

# Computational Aspects in Econometrics - Python II module

Pieter Kleer

# Table of contents

<b>1 About</b>	<b>4</b>
1.1 Welcome . . . . .	4
1.2 Goal . . . . .	4
1.3 Use of Spyder . . . . .	4
<b>2 Good coding practices</b>	<b>5</b>
2.1 Efficient computations . . . . .	5
2.2 No hard coding . . . . .	7
2.3 Don't repeat yourself (DRY) . . . . .	8
2.4 Single responsibility . . . . .	9
2.5 Documentation . . . . .	10
<b>3 NumPy arrays</b>	<b>12</b>
3.1 Introduction . . . . .	12
3.2 Creating arrays . . . . .	12
3.2.1 Lists . . . . .	12
3.2.2 Arrays from functions . . . . .	15
3.2.3 Reading data from files . . . . .	17
3.3 Accessing . . . . .	17
3.3.1 Basic indexing . . . . .	18
3.3.2 Index slicing . . . . .	18
3.3.3 Fancy indexing . . . . .	20
3.4 Modifying . . . . .	21
3.4.1 Elements, rows or columns . . . . .	21
3.4.2 Broadcasting . . . . .	22
3.4.3 Transpose . . . . .	23
3.5 Repeating and stacking . . . . .	23
3.6 Reshaping . . . . .	24
3.7 Copy vs. view . . . . .	27
3.7.1 View . . . . .	27
3.7.2 Copy . . . . .	28
<b>4 Vectorization</b>	<b>30</b>
4.1 Arithmetic operations . . . . .	32
4.1.1 Multiplication broadcasting . . . . .	35
4.2 Mathematical functions . . . . .	35
4.3 Operations along array axes . . . . .	36
4.3.1 Sorting and searching . . . . .	37
4.3.2 Summary statistics . . . . .	39
<b>5 Linear algebra and optimization</b>	<b>42</b>
5.1 Linear algebra . . . . .	42

5.1.1	Matrix multiplications . . . . .	42
5.1.2	Matrix properties . . . . .	44
5.1.3	Equation solving . . . . .	46
5.2	Linear optimization . . . . .	47
5.2.1	Explicit input data . . . . .	48
5.2.2	Implicit input data . . . . .	51
5.2.3	Remarks . . . . .	55
<b>6</b>	<b>Nonlinear algebra and optimization</b>	<b>56</b>
6.1	Root finding . . . . .	56
6.1.1	Univariate function . . . . .	56
6.1.2	Multivariate functions . . . . .	61
6.1.3	Least squares method . . . . .	64
6.2	Nonlinear optimization . . . . .	67
6.2.1	Univariate function . . . . .	68
6.2.2	Multivariate function . . . . .	69
6.2.3	Constrained optimization . . . . .	69
6.2.4	Remarks . . . . .	71
<b>7</b>	<b>Visualization</b>	<b>72</b>
7.1	Basic plotting . . . . .	72
7.2	Subplots . . . . .	80
7.2.1	Fixed grid . . . . .	80
7.2.2	Iterative adding . . . . .	84
7.3	Bivariate functions . . . . .	86
7.3.1	Contour plot . . . . .	89
7.3.2	3D plot . . . . .	94
<b>8</b>	<b>Probability theory</b>	<b>96</b>
8.1	Randomness . . . . .	96
8.1.1	Samples . . . . .	96
8.1.2	Subsets . . . . .	99
8.1.3	Seed . . . . .	100
8.2	Probability distributions . . . . .	101
8.2.1	Distributions as input arguments . . . . .	105
<b>9</b>	<b>Statistics and data fitting</b>	<b>107</b>
9.1	Correlation coefficients . . . . .	107
9.1.1	Pearson coefficient . . . . .	107
9.1.2	Spearman rank coefficient . . . . .	108
9.1.3	Other coefficients . . . . .	111
9.2	Data fitting . . . . .	111
9.2.1	Regression . . . . .	111
9.2.2	Interpolation . . . . .	117
9.2.3	Distributional fitting . . . . .	120
<b>10</b>	<b>Learning problems</b>	<b>123</b>
10.1	Binary logistic regression . . . . .	123
10.1.1	Input data . . . . .	123
10.1.2	Classification model . . . . .	125
10.1.3	Visualization . . . . .	129
10.2	Clustering . . . . .	131
10.2.1	Input data . . . . .	131
10.2.2	Clustering algorithm . . . . .	133
10.2.3	Visualization . . . . .	135

10.3 Support vector machine (SVM) . . . . .	137
10.3.1 Input data . . . . .	137
10.3.2 Classification model . . . . .	140
10.3.3 Visualization . . . . .	143
<b>11 Higher-dimensional arrays</b>	<b>145</b>
11.1 Creating arrays . . . . .	145
11.2 Itertools . . . . .	149
11.3 Axis operations . . . . .	152
11.3.1 Arithmetic operations . . . . .	153
11.3.2 Reshaping . . . . .	154
11.4 Unpacking . . . . .	156
<b>Appendices</b>	<b>159</b>
<b>A Corrections and changes</b>	<b>159</b>
A.1 Chapter 11 . . . . .	159
A.2 Section 8.2.1 . . . . .	159
A.3 Section 3.2.2 . . . . .	159
A.4 Section 4.3.1 . . . . .	159
A.5 Section 3.5 . . . . .	159
<b>B Function basics</b>	<b>160</b>
B.1 Output arguments . . . . .	160

# Chapter 1

## About

### 1.1 Welcome

Welcome to the online “book” for the Python II module of Computational Aspects in Econometrics. We will follow the content in this book during the lectures and it is the basis of the material that will appear on the exam, so you should read through this book carefully. Because this book is new, it is likely that we will make some edits throughout the course.

Please note that this is an advanced Python module. We assume familiarity with the basics of programming in Python. For students enrolled in the bachelor Econometrics and Operations Research, the topics of the course Programming for EOR is a good example of what I expect you to be familiar with. An online book covering most of these topics can be found here. This book also contains some topics not covered in Programming for EOR.

### 1.2 Goal

The goal of this module is to teach you the basics of scientific computing with Python. Here you should think mostly of implementing algorithmic tasks that you encounter during your Econometrics and Operations Research courses, such as, linear algebra, optimization, statistics and machine learning. We hope that the skills you are taught here can be useful for, e.g., numerical work in your bachelor or (perhaps later) master thesis. Furthermore, many companies nowadays program in Python, so the topics of this module can also be useful in your professional career later in life.

Next to teaching you how to implement certain mathematical tasks in a correct manner in Python, we also put emphasis on good coding practices. Especially if you start to write scripts with hundreds of lines of code, it is important that you learn how to do this in a structured fashion using efficient Python functionality. Good coding practices are the topic of the next chapter. The idea is that you use these practices when doing the exercises corresponding to every lecture, as well as the group assignment.

### 1.3 Use of Spyder

This course document is based on the use of Spyder as integrated development environment (IDE) for creating Python code, i.e., the program that the code is written in. You can also use VS code or any other IDE to do the exercises and/or assignment in. Whenever this book contains screenshots to illustrate something, they will have been taken in Spyder.

To install the Anaconda distribution containing Spyder, follow the steps here. This is the installation that was also recommended in the Python I module.

# Chapter 2

## Good coding practices

In this chapter we will discuss the good coding practices that have to be applied when writing Python code: efficient computations, no hard coding, don't repeat yourself (DRY), single responsibility, and documentation. Overall, always try to keep your code simple and structured.

### 2.1 Efficient computations

Perhaps the most important topic of this course is that of efficient computation, i.e., to make efficient use of the mathematical functionality that Python has to offer, in particular the functionality of the NumPy package.

The way to think of this is as follows: Many of the mathematical tasks and exercises that we will see could, in theory, be solved using for- and/or while-loops, as well as if/else-statements. However, there are often more efficient functions programmed in the NumPy package in Python that can carry out these task in a quicker way using less code!

