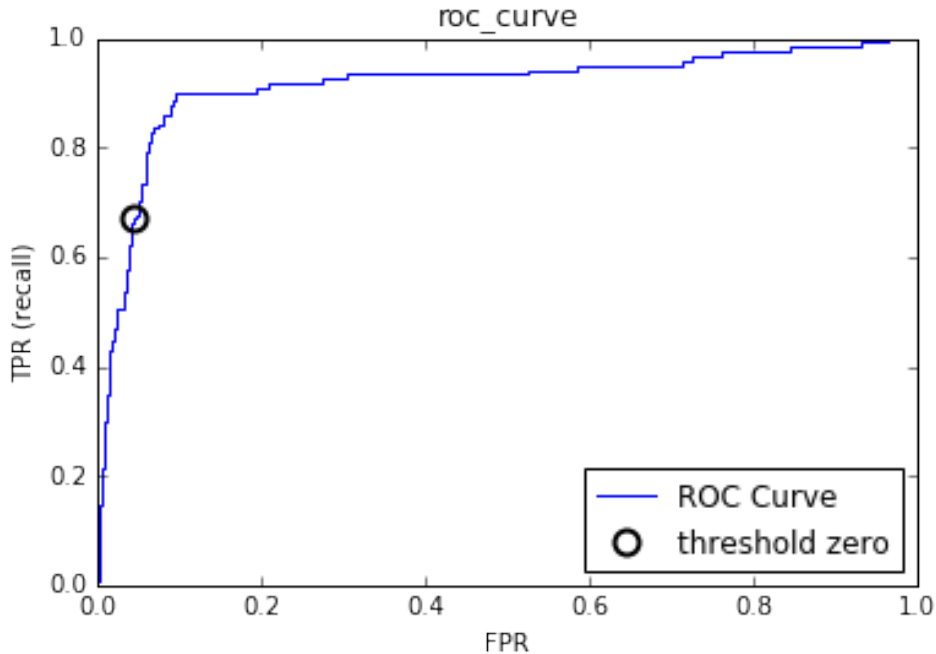
```
\begin{equation}
\text{FPR} = \frac{\text{FP}}{\text{FP} + \text{TN}}
\end{equation}
```

The ROC curve can be computed using the `roc_curve` function:

```
from sklearn.metrics import roc_curve
fpr, tpr, thresholds = roc_curve(y_test, svc.decision_function(X_test))

plt.plot(fpr, tpr, label="ROC Curve")
plt.xlabel("FPR")
plt.ylabel("TPR (recall)")
plt.title("roc_curve");
# find threshold closest to zero:
close_zero = np.argmin(np.abs(thresholds))
plt.plot(fpr[close_zero], tpr[close_zero], 'o', markersize=10,
```

```
label="threshold zero", fillstyle="none", c='k', mew=2)
plt.legend(loc=4)
```



For the ROC curve, the ideal curve is close to the top left: you want a classifier that produces a *high recall* while keeping a *low false positive rate*. Compared to the default threshold of zero, the curve shows that we could achieve a significant higher recall (around 0.9) while only increasing the FPR slightly. The point close to the top left might be a better operating point than the one chosen by default. Again, be aware that choosing a threshold should not be done on the test set, but on a separate validation set.

You can find a comparison of the Random Forest and the SVC using ROC curves in Figure `roc_curve_comparison`.

```
from sklearn.metrics import roc_curve
fpr_rf, tpr_rf, thresholds_rf = roc_curve(y_test, rf.predict_proba(X_test)[: , 1])

plt.plot(fpr, tpr, label="ROC Curve SVC")
plt.plot(fpr_rf, tpr_rf, label="ROC Curve RF")

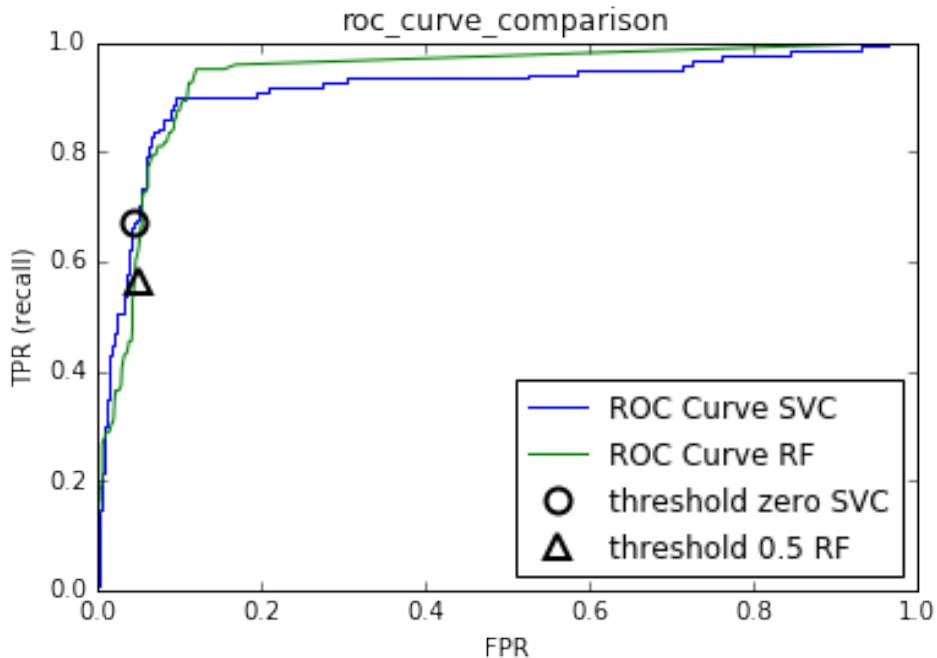
plt.xlabel("FPR")
plt.ylabel("TPR (recall)")
plt.title("roc_curve_comparison");
plt.plot(fpr[close_zero], tpr[close_zero], 'o', markersize=10,
        label="threshold zero SVC", fillstyle="none", c='k', mew=2)
```

```

close_default_rf = np.argmin(np.abs(thresholds_rf - 0.5))
plt.plot(fpr_rf[close_default_rf], tpr[close_default_rf], '^', markersize=10,
         label="threshold 0.5 RF", fillstyle="none", c='k', mew=2)

plt.legend(loc=4)

```



As for the precision-recall curve, we often want to summarize the ROC curve using a single number, the area under the curve. Often the area under the ROC-curve is just called *AUC (area under the curve)* and it is understood that the curve in question is the ROC curve. We can compute the area under the ROC curve using the `roc_auc_score` function:

```

from sklearn.metrics import roc_auc_score
rf_auc = roc_auc_score(y_test, rf.predict_proba(X_test)[: , 1])
svc_auc = roc_auc_score(y_test, svc.decision_function(X_test))
print("AUC for Random Forest: %f" % rf_auc)
print("AUC for SVC: %f" % svc_auc)

```

AUC for Random Forest: 0.936695

AUC for SVC: 0.916294

Comparing random forest and SVC using the AUC score, we find that Random Forest performs quite a bit better than SVC.



Because average precision is the area under a curve that goes from 0 to 1, average precision always returns a value between 0 (worst) and 1 (best). Predicting randomly always produces an AUC of 0.5, not matter how imbalanced the classes in a dataset are. This makes it a much better metric for imbalanced classification problems than accuracy.

The AUC can be interpreted as evaluating the *ranking* of positive samples. The AUC is equivalent to the probability that a randomly picked point of the positive class will have a higher score according to the classifier than a randomly picked point from the negative class. So an perfect AUC of 1 means that all positive points have a higher score than all negative points.

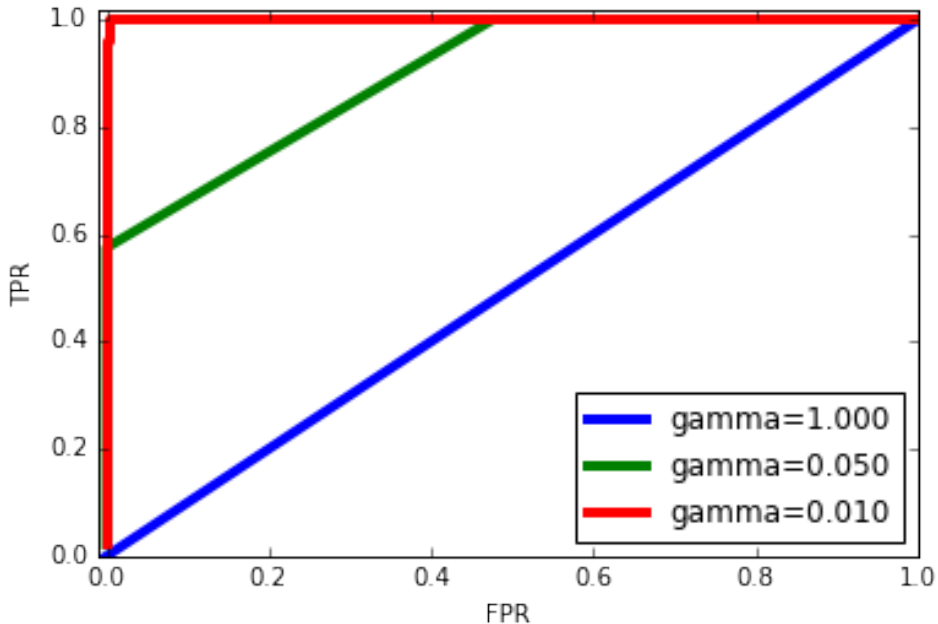
For classification problems with imbalanced classes, using AUC for model-selection is often much more meaningful than using accuracy. Let's go back to the problem we studied above of classifying all nines in the `digits` dataset versus all other digits. We will classify the dataset with an SVM with three different settings of the kernel bandwidth `gamma`:

```
y = digits.target == 9

X_train, X_test, y_train, y_test = train_test_split(
    digits.data, y, random_state=0)

plt.figure()

for gamma in [1, 0.05, 0.01]:
    svc = SVC(gamma=gamma).fit(X_train, y_train)
    accuracy = svc.score(X_test, y_test)
    auc = roc_auc_score(y_test, svc.decision_function(X_test))
    fpr, tpr, _ = roc_curve(y_test, svc.decision_function(X_test))
    print("gamma = %.02f accuracy = %.02f AUC = %.02f" % (gamma, accuracy, auc))
    plt.plot(fpr, tpr, label="gamma=%.03f" % gamma, linewidth=4)
plt.xlabel("FPR")
plt.ylabel("TPR")
plt.xlim(-0.01, 1)
plt.ylim(0, 1.02)
plt.legend(loc="best")
```



gamma = 1.00 accuracy = 0.90 AUC = 0.50

gamma = 0.05 accuracy = 0.90 AUC = 0.90

gamma = 0.01 accuracy = 0.90 AUC = 1.00

The accuracy of all three settings of gamma is the same, 90%. This could either be chance performance, or it could be not. Looking at the AUC and the corresponding curve, however, we see a clear distinction between the three models: With gamma=1.0, the AUC is actually at chance level, meaning that the output of the decision\_function is as good as random. With gamma=0.05, performance drastically improves to an AUC of 0.5. Finally with gamma=0.01, we get a perfect AUC of 1.0. That means that all positive points are ranked higher than all negative points according to the decision function. In other words, with the right threshold, this model can classify the data perfectly! [Footnote: Looking at the curve for gamma=0.01 in detail you can see a small kink close to the top left. That means that at least one point was not ranked correctly. The AUC of 1.0 is a consequence of rounding to the second decimal.] Knowing this, we can adjust the threshold on this model, and obtain great predictions.

If we only used accuracy, we would have never discovered this.

For this reason, we highly recommend using AUC when evaluating models on imbalanced data. Keep in mind that AUC does not make use of the default threshold, so

adjusting the decision threshold might be necessary to obtain useful classification results from a model with high AUC.

## Multi-class classification

Now that we have discussed evaluation of binary classification tasks in-depth, let's move on to metrics to evaluate multi-class classification. Basically all metrics for multi-class classification are derived from binary classification metrics, but averaged over all classes.

Accuracy for multi-class classification is again defined as the fraction of correctly classified examples. And again, when classes are imbalanced, accuracy is not a great evaluation measure. Imagine a three-class classification problem with 85% of points belonging to class A, 10% belonging to class B and 5% belonging to class C. What does being 85% accurate mean on this dataset?

In general, multi-class classification results are harder to understand than binary classification results.

Apart from accuracy, common tools are the confusion matrix and the classification report we saw in the binary case above.

Let's apply these two detailed evaluation methods on the task of classifying the 10 different hand-written digits in the `digits` dataset:

```
from sklearn.metrics import accuracy_score
X_train, X_test, y_train, y_test = train_test_split(
    digits.data, digits.target, random_state=0)
lr = LogisticRegression().fit(X_train, y_train)
pred = lr.predict(X_test)
print("accuracy: %0.3f" % accuracy_score(y_test, pred))
print("confusion matrix:")
print(confusion_matrix(y_test, pred))
```

```
accuracy: 0.953
```

```
confusion matrix:
```

```
[[37  0  0  0  0  0  0  0  0  0]
```

```
 [ 0 39  0  0  0  0  2  0  2  0]
```

```
 [ 0  0 41  3  0  0  0  0  0  0]
```

```
 [ 0  0  1 43  0  0  0  0  0  1]
```

```
 [ 0  0  0  0 38  0  0  0  0  0]
```

```
 [ 0  1  0  0  0 47  0  0  0  0]
```

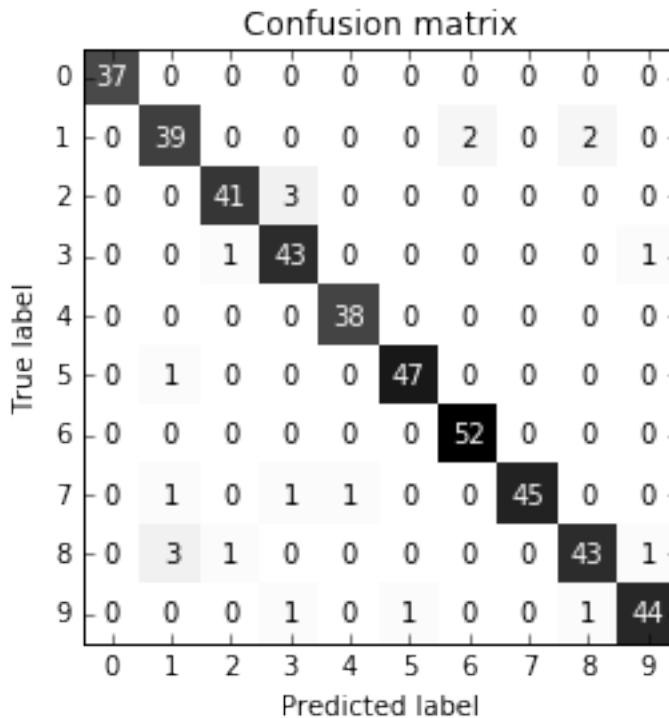
```
 [ 0  0  0  0  0  0 52  0  0  0]
```

```

[ 0  1  0  1  1  0  0 45  0  0]
[ 0  3  1  0  0  0  0  0 43  1]
[ 0  0  0  1  0  1  0  0  1 44]]
scores_image = mglearn.tools.heatmap(confusion_matrix(y_test, pred), xlabel='Predicted label', yla
                                xticklabels=digits.target_names, yticklabels=digits.target_na
                                cmap=plt.cm.gray_r, fmt="%d")

plt.title("Confusion matrix")
plt.gca().invert_yaxis()

```



The model has an accuracy of 95.6%, which already tells us that we are doing pretty well. The confusion matrix provides us with some more detail. As for the binary case, each row corresponds to a true label, and each column corresponds to a predicted label. You can find a visually more appealing plot in Figure `multi_class_confusion_matrix`. For the first class, the digit 0, there are 37 samples in the class, and all of these samples were classified as class 0 (no false negatives for the zero class). We can see that because all other entries in the first row of the confusion matrix are zero. We can also see that no other digits was mistakenly classified as zero, because all other

entries in the first column of the confusion matrix are zero (no false positives for class zero).

Some digits that were confused with others are the digit two (third row), three of which were classified as the digit three (fourth column). There was also one digit three that was classified as two (third column, fourth row) and one digit eight that was classified as two (third column, fourth row).

With the `classification_report` function, we can compute the precision, recall and f-score for each class:

```
print(classification_report(y_test, pred))
```

	precision	recall	f1-score	support
0	1.00	1.00	1.00	37
1	0.89	0.91	0.90	43
2	0.95	0.93	0.94	44
3	0.90	0.96	0.92	45
4	0.97	1.00	0.99	38
5	0.98	0.98	0.98	48
6	0.96	1.00	0.98	52
7	1.00	0.94	0.97	48
8	0.93	0.90	0.91	48
9	0.96	0.94	0.95	47
avg / total	0.95	0.95	0.95	450

Unsurprisingly, precision and recall are a perfect 1 for class zero, as there are no confusions with this class. For class seven on the other hand, precision is 1 because no other class was mistakenly classified as seven, while for class six, there are not false negatives, so the recall is 1. We can also see that the model has particular difficulties with classes eight and three.

The most commonly used metric for imbalanced datasets in the multi-class setting is the multi-class version of the f-score. The idea behind multi-class F-score is to compute one binary F-score per class, with that class being the positive class, and the

other classes making up the negative classes. Then, these per-class F-scores are averaged using one of the following strategies:

- “macro” averaging computes the unweighted the per-class f-scores. This gives equal weight to all classes, no matter what their size is.
- “weighted” averaging computes the mean of the per-class f-scores, weighted by their support. This is what is reported in the classification report.
- “micro” averaging computes total number of false positives, false negatives and true positives over all classes, and then compute precision, recall and f-score using these counts.

If you care about each *sample* equally much, it is recommended to use "micro" average f1-score, if you care about each *class* equally much, it is recommended to use the "macro" average f1-score:

```
print("micro average f1 score: %f" % f1_score(y_test, pred, average="micro"))
print("macro average f1 score: %f" % f1_score(y_test, pred, average="macro"))
```

```
micro average f1 score: 0.953333
```

```
macro average f1 score: 0.954000
```

## Regression metrics

Evaluation for regression can be done in similar detail as we did for classification above, for example by analyzing over-predicting the target versus under-predicting the target. However, in most application we’ve seen, using the default  $R^2$  used in the score method of all regressors is enough. Sometimes business decisions are made on the basis of mean squared error or mean absolute error, which might give incentive to tune models using these metrics. In general, though, we have found  $R^2$  to be a more intuitive metric to evaluate regression models.

## Using evaluation metrics in model selection

We now discussed many evaluation methods in detail, and how to apply them given the ground truth and a model.

However, we often want to use metrics like AUC in model selection using `GridSearchCV` or `cross_val_score`.

Luckily scikit-learn provides a very simple way to achieve this, via the `scoring` argument that can be used in both `GridSearchCV` and `cross_val_score`. You can simply provide a string describing the desired evaluation metric you want to use. Say, for example, we want to evaluate the SVC classifier on the “nine vs rest” task on the digits

dataset, using the AUC score. Changing the score from the default (accuracy) to AUC can be done by providing "roc\_auc" as the scoring parameter:

```
# default scoring for classification is accuracy
print("default scoring ", cross_val_score(SVC(), digits.data, digits.target == 9))
# providing scoring="accuracy" doesn't change the results
explicit_accuracy = cross_val_score(SVC(), digits.data, digits.target == 9, scoring="accuracy")
print("explicit accuracy scoring ", explicit_accuracy)
roc_auc = cross_val_score(SVC(), digits.data, digits.target == 9, scoring="roc_auc")
print("AUC scoring ", roc_auc)

default scoring [ 0.9  0.9  0.9]

explicit accuracy scoring [ 0.9  0.9  0.9]

AUC scoring [ 0.994  0.99  0.996]
```

Similarly we can change the metric used to pick the best parameters in GridSearchCV:

```
X_train, X_test, y_train, y_test = train_test_split(
    digits.data, digits.target == 9, random_state=0)

# we provide a somewhat bad grid to illustrate the point:
param_grid = {'gamma': [0.0001, 0.01, 0.1, 1, 10]}
# using the default scoring of accuracy:
grid = GridSearchCV(SVC(), param_grid=param_grid)
grid.fit(X_train, y_train)
print("Grid-Search with accuracy")
print("Best parameters:", grid.best_params_)
print("Best cross-validation score (accuracy):", grid.best_score_)
print("Test set AUC: %.3f" % roc_auc_score(y_test, grid.decision_function(X_test)))
print("Test set accuracy %.3f: " % grid.score(X_test, y_test))

# using AUC scoring instead:
grid = GridSearchCV(SVC(), param_grid=param_grid, scoring="roc_auc")
grid.fit(X_train, y_train)
print("\nGrid-Search with AUC")
print("Best parameters:", grid.best_params_)
print("Best cross-validation score (AUC):", grid.best_score_)
print("Test set AUC: %.3f" % roc_auc_score(y_test, grid.decision_function(X_test)))
print("Test set accuracy %.3f: " % grid.score(X_test, y_test))

Grid-Search with accuracy

Best parameters: {'gamma': 0.0001}

Best cross-validation score (accuracy): 0.970304380104

Test set AUC: 0.992

Test set accuracy 0.973:
```

```
Grid-Search with AUC
```

```
Best parameters: {'gamma': 0.01}
```

```
Best cross-validation score (AUC): 0.997467845028
```

```
Test set AUC: 1.000
```

```
Test set accuracy 1.000:
```

When using accuracy, the parameter `gamma=0.0001` is selected, while `gamma=0.01` is selected when using AUC. The cross-validation accuracy is consistent with the test set accuracy in both cases. However, using AUC found a better parameter setting, both in terms of AUC and even in terms of accuracy [Footnote: Finding a higher accuracy solution using AUC is likely a consequence of accuracy being a bad measure of model performance on imbalanced data].

The most important values for the `scoring` parameter for classification are `accuracy` (the default), `roc_auc` for the area under the ROC curve, `average_precision` for the area under the precision-recall curve, `f1`, `f1_macro`, `f1_micro` and `f1_weighted` for the binary F1 score and the different weighted variants.

For regression, the most commonly used values are `r2` for the  $R^2$  score, `mean_squared_error` for mean squared error and `mean_absolute_error` for mean absolute error.

You can find a full list of supported arguments in the documentation or by looking at the `SCORER` dictionary defined in the `metrics.scorer` module:

```
from sklearn.metrics.scorer import SCORERS
print(sorted(SCORERS.keys()))

['accuracy', 'adjusted_rand_score', 'average_precision', 'f1', 'f1_macro', 'f1_micro', 'f1_samples
```

## Summary and outlook

In this chapter we discussed cross-validation, grid-search and evaluation metrics, the corner-stones of evaluating and improving machine learning algorithms. The tools described in this chapter, together with the algorithms described in Chapters 2 and 3 are the bread and butter of every machine learning practitioner. There are two particular points that we made in this chapter that warrant repeating, because they are often overlooked by new practitioners: Cross-validation or the use of a test set allow us to evaluate a machine learning model as it will perform in the future. However, if we use the test-set or cross-validation to select a model or select model parameters, we “used up” the test data, and using the same data to evaluate how well our model will do in the future will lead to overly optimistic estimates. We therefore need to resort to a split into training data for model building, validation data for model and parameter



selection, and test data for model evaluation. Instead of a simple split, we can replace each of these splits with cross-validation. The most commonly used form as described above is a train-test split for evaluation, and using cross-validation on the training set for model and parameter selection.

The second important point is the importance of the evaluation metric or scoring function used for model selection and model evaluation. The theory of how to make business decisions from the predictions of a machine learning model is somewhat beyond the scope of this book. However, it is rarely the case that the end goal of a machine learning task is building a model with a high accuracy. Make sure that the metric you choose to evaluate and select a model is a good stand-in for what the model will actually be used for. In reality, classification problems rarely have balanced classes, and often false positives and false negatives have very different consequences. Make sure you understand what these consequences are, and pick an evaluation metric accordingly.

The techniques model evaluation and selection techniques we described so far are the most important tools in a data scientist's toolbox. However, grid search and cross validation as we described it in this chapter can only be applied to a single supervised model. We have seen before, however, that many models require preprocessing, and that in some applications, like the face recognition example in Chapter 3, extracting a different representation of the data can be useful. In the next chapter, we will introduce the `Pipeline` class, which allows us to use grid-search and cross-validation on these complex chains of algorithms.



---

# Algorithm Chains and Pipelines

For many machine learning algorithms, the particular representation of the data that you provide is very important, as we discussed in Chapter 5. This starts with scaling the data and combining features by hand and goes all the way to learning features using unsupervised machine learning as we saw in Chapter 3.

Consequently, most machine learning applications require not only the application of a single algorithm, but the chaining together of many different processing steps and machine learning models.

For example we noticed that we can greatly improve the performance of a kernel SVM on the cancer dataset by using the `MinMaxScaler` for preprocessing. The code for splitting the data, computing minimum and maximum, scaling the data, and training the SVM is shown below:

```
from sklearn.svm import SVC
from sklearn.datasets import load_breast_cancer
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import MinMaxScaler

# load and split the data
cancer = load_breast_cancer()
X_train, X_test, y_train, y_test = train_test_split(
    cancer.data, cancer.target, random_state=0)

# compute minimum and maximum on the training data
scaler = MinMaxScaler().fit(X_train)
# rescale training data
X_train_scaled = scaler.transform(X_train)

svm = SVC()
# learn an SVM on the scaled training data
svm.fit(X_train_scaled, y_train)
```

```
# scale test data and score the scaled data
X_test_scaled = scaler.transform(X_test)
svm.score(X_test_scaled, y_test)

0.95104895104895104
```

## Parameter Selection with Preprocessing

Now let's say we want to find better parameters for SVC using GridSearchCV, as discussed in Chapter 6.

How should we go about doing this? A naive approach might look like this:

```
from sklearn.model_selection import GridSearchCV
# illustration purposes only, don't use this code
param_grid = {'C': [0.001, 0.01, 0.1, 1, 10, 100],
              'gamma': [0.001, 0.01, 0.1, 1, 10, 100]}
grid = GridSearchCV(SVC(), param_grid=param_grid, cv=5)
grid.fit(X_train_scaled, y_train)
print("best cross-validation accuracy:", grid.best_score_)
print("test set score: ", grid.score(X_test_scaled, y_test))
print("best parameters: ", grid.best_params_)

best cross-validation accuracy: 0.981220657277

test set score: 0.972027972028

best parameters: {'gamma': 1, 'C': 1}
```

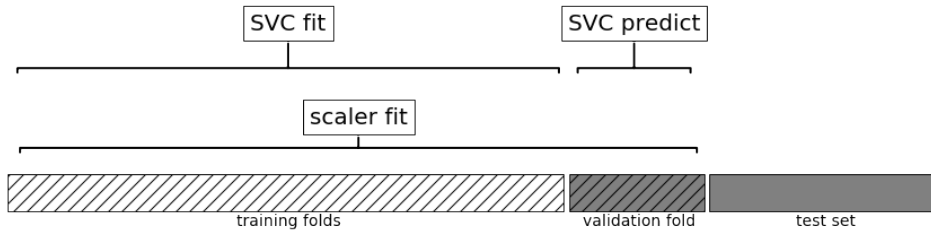
Here, we ran the grid-search over the parameters of the SVC using the scaled data. However, there is a subtle catch in what we just did. When scaling the data, we used *all data in the training set* to find out how to train it.

We then use the *scaled training data* to run our grid-search using cross-validation. For each split in the cross-validation, some part of the original training set will be declared the training part of this split, and some the test part of the split. The test part is used to measure how new data will look like to a model trained on the training part. However, we already used the information contained in the test part of the split, when scaling the data. Remember that the test part in each split in the cross-validation is part of the training set, and we used *the information from the whole training data* to find the right scaling of the data. *This is fundamentally different to how new data looks to the model.* If we observe new data (say in form of our test set), this data will not have been used to scale the training data. This data might have a different minimum and maximum than the training data.