Let us look at an example. Suppose I am given a vector  $x = [x_1, \dots, x_n] \in \mathbb{R}^n$ , and I want to compute the  $L^2$ -norm

$$\|x\|_2 = \sqrt{\sum_{i=1}^n x_i^2}$$

of this vector. One way to solve this directly would be by using a for-loop to compute the sum inside the square root, and then take the square root of this number. We will illustrate this next for the vector  $x = [1, 2, 3, \dots, 300.000]$ .

```
# Length of vector
n = 300000

# Compute inner summation of ||x||_2
inner_sum = 0
for i in range(1,n+1):
    inner_sum = inner_sum + i**2

# Take square root
two_norm = (inner_sum)**(0.5)

# Print value of two-norm
print(two_norm)
```

94868566.97584295

Another way to do this is to define the vector  $x$  efficiently making use of the `arange()` function in Numpy, followed by the `linalg.norm()` function that can compute the  $L^2$ -norm for us directly. We will see these functions in more detail in a subsequent chapter.

It is standard convention to import the Numpy package under the alias `np`.

```
#Import Numpy package under the alias np
import numpy as np

# Length of vector
n = 300000

# Define vector x as array using arange() function
x = np.arange(1,n+1)

# Compute two-norm with built-in function
two_norm = np.linalg.norm(x)

# Print value of two-norm
print(two_norm)
```

94868566.97584295

This is a much cleaner, and in fact faster, way to compute the  $L^2$ -norm of the vector  $x$ . Especially for large values of  $n$ , the second piece of code that exploits the Numpy functionality can be much faster! The Python code below (which we will not discuss) illustrates this comparison by timing how long both approaches require to compute the norm for  $n = 30.000.000$  (i.e., thirty million). If you run the code below on your own device, you might get different outputs, but, in general, there should be a significant (multiplicative) difference in execution time.

```
import numpy as np
import time

## Computing norm with for-loop

# We determine the time it takes to input the code between start and end
start = time.time()

# Length of vector
n = 30000000

# Compute inner summation of ||x||_2
inner_sum = 0
for i in range(1,n+1):
    inner_sum = inner_sum + i**2

# Take square root
two_norm = (inner_sum)**(0.5)

end = time.time()

# Time difference
```

```

loop_time = end - start
print('%.10f seconds needed for computing norm' % (loop_time),
      'with for-loop')

## Computing norm with Numpy functions

#We determine the time it takes to input the code between start and end
start = time.time()

# Length of vector
n = 30000000

# Define vector x as array using arange() function
x = np.arange(1,n+1)

# Compute two-norm with built-in function
two_norm = np.linalg.norm(x)

end = time.time()

# Time difference
numpy_time = end - start
print('%.10f seconds needed for computing norm' % (numpy_time),
      'with Numpy functions')

#This shows how many times faster Numpy approach is faster than for-loop solution
if numpy_time != 0:
    (print('NumPy\'s approach is %i times more efficient than for-loop approach.' %
          ((loop_time)/(numpy_time))))

```

10.0970709324 seconds needed for computing norm with for-loop  
0.1190447807 seconds needed for computing norm with Numpy functions  
NumPy's approach is 84 times more efficient than for-loop approach.

One important take-away of the above comparison is the following.

When performing mathematical tasks, avoid the use of for- and while-loops, as well as if/else-statements, by efficient use of Python functionality.

## 2.2 No hard coding

Suppose we are given the function  $f(x) = a \cdot x^2 + a \cdot b \cdot x - a \cdot b \cdot c$  and the goal is to compute  $f(10)$  for  $a = 3, b = 4$  and  $c = -10$ . One way of doing this would be to plug in all the variables and return the resulting function value.

```

# Hard coding
print(3*(10**2) + 3*4*10 + 4*-2*3)

```

396

However, this is inefficient for the following reason: If we would want to change the number  $x = 10$  to, e.g.,  $x = 20$ , we would have to twice replace 10 by 20. The same is true for the variable  $a$ , which appears in even three places. In general, in large scripts, variables can appear in more than a hundred places. To overcome

this inefficiency issue, it is always better to separate the input data (the  $x, a, b$  and  $c$  in this case) from the function execution

```
# No hard coding
def f(x, a, b, c):
    return a*x**2 + a*b*x + b*c*a

x = 10
a, b, c = 3, 4, -2
print(f(x, a, b, c))
```

396

The take-away of the above comparison is the following.

Separate input data from the execution of functions and commands.

## 2.3 Don't repeat yourself (DRY)

If you have to carry out a piece of code for multiple sets of input data, always avoid copy-pasting the code. As a first step, try to do the repeated execution using a for-loop. For example, suppose we want to print the function values  $f(x, 3, 4, -2)$  for  $x = 1, 2, 3, 4$ , with  $f$  as in the previous section. We can do this as follows.

```
def f(x, a, b, c):
    return a*x**2 + a*b*x + b*c*a

a, b, c = 3, 4, -2

# With repetition
x = 1
print('%.2f' % f(x,a,b,c))
x = 2
print('%.2f' % f(x,a,b,c))
x = 3
print('%.2f' % f(x,a,b,c))
x = 4
print('%.2f' % f(x,a,b,c))
```

-9.00  
12.00  
39.00  
72.00

A more efficient way of typing this, is by using a for-loop that repeatedly executes the print statement.

```
import numpy as np

a, b, c = 3, 4, -2
x = [1,2,3,4]
# Determine all function values with list comprehension
y = [f(i,a,b,c) for i in x]

# Print values in y (could also print the whole vector y right away)
for j in y:
```

```
print(j)
```

```
-9  
12  
39  
72
```

The take-away of the above comparison is the following.

Don't carry out the same task on different inputs twice by copy-pasting code, but use, e.g., a for-loop in which you iterate over the inputs.

In fact, later on in the course we will explain the concept of vectorizing a function, to make sure it can handle multiple inputs simultaneously. This is another way to avoid unnecessary repetition and in fact also the use of loops.

## 2.4 Single responsibility

When you write larger pieces of codes, it is often useful to split it up in smaller parts that all serve their own purpose. Suppose we want to implement Newton's method for finding a root  $x$  of a function  $f : \mathbb{R} \rightarrow \mathbb{R}$ , i.e., a point  $x$  that satisfies  $f(x) = 0$ .

Newton's methods starts with a (suitably chosen) initial guess  $x_0 \in \mathbb{R}$  and repeatedly computes better approximations using the recursive formula

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

The goal is to implement this formula for the function  $f(x) = (x-1)^2 - 1$ , whose derivative is  $f'(x) = 2(x-1)$ . The roots of this function are  $x = 0$  and  $x = 2$ .

```
# We implement the function y = x - f(x)/f'(x)  
def y(x):  
    return x - ((x-1)**2 - 1)/(2*(x-1))  
  
x0 = 3  
x1 = y(x0)  
  
print(x1)
```

```
2.25
```

A clearer way to implement the formula  $x_{i+1} = x_i - f(x_i)/f'(x_i)$  is to define separate functions for the evaluation of the functions  $f$  and  $f'$ , and then combine these to create the recursive formula. In this way, we get three functions that are each responsible for one aspect of Newton's formula, namely implementing the function  $f$ , implementing the function  $f'$  and computing the recursive formula. This also makes it easier for a user of the code to understand what is happening.

```
# Single responsibility version  
  
# Define f  
def f(x):  
    return (x-1)**2 - 1  
  
# Define f'  
def f_prime(x):  
    return 2*(x-1)
```

```

def fprime(x):
    return 2*(x-1)

# Implement function y = x - f(x)/f'(x)
def y(x):
    return x - f(x)/fprime(x)

x0 = 3
x1 = y(x0)

print(x1)

```

2.25

The take-away of the above comparison is the following.

If you are implementing a complex mathematical task involving multiple aspects, try to separate these aspects in different functions.

## 2.5 Documentation

The final good coding practice that we discuss is documentation. Ideally, you should always explain inside a function what the inputs and outputs are, and for larger scripts it is good to indicate what every part of the script does. For smaller functions and scripts this is not always necessary. We will next give an example for Newton's method as in the previous section

```

## Function that implements Newton's method
def newton(f,fprime,x0,iters):
    """
    This function implements Newton's iterative method
    x_{i+1} = x_i - f(x_i)/f'(x_i) for finding root of f.

    Input parameters
    -----
    f : Function f
    fprime : Derivative of the function f
    x0 : Initial estimate for root x of f.
    iters : Number of iterations that we run Newton's method.

    Returns
    -----
    Approximation for x satisfying f(x) = 0.
    """

    # Initial guess
    x = x0

    # Repeatedly compute the recursive formula
    # by overwriting x for 'iters' iterations
    for i in range(iters):
        x_new = x - f(x)/fprime(x)
        x = x_new
    return x

```

```

## An example of Newton's method as implemented above

# Define f
def f(x):
    return (x-1)**2 - 1

# Define f'
def fprime(x):
    return 2*(x-1)

# Define intial guess and number of iterations
x0 = 10
iters = 6

# Run Newton's method
root = newton(f,fprime,x0,iters)

# Print output and explain what has been computed
print('Running Newton\'s method for %.i iterations with initial' % iters,
      'estimate %.2f' % x0,'\\n','gives (estimated) root x = %.7f' % root,
      'with f(x) = %.7f' % f(root))

```

```

Running Newton's method for 6 iterations with initial estimate 10.00
gives (estimated) root x = 2.0000013 with f(x) = 0.0000025

```

The following is a set of guidelines regarding how to add documentation to a function.

Try to adhere to the following documentation rules when writing complex functions:

1. Function documentation between triple double-quote characters.
2. Clearly describe what a function does and what its input and output arguments are.
3. Choose descriptive variable names, lines not longer than 80 characters.
4. Don't add comments for every line. Add comments for main ideas and complex parts.
5. A comment should not repeat the code as text (e.g. "time = time + 1 # increase time by one).

# Chapter 3

## NumPy arrays

### 3.1 Introduction

The NumPy package (module) is used in almost all numerical computations using Python. It is a package that provides high-performance vector, matrix and higher-dimensional data structures for Python. High-performance here refers to the fact that Python can perform computations on such data structures very quickly if appropriate functions are used for this.

To use NumPy you need to import the `numpy` module. This is typically done under the alias `np` so that you don't have to type `numpy` all the time when using a function from the module.

```
import numpy as np
```

We emphasize at this point that there is often not a unique way or command to achieve a certain outcome. When doing the exercises corresponding to the theory given in this chapter, it is, however, recommended to find a solution using the presented functionality.

### 3.2 Creating arrays

In the NumPy package the data type used for vectors, matrices and higher-dimensional data sets is an array. There are a number of ways to initialize new arrays, for example from

- a Python list or tuples;
- using functions that are dedicated to generating numpy arrays, such as `arange()` and `linspace()` (we will see those later);
- reading data from files.

#### 3.2.1 Lists

For example, to create new vector and matrix arrays from Python lists we can use the `numpy.array()` function. Since we imported NumPy under the alias `np`, we use `np.array()` for this.

To create a vector, the argument to the array function is a Python list

```
v = np.array([1,2,3,4]) #Array creation from list [1,2,3,4]
print(v)
```

[1 2 3 4]

To create a matrix, the argument to the array function is a nested Python list. Every element of the outer list is a list corresponding to a row of the matrix. For example, the matrix

$$M = \begin{bmatrix} 1 & 2 & 7 \\ 3 & -4 & 4 \end{bmatrix}$$

is created as follows.

```
M = np.array([[1, 2, 7], [3, -4, 4]])
print(M)
```

```
[[ 1  2  7]
 [ 3 -4  4]]
```

You can access the shape (number of rows and columns) , size (number of elements) and number of dimensions (number of axes in matrix) of the array with the `shape`, `size` and `ndim` attributes, respectively. Note that the size is simply the product of the numbers in the shape tuple, and the number of dimensions is the size of the shape tuple.

```
# Shape of matrix M
shape_M = M.shape #np.shape(M) also works
print(shape_M)
```

```
(2, 3)
```

```
# Size of matrix M
size_M = M.size #np.size(M) also works
print(size_M)
```

```
6
```

```
# Number of dimensions
ndim_M = M.ndim #np.ndim(M) also works
print(ndim_M)
```

```
2
```

NumPy arrays are of the data type `ndarray` (short for *n*-dimensional array). You can access the type through the `type()` function.

```
# Type of matrix M
type_M = type(M)
print(type_M)
```

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

So far a NumPy array looks awfully much like a Python list (or nested list). Why not simply use Python lists for computations instead of creating a new array type?

There are several reasons:

- Python lists are very general. They can contain any kind of object. They are dynamically typed. They do not support mathematical functions such as matrix and dot multiplications.
- Numpy arrays are statically typed and homogeneous. The type of the elements is determined when the array is created.
- Numpy arrays are memory efficient.

- Because of the static typing, fast implementation of mathematical functions such as multiplication and addition of numpy arrays can be implemented in a compiled language (C and Fortran are used).

Using the `dtype` (data type) attribute of an array, we can see what type the data inside an array has.

```
# Data type of elements in array
dtype_M = M.dtype
print(dtype_M)
```

`int32`

If we want, we can explicitly define the type of the array data when we create it, using the `dtype` keyword argument:

```
# Define data as integers
M = np.array([[1, 2], [3, 4]], dtype=int)
print('M = \n', M)
```

```
M =
[[1 2]
[3 4]]
```

```
# Define data as floats
N = np.array([[1, 2], [3, 4]], dtype=float)
print('N = \n', N)
```

```
N =
[[1. 2.]
[3. 4.]]
```

```
# Define data as complex floats
O = np.array([[1, 2], [3, 4]], dtype=complex)
print('O = \n', O)
```

```
O =
[[1.+0.j 2.+0.j]
[3.+0.j 4.+0.j]]
```

Common data types that can be used with `dtype` are: `int`, `float`, `complex`, `bool`, `object`, etc.

We can also explicitly define the bit size of the data types, such as: `int64`, `int16`, `float128`, `complex128`. For example, `int64` allows us to define an integer variable in the range  $[-2^{64}, \dots, 2^{64}]$ .

You can also change the data type of the elements using the `astype()` method.

```
M = np.array([[1,2], [3,4]])
print(M.dtype)
```

`int32`

```
# Define M_float as matrix whose elements are those of
# the matrix M, but then as floats.
M_float = M.astype(float)
print(M_float)
```

```
[[1. 2.  
[3. 4.]
```

```
print(M_float.dtype)
```

```
float64
```

### 3.2.2 Arrays from functions

There are various useful arrays that can be automatically created using functions from the NumPy package. These arrays are typically hard to implement directly as a list.

`arange(n)`: This function creates the array  $[0, 1, 2, \dots, n - 1]$  whose elements range from 0 to  $n - 1$ .

```
n = 10  
x = np.arange(n)  
  
print(x)
```

```
[0 1 2 3 4 5 6 7 8 9]
```

If you want to explicitly define the data type of the elements, you can add the `dtype` keyword argument (the same applies for all functions that are given below).

```
n = 10  
x = np.arange(n, dtype=float)  
  
print(x)
```

```
[0. 1. 2. 3. 4. 5. 6. 7. 8. 9.]
```

`arange(a,b)`: This function creates the array  $[a, a + 1, a + 2, \dots, b - 2, b - 1]$ .

```
a, b = 5,11  
x = np.arange(a,b)  
  
print(x)
```

```
[ 5  6  7  8  9 10]
```

`arange(a,b,step)`: This function creates the array  $[a, a + step, a + 2 \cdot step, \dots, b - 2 \cdot step, b - step]$ . That is, the array ranges from  $a$  to  $b$  (but not including  $b$  itself), in steps of size `step`.

```
a, b, step = 5, 11, 0.3  
x = np.arange(a,b,step)  
  
print(x)
```

```
[ 5.   5.3  5.6  5.9  6.2  6.5  6.8  7.1  7.4  7.7  8.   8.3  8.6  8.9  
 9.2  9.5  9.8 10.1 10.4 10.7]
```

`linspace(a,b,k)`: Create a discretization of the interval  $[a, b]$  containing  $k$  evenly spaced points, including  $a$  and  $b$  as the first and last element of the array.

```

a,b,k = 5,10,20
x = np.linspace(a,b,k)

print(x)

```

[ 5. 5.26315789 5.52631579 5.78947368 6.05263158 6.31578947  
6.57894737 6.84210526 7.10526316 7.36842105 7.63157895 7.89473684  
8.15789474 8.42105263 8.68421053 8.94736842 9.21052632 9.47368421  
9.73684211 10. ]

`diag(x)`: This function creates a matrix whose diagonal contains the list/vector/array `x`.

```

x = np.array([1,2,3])
D = np.diag(x)

print(D)

```

[[1 0 0]  
[0 2 0]  
[0 0 3]]

`np.zeros(n)`: This function create a vector of length `n` with zeros.

```

n = 5
x = np.zeros(n)

print(x)

```

[0. 0. 0. 0. 0.]