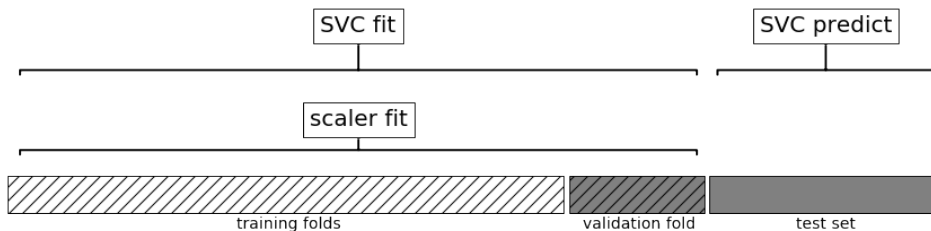
The illustration below shows how the data processing during cross-validation and the final evaluation differ:

```
mglearn.plots.plot_improper_processing()
```

### Cross validation



### Test set prediction



So the splits in the cross-validation no longer correctly mirror how new data will look to the modeling process. We already leaked information from these parts of the data into our modeling process. This will lead to overly optimistic results during cross-validation, and possibly the selection of suboptimal parameters.

To get around this problem, the splitting of the data set during cross-validation should be done *before doing any preprocessing*. Any process that extracts knowledge from the dataset should only ever be applied to the training portion of the data set, so any cross-validation should be the “outermost loop” in your processing.

To achieve this in scikit-learn with the `cross_val_score` function and the `GridSearchCV` function, we can use the `Pipeline` class. The `Pipeline` class is a class that allows “gluing” together multiple processing steps into a single scikit-learn estimator. The `Pipeline` class itself has `fit`, `predict` and `score` methods and behaves just like any other model in scikit-learn. The most common use-case of the pipeline class is in chaining preprocessing steps (like scaling of the data) together with a supervised model like a classifier.

## Building Pipelines

Let’s look at how we can use the `Pipeline` to express the work-flow for training an SVM after scaling the data `MinMaxScaler` (for now without the grid-search). First, we build a pipeline object, by providing it with a list of steps. Each step is a tuple contain-

ing a name (any string of your choosing [Footnote: With one exception: the name may not contain a double underscore "\_\_".]) and an instance of an estimator:

```
from sklearn.pipeline import Pipeline
pipe = Pipeline([("scaler", MinMaxScaler()), ("svm", SVC())])
```

Here, we created two steps, the first called "scaler" is a `MinMaxScaler`, the second, called "svm" is an `SVC`. Now, we can fit the pipeline, like any other scikit-learn estimator:

```
pipe.fit(X_train, y_train)

Pipeline(steps=[('scaler', MinMaxScaler(copy=True, feature_range=(0, 1))), ('svm', SVC(C=1.0, cache_size=10240, class_weight=None, coef0=0.0,
decision_function_shape=None, degree=3, gamma='auto', kernel='rbf',
max_iter=-1, probability=False, random_state=None, shrinking=True,
tol=0.001, verbose=False))])
```

Here, `pipe.fit` first calls `fit` on the first step, the scaler, then transforms the training data using the scaler, and finally fits the SVM with the scaled data. To evaluate on the test data, we simply call `pipe.score`:

```
pipe.score(X_test, y_test)
0.95104895104895104
```

Calling the `score` method on the pipeline first transforms the test data using the scaler, and then calls the `score` method on the SVM using the scaled test data. As you can see, the result is identical to the one we got from the code above, doing the transformations “by hand”.

Using the pipeline, we reduced the code needed for our “preprocessing + classification” process.

The main benefit of using the pipeline, however, is that we can now use this single estimator in `cross_val_score` or `GridSearchCV`.

## Using Pipelines in Grid-searches

Using a pipeline in a grid-search works the same way as using any other estimator. We define a parameter grid to search over, and construct a `GridSearchCV` from the pipeline and the parameter grid. When specifying the parameter grid, there is a slight change, though. We need to specify for each parameter which step of the pipeline it belongs to.

Both parameters that we want to adjust, `C` and `gamma` are parameters of `SVC`, the second step. We gave this step the name "svm". The syntax to define the a parameter grid for a pipeline is to specify for each parameter the step name, followed by "\_\_" (dou-

ble underscore), followed by the parameter name. To search over the C parameter of the SVC we therefore have to use "svm\_\_C" as the key in the parameter grid dictionary, and similarly for gamma:

```
param_grid = {'svm__C': [0.001, 0.01, 0.1, 1, 10, 100],
              'svm__gamma': [0.001, 0.01, 0.1, 1, 10, 100]}
```

Using this parameter grid we can use GridSearchCV as usual:

```
grid = GridSearchCV(pipe, param_grid=param_grid, cv=5)
grid.fit(X_train, y_train)
print("best cross-validation accuracy:", grid.best_score_)
print("test set score: ", grid.score(X_test, y_test))
print("best parameters: ", grid.best_params_)

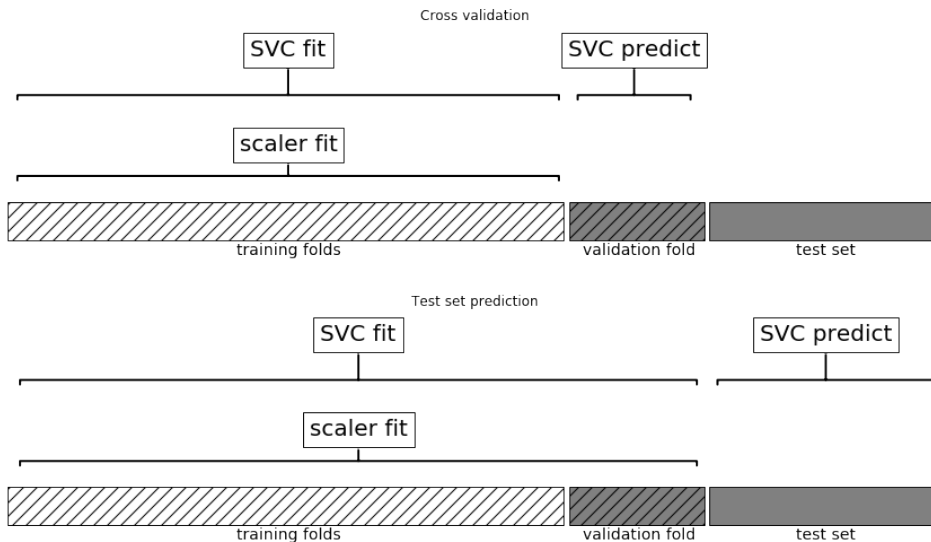
best cross-validation accuracy: 0.981220657277

test set score: 0.972027972028

best parameters: {'svm__C': 1, 'svm__gamma': 1}
```

In contrast to the grid-search we did before, now for each split in the cross-validation, the `MinMaxScaler` is refit with only the training splits, not leaking any information of the test split into the parameter search, as illustrated below. Compare this with Figure `improper_preprocessing` above.

```
mglearn.plots.plot_proper_processing()
```



The impact of leaking information in the cross-validation varies depending on the nature of the preprocessing step. Estimating the scale of the data using the test fold

usually doesn't have a terrible impact, while using the test fold in feature extraction and feature selection can lead to substantial differences in outcomes.

[FIXME info box] Illustrating information leakage

A great example of leaking information in cross-validation is given in Hastie et al. (FIXME insert cite) and we reproduce an adapted version here.

Let us consider a synthetic regression task with 100 samples and 1000 features that are sampled independently from a Gaussian distribution. We also sample the response from a Gaussian distribution:

```
rnd = np.random.RandomState(seed=0)
X = rnd.normal(size=(100, 10000))
y = rnd.normal(size=(100,))
```

Given the way we created the dataset, there is no relation between the data  $X$  and the target  $y$  (they are independent), so it should not be possible to learn anything from this data set.

We will now do the following: First select the most informative of the ten features using `SelectPercentile` feature selection, and then evaluate a `Ridge` regressor using cross-validation:

```
from sklearn.feature_selection import SelectPercentile, f_regression

select = SelectPercentile(score_func=f_regression, percentile=5).fit(X, y)
X_selected = select.transform(X)
print(X_selected.shape)

(100, 500)

from sklearn.model_selection import cross_val_score
from sklearn.linear_model import Ridge
np.mean(cross_val_score(Ridge(), X_selected, y, cv=5))

0.90579530652398221
```

The mean  $R^2$  computed by cross-validation is 0.9, indicating a very good model. This can clearly not be right, as our data is entirely random. What happened here is that our feature selection picked out some features among the 10000 random features that are (by chance) very well correlated with the target. Because we fit the feature selection *outside* of the cross-validation, it could find features that are correlated both on the training and the test folds. The information we leaked from the test-folds was very informative, leading to highly unrealistic results.

Let's compare this to a proper cross-validation using a pipeline:

```
pipe = Pipeline([("select", SelectPercentile(score_func=f_regression, percentile=5)), ("ridge", Ridge())])
np.mean(cross_val_score(pipe, X, y, cv=5))

-0.24655422384952805
```



This time, we get a *negative*  $R^2$  score, indicating a very poor model.

Using the pipeline, the feature selection is now *inside* the cross-validation loop. This means features can only be selected using the training folds of the data, not the test fold. The feature selection finds features that are correlated with the target on the training set. But because the data is entirely random, these features are not correlated with the target on the test set.

In this example, rectifying the data leakage issue in the feature selection makes the difference between concluding that a model works very well and concluding that a model works not at all.

[end infobox]

## The General Pipeline Interface

The `Pipeline` class is not restricted to preprocessing and classification, but can in fact join any number of estimators together.

For example, you could build a pipeline containing feature extraction, feature selection, scaling and classification, for a total of four steps. Similarly the last step could be regression or clustering instead of classification.

The only requirement for estimators in a pipeline is that all but the last step need to have a `transform` method, so they can produce a new representation of the data that can be used in the next step.

Internally, during the call to `Pipeline.fit`, the pipeline calls first `fit` and then `transform` on each step in turn [Footnote: or just `fit_transform`], with the input given by the output of the `transform` method of the previous step. For the last step in the pipeline, just `fit` is called. Brushing over some finer details, this is implemented as follows. Remember that `pipeline.steps` is a list of tuples, so `pipeline.steps[0][1]` is the first estimator, `pipeline.steps[1][1]` is the second estimator, and so on.

```
def fit(self, X, y):
    X_transformed = X
    for step in self.steps[:-1]:
        # iterate over all but the final step
        # fit and transform the data
        X_transformed = step[1].fit_transform(X_transformed, y)
    # fit the last step
    self.steps[-1][1].fit(X_transformed, y)
    return self
```

When predicting using `Pipeline`, similarly we transform the data using all but the last step, and then call `predict` on the last step:

```
def predict(self, X):
    X_transformed = X
```

```

for step in self.steps[:-1]:
    # iterate over all but the final step
    # transform the data
    X_transformed = step[1].transform(X_transformed)
# fit the last step
return self.steps[-1][1].predict(X_transformed)

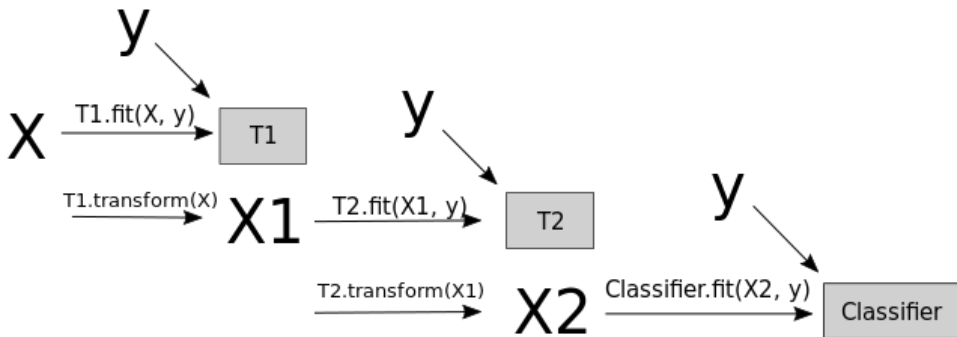
```

The process is illustrated below for two transformers T1 and T2 and a classifier Clf:

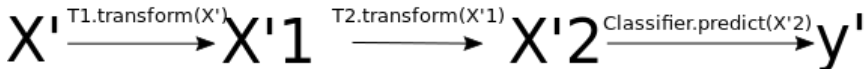
```
pipe = make_pipeline(T1(), T2(), Classifier())
```



```
pipe.fit(X, y)
```



```
pipe.predict(X')
```



The pipeline is actually even more general than this. There is no requirement for the last step in a pipeline to have a `predict` function, and we could create a pipeline just containing, for example, a scaler and PCA. Then, because the last step PCA has a `transform` method, we could call `transform` on the pipeline to get the output of PCA. `transform` applied to the data that was processed by the previous step. The last step of a pipeline is only required to have a `fit` method.

## Convenient Pipeline creation with `make_pipeline`

Creating a Pipeline using the syntax described above is sometimes a bit cumbersome, and we often don't need user-specified names for each step. There is a convenience

function `make_pipeline` that will create a pipeline for us and automatically name each step based on its class. The syntax for `make_pipeline` is as follows:

```
from sklearn.pipeline import make_pipeline
# standard syntax
pipe_long = Pipeline([("scaler", MinMaxScaler()), ("svm", SVC(C=100))])
# abbreviated syntax
pipe_short = make_pipeline(MinMaxScaler(), SVC(C=100))
```

The pipeline objects `pipe_long` and `pipe_short` do exactly the same, only that `pipe_short` has steps that were automatically named. We can see the name of the steps by looking at the `steps` attribute:

```
pipe_short.steps
[('minmaxscaler', MinMaxScaler(copy=True, feature_range=(0, 1))),
 ('svc', SVC(C=100, cache_size=200, class_weight=None, coef0=0.0,
            decision_function_shape=None, degree=3, gamma='auto', kernel='rbf',
            max_iter=-1, probability=False, random_state=None, shrinking=True,
            tol=0.001, verbose=False))]
```

The steps are named `minmaxscaler` and `svc`. In general the step names are just lower-case version of the class names. If multiple steps have the same class, a number is appended:

```
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA

pipe = make_pipeline(StandardScaler(), PCA(n_components=2), StandardScaler())
pipe.steps
[('standardscaler-1',
 StandardScaler(copy=True, with_mean=True, with_std=True)),
 ('pca', PCA(copy=True, iterated_power=4, n_components=2, random_state=None,
            svd_solver='auto', tol=0.0, whiten=False)),
 ('standardscaler-2',
 StandardScaler(copy=True, with_mean=True, with_std=True))]
```

As you can see, the first `StandardScaler` was named "standardscaler-1" and the second "standardscaler-2". However, in such settings it might be better to use the Pipeline construction with explicit names, to give more semantic names to each step.