`np.zeros((m,n))`: This function create a matrix of size  $m \times n$  with zeros. Note that we have to input the size of the matrix as a tuple `(m,n)`; using `np.zero(m,n)`

```

m, n = 2, 5
M = np.zeros((m,n))

print(M)

```

[[0. 0. 0. 0. 0.]  
[0. 0. 0. 0. 0.]]

`np.ones(n)` and `np.ones((m,n))`: These functions create a vector of length `n` with ones, and a matrix of size  $m \times n$  with ones, respectively.

```

m, n = 2, 5
x = np.ones(n)

print(x)

```

[1. 1. 1. 1. 1.]

```

M = np.ones((m,n))

print(M)

```

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

### 3.2.3 Reading data from files

The third option, which you might use most often in a professional context, is to read in data from a file directly into a NumPy array. You can do this using the `loadtxt()` function.

If you want to try this yourself, download the file `numerical_data.dat` here and store it in the same folder as where you are storing the Python script in which you execute the code snippet below.

```
# Load data into NumPy array
data_dat = np.loadtxt('numerical_data.dat')

# Print the data
print(data_dat)
```

```
[[ 1.    5.    4.   -9.    1. ]
 [ 3.    5.    6.    7.    7. ]
 [ 4.    3.    2.    1.    0.5]]
```

Python puts every row in the data (DAT) file into a separate row of the NumPy array; note that the numbers in the data file are separated by a whitespace character.

We can also save data from a Numpy array into a DAT-file using the `savetxt()` function. The first argument of this function is the name of the file in which you want to store the array, and the second argument is the array to be stored.

```
# Matrix M
M = np.array([[1,2,3],[5,6,7],[10,11,12],[14,15,16]])

# Save matrix to DAT file
np.savetxt('matrix.dat', M)
```

This should have created the file `matrix.dat` in the same folder as where you stored the Python script that ran the code above. You might notice that the numbers are stored using the scientific notation. For example, the number 1 appears as `1.000000000000000e+00` in the CSV-file.

You can suppress this behaviour by explicitly specifying the data type in which you want the numbers in the matrix to be stored using the `fmt` keyword argument. For example, `fmt = '%i'` stores the numbers as integers.

```
# Matrix M
M = np.array([[1,2,3],[5,6,7],[10,11,12],[14,15,16]])

# Save matrix to DAT file
np.savetxt('matrix_int.dat', M, fmt='%i')
```

This should have created the file `matrix_int.dat` in the same folder as where you stored the Python script that ran the code above.

## 3.3 Accessing

In this section we will describe how you can access, or index, the data in a NumPy array.

We can index elements in an array using square brackets and indices, just like as with lists. In NumPy

indexing starts at 0, just like with a Python list.

```
v = np.array([12,4,1,9])

# Element in position 0
print(v[0])

# Element in position 2
print(v[2])

# Element in position -1 (last element)
print(v[-1]) # Same as v[3]

# Element in position -3 (counted backwards)
print(v[-3]) # Same as v[1]
```

```
12
1
9
4
```

### 3.3.1 Basic indexing

If you want to access the element at position  $(i,j)$  from a two-dimensional array, you can use the double bracket notation `[i][j]`, but with arrays you can also use the more compact syntax `[i,j]`.

```
M = np.array([[10,2,6,7], [-15,6,7,-8], [9,10,11,12],[3,10,6,1]])

# Element at position (1,1)
print('List syntax:',M[1][1])

# Element at position (1,1)
print('Array syntax', M[1,1])
```

```
List syntax: 6
Array syntax 6
```

If you want to access row  $i$  you can use `M[i]` or `M[i,:]`.

```
print(M[2]) # Gives last row

print(M[2,:]) # Gives last row
```

```
[ 9 10 11 12]
[ 9 10 11 12]
```

If you want to access column  $j$  you can use `M[:,j]`. Both here and in the previous command, the colon `:` is used to indicate that we want all the elements in the respective dimension. So `M[:,j]` should be interpreted as, we want the elements from all rows in the  $j$ -th column.

### 3.3.2 Index slicing

Index slicing is the technical name for the index syntax that returns a slice, a consecutive part of an array.

```
v = np.array([12,4,1,9,11,14,17,98])  
print(v)
```

```
[12  4   1   9  11  14  17  98]
```

`v[lower:upper]`: This return the elements in `v` at positions `lower`, `lower+1`, ..., `upper-1`. Note that the element at position `upper` is not included.

```
# Returns v[1], v[2], v[3], v[4], v[5]  
print(v[1:6])
```

```
[ 4   1   9  11  14]
```

You can also omit the `lower` or `upper` value, in which case it is set to be position 0 or the last position `-1`, respectively.

```
# Returns v[3],...,v[8]  
print(v[3:])  
  
# Returns v[0],...,v[4]  
print(v[:5])
```

```
[ 9  11  14  17  98]  
[12  4   1   9  11]
```

`v[lower:upper:step]`: This returns the elements in `v` at position `lower`, `lower+step`, `lower+2*step`, ..., `(upper-1)-step`, `(upper-1)`. It does the same as `[lower:upper]`, but now in steps of size `step`.

```
v = np.array([12,4,1,9,11,14,17,98])  
  
# Returns v[1], v[3], v[5]  
print(v[1:6:2])
```

```
[ 4   9  14]
```

You can omit any of the three parameters `lower`, `upper` and `step`

```
# lower, upper, step all take the default values  
print(v[:])  
  
# Index in step is 2 with lower and upper defaults  
print(v[::-2])  
  
# Index in steps of size 2 starting at position 3  
print(v[3::-2])
```

```
[12  4   1   9  11  14  17  98]  
[12  1   11  17]  
[ 9  14  98]
```

You can also use slicing with negative index values.

```
# The last three elements of v
print(v[-3:])
```

[14 17 98]

Furthermore, the same principles apply to two-dimensional arrays, where you can specify the desired indices for both dimensions

```
M = np.array([[10,2,6,7], [-15,6,7,-8], [9,10,11,12],[3,10,6,1]])

print(M)
```

```
[[ 10   2   6   7]
 [-15   6   7  -8]
 [  9   10  11  12]
 [  3   10   6   1]]
```

`[a:b, c:d]`: This returns the submatrix consisting of the rows `a,a+1,...,b-1` and rows `c,c+1,...,d`. You can also combine this with a step argument, i.e., use `[a:b:step1, c:d:step2]`.

```
# Returns elements in submatrix formed by rows 2,3 (excluding 4)
# and columns 1,2 (excluding 3)
print(M[2:4,1:3])
```

```
[[10 11]
 [10  6]]
```

If you want to obtain a submatrix whose rows and/or columns do not form a consecutive range, or if you want to specify these lists manually, you can use the `ix_()` function from NumPy. Its arguments should be a list of row indices, and a list of column indices specifying the indices of the desired submatrix.

```
i = [0,2,3]
j = [0,3]

# Returns submatrix formed by rows 0,2,3 and columns 0,3
print(M[np.ix_(i,j)])
```

```
[[10  7]
 [ 9 12]
 [ 3  1]]
```

### 3.3.3 Fancy indexing

Fancy indexing is the name for when an array or list is used instead of indices, to access part of an array. For example, if you want to access elements in the locations  $(0,3), (1,2)$  and  $(1,3)$ , you can define a list of row indices `[0,1,1]` and columns indices `[3,2,3]` and access the matrix with these lists.

```
i = [0,1,1]
j = [3,2,3]

# Returns M[0,3] = 7, M[1,2] = 7, M[1,3] = -8
print(M[i,j])
```

[ 7 7 -8]

Another way of fancy indexing is by using a Boolean list, that indicates for every element whether it should be indexed (True) or not (False). Such a list is sometimes called a mask.

```
v = np.array([1,6,2,3,9,3,6])

# Tell for every element whether it should be indexed
mask = [False, True, True, True, False, True, False]

print(v[mask])
```

```
[6 2 3 3]
```

Typically, the mask is generated from a Boolean statement. For example, suppose we want to select all elements strictly smaller than 3 and greater or equal than 7 from the array v.