## Accessing step attributes

Often you might want to inspect attributes of one of the steps of the pipeline, say the coefficients of a linear model or the components extracted by PCA. The easiest way to access the step in a pipeline is the `named_steps` attribute, which is a dictionary from step names to the estimators:

```
# fit the pipeline defined above to the cancer dataset
pipe.fit(cancer.data)
# extract the first two principal components from the "pca" step
components = pipe.named_steps["pca"].components_
print(components.shape)

/home/andy/checkout/scikit-learn/sklearn/utils/extmath.py:368: UserWarning: The number of power it
warnings.warn("The number of power iterations is increased to ")
```

## Accessing attributes in grid-searched pipeline.

As we discussed above, one of the main reasons to use pipelines is for doing grid-searches. A common task then is to access some of the steps of a pipeline inside a grid-search.

Let's grid-search a `LogisticRegression` classifier on the cancer dataset, using `Pipeline` and `StandardScaler` to scale the data before passing it to the `LogisticRegression` classifier.

First we create a pipeline using the `make_pipeline` function:

```
from sklearn.linear_model import LogisticRegression

pipe = make_pipeline(StandardScaler(), LogisticRegression())
```

Next, we create a parameter grid. The regularization parameter to tune for `LogisticRegression` is the parameter `C` as explained in Chapter 2. We use a logarithmic grid for this parameter, searching between 0.01 and 100. Because we used the `make_pipeline` function, the name of the `LogisticRegression` step in the pipeline is the lower-cased class-name `"logisticregression"`. To tune the parameter `C`, we therefore have to specify a parameter grid for `"logisticregression__C"`:

```
param_grid = {'logisticregression__C': [0.01, 0.1, 1, 10, 100]}
```

We split the cancer dataset into training and test set, and fit a grid-search as usual:

```
X_train, X_test, y_train, y_test = train_test_split(
    cancer.data, cancer.target, random_state=4)
grid = GridSearchCV(pipe, param_grid, cv=5)
grid.fit(X_train, y_train)

GridSearchCV(cv=5, error_score='raise',

    estimator=Pipeline(steps=[('standardscaler', StandardScaler(copy=True, with_mean=True, with
```

```

        intercept_scaling=1, max_iter=100, multi_class='ovr', n_jobs=1,
        penalty='l2', random_state=None, solver='liblinear', tol=0.0001,
        verbose=0, warm_start=False))]),
    fit_params={}, iid=True, n_jobs=1,
    param_grid={'logisticregression__C': [0.01, 0.1, 1, 10, 100]},
    pre_dispatch='2*n_jobs', refit=True, scoring=None, verbose=0)

```

So how do we access the coefficients of the best LogisticRegression model that was found by GridSearchCV? From Chapter 6 we know that the best model found by Grid SearchCV, trained on all the training data, is stored in `grid.best_estimator_`:

```

print(grid.best_estimator_)
Pipeline(steps=[('standardscaler', StandardScaler(copy=True, with_mean=True, with_std=True)), ('logisticregression', LogisticRegression(C=0.1, class_weight=None, dual=False, fit_intercept=True, intercept_scaling=1, max_iter=100, multi_class='ovr', n_jobs=1, penalty='l2', random_state=None, solver='liblinear', tol=0.0001, verbose=0, warm_start=False))])

```

This `best_estimator_` in our case is a pipeline with two steps, "standardscaler" and "logisticregression". To access the logisticregression step, we can use the `named_steps` attribute of the pipeline that we explained above:

```

print(grid.best_estimator_.named_steps["logisticregression"])
LogisticRegression(C=0.1, class_weight=None, dual=False, fit_intercept=True, intercept_scaling=1, max_iter=100, multi_class='ovr', n_jobs=1, penalty='l2', random_state=None, solver='liblinear', tol=0.0001, verbose=0, warm_start=False)

```

Now that we have the trained LogisticRegression instance, we can access the coefficients (weights) associated with each input feature:

```

print(grid.best_estimator_.named_steps["logisticregression"].coef_)
[[-0.389 -0.375 -0.376 -0.396 -0.115  0.017 -0.355 -0.39  -0.058  0.209
 -0.495 -0.004 -0.371 -0.383 -0.045  0.198  0.004 -0.049  0.21  0.224
 -0.547 -0.525 -0.499 -0.515 -0.393 -0.123 -0.388 -0.417 -0.325 -0.139]]

```

This might be a somewhat lengthy expression, but often comes in handy in understanding your models.

## Grid-searching preprocessing steps and model parameters

Using pipelines, we can encapsulate all processing steps in our machine learning work flow in a single scikit-learn estimator. Another benefit of doing this is that we can now *adjust the parameters of the preprocessing* using the outcome of a supervised task like regression or classification.

In previous chapters, we used polynomial features on the boston dataset before applying the ridge regressor. Let's model that using a pipeline. The pipeline contains three steps: scaling the data, computing polynomial features, and ridge regression:

```
from sklearn.datasets import load_boston
boston = load_boston()
X_train, X_test, y_train, y_test = train_test_split(boston.data, boston.target, random_state=0)

from sklearn.preprocessing import PolynomialFeatures
pipe = make_pipeline(
    StandardScaler(),
    PolynomialFeatures(),
    Ridge())
```

But how do we know which degree of polynomials to choose, or whether to choose any polynomials or interactions at all? Ideally we want to select the degree parameter based on the outcome of the classification.

Using our pipeline, we can search over the degree parameter together with the parameter alpha of Ridge. To do this, we define a `param_grid` that contains both, appropriately prefixed by the step names:

```
param_grid = {'polynomialfeatures__degree': [1, 2, 3],
              'ridge__alpha': [0.001, 0.01, 0.1, 1, 10, 100]}
```

Now we can run our grid-search again:

```
grid = GridSearchCV(pipe, param_grid=param_grid, cv=5, n_jobs=-1)
grid.fit(X_train, y_train)

GridSearchCV(cv=5, error_score='raise',

             estimator=Pipeline(steps=[('standardscaler', StandardScaler(copy=True, with_mean=True, with
normalize=False, random_state=None, solver='auto', tol=0.001))]),

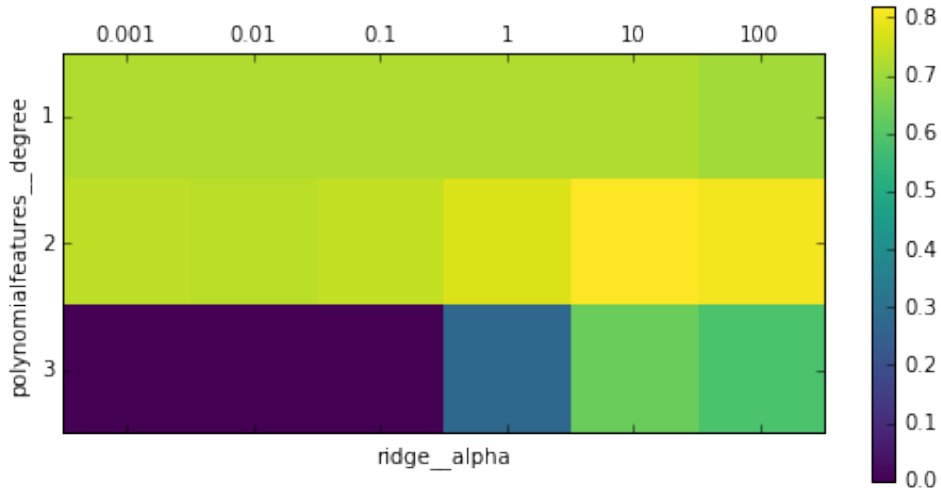
             fit_params={}, iid=True, n_jobs=-1,

             param_grid={'ridge__alpha': [0.001, 0.01, 0.1, 1, 10, 100], 'polynomialfeatures__degree': [
pre_dispatch='2*n_jobs', refit=True, scoring=None, verbose=0)
```

We can visualize the outcome of the cross-validation using a heatmap, as we did in Chapter 6:

```
plt.matshow(np.array([s.mean_validation_score for s in grid.grid_scores_]).reshape(3, -1),
            vmin=0, cmap="viridis")
plt.xlabel("ridge__alpha")
plt.ylabel("polynomialfeatures__degree")
plt.xticks(range(len(param_grid['ridge__alpha']), param_grid['ridge__alpha'])
plt.yticks(range(len(param_grid['polynomialfeatures__degree']), param_grid['polynomialfeatures__c

plt.colorbar()
```



Looking at the results produced by the cross-validation, we can see that using polynomials of degree two helps, but that degree three polynomials are much worse than either degree one or two.

This is reflected in the best parameters that were found:

```
print(grid.best_params_)
{'ridge__alpha': 10, 'polynomialfeatures__degree': 2}
```

Which lead to the following score:

```
grid.score(X_test, y_test)
0.76735803503061784
```

Let's run a grid-search without polynomial features for comparison:

```
param_grid = {'ridge__alpha': [0.001, 0.01, 0.1, 1, 10, 100]}
pipe = make_pipeline(StandardScaler(), Ridge())
grid = GridSearchCV(pipe, param_grid, cv=5)
grid.fit(X_train, y_train)
grid.score(X_test, y_test)
0.62717803817745799
```

As we had expected from the grid-search results visualized above, using no polynomial features leads to decidedly worse results. Searching over preprocessing parameters together with model parameters is a very powerful strategy. However, keep in mind that `GridSearchCV` tries *all possible combinations* of the specified parameters. Adding more parameters to your grid therefore increases the number of models that need to be built exponentially.

## Summary and Outlook

In this chapter we introduced the `Pipeline` class a general purpose tool to chain together multiple processing steps in a machine learning work flow. Real-world applications of machine learning are rarely an isolated use of a model, and instead a sequence of processing steps. Using pipelines allows us to encapsulate multiple steps into a single python object that adheres to the familiar scikit-learn interface of `fit`, `predict` and `transform`.

In particular when doing model evaluation using cross-validation and parameter selection using grid-search, using the `Pipeline` class to capture all processing steps is essential for proper evaluation.

The `Pipeline` class also allows writing more succinct code, and reduces the likelihood of mistakes that can happen when building processing chains without the pipeline class (like forgetting to apply all transformers on the test set, or maybe not applying them in the right order).

Choosing the right combination of feature extraction, preprocessing and models is somewhat of an art, that often requires some trial-and-error. However, using pipelines, this “trying out” of many different processing steps is quite simple. When experimenting, be careful not to over-complicate your processes, and make sure to evaluate whether every component your are including in your model is necessary.

With this chapter, we complete our survey of general purpose tools and algorithms provided by scikit-learn. You now possess all the required skills and know the necessary mechanisms to apply machine learning in practice. In the next chapter, we will dive in more detail into one particular type of data that is commonly seen in practice, and that requires some special expertise to handle correctly: text data.



---

# Working with Text Data

In Chapter 5, we talked about two kinds of features that can represent properties of the data: continuous features that describe a quantity, and categorical features that are items from a fixed list. There is a third kind of feature that can be found in many applications, which is text.

For example, if we want to classify an email into whether it is a legitimate email or spam, the content of the email will certainly contain important information for this classification task. Or maybe we want to learn about the opinion of a politician on the topic of immigration. Here, their speeches or tweets might provide useful information.

In customer services, we often want to find out if a message is a complaint or an inquiry. And depending on the kind of complaint, we might be able to provide automatic advice or forward it to a specific department. These decisions can all be supported by the content of the message that was sent to customer service.

Text data is usually represented as strings, made up of characters. In any of the examples above, the length of the text of each text will be different.

This feature is clearly very different from the numeric features that we discussed so far, and we need to process the text data before we can apply our machine learning algorithms to the text data.

## Types of data represented as strings

Before we dive into the processing steps that go into representing text data for machine learning, we want to briefly discuss different kinds of text data that you might encounter. Text is usually just a string in your dataset, but not each string feature should be treated as text. A string feature can sometimes represent categorical

variables, as we discussed in Chapter 5. There is no way to know how to treat a string feature before looking at the data.

There are four kinds of string data you might see:

- Categorical data
- Free strings that can be semantically mapped to categories
- Structured string data
- Text data

*Categorical data* is data that comes from a fixed list. Say you collect data via a survey where you ask people their favorite color, with a drop-down menu that allows them to select from “red”, “green”, “blue”, “yellow”, “black”, “white”, “purple” and “pink”. This will result in a dataset with exactly 8 different possible values, which clearly encode a categorical variable. You can check whether this is the case for your data by eyeballing it (if you see very many different strings it is unlikely that this is a categorical variable), and confirming it by computing the unique values over the dataset, and possibly a histogram over how often each appears. You also might want to check whether each variable actually corresponds to a category that makes sense for your application. Maybe half-way through the existence of your survey, someone found that “black” was misspelled as “blak” and subsequently fixed the survey. As a result your dataset contains both “blak” and “black”, which correspond to the same semantic meaning, and should be consolidated.

Now imagine instead of providing a drop-down menu, you provide a text field for the user to provide their own favorite color. Many people might respond with a color name like “black” or “blue”. Others might have typographic errors, or use aliases, or different spellings like “gray” and “grey”, use more evocative names like “midnight blue”, and there will certainly be answers that can not reasonably be related to any color, say “calmly checkered hissing” or “asdfasdfasdf”.

The responses you can obtain from a text field belong to the second category, *free strings that correspond to a set of categories*. It will probably be best to encode this data as a categorical variable, where you can select the categories either using the most common entries, or by defining categories that will capture responses in a way that makes sense for your application.

You might then have some categories for standard colors, maybe a category “multi-colored” for people that gave answers like “green and red stripes” and an “other” category, for things that can not be encoded otherwise. This kind of preprocessing of strings can take a lot of manual effort, and is not easily automated.

If you are in a position where you can influence data collection, we highly recommend avoiding manually entered values for concepts that are better captured using categorical variables.