The following statements achieve this. Recall that you can use & if you want the first AND the second statement to be satisfied, and | if either the first OR the second has to be satisfied (or both).

```
mask_37 = (v < 3) | (v >= 7)

# Boolean vector indicating for every element in v
# whether the conditions v < 3 and v >= 7 are satisfied
print(mask_37)
```

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

We can now access the elements satisfying these conditions by indexing v with this mask

```
print(v[mask_37])
```

```
[1 2 9]
```

## 3.4 Modifying

### 3.4.1 Elements, rows or columns

Using similar ways of indexing as in the previous section, we can also modify the elements of an array

```
M = np.array([[1,1,1,1], [2,2,2,2], [3,3,3,3],[4,4,4,4]])
```

```
print(M)
```

```
[[1 1 1 1]
 [2 2 2 2]
 [3 3 3 3]
 [4 4 4 4]]
```

```
# Modify individual element
M[0,1] = -1
```

```
print(M)
```

```
[[ 1 -1  1  1]
 [ 2  2  2  2]
```

```
[ 3  3  3  3]
[ 4  4  4  4]]
```

```
# Modify (part of a) row
M[1,[1,2,3]] = [-2,-2,-2]

print(M)
```

```
[[ 1 -1  1  1]
 [ 2 -2 -2 -2]
 [ 3  3  3  3]
 [ 4  4  4  4]]
```

```
# Modify third column to ones
M[:,3] = np.ones(4)

print(M)
```

```
[[ 1 -1  1  1]
 [ 2 -2 -2  1]
 [ 3  3  3  1]
 [ 4  4  4  1]]
```

### 3.4.2 Broadcasting

There does not necessarily have to be a match between the part of the matrix that we index, and the dimensions of the data that we want to overwrite that part with.

```
M = np.array([[1,1,1,1], [2,2,2,2], [3,3,3,3], [4,4,4,4]])

print(M)
```

```
[[1 1 1 1]
 [2 2 2 2]
 [3 3 3 3]
 [4 4 4 4]]
```

For example, in order to replace the third column of  $M$  by ones, we can also do the command below, instead of using `np.ones(4)`.

```
# Modify third column to ones
M[:,3] = 1

print(M)
```

```
[[1 1 1 1]
 [2 2 2 1]
 [3 3 3 1]
 [4 4 4 1]]
```

Although there is a mismatch between the indexed part on the left (a column) and the data on the right (single number), Python broadcasts the data to an appropriate format by copying it to the correct size. That is, it copies the 1 to an array  $[1,1,1,1]$  of ones, which it then places in the third column.

This works similar in higher dimensions. Suppose we want to overwrite the second and third row with  $[1, 6, 2, 3]$ . Then the indexed part is a  $2 \times 4$  array, but the data a  $1 \times 4$  array.

```
# Modify second and third row
M[2:4,:] = [1,6,2,3]

print(M)

[[1 1 1 1]
 [2 2 2 1]
 [1 6 2 3]
 [1 6 2 3]]
```

Python here first copies the data to  $[[1, 6, 2, 3], [1, 6, 2, 3]]$  and then modifies  $M$  with this array.

### 3.4.3 Transpose

Another useful function, in the context of linear algebra, is to take the transpose of a two-dimensional array  $M$ , which modifies the entries along the diagonal.

```
M = np.array([[1,2,3],[3,4,-1]])

print(M)

[[ 1   2   3]
 [ 3   4  -1]]

transpose_M = M.T #np.transpose(M) also works
print(transpose_M)

[[ 1   3]
 [ 2   4]
 [ 3  -1]]
```

## 3.5 Repeating and stacking

We can also use existing matrices and build new ones from it by stacking them either horizontally or vertically.

`tile(M, (k, r))`: This function takes an array  $M$  and copies it  $k$  times vertically and  $r$  times horizontally, resulting in a “tiling” of the original array  $M$ .

```
M = np.array([[1,2],[3,4]])

M_tile = np.tile(M, (2,3))
print(M_tile)

[[1 2 1 2 1 2]
 [3 4 3 4 3 4]
 [1 2 1 2 1 2]
 [3 4 3 4 3 4]]
```

If you do not input a tuples with two arguments, but only a number, then `tile()` does the tiling only horizontally.

```
M = np.array([[1,2],[3,4]])

M_tile = np.tile(M,4)
print(M_tile)
```

```
[[1 2 1 2 1 2 1 2]
 [3 4 3 4 3 4 3 4]]
```

`repeat(M,k)`: This function takes every element of `M`, repeats it  $k$  times, and puts all these numbers in a one-dimension array.

```
M = np.array([[1,2],[3,4]])

M_repeat = np.repeat(M,3)
print(M_repeat)
```

```
[1 1 1 2 2 2 3 3 3 4 4 4]
```

`vstack((a,b))`: This stacks two arrays `a` and `b` vertically, provided they have the correct dimensions to do this. Note that `a` and `b` should be inputted as a tuple `(a,b)`.

```
a = np.array([7,8])
M = np.array([[1,2],[3,4]])

M_a = np.vstack((M,a))
print(M_a)
```

```
[[1 2]
 [3 4]
 [7 8]]
```

`hstack((a,b))`: This stacks two arrays `a` and `b` horizontally, provided they have the correct dimensions to do this.

Note that in the example below we define `a` as a  $1 \times 2$  array, i.e., a column array, to make sure we can stack it right of `M`. If we would have kept `a = np.array([7,8])` then Python will give an error, because it cannot stack a row vector next to a two-dimensional array.

```
a = np.array([[7],[8]])
M = np.array([[1,2],[3,4]])

M_a = np.hstack((M,a))
print(M_a)
```

```
[[1 2 7]
 [3 4 8]]
```

## 3.6 Reshaping

It is possible to adjust the shape of an array, while keeping the data of the array the same. For example, consider the  $x = [1, 2, 3, \dots, 12]$ .

```

x = np.arange(1,13)

print(x)

```

[ 1 2 3 4 5 6 7 8 9 10 11 12]

We can reshape it into the  $3 \times 4$  matrix

$$M = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 11 & 10 & 11 & 12 \end{bmatrix}$$

by using the `reshape(a,b)` method. It reshapes  $x$  to an  $a \times b$  array provided that  $a \cdot b$  equal the size (i.e., number of elements) of  $x$ .

```

# Reshape x to a 3-by-4 matrix
M = x.reshape(3,4)

print(M)

```

[[ 1 2 3 4]  
 [ 5 6 7 8]  
 [ 9 10 11 12]]

We can also reshape two-dimensional arrays, for example, we can reshape  $M$  again to a  $2 \times 6$  matrix.

```

# Reshape M to a 2-by-6 matrix
N = M.reshape(2,6)

print(N)

```

[[ 1 2 3 4 5 6]  
 [ 7 8 9 10 11 12]]

You should observe that Python does the reshaping in a very specific way: When we transform  $x$  to  $M$  above, Python fills the matrix  $M$  in a row-by-row fashion (instead of column-by-column). This is because of what is called the largest (axis) index change fastest principle.

To understand this idea, recall that we can access the element at position  $(i,j)$  of a matrix  $M$  with `M[i,j]`. Here  $i$  is the row-index at position 0 of the index list `[i,j]`, and  $j$  is the column index at position 1 of the index list `[i,j]`. We said that the row indices form the 0-axis of the matrix, and the column indices the 1-axis.