Often, manually entered values do not correspond to fixed categories, but still have some *underlying structure*, like addresses, names of places or people, dates, telephone numbers or other identifiers. These kind of strings are often very hard to parse, and their treatment is highly dependent on context and domain. A systematic treatment of these cases is beyond the scope of this book.

The final category of string data is *free form text that consists of phrases or sentences*. Examples of these include tweets, chat logs, hotel reviews, but also the collected works of Shakespeare, the content of Wikipedia or the project Gutenberg collection of 50.000 e-books. All of these collections contain information mostly as sentences of words[footnote: arguably the content of websites linked to in tweets contain more information than the text of the tweet]. For simplicity's sake, let's assume all our documents are in one language, English [footnote: most of what we will talk about in the rest of the chapter also applies to other languages that use the Roman alphabet, and partially also to other alphabets with word boundary delimiters. Chinese for example does not delimit word boundaries, and has other challenges that make applying the techniques of this chapter difficult]. In the context of text analysis, the dataset is often called the *corpus*, and each data point, represented as a single text, is called a *document*.

These terms come from the *information retrieval* (IR) and *natural language processing* (NLP) community, which both deal mostly in text data.

## Example application: Sentiment analysis of movie reviews

As a running example in this chapter, we will use a data set of movie reviews collected from the IMDb (Internet Movie Database) website collected by Stanford Researcher Andrew Maas [footnote: The dataset is available at <http://ai.stanford.edu/~amaas/data/sentiment/>]. This dataset contains the text of the reviews, together with a label that indicates “positive” and “negative” reviews. The IMDb website itself contains ratings from one to ten. To simplify the modeling, this annotation is summarized as a two-class classification dataset where reviews with a score of 6 or higher are labeled as positive, and the rest as negative. We will leave the question of whether this is a good representation of the data open, and simply use the data as provided by Andrew Maas.

After unpacking the data, the data set is provided as text files in two separate folders, one for the training data, and one for the test data. Each of these in turn has two sub-folders, one called “positive” and one called “negative”:

```
!tree -L 2 data/acLImdb
```

```

data/aclImdb
├── test
│   ├── neg
│   └── pos
└── train
    ├── neg
    └── pos

```

6 directories, 0 files

The “positive” folder contains all the positive documents, each as a separate text file, and similarly for the “negative” folder. There is a helper function in scikit-learn to load files stored in such a folder-structure, where each subfolder corresponds to a label, called `load_files`. We apply the `load_files` function first to the training data:

```

from sklearn.datasets import load_files

reviews_train = load_files("data/aclImdb/train/")
# load_files returns a bunch, containing training texts and training labels
text_train, y_train = reviews_train.data, reviews_train.target
print("type of text_train: ", type(text_train))
print("length of text_train: ", len(text_train))
print("text_train[1]:")
# print review number 1
print(text_train[1])

type of text_train: <class 'list'>

length of text_train: 25000

text_train[1]:

```

```

b'Words can\'t describe how bad this movie is. I can\'t explain it by writing only. You have too s

```

We can see that `text_train` is a list of length 25,000, where each entry is a string containing a review. We printed the review with index one. You can see that the review contains some HTML line breaks ("`<br />`"). While these are unlikely to have a large impact on our machine learning models, it is better to clean the data from this formatting before we proceed:

```

text_train = [doc.replace(b"<br />", b" ") for doc in text_train]

```

The type of the entries of `text_train` depends on your Python version. In Python3, they will be of type “bytes” which represents a binary encoding of the string data. In

Python2, `text_train` contains strings. We won't go into the details of the different string types in Python here, but recommend that you read the documentation regarding strings and unicode in Python [Footnote: <https://docs.python.org/3/howto/unicode.html> for Python 3 and <https://docs.python.org/2/howto/unicode.html> for Python 2].

The dataset was collected such that the positive class and the negative class balanced, so that there are as many positive as negative strings:

```
print(np.bincount(y_train))  
[12500 12500]
```

We load the test dataset in the same manner:

```
reviews_test = load_files("data/aclImdb/test/")  
text_test, y_test = reviews_test.data, reviews_test.target  
print("Number of documents in test data: %d" % len(text_test))  
print(np.bincount(y_test))  
text_test = [doc.replace(b"<br />", b" ") for doc in text_test]  
  
Number of documents in test data: 25000  
  
[12500 12500]
```

The task we want to solve is given a review, we want to assign the labels “positive” and “negative” based on the text content of the review. This is a standard binary classification task. However, the text data is not in a format that a machine learning model can handle. We need to convert the string representation of the text into a numeric representation that we can apply our machine learning algorithms to.

## Representing text data as Bag of Words

One of the most simple, but effective and commonly used ways to represent text for machine learning is using the *bag-of-words* representation. When using bag-of-words, we discard most of the structure of the input text, like chapters, paragraphs, sentences and formatting, and only count *how often each word appears in each text*. Discarding all this structure and counting only occurrence leads to the mental image of representing text as a “bag”.

Computing the bag-of-word representation for a corpus of documents consists of the following three steps:

- 1) Tokenization: Split each document into the words that appear in it (called *tokens*), for example by splitting them by whitespace and punctuation.
- 2) Vocabulary building: Collect a vocabulary of all words that appear in any of the documents, and number them (say in alphabetical order).

3) Encoding: For each document, count how often each of the words in the vocabulary appear in this document.

bag\_of\_words

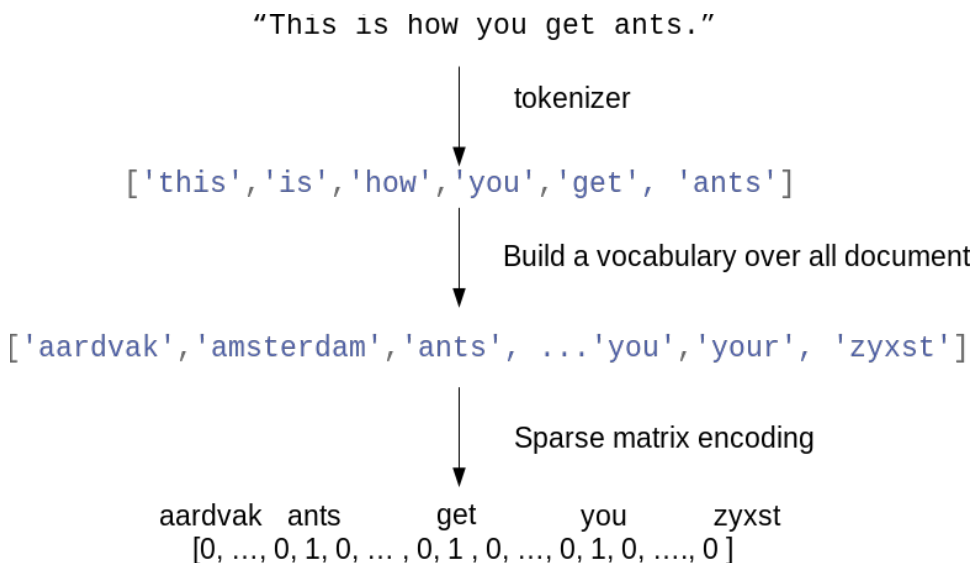


Figure bag\_of\_words illustrates the process on the string “This is how you get ants”. The output of the process is one vector of word-counts for each document. For each word in the vocabulary, we have a count of how often it appears in each document. That means our numeric representation has one feature for each unique word in the whole dataset. Note how the order of the words in the original string is completely irrelevant to the bag of words feature representation. There are some subtleties involved in step 1 and step 2 above, which we will discuss in more detail later in this chapter.

For now, let’s look at how we can apply the bag-of-word processing using scikit-learn.

### Applying bag-of-words to a toy dataset

The bag-of-word representation is implemented in the `CountVectorizer`, which is a transformer. Let’s first apply it to a toy dataset, consisting of two samples, to see it working:

```
bards_words = ["The fool doth think he is wise,",
               "but the wise man knows himself to be a fool"]
```

We import and instantiate the `CountVecorizer` and fit it to our toy data:

```
from sklearn.feature_extraction.text import CountVectorizer
vect = CountVectorizer()
vect.fit(bards_words)
```

```

CountVectorizer(analyzer='word', binary=False, decode_error='strict',
               dtype=<class 'numpy.int64'>, encoding='utf-8', input='content',
               lowercase=True, max_df=1.0, max_features=None, min_df=1,
               ngram_range=(1, 1), preprocessor=None, stop_words=None,
               strip_accents=None, token_pattern='(?u)\\b\\w\\w+\\b',
               tokenizer=None, vocabulary=None)

```

Fitting the `CountVectorizer` consists of the tokenization of the training data and building of the vocabulary, which we can access as the `vocabulary_` attribute:

```

print(len(vect.vocabulary_))
print("vocabulary content:")
vect.vocabulary_
{'be': 0,
 'but': 1,
 'doth': 2,
 'fool': 3,
 'he': 4,
 'himself': 5,
 'is': 6,
 'knows': 7,
 'man': 8,
 'the': 9,
 'think': 10,
 'to': 11,
 'wise': 12}
13

```

vocabulary content:

The vocabulary consists of 13 words, from “be” to “wise”.

To create the bag-of-words representation for the training data, we call the `transform` method:

```
bag_of_words = vect.transform(bards_words)
bag_of_words
<2x13 sparse matrix of type '<class 'numpy.int64'>'
```

with 16 stored elements in Compressed Sparse Row format>

The bag of word representation is stored in a SciPy sparse matrix that only stores the entries that are non-zero (see Chapter 1). The matrix is of shape 2 x 13, one row for each of the two data points, and one feature for each of the words in the vocabulary. A sparse matrix is used as most documents only contain a small subset of the words in the vocabulary, meaning most entries in the feature array are zero. Think about how many different words might appear in a movie review compared to all the words in the English language (which is what the vocabulary models). Storing all these zeros would be prohibitive, and a waste of memory.

To look at the actual content of the sparse matrix, we can convert it to a “dense” NumPy array (that also stores all the zero entries) using the `toarray` method. This is possible because we are using a small toy dataset that contains only 13 words. For any real dataset, this would result in a `MemoryError`.

```
print(bag_of_words.toarray())
[[0 0 1 1 1 0 1 0 0 1 1 0 1]
 [1 1 0 1 0 1 0 1 1 1 0 1 1]]
```

We can see that the word counts for each word are either zero or one, none of the two strings in `bards_words` contain a word twice. You can read these feature vectors as follows: The first string "The fool doth think he is wise," is represented as the first row in, and it contains the first word in the vocabulary, "be", zero times. It also contains the second word in the vocabulary, "but", zero times. It does contain the third word, "doth", once, and so on. Looking at both rows, we can see that the fourth word, "fool", the tenth word "the" and the thirteenth word "wise" appear in both strings.

## Bag-of-word for movie reviews

Now that we went through the bag-of-word process in detail, let's apply it to our task of sentiment analysis for movie reviews. Above, we already loaded our training and test data from the IMDb reviews into lists of strings (`text_train` and `text_test`), which we will now process:

```
vect = CountVectorizer().fit(text_train)
X_train = vect.transform(text_train)
print(repr(X_train))
```



```
<25000x74849 sparse matrix of type '<class 'numpy.int64'>
```

```
with 3431196 stored elements in Compressed Sparse Row format>
```

The shape of  $X_{\text{train}}$ , the bag-of-words representation of the training data, is 25,000 x 74,849, indicating that the vocabulary contains 74,849 entries. Again, the data is stored as a SciPy sparse matrix. Let's look in a bit more detail at the vocabulary. Another way to access the vocabulary is using the `get_feature_name` method of the vectorizer, which returns a convenient list where each entry corresponds to one feature:

```
feature_names = vect.get_feature_names()
print(len(feature_names))
# print first fifty features
print(feature_names[:20])
# print feature 20010 to 20030
print(feature_names[20010:20030])
# get every 2000th word to get an overview
print(feature_names[::2000])
```

```
74849
```

```
['00', '000', '0000000000001', '00001', '00015', '000s', '001', '003830', '006', '007', '0079', '0
```

```
['dratted', 'draub', 'draught', 'draughts', 'draughtswoman', 'draw', 'drawback', 'drawbacks', 'dra
```

```
['00', 'aesir', 'aquarian', 'barking', 'blustering', 'bête', 'chicanery', 'condensing', 'cunning',
```

As you can see, possibly a bit surprisingly, is that the first ten entries in the vocabulary are all numbers. All these numbers appear somewhere in the reviews, and are therefore extracted as words. Most of these numbers don't have any immediate semantic meaning---apart from "007", which, in particular in the context of movies, is likely to refer to the James Bond character [footnote: A quick analysis of the data confirms that this is indeed the case. Try confirming it yourself.]. Weeding out the meaningful from the non-meaningful "words" is sometimes tricky. Looking at some words further along in the vocabulary, we find a collection of English words starting with "dra". You might notice that for "draught", "drawback" and "drawer" both the singular and plural form are contained in the vocabulary as distinct words. These words have very closely related semantic meanings, and counting them as different words, corresponding to different features, might not be ideal.