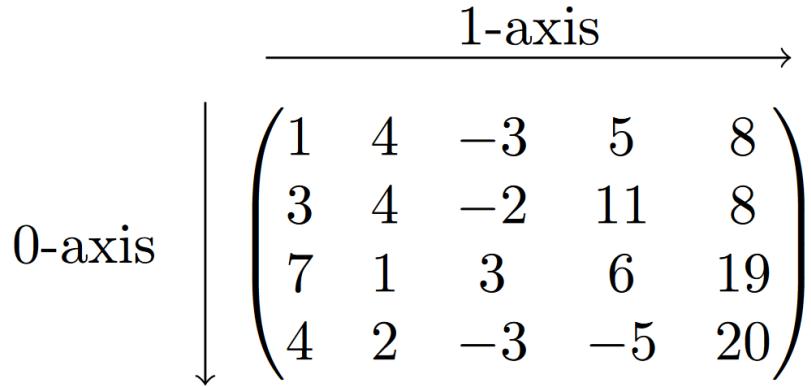


Figure 3.1: Axes of a two-dimensional array

Largest (axis) index changing fastest means that an  $m \times n$  matrix gets filled first along the 1-axis, i.e., it fills the positions  $(0, 0), (0, 1), \dots, (0, n)$  while keeping the row index 0 fixed. It then moves up one row index, i.e., one position along the 0-axis and fills the elements  $(1, 0), (1, 1), \dots, (1, n)$ , i.e., the elements along the 1-axis. It continues in this fashion until the complete matrix is full.

Another convenient method for reshaping is `flatten()`, which turns a matrix of any size into a one-dimensional array.

```
# Define 2-by-3 matrix
M = np.array([[9,1,3],[2,4,3]])

# Turn into one-dimensional array
x = M.flatten()
print(x)
```

[9 1 3 2 4 3]

If you want to turn a one-dimensional array  $x = [x_0, \dots, x_{n-1}]$  into a column array of shape  $(n, 1)$ , you can do this as follows.

```
x = np.array([1,2,4,3,8])
n = np.size(x)

x = x.reshape(n,1)
print(x)
```

[[1]
 [2]
 [4]
 [3]
 [8]]

A more direct way of doing this, is by using `x[:, None]`.

```
x = np.array([1,2,4,3,8])
x = x[:,None] # Turns x into column array of shape (n,1)

print(x)
```

```
[[1]
 [2]
 [4]
 [3]
 [8]]
```

## 3.7 Copy vs. view

In the last sections we have seen various ways of using arrays to create other arrays. One point of caution here is whether or not the new array is a view or a copy of the original array.

### 3.7.1 View

A view  $y$  of an array  $x$  is another array that simply displays the elements of the array  $x$  in a different array, but the elements will always be the same. This means that if we would change an element in the array  $x$ , the same element will change in  $y$  and vice versa.

```
x = np.array([[4,2,6],[7,11,0]])
y = x # This create a view of x

print('y = \n', y)
```

```
y =
[[ 4  2  6]
 [ 7 11  0]]
```

We next change an element in  $x$ . Note that the same element changes in  $y$ .

```
# Change element in x
x[0,2] = -30

# y now also changes in that position
print('y = \n', y)

y =
[[ 4  2 -30]
 [ 7 11  0]]
```

The same happens the other way around: If we change an element in  $y$ , then the corresponding element in  $x$  also changes.

```
# Change element in y
y[1,1] = 100

# x now also changes in that position
print('x = \n', x)

x =
[[ 4  2 -30]
 [ 7 100  0]]
```

Note that the same behaviour occurs in we apply the `reshape()` method.

```

# Define x = [1,2,...,12]
x = np.arange(1,13)

# Reshape x to a 3-by-4 matrix
M = x.reshape(3,4) # Creates view of x

print(M)

```

```

[[ 1  2  3  4]
 [ 5  6  7  8]
 [ 9 10 11 12]]

```

If we now change an element in  $M$ , then the corresponding element changes in  $x$ . This mean that  $M$  is a view of the original array  $x$ .

```

# Change element in M
M[1,3] = 50

# x now also changes in that position
print(x)

```

```
[ 1  2  3  4  5  6  7 50  9 10 11 12]
```

### 3.7.2 Copy

A copy of an array  $x$  is an array  $z$  that is completely new and independent of  $x$ , meaning that if we change an element in  $x$ , then the corresponding element in  $z$  does not change, and vice versa. To obtain a copy of  $x$ , we can simply apply the `copy()` method to it.

```

# Define x = [1,2,...,12]
x = np.arange(1,13)

z = x.copy() # Create copy of x
z[0] = -10 # Change element of z

print('z = \n', z)
print('x = \n', x) # x has not changed

z =
[-10   2   3   4   5   6   7   8   9   10  11  12]
x =
[ 1  2  3  4  5  6  7  8  9 10 11 12]

```

Note that in the above example,  $x$  remains unchanged when we modify the element of  $z$  at position 0.

Similarly, to turn a reshaped array into a copy, we can apply the `copy()` method to it.

```

# Define x = [1,2,...,12]
x = np.arange(1,13)

# Reshape x to a 3-by-4 matrix
M = x.reshape(3,4).copy() # Create copy
M[0,0] = -10 # Change element of x

```

```
print('M = \n', M)
print('x = \n', x) # x has not changed
```

```
M =
[[-10   2   3   4]
 [ 5   6   7   8]
 [ 9  10  11  12]]
x =
[ 1  2  3  4  5  6  7  8  9 10 11 12]
```

The `flatten()` method actually directly creates a copy of the original array.

```
# Define 2-by-3 matrix
M = np.array([[9,1,3],[2,4,3]])

# Turn into one-dimensional array
x = M.flatten() # Creates copy of M
x[0] = 100 # Change element in x

print('x = \n', x)
print('M = \n', M) # M has not changed
```

```
x =
[100   1   3   2   4   3]
M =
[[9 1 3]
[2 4 3]]
```

It is important to know whether a Python function or command creates a copy or a view of the original array. You can typically look this up in the documentation of Python. Otherwise, experiment with the function or command to be sure how it behaves.

# Chapter 4

## Vectorization

In this chapter we will explore the power of NumPy arrays by studying the concept of vectorization. Let us first import the NumPy package.

```
import numpy as np
```

The idea of vectorization is that functions are designed so that they can efficiently handle multiple inputs simultaneously.

As an example, let's implement the Heavyside function  $H$ , which is defined by

$$H(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{if } x < 0 \end{cases} .$$

That is, the function returns 1 if  $x$  is nonnegative, and 0 otherwise. If we are only interested in computing  $H(x)$  for a single value  $x$ , then the following function suffices.

```
# Heavyside function
def Heavyside(x):
    if x >= 0:
        return 1
    else:
        return 0

print('H(2) =', Heavyside(2))
print('H(-3) =', Heavyside(-3))
```

```
H(2) = 1
H(-3) = 0
```

Suppose now that we would want to compute the value  $H(x)$  for many values given in an array  $x = [x_0, \dots, x_{n-1}]$ ; this you would need to do, e.g., if you want to visualize a function. One way to do this is to use a for-loop and append the value of  $H(x_i)$  to an (initially empty) list in iteration  $i$ .

```
n = 8
x = np.arange(-n,n)

h_values = []
for i in x:
    h_values.append(Heavyside(i)) # append H(i) to list h_values
```

```
print(h_values)
```

```
[0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1]
```

As mentioned earlier, for-loops are typically very time-inefficient and should be avoided whenever possible. It would be better if we could instead use another approach that can compute the function values more efficiently.

One approach to avoid the for-loop is with a Boolean statement. Recall from Chapter 2 that for an array  $x$ , the command  $x \geq 0$  will return a Boolean array containing True at position  $i$  if  $x_i \geq 0$ , and False if not. This command is an example of a vectorized operation: Although, mathematically speaking, it is defined to compare a number  $x$  with 0, the command also works if  $x$  is an array, in which case each of its elements get compared to 0.

```
comparison = (x >= 0) # Compare each element in x with 0
print(comparison)
```

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

The statement  $x \geq 0$  returns a Boolean array containing True and False, but the Heavyside function should output 1 and 0, respectively. To achieve this, we can convert the Boolean array to an array with ones and zeros.