Before we try to improve our feature extraction, let us obtain a quantitative measure of performance by actually building a classifier. We have the training labels stored in  $y_{\text{train}}$  and the bag-of-word representation of the training data in  $X_{\text{train}}$ , so we can train a classifier on this data. For high-dimensional, sparse data like this, linear models, like `LogisticRegression` often work best. Let's start by evaluating `LogisticRegression` using cross-validation[footnote: The attentive reader might notice that we violate our lesson from Chapter 7 on cross-validation with preprocessing. Using

the default settings of `CountVectorizer`, it actually does not collect any statistics, so our results are valid. Using `Pipeline` from the start would be a better choice for applications, but we defer it for ease of exposure.]

```
from sklearn.model_selection import cross_val_score
from sklearn.linear_model import LogisticRegression

scores = cross_val_score(LogisticRegression(), X_train, y_train, cv=5)
np.mean(scores)

0.8813199999999999
```

We obtain a mean cross-validation score of 88.2%, which indicates reasonable performance for a balanced binary classification task. We know that `LogisticRegression` has a regularization parameter `C` which we can tune via cross-validation:

```
from sklearn.model_selection import GridSearchCV
param_grid = {'C': [0.001, 0.01, 0.1, 1, 10]}
grid = GridSearchCV(LogisticRegression(), param_grid, cv=5)
grid.fit(X_train, y_train)
print("Best cross-validation score: ", grid.best_score_)
print("Best parameters: ", grid.best_params_)

Best cross-validation score: 0.88816

Best parameters: {'C': 0.1}
```

We obtain a cross-validation score of 88.8% using `C=0.1`. We can now assess the generalization-performance of this parameter setting on the test set:

```
X_test = vect.transform(text_test)
grid.score(X_test, y_test)

0.8789599999999999
```

Now, let's see if we can improve the extraction of words. The way the `CountVectorizer` extracts tokens is using a regular expression. By default, the regular expression that is used is `"\b\w\w+\b"`. If you are not familiar with regular expressions, this means it finds all sequences of characters that consist of at least two letters or numbers (`"\w"`) and that are separated by word boundaries (`"\b"`), in particular it does not find single-letter words, and it splits up contractions like “doesn't” or “bit.ly”, but matches “h8ter” as a single word. The `CountVectorizer` then converts all words to lower-case characters, so that “soon”, “Soon” and “sOon” all correspond to the same token (and therefore feature).

This simple mechanism works quite well in practice, but as we saw above, we get many uninformative features like the numbers. One way to cut back on these is to only use tokens that appear in at least 2 documents (or at least 5 documents etc). A token that appears only in a single document is unlikely to appear in the test set and is therefore not helpful.



```
print(len(ENGLISH_STOP_WORDS))
# print some of the stop words
print(list(ENGLISH_STOP_WORDS)[:10])

318
```

```
['show', 'however', 'something', 'is', 'of', 'are', 'about', 'least', 'eight', 'thereupon', 'always']
```

Clearly, removing the stop-words in the list can only decrease the number of features by the length of the list, here 318, but it might lead to an improvement in performance. Let's give it a try:

```
# specifying "english" uses the build-in list. We could also augment it and pass our own.
vect = CountVectorizer(min_df=5, stop_words="english").fit(text_train)
X_train = vect.transform(text_train)
print(repr(X_train))

<25000x26966 sparse matrix of type '<class 'numpy.int64'>'
      with 2149958 stored elements in Compressed Sparse Row format>
```

There are now 305 (=27272 - 26967) less features in the dataset, which means that most, but not all of the stop-words appeared. Let's run the grid-search again:

```
grid = GridSearchCV(LogisticRegression(), param_grid, cv=5)
grid.fit(X_train, y_train)
print("Best cross-validation score: ", grid.best_score_)

Best cross-validation score: 0.88296
```

The grid-search performance decreased slightly using the stop words. The change is very slight, but given that excluding 305 features is unlikely to change performance or interpretability a lot, it doesn't seem worth using this list. Fixed lists are mostly helpful for small datasets, that might not contain enough information for the model to determine which words are stop words from the data itself. As an exercise, you can try out the other approach, discarding frequently appearing words, by setting the `max_df` option of `CountVectorizer` and see how it influences the number of features and the performance.

## Rescaling the data with TFIDF

Instead of dropping features that are deemed unimportant, another approach is to rescale features by how informative we expect them to be. One of the most common ways to do this is using the term frequency-inverse document frequency (tf-idf) method. The intuition of this method is to give high weight to a term that appears often in a particular document, but not in many documents in the corpus. If a word appears often in a particular document, but not in very many documents, it is likely to be very descriptive of the content of that document.

Scikit-learn implements the tf-idf method in two classes, the `TfidfTransformer`, which takes in the sparse matrix output produced by `CountVectorizer` and transforms it, or `TfidfVectorizer`, which takes in the text data and does both the bag-of-words feature extraction and the tf-idf transformation.

There are several variants of the tf-idf rescaling scheme, which you can find on the wikipedia page [footnote: <https://en.wikipedia.org/wiki/Tf-idf>]. The tf-idf score for word  $w$  in document  $d$  as implemented in both the `TfidfTransformer` and `TfidfVectorizer` is given by:

$$\text{tfidf}(w, d) = \text{tf} \log\left(\frac{N + 1}{N_w + 1}\right) + 1$$

where  $N$  is the number of documents in the training set,  $N_w$  is the number of documents in the training set that the word  $d$  appears in, and  $\text{tf}$ , the term frequency, is the number of times that the word  $w$  appears in the query document (the document you want to transform or encode). Both classes also apply  $l_2$  normalization after computing the tf-idf representation, in other words they rescale the representation of each document to have euclidean norm 1. Rescaling in this way means that the length of a document (the number of words) does not change the vectorized representation. We provide this formula here mostly for completeness, and you don't need to remember it to use the tf-idf encoding.

Because tf-idf actually makes use of the statistical properties of the training data, we will use a pipeline, as described in Chapter 7, to ensure the results of our grid-search are valid. This leads to the following code:

```
from sklearn.feature_extraction.text import TfidfVectorizer
from sklearn.pipeline import make_pipeline
pipe = make_pipeline(TfidfVectorizer(min_df=5, norm=None), LogisticRegression())
param_grid = {'logisticregression__C': [0.001, 0.01, 0.1, 1, 10]}

grid = GridSearchCV(pipe, param_grid, cv=5)
grid.fit(text_train, y_train)
print("Best cross-validation score: ", grid.best_score_)

Best cross-validation score: 0.89392
```

As you can see, there is some improvement of using tf-idf instead of using just word counts. We can also inspect which words tf-idf found most important. Keep in mind that the tf-idf scaling is meant to find words that distinguish documents, but it is a purely unsupervised technique. So “important” here does not necessarily related to the “positive review” and “negative review” labels we are interested in. First we extract the `TfidfVectorizer` from the pipeline:

```

vectorizer = grid.best_estimator_.named_steps["tfidfvectorizer"]
# transform the training dataset:
X_train = vectorizer.transform(text_train)
# find maximum value for each of the features over dataset:
max_value = X_train.max(axis=0).toarray().ravel()
sorted_by_tfidf = max_value.argsort()
# get feature names
feature_names = np.array(vectorizer.get_feature_names())

print("features with lowest tfidf")
print(feature_names[sorted_by_tfidf[:20]])

print("features with highest tfidf")
print(feature_names[sorted_by_tfidf[-20:]])

features with lowest tfidf

['poignant' 'disagree' 'instantly' 'importantly' 'lacked' 'occurred'

 'currently' 'altogether' 'nearby' 'undoubtedly' 'directs' 'fond' 'stinker'

 'avoided' 'emphasis' 'commented' 'disappoint' 'realizing' 'downhill'

 'inane']

features with highest tfidf

['coop' 'homer' 'dillinger' 'hackenstein' 'gadget' 'taker' 'macarthur'

 'vargas' 'jesse' 'basket' 'dominick' 'the' 'victor' 'bridget' 'victoria'

 'khouri' 'zizek' 'rob' 'timon' 'titanic']

```

Features with low tf-idf are those that are either very commonly used across documents, or are only used sparingly, and only in very long documents. Interestingly, many of the high tf-idf features actually identify certain shows or movies. These terms only appear in reviews for this particular show or franchise, but tend to appear very often in these particular reviews. This is very clear for example for “pokemon”, “smallville” and “doodlebops”, but “scanners” here actually also refers to a movie title. These words are unlikely to help us in our sentiment classification task (unless maybe some franchises are universally reviewed positively or negatively) but certainly contain a lot of specific information about the review.

We can also find the words that have low inverse document frequency, that is those that appear frequently and are therefore deemed less important. The inverse document frequency values found on the training set are stored in the `idf_` attribute:

```

sorted_by_idf = np.argsort(vectorizer.idf_)
print("features with lowest idf")
print(feature_names[sorted_by_idf[:100]])

```

features with lowest idf

```
['the' 'and' 'of' 'to' 'this' 'is' 'it' 'in' 'that' 'but' 'for' 'with'
 'was' 'as' 'on' 'movie' 'not' 'have' 'one' 'be' 'film' 'are' 'you' 'all'
 'at' 'an' 'by' 'so' 'from' 'like' 'who' 'they' 'there' 'if' 'his' 'out'
 'just' 'about' 'he' 'or' 'has' 'what' 'some' 'good' 'can' 'more' 'when'
 'time' 'up' 'very' 'even' 'only' 'no' 'would' 'my' 'see' 'really' 'story'
 'which' 'well' 'had' 'me' 'than' 'much' 'their' 'get' 'were' 'other'
 'been' 'do' 'most' 'don' 'her' 'also' 'into' 'first' 'made' 'how' 'great'
 'because' 'will' 'people' 'make' 'way' 'could' 'we' 'bad' 'after' 'any'
 'too' 'then' 'them' 'she' 'watch' 'think' 'acting' 'movies' 'seen' 'its'
 'him']
```

As expected, these are mostly English stop words like “the” and “no”. But some are clearly domain specific to the movie reviews, like “movie”, “film”, “time”, “story” and so on. Interestingly, “good”, “great” and “bad” are also among the most frequent, and therefore “least relevant” words, even though we might expect these to be very important for our sentiment analysis task.

## Investigating model coefficients

Finally, let us look into a bit more detail into what our logistic regression model actually learned from the data.

Because there are so many features, 27.272 after removing the infrequent ones, we can clearly not look at all of the coefficients at the same time. However, we can look at the largest coefficients, and see which words these correspond to.

We will use the last model that we trained, based on the tf-idf features.

```
mglearn.tools.visualize_coefficients(grid.best_estimator_.named_steps["logisticregression"].coef_,
                                     feature_names, n_top_features=40)
plt.title("tfidf-coefficient")
```





```
cv = CountVectorizer(ngram_range=(1, 1)).fit(bards_words)
print(len(cv.vocabulary_))
print(cv.get_feature_names())
```

13

```
['be', 'but', 'doth', 'fool', 'he', 'himself', 'is', 'knows', 'man', 'the', 'think', 'to', 'wise']
```

To look only at bigrams, that is only at sequences of two tokens following each other, we can set `ngram_range` to `(2, 2)`:

```
cv = CountVectorizer(ngram_range=(2, 2)).fit(bards_words)
print(len(cv.vocabulary_))
print(cv.get_feature_names())
```

14

```
['be fool', 'but the', 'doth think', 'fool doth', 'he is', 'himself to', 'is wise', 'knows himself']
```

Using longer sequences of tokens usually results in many more features, and in more specific features. There is no common bigram between the two phrases in `bard_words`:

```
cv.transform(bards_words).toarray()
array([[0, 0, 1, 1, 1, 0, 1, 0, 0, 1, 0, 1, 0, 0],
       [1, 1, 0, 0, 0, 1, 0, 1, 1, 0, 1, 0, 1, 1]])
```

For most applications, the minimum number of tokens should be one, as single words often capture a lot of meaning. Adding bigrams helps in most cases, and adding longer sequences, up to 5-grams, might help, but will lead to an explosion of the number of features, and might lead to overfitting, as there are many very specific features.

Here is what using unigrams, bigrams and trigrams on `bards_words` looks like:

```
cv = CountVectorizer(ngram_range=(1, 3)).fit(bards_words)
print(len(cv.vocabulary_))
print(cv.get_feature_names())
```

39

```
['be', 'be fool', 'but', 'but the', 'but the wise', 'doth', 'doth think', 'doth think he', 'fool',
```

Let's use the `TfidfVectorizer` on the IMDb movie review data and find the best setting of `n-gram` range using grid-search:

```
pipe = make_pipeline(TfidfVectorizer(min_df=5), LogisticRegression())
param_grid = {'logisticregression__C': [0.001, 0.01, 0.1, 1, 10, 100, 1000],
              "tfidfvectorizer__ngram_range": [(1, 1), (1, 2), (1, 3)]}

grid = GridSearchCV(pipe, param_grid, cv=5)
grid.fit(text_train, y_train)
```

```
print("Best cross-validation score: ", grid.best_score_)
grid.best_params_

{'logisticregression__C': 1000, 'tfidfvectorizer__ngram_range': (1, 3)}

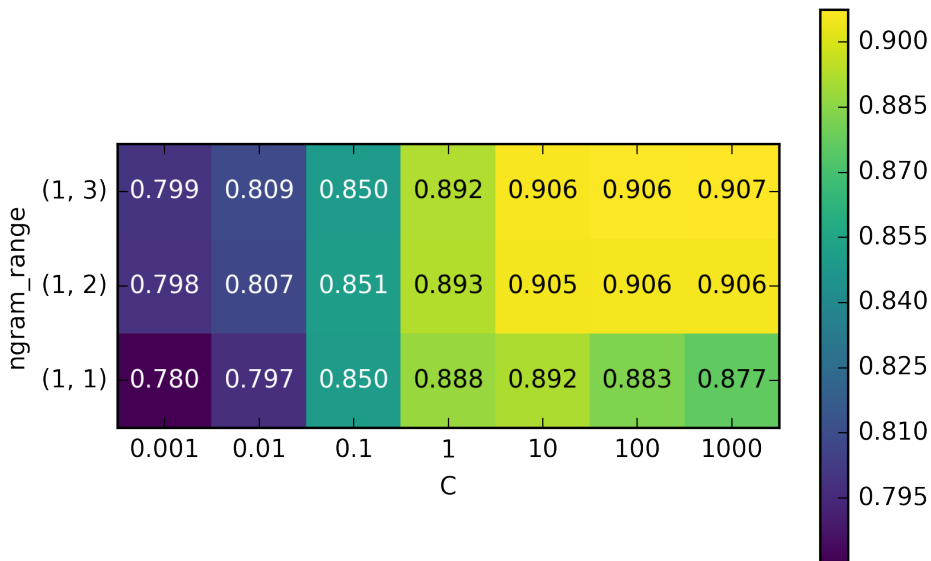
Best cross-validation score: 0.9074
```

As you can see from the results, we improved performance a bit more than a percent by adding bigram and trigram features.

We can visualize the cross-validation accuracy as a function of the `ngram_range` and `C` parameter as a heat map, as we did in Chapter 6:

```
# extract scores from grid_search
scores = [s.mean_validation_score for s in grid.grid_scores_]
scores = np.array(scores).reshape(-1, 3).T
# visualize heatmap
heatmap = mglearn.tools.heatmap(scores, xlabel="C", ylabel="ngram_range",
                                xticklabels=param_grid['logisticregression__C'],
                                yticklabels=param_grid['tfidfvectorizer__ngram_range'],
                                cmap="viridis", fmt="%.3f")

plt.colorbar(heatmap);
```



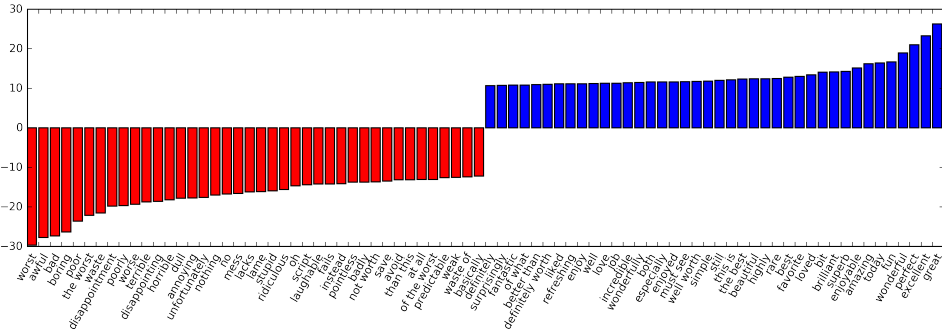
From the heat map we can see that using bigrams increases performance quite a bit, while adding three-grams only provides a very small benefit in terms of accuracy. To understand better how the model improved, we visualize the important coefficient for the best model (which includes unigrams, bigrams and trigrams):

```
# extract feature names and coefficients
feature_names = np.array(grid.best_estimator_.named_steps['tfidfvectorizer'].get_feature_names())
coef = grid.best_estimator_.named_steps['logisticregression'].coef_
```

```

mglearn.tools.visualize_coefficients(coef, feature_names, n_top_features=40)
plt.title("ngram-coefficient")

```



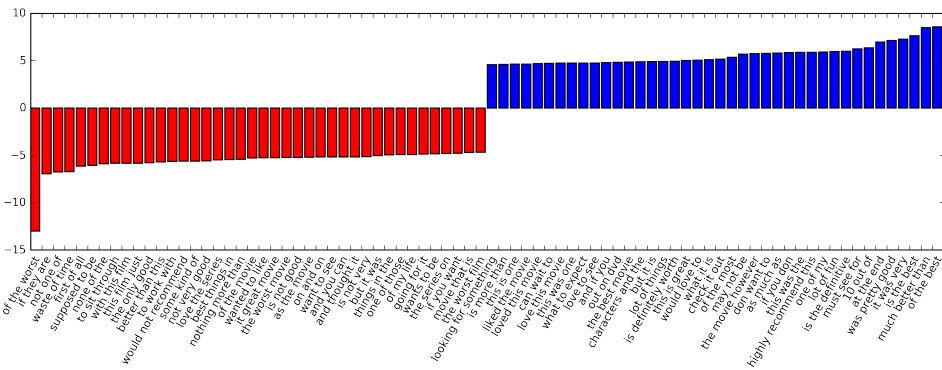
There are particularly interesting features containing the word “worth” that were not present in the unigram model: “not worth” is indicative of a negative review, while “definitely worth” and “well worth” are indicative of a positive review. This is a prime example of context influencing the meaning of the word “worth”.

Below, we visualize only bigrams and trigrams, to provide further insight into why these features are helpful. Many of the useful bigrams and trigrams consist of common words that would not be informative on their own, as in the phrases “none of the”, “the only good”, “on and on”, “this was one of”, “of the most” and so on. However, the impact of these features is quite limited compared to the importance of the unigram features.

```

# find 3-gram features
mask = np.array([len(feature.split(" ")) for feature in feature_names]) == 3
# visualize only 3-gram features:
mglearn.tools.visualize_coefficients(coef.ravel()[mask],
                                     feature_names[mask], n_top_features=40)

```



## Advanced tokenization, stemming and lemmatization

We mentioned above that the feature extraction in the `CountVectorizer` and `TfidfVectorizer` is relatively simple, and much more elaborate methods are possible. One particular step that is often improved in more sophisticated text processing applications is the first step in the bag-of-words model, the tokenization, the step defines what constitutes a word for the purpose of feature extraction.

We saw above that the vocabulary often contains singular and plural version of words as in 'drawback', 'drawbacks', 'drawer', 'drawers', 'drawing', 'drawings'. For the purpose of a bag-of-words model, the semantics of “drawback” and “drawbacks” are so close that distinguishing them will only increase overfitting, and not allow the model to fully exploit the training data. Similarly, we found the vocabulary includes words like 'replace', 'replaced', 'replacement', 'replaces', 'replacing', which are different verb forms and a nouns relating to the verb “to replace”.

Similarly to having singular and plural of a noun, treating different verb-forms and related words as distinct tokens is disadvantageous for building a model that generalizes well. This problem can be overcome by representing each word using its *word stem*, identifying (or *conflating*) all the words that have the same word stem. If this is done by using a rule-based heuristic, like dropping common suffixes, this is usually referred to as *stemming*. If instead a dictionary of known word forms is used (that is using an explicit and human-verified system), and the role of the word in the sentence taken into account, the process is referred to as *lemmatization* and the standardized form of the word is referred to as *lemma*. Both processing methods, lemmatization and stemming, are forms of *normalization* that try to extract some normal form of a word. Another interesting case of normalization is spell correction, which can be helpful in practice, but is outside of the scope of this book.

To get a better feeling for normalization, let's compare a method for stemming, the Porter stemmer, a widely used collection of heuristics (here imported from the `nltk` package) to lemmatization as implemented in the `SpaCy` package. For details of the interface, consult the `nltk` and `SpaCy` documentations. We are more interested in the general principles here.

```
import spacy
import nltk

# load spacy's English language models
en_nlp = spacy.load('en')
# instantiate NLTK's Porter stemmer
stemmer = nltk.stem.PorterStemmer()

# define function to compare lemmatization in spacy with stemming in NLTK
def compare_normalization(doc):
```

```

# tokenize document in spacy:
doc_spacy = en_nlp(doc)
# print lemmas found by spacy
print("Lemmatization:")
print([token.lemma_ for token in doc_spacy])
# print tokens found by Porter stemmer
print("Stemming:")
print([stemmer.stem(token.norm_.lower()) for token in doc_spacy])

```

We will compare lemmatization and the Porter stemmer on a sentence designed to show some of the differences:

```
compare_normalization(u"Our meeting today was worse than yesterday, I'm scared of meeting the client")
```

```
Lemmatization:
```

```
['our', 'meeting', 'today', 'be', 'bad', 'than', 'yesterday', ',', 'i', 'be', 'scared', 'of', 'meeting']
```

```
Stemming:
```

```
['our', 'meet', 'today', 'wa', 'wors', 'than', 'yesterday', ',', 'i', 'm', 'scare', 'of', 'meet']
```

Stemming is always restricted to trimming the word to a stem, so “was” becomes “wa”, while lemmatization can retrieve the correct base verb form, “be”. Similarly, lemmatization can normalize “worse” to “bad”, while stemming produces “wors”. Another major difference is that stemming reduces both occurrences of “meeting” to “meet”. Using lemmatization, the first occurrence of “meeting” is recognized as a noun, and left as-is, while the second occurrence is recognized as verb, and reduced to “meet”. In general, lemmatization is a much more involved process than stemming, but usually produces better results when used for normalizing tokens for machine learning.

While scikit-learn implements neither form of normalization, CountVectorizer allows specifying your own tokenizer to convert each document into a list of tokens using the tokenizer parameter. We can use the lemmatization from SpaCy to create a callable that will take a string and produce a list of lemmas:

```

# Technicality: we want to use the regexp based tokenizer that is used by CountVectorizer
# and only use the lemmatization from SpaCy. To this end, we replace en_nlp.tokenizer (the SpaCy tokenizer)
# with the regexp based tokenization
import re
# regexp used in CountVectorizer:
regexp = re.compile('(?!u)\b\w+\b')

# load spacy language model and save old tokenizer
en_nlp = spacy.load('en')
old_tokenizer = en_nlp.tokenizer
# replace the tokenizer with the regexp above
en_nlp.tokenizer = lambda string: old_tokenizer.tokens_from_list(regexp.findall(string))

# create a custom tokenizer using the SpaCy document processing pipeline
# (now using our own tokenizer)

```

```

def custom_tokenizer(document):
    doc_spacy = en_nlp(document, entity=False, parse=False)
    return [token.lemma_ for token in doc_spacy]

# define a count vectorizer with the custom tokenizer
lemma_vect = CountVectorizer(tokenizer=custom_tokenizer, min_df=5)

```

Let's transform the data and inspect the vocabulary size:

```

# transform text_train using CountVectorizer with lemmatization
X_train_lemma = lemma_vect.fit_transform(text_train)
print("X_train_lemma.shape: ", X_train_lemma.shape)

# Standard CountVectorizer for reference
vect = CountVectorizer(min_df=5).fit(text_train)
X_train = vect.transform(text_train)
print("X_train.shape: ", X_train.shape)

X_train_lemma.shape: (25000, 21596)

X_train.shape: (25000, 27271)

```

As you can see from the output above, lemmatization reduced the number of features from 27,272 (with the standard `CountVectorizer` processing) to 21,596. Lemmatization can be seen as a kind of regularization, as it conflates certain features. Therefore, we expect lemmatization to improve performance most when the dataset is small. To illustrate how lemmatization can help, we will use `StratifiedShuffleSplit` for cross-validation, using only 1% of the data as training data, and the rest as test data:

```

# build a grid-search using only 1% of the data as training set:
from sklearn.model_selection import StratifiedShuffleSplit

param_grid = {'C': [0.001, 0.01, 0.1, 1, 10]}
cv = StratifiedShuffleSplit(n_iter=5, test_size=0.99, train_size=0.01, random_state=0)
grid = GridSearchCV(LogisticRegression(),
                    param_grid, cv=cv)

# Perform grid-search with standard CountVectorizer
grid.fit(X_train, y_train)
print("Best cross-validation score (standard CountVectorizer): {:.3f}".format(grid.best_score_))
# Perform grid-search with Lemmatization
grid.fit(X_train_lemma, y_train)
print("Best cross-validation score (lemmatization): {:.3f}".format(grid.best_score_))

Best cross-validation score (standard CountVectorizer): 0.721

Best cross-validation score (lemmatization): 0.731

```

In this case, lemmatization provided a modest improvement in performance. As with many of the different feature extraction techniques, the result varies depending on the dataset. Lemmatization and stemming can sometimes help in building better, or at least more compact models, so we suggest you give these techniques a try when trying to squeeze out the last bit of performance on a particular task.

# Topic Modeling and Document Clustering

One particular technique that is often applied to text data is *topic modeling*, which is an umbrella term, describing the task of assigning each document to one or multiple *topics*, usually without supervision. A good example for this is news data, which might be categorized into topics like “politics”, “sports”, “finance” and so on. If each document is assigned a single topic, this is the task of clustering the documents, as discussed in Chapter 3.

If each document can have more than one topic, the task relates to decomposition methods from Chapter 3. Each of the components we learn then corresponds to one topic, and the coefficient of the components in the representation of a document tells us how much each document is about a particular topic.

Often, when people talk about topic modeling, they refer to one particular decomposition method called Latent Dirichlet Allocation (often LDA for short [footnote: There is another machine learning model called LDA, which is Linear Discriminant Analysis, a linear classification model. This leads to quite some confusion. In this book, LDA refers to Latent Dirichlet Allocation]).

Intuitively, the LDA model tries to find groups of words (the topics) that appear together frequently. LDA also requires that each document can be understood as a “mixture” of a subset of the topics. It is important to understand that for the machine learning model a “topic” might not be what we would normally call a topic in everyday speech, but that it resembles more the components extracted by PCA or NMF, which might or might not have a semantic meaning.

Even if there is a semantic meaning for an LDA “topic”, it might not be something we’d usually call a topic. Going back to the example of news articles, we might have a collection of articles about sports, politics and finance, written by two specific authors. In a politics article, we might expect words like “governor”, “vote”, “party” etc, while in a sports article we might expect words like “team”, “score” and “season”. Each of these groups will likely appear together, while it’s less likely that “team” and “governor” appear together.

However, these are not the only groups of words we might expect to appear together. The two reporters might prefer different phrases or different choices of words. Maybe one of them likes to use the word “demarcate” and one likes the word “polarize”. Another “topic” would then be “words often used by reporter A” and “words often used by reporter B”, though these are not topics in the usual sense of the word.

Let’s apply LDA to our movie review dataset to see how it works in practice. For unsupervised text document models, it is often good to remove very common words, as they might otherwise dominate the analysis. We remove words that appear in at

least 20 percent of the documents, and we limit the bag-of-words model to the 10,000 that are most common after removing the top 20 percent:

```
vect = CountVectorizer(max_features=10000, max_df=.15)
X = vect.fit_transform(text_train)
```

We learn a topic model with 10 topics, which is few enough that we can look at all of them.

Similarly to the components in NMF, topics don't have an inherent ordering, and changing the number of topics will change all of the topics. [footnote: In fact, NMF and LDA solve quite related problems, and we could also use NMF to extract "topics".]