This can be done with the `astype()` method, or by a clever multiplication: In Python, multiplying True with 1 gives 1, and False with 1 gives 0. Note that these are also examples of vectorized operations. For example, in the latter case, we multiply an array with one number, which Python executes by multiplying every element in the array with that number.

```
# Convert Boolean values to integers (True becomes 1, False becomes 0)
H = comparison.astype('int')
print(H)

# Multiply Boolean array with 1 (True*1 = 1, and False*1 = 0)
H2 = comparison*1
print(H2)
```

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

This means we can define the vectorized Heavyside function as follows, using the “multiplication with one” approach. We actually need less code for the vectorized version than in the original approach.

```
# Vectorized Heavyside function
def Heavyside(x):
    return (x >= 0)*1

print(x)
print(Heavyside(x))
```

```
[-8 -7 -6 -5 -4 -3 -2 -1  0  1  2  3  4  5  6  7]
[0 0 0 0 0 0 0 1 1 1 1 1 1 1 1]
```

A vectorized function can handle higher-dimensional inputs. For example, a function that is (mathematically speaking) defined for a single number can also handle one- or two-dimensional

arrays as input, in which case the function computes the function value for every number in the array. Or a function that is defined for a one-dimensional array, can also handle two-dimensional arrays as input, in which case it computes the function value for every (one-dimensional) row (inner list) of the two-dimensional array.

We remark that vectorizing a function should not result in additional for-loops, but should exploit the functionality that Python, and in particular NumPy, have to offer. We will see many examples of this later in this chapter.

In this course, you will typically be told which types of input data your function should be able to handle, so, e.g., it could be that you have to write a function that performs mathematical operations on a one-dimensional array, but that it should be able to handle two-dimensional arrays as well (again, in which case your function should compute the function value for every row of that array).

As an example of what you should not do, the following definition of the Heavyside function is also able to handle “higher dimensional” inputs, but it does so by looping over the elements of the input, which makes it again a slow function. To summarize, you should not “hide” additional for-loops in the function itself.

```
# Heavyside function
def Heavyside(x):
    h = []
    for i in x:
        if i >= 0:
            h.append(0)
        else:
            h.append(1)
    return h

x = np.array([-2,-1,0,1,2])
print(Heavyside(x))
```

[1, 1, 0, 0, 0]

Also, it is not allowed to use functions like `vectorize()` from NumPy, because these are implemented essentially as a loop (as stated in the documentation of that function).

We continue with exploring vectorized functions within Python and NumPy.

## 4.1 Arithmetic operations

All basic arithmetic operations (addition, subtraction, division, multiplication and comparison) are vectorized in Python. We will illustrate this with the addition operation `+`, but the same commands can be applied to the other arithmetic operations `-`, `/`, `*`, and `>=`, `==`, `<=`, `!=`.

The addition operation `+` can be used to add two numbers together, as you well know. It can also add two arrays, i.e., it works as well for one- and two-dimensional arrays if they have the same shape. This is the usual addition operation you learn about when studying linear algebra.

```
x = np.array([1,4,7])
y = np.array([2,4,3])

print('x + y =\n',x+y)

x + y =
[ 3  8 10]
```

```

A = np.array([[1,2],[1,4]])
N = np.array([[7,9],[3,4]])

print('A + N = \n', A+N)

```

```

A + N =
[[ 8 11]
 [ 4  8]]

```

Python is also able to handle addition of arrays of different shapes in certain cases, using the concept of broadcasting that we have seen before. For example, we can add a single number to any array, in which case Python adds this number to every element in the array. This can be seen as an instance of vectorization.

```

c = 5

print('A + c =\n', A+c)

```

```

A + c =
[[6 7]
 [6 9]]

```

We can also add either a one-dimensional array  $x$  of size  $n$  to an  $m \times n$  matrix  $A$ . In this case, the array  $x$  gets added to every row of  $A$ :

$$\begin{aligned}
A + x &= \begin{bmatrix} a_{00} & a_{01} & \cdots & a_{0(n-1)} \\ a_{10} & a_{11} & \cdots & a_{1(n-1)} \\ \vdots & \vdots & \ddots & \vdots \\ a_{(m-1)0} & a_{(m-1)1} & \cdots & a_{(m-1)(n-1)} \end{bmatrix} + \begin{bmatrix} x_0 & x_1 & \cdots & x_{(n-1)} \end{bmatrix} \\
&= \begin{bmatrix} a_{00} + x_0 & a_{01} + x_1 & \cdots & a_{0(n-1)} + x_{n-1} \\ a_{10} + x_0 & a_{11} + x_1 & \cdots & a_{1(n-1)} + x_{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ a_{(m-1)0} + x_0 & a_{(m-1)1} + x_1 & \cdots & a_{(m-1)(n-1)} + x_{n-1} \end{bmatrix}
\end{aligned}$$

In the example below, we have  $m = 3$  and  $n = 2$ .

```

x = np.array([10,12])
print('Shape of x:', np.shape(x))

A = np.array([[1,2],[1,4],[3,1]])
print('Shape of A:', np.shape(A))

print('A + x = \n', A + x)

```

```

Shape of x: (2,)
Shape of A: (3, 2)
A + x =
[[11 14]
 [11 16]
 [13 13]]

```

Again, this can be seen as an instance of vectorization, since Python automatically adds  $x$  to every row of the matrix  $A$ .

Note that the shape of  $x$  is  $(n,)$  which is the syntax that Python uses to denote that  $x$  only has one dimension. You can define  $x = [x_0, \dots, x_{n-1}]$  explicitly as a row vector of shape  $(1, n)$  by defining `x = np.array([[x_0, ..., x_{n-1}]])`, that is, with double brackets. It is sometimes needed to change the shape of an array from  $(n,)$  to  $(1, n)$  or  $(n, 1)$  to be able to use a function from NumPy.

Addition works in the same way if we define  $x$  explicitly as an array of shape  $(1, n)$ .

```
x = np.array([[10,12]])
print('Shape of x:', np.shape(x))

A = np.array([[1,2],[1,4],[3,1]])
print('Shape of A:', np.shape(A))

print('A + x =\n', A + x)
```

```
Shape of x: (1, 2)
Shape of A: (3, 2)
A + x =
[[11 14]
 [11 16]
 [13 13]]
```

The same works if we define  $x = [x_0, \dots, x_{m-1}]^T$  as a column array of shape  $(m, 1)$ , in which case it gets added to every column of the matrix  $A$  of shape  $(m, n)$ :

$$\begin{aligned} A + x &= \begin{bmatrix} a_{00} & a_{01} & \cdots & a_{0(n-1)} \\ a_{10} & a_{11} & \cdots & a_{1(n-1)} \\ \vdots & \vdots & \ddots & \vdots \\ a_{(m-1)0} & a_{(m-1)1} & \cdots & a_{(m-1)(n-1)} \end{bmatrix} + \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_{(m-1)} \end{bmatrix} \\ &= \begin{bmatrix} a_{00} + x_0 & a_{01} + x_0 & \cdots & a_{0(n-1)} + x_0 \\ a_{10} + x_1 & a_{11} + x_1 & \cdots & a_{1(n-1)} + x_1 \\ \vdots & \vdots & \ddots & \vdots \\ a_{(m-1)0} + x_{m-1} & a_{(m-1)1} + x_{m-1} & \cdots & a_{(m-1)(n-1)} + x_{m-1} \end{bmatrix} \end{aligned}$$

```
x = np.array([[10],[12],[14]])
print('Shape of x:', np.shape(x))

A = np.array([[1,2],[1,4],[3,1]])
print('Shape of A:', np.shape(A))

print('A + x =\n', A + x)
```

```
Shape of x: (3, 1)
Shape of A: (3, 2)
A + x =
[[11 12]
 [13 16]
 [17 15]]
```

We cannot add arrays of any dimensions to each other. For example, if we would try to add a  $2 \times 2$  array to a  $4 \times 2$  array, then Python will return `ValueError: operands could not be broadcast together with shapes (4,2) (2,2)`, i.e., Python cannot perform this addition.