We choose the "batch" learning method, which is somewhat slower than the default, but usually provides better results, and increase "max\_iter", which can also lead to better models.

```
from sklearn.decomposition import LatentDirichletAllocation
lda = LatentDirichletAllocation(n_topics=10, learning_method="batch", max_iter=25, random_state=0)
# be build the model and transform the data in one step
# computing transform takes some time, and we can save time by doing both at once.
document_topics = lda.fit_transform(X)
```

As in the decomposition methods we saw in Chapter 3, LDA has a `components_` attribute, that stores how important each word is for each topic. The size of `components_` is `(n_topics, n_words)`.

```
lda.components_.shape
(10, 10000)
```

To understand better what the different topics mean, we will look at the most important word for each of the topics. The `print_topics` function we use below provides a nice formatting for these features.

```
# for each topic (a row in the components_), sort the features (ascending).
# Invert rows with[:,::-1] to make sorting descending
sorting = np.argsort(lda.components_, axis=1)[::-1]
# get the feature names from the vectorizer:
feature_names = np.array(vect.get_feature_names())

# print out the 10 topics:
mglearn.tools.print_topics(topics=range(10), feature_names=feature_names,
                           sorting=sorting, topics_per_chunk=5, n_words=10)
```

topic 0	topic 1	topic 2	topic 3	topic 4
-----	-----	-----	-----	-----
between	war	funny	show	did
young	world	worst	series	saw



family	us	comedy	episode	am
real	our	thing	tv	thought
performance	american	guy	episodes	years
beautiful	documentary	re	shows	book
work	history	stupid	season	watched
each	new	actually	new	now
both	own	nothing	television	dvd
director	point	want	years	got

topic 5	topic 6	topic 7	topic 8	topic 9
-----	-----	-----	-----	-----
horror	kids	cast	performance	house
action	action	role	role	woman
effects	animation	john	john	gets
budget	game	version	actor	killer
nothing	fun	novel	oscar	girl
original	disney	both	cast	wife
director	children	director	plays	horror
minutes	10	played	jack	young
pretty	kid	performance	joe	goes
doesn	old	mr	performances	around

Judging from the important words, topic 1 seems to be about historical and war movies, topic 2 might be about bad comedy, topic 3 might be about tv series, topic 4 seems to capture some very common words, topic 6 seem to capture children's movies, and topic 8 seems to capture award-related reviews. Using only ten topics, each of the topics needs to be very broad, so that they can together cover all the different kinds of reviews in our dataset.

Next, we will learn another model, this time with 100 topics. Using more topics makes the analysis much harder, but makes it more likely that topics can specialize to interesting subsets of the data.

```
lda100 = LatentDirichletAllocation(n_topics=100, learning_method="batch", max_iter=25, random_state=1)
document_topics100 = lda100.fit_transform(X)
```

Looking at all 100 topics would be a bit overwhelming, so we selected some interesting and representative topics.

```
topics = np.array([7, 16, 24, 25, 28, 36, 37, 45, 51, 53, 54, 63, 89, 97])
sorting = np.argsort(lda100.components_, axis=1)[: , :-1]
feature_names = np.array(vect.get_feature_names())
mglearn.tools.print_topics(topics=topics, feature_names=feature_names, sorting=sorting,
                           topics_per_chunk=7, n_words=20)
```

topic 7	topic 16	topic 24	topic 25	topic 28	topic 36	topic 37
thriller	worst	german	car	beautiful	performance	excellent
suspense	awful	hitler	gets	young	role	highly
horror	boring	nazi	guy	old	actor	amazing
atmosphere	horrible	midnight	around	romantic	cast	wonderful
mystery	stupid	joe	down	between	play	truly
house	thing	germany	kill	romance	actors	superb
director	terrible	years	goes	wonderful	performances	actors
quite	script	history	killed	heart	played	brilliant
bit	nothing	new	going	feel	supporting	recommend
de	worse	modesty	house	year	director	quite
performances	waste	cowboy	away	each	oscar	performance
dark	pretty	jewish	head	french	roles	performances
twist	minutes	past	take	sweet	actress	perfect
hitchcock	didn	kirk	another	boy	excellent	drama
tension	actors	young	getting	loved	screen	without
interesting	actually	spanish	doesn	girl	plays	beautiful

mysterious	re	enterprise	now	relationship	award	human
murder	supposed	von	night	saw	work	moving
ending	mean	nazis	right	both	playing	world
creepy	want	spock	woman	simple	gives	recommended
topic 45	topic 51	topic 53	topic 54	topic 63	topic 89	topic 97
-----	-----	-----	-----	-----	-----	-----
music	earth	scott	money	funny	dead	didn
song	space	gary	budget	comedy	zombie	thought
songs	planet	streisand	actors	laugh	gore	wasn
rock	superman	star	low	jokes	zombies	ending
band	alien	hart	worst	humor	blood	minutes
soundtrack	world	lundgren	waste	hilarious	horror	got
singing	evil	dolph	10	laughs	flesh	felt
voice	humans	career	give	fun	minutes	part
singer	aliens	sabrina	want	re	body	going
sing	human	role	nothing	funniest	living	seemed
musical	creatures	temple	terrible	laughing	eating	bit
roll	miike	phantom	crap	joke	flick	found
fan	monsters	judy	must	few	budget	though
metal	apes	melissa	reviews	moments	head	nothing
concert	clark	zorro	imdb	guy	gory	lot
playing	burton	gets	director	unfunny	evil	saw
hear	tim	barbra	thing	times	shot	long
fans	outer	cast	believe	laughed	low	interesting

prince	men	short	am	comedies	fulci	few
especially	moon	serial	actually	isn	re	half

The topics we extracted this time seem to be more specific, though many are hard to interpret. Topic 7 seems to be about horror movies and thrillers, topics 16 and 54 see, to capture bad reviews, while topic 63 mostly seems to be capturing positive reviews of comedies.

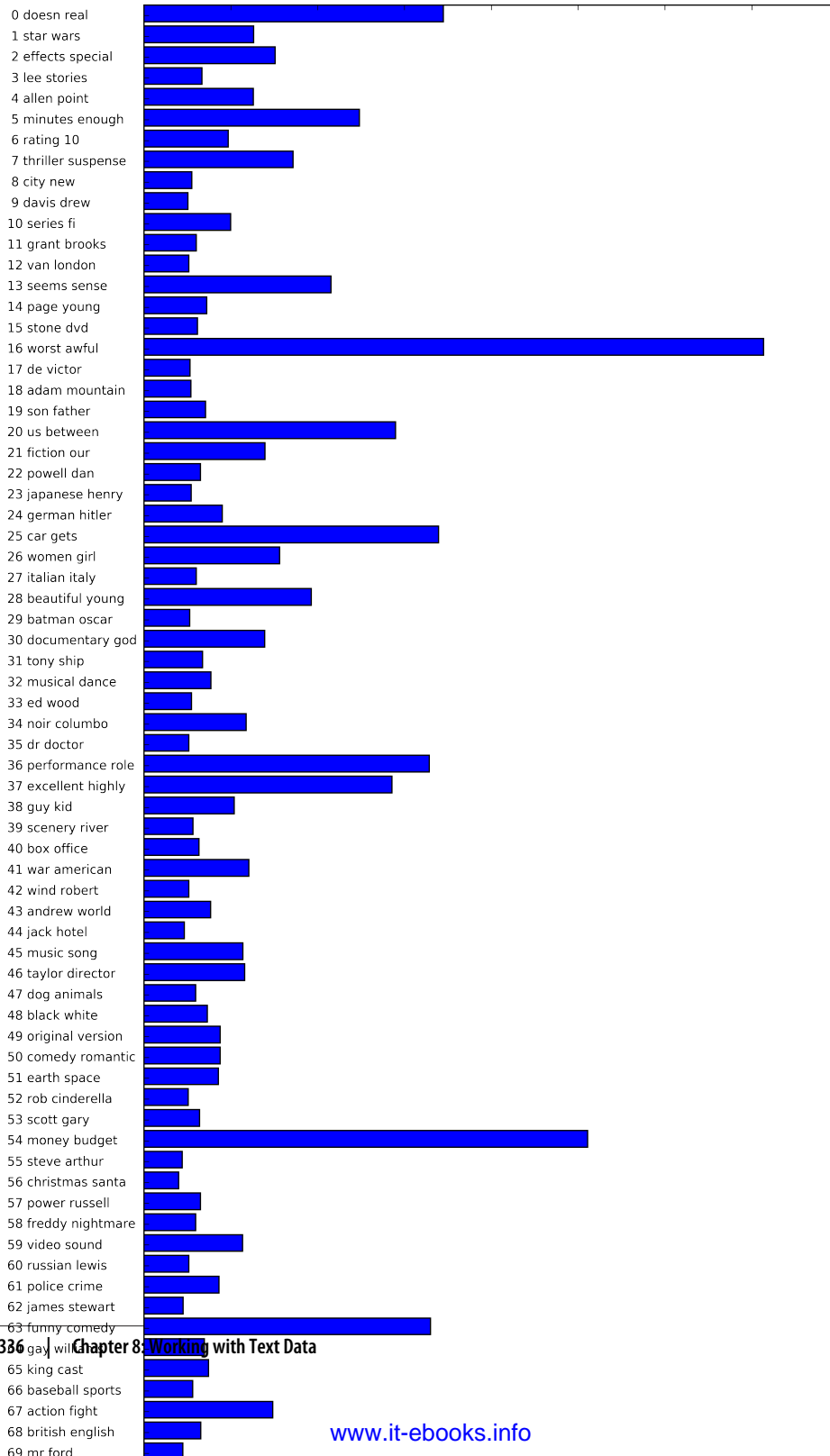
If you want to make further inferences using the topics that were discovered, it is good to confirm the intuition we gained from looking the highest ranking words for each topic, by looking at the documents that are assigned to these topics. For example, topic 45 seems to be about music. Let's check which kind of reviews are assigned this topic:

```
# sort by weight of "music" topic 45
music = np.argsort(document_topics100[:, 45])[:-1]
# print the five documents where the topic is most important
for i in music[:10]:
    # pshow first two sentences
    print(b".".join(text_train[i].split(b".")[:2]) + b".\n")
b'I love this movie and never get tired of watching. The music in it is great.\n'
b'I enjoyed Still Crazy more than any film I have seen in years. A successful band from the 70's c
b'Hollywood Hotel was the last movie musical that Busby Berkeley directed for Warner Bros. His dir
b"What happens to washed up rock-n-roll stars in the late 1990's? They launch a comeback / reunio
b'As a big-time Prince fan of the last three to four years, I really can't believe I've only jus
b"This film is worth seeing alone for Jared Harris' outstanding portrayal of John Lennon. It does
b"The funky, yet strictly second-tier British glam-rock band Strange Fruit breaks up at the end of
b'I just finished reading a book on Anita Loos' work and the photo in TCM Magazine of MacDonald in
b'I love this movie!!! Purple Rain came out the year I was born and it has had my heart since I ca
b"This movie is sort of a Carrie meets Heavy Metal. It's about a highschool guy who gets picked on
```

As we can see, this topic covers a wide variety of music-centered reviews, from musicals, to biographic movies, to some hard-to-specify genre in the last review. Another interesting way to inspect the topics is to see how much weight each topic gets overall, by summing the document\_topics over all reviews. We name each topic by the two most comen words:

```
plt.figure(figsize=(10, 30))
plt.barh(np.arange(100), np.sum(document_topics100, axis=0))
topic_names = [{">2} ".format(i) + " ".join(words) for i, words in enumerate(feature_names[sortin
```

```
plt.yticks(np.arange(100) + .5, topic_names, ha="left");  
ax = plt.gca()  
ax.invert_yaxis()  
yax = ax.get_yaxis()  
yax.set_tick_params(pad=110)
```



The most important topics are 97, which seems to consist mostly of stop-words, possibly with a slight negative direction, topic 16, which is clearly about bad reviews, followed by some genre-specific and 36 and 37, both of which seem to contain laudatory words.

It seems like LDA mostly discovered two kind of topics: genre-specific and rating-specific, in addition to several more unspecific topics. This seems like an interesting discovery, as most reviews are made of some movie-specific comments, and some comments that justify or emphasize the rating.

Topic models like LDA are an interesting methods to understand large text corpora in the absence of labels --- or, as here, even if labels are available. The LDA algorithms is randomized, though, and changing the `random_state` parameter can lead to quite different outcomes. While identifying topics can be helpful, any conclusions you draw from an unsupervised model should be taken with a grain of salt, and we recommend verifying your intuition by looking at the documents in a specific topic.

## Summary and Outlook

In this chapter we talked about the basics of processing text, also known as *natural language processing* (NLP) with an example application classifying movie reviews. The tools discussed here should serve as a great starting point when trying to process text data. In particular for text classification such as spam and fraud detection or sentiment analysis, bag of word representations provide a simple and powerful solution. As so often in machine learning, the representation of the data is key in NLP applications, and inspecting the tokens and n-grams that are extracted can give powerful insights into the modeling process. In text processing applications, it is often possible to introspect models in a meaningful way, as we saw above, both for supervised and unsupervised tasks. You should take full advantage of this ability when using NLP based methods in practice.

NLP and text processing is a large research field, and discussing the details of advanced methods is far beyond the scope of this book. If you want to learn more about text processing and natural language processing, we recommend the O'Reilly book *Natural Language Processing with Python* by Bird, Klein and Loper, which provides an overview of NLP together with an introduction to the `nltk` python package for NLP. Another great and more conceptual book is the standard reference *Introduction to information retrieval* by Manning, Raghavan and Sch&uuml;tze, which describes fundamental algorithms in information retrieval, NLP and machine learning. Both books have online versions that can be accessed free of charge.

As we discussed above, the classes `CountVectorizer` and `TfidfVectorizer` only implement relatively simple text processing methods. For more advanced text processing methods, we recommend the Python packages `SpaCy`, a relatively new, but

very efficient and well-designed package, `nltk`, a very well-established and complete, but somewhat dated library, and `gensim`, an NLP package with an emphasis on topic modelling.

There have been several very exciting new developments in text processing in recent years, which are outside of the scope of this book and relate to neural networks. The first is the use of continuous vector representations, also known as word vectors or distributed word representations, as implemented in the `word2vec` library. The original paper “Distributed representations of words and phrases and their compositionality” by Mikolov, Suskever, Chen, Corrado and Dean is a great introduction to the subject. Both `SpaCy` and `gensim` provide functionality for the techniques discussed in this paper and its follow-ups.

Another direction in NLP that has picked up momentum in recent years are *recurrent neural networks* (RNNs) for text processing. RNNs are a particularly powerful type of neural network that can produce output that is again text, in contrast to classification models that can only assign class labels. The ability to produce text as output makes RNNs well-suited for automatic translation and summarization. An introduction to the topic can be found in the relatively technical paper “Sequence to Sequence Learning

with Neural Networks” by Suskever, Vinyals and Le. A more practical tutorial using `tensorflow` framework can be found on the `tensorflow` website [footnote <https://www.tensorflow.org/versions/r0.8/tutorials/seq2seq/index.html>].