### 4.1.1 Multiplication broadcasting

We emphasize that the broadcasting concepts above also apply to the multiplication operator `*`. That is, if  $x$  is a column array then  $A*x$  multiplies every column of  $A$  in a pointwise fashion with the array  $x$ . Similarly, for two matrix  $A$  and  $B$ , the syntax  $A*B$  returns a matrix in which all elements of  $A$  and  $B$  are pointwise multiplied with each other, that is, entry  $(i, j)$  contains  $a_{ij} \cdot b_{ij}$ .

This is not the same as, e.g., the matrix-vector multiplication  $Ax$  in the linear algebra sense, i.e,

$$\begin{aligned} Ax &= \begin{bmatrix} a_{00} & a_{01} & \cdots & a_{0(n-1)} \\ a_{10} & a_{11} & \cdots & a_{1(n-1)} \\ \vdots & \vdots & \ddots & \vdots \\ a_{(m-1)0} & a_{(m-1)1} & \cdots & a_{(m-1)(n-1)} \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_{(m-1)} \end{bmatrix} \\ &= \begin{bmatrix} a_{00}x_0 + a_{01}x_1 + \cdots + a_{0(n-1)}x_{n-1} \\ a_{10}x_0 + a_{11}x_1 + \cdots + a_{1(n-1)}x_{n-1} \\ \vdots \\ a_{(m-1)0}x_0 + a_{(m-1)1}x_1 + \cdots + a_{(m-1)(n-1)}x_{n-1} \end{bmatrix} \end{aligned}$$

We will see matrix-vector and matrix-matrix multiplications in the linear algebra sense later in this book.

## 4.2 Mathematical functions

Many mathematical functions in NumPy are also vectorized by default. Here you should think of functions like

- Trigonometry: `sin()`, `cos()`, `tan()`
- Exponentiation and logarithms: `exp()`, `log()`, `log10()`, `log2()`
- Rounding: `around()`, `floor()`, `ceil()`
- Division with remainder: `mod()`, `divmod()`
- Power computation: `sqrt()`, `abs()`, `power()`

You access them using `np.function_name()`. Let us look at some examples; you can check out the documentation of the other functions yourself.

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

# Compute sin(i) for every element i in x
y = np.sin(x)
print(y)
```

```
[ 0.90929743  0.84147098 -0.2794155 ]
```

```
A = np.array([[2, 1, 6], [1, 1, 3]])

# Compute e^i for every element i in A
y = np.exp(A)
print(y)
```

```
[[ 7.3890561   2.71828183 403.42879349]
 [ 2.71828183   2.71828183  20.08553692]]
```

```

x = np.array([1.249583, 3.110294, 4.51139])

# Round every number in x to two decimals
x = np.around(x, decimals=2)
print(x)

```

[1.25 3.11 4.51]

```

x = np.array([10,9,4])
y = np.array([2,4,5])

# Compute x_i (mod y_i) for all i
# and output divisor and remainder
z = np.divmod(x,y)
print(z)

```

(array([5, 2, 0]), array([0, 1, 4]))

`np.divmod()` outputs two arrays: the divisors and the remainder. For example, looking at  $x[1] = 9$  and  $y[1] = 4$ : the number 4 fits twice in 9, after which 1 is left, i.e.,  $9 = 2 \cdot 4 + 1$ . The number 2 appears in the second position of the first array, and the remainder 1 in the second position of the second array.

```

A = np.array([[2,3,6],[4,2,3]])
N = np.array([[1,2,3],[1,2,3]])

# Pointwise compute a_{ij}^{n_{ij}} for all i,j
P = np.power(A,N)
print(P)

```

[[ 2 9 216]  
 [ 4 4 27]]

## 4.3 Operations along array axes

Another efficient way to perform vectorized operations is to exploit the fact that many NumPy functions that perform an operation on a one-dimensional array, can also be used for two-dimensional arrays where the operation is then either performed on every column (i.e., along the 0-axis), or on every row (i.e., along the 1-axis).

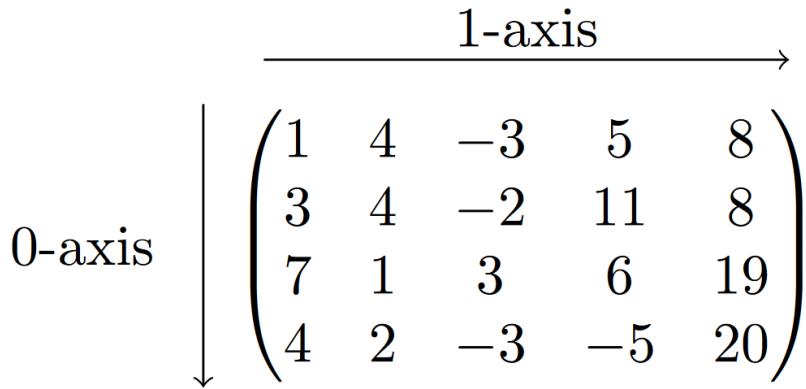


Figure 4.1: Axes of a two-dimensional array

We will look at some examples of this in the next sections.

### 4.3.1 Sorting and searching

The function `sort()` can be used to sort the elements in a one-dimensional array in ascending order, i.e., smallest to largest.

```
x = np.array([0.89, 0.5, 0.57, 0.34])

# Sort and print the elements in x
xAscending = np.sort(x)
print(xAscending)
```

[0.34 0.5 0.57 0.89]

It is not possible to use `sort()` to sort in descending order, i.e., largest to smallest, but this can be accomplished by reversing the sorted array. We can do this using index slicing with a step size of  $-1$ , starting at position  $-1$ , meaning that Python goes backwards through the array.

```
# Access x from beginning till end with step size -1
xDescending = xAscending[-1::-1]

print(xDescending)
```

[0.89 0.57 0.5 0.34]

Vectorizing the (ascending) sort operation means we want to have a function that can take as input a two-dimensional array, and return for every row (or column) the sorted list of numbers. It turns out that `sort()` can do this right away, by adding an additional keyword argument `axis`.

Adding `axis=0` means that Python will sort the numbers in every column, i.e., along the 0-axis, and `axis=1` will sort numbers in every row, i.e., along the 1-axis.

```
A = np.array([
    [0.89, 0.5, 0.57, 0.34],
    [0.61, 0.12, 0.04, 1. ],
    [0.27, 0.26, 0.28, 0.25],
    [0.9, 0.84, 0.15, 1. ]])
```

```
# Sort elements in every column
A_col_ordered = np.sort(A, axis=0)
print(A_col_ordered)
```

```
[[0.27 0.12 0.04 0.25]
 [0.61 0.26 0.15 0.34]
 [0.89 0.5  0.28 1.  ]
 [0.9  0.84 0.57 1.  ]]
```

```
# Sort elements in every row
A_row_ordered = np.sort(A, axis=1)
print(A_row_ordered)
```

```
[[0.34 0.5  0.57 0.89]
 [0.04 0.12 0.61 1.  ]
 [0.25 0.26 0.27 0.28]
 [0.15 0.84 0.9  1.  ]]
```

We remark that `sort()` creates a copy, and not a view of the original matrix (see Chapter 3.7).

Another useful sorting function is `argsort()` that, for a given array  $x = [x_0, \dots, x_{n-1}]$  outputs an array whose  $i$ -th element is the position of the number in  $x$  that appears in place  $i$  in the ordered array `np.sort(x)`.

```
x = np.array([0.89, 0.5, 0.57, 0.34])

# Position in original array or elements in ordered list
order = np.argsort(x) # np.sort(x) = [0.34, 0.5, 0.57, 0.89]
print(order)

# Obtaining sort() from argsort()
print(x[order])
```

```
[3 1 2 0]
[0.34 0.5  0.57 0.89]
```

In the example above, in the ordered list `np.sort(x)` the first number is 0.34, which appears at position 3 in  $x$ ; the second number is 0.5, which appears at position 1 in  $x$ , the third number is 0.57 which appears in position 2 in  $x$ ; and the fourth number is 0.89, which appears in position 0 in  $x$ .

This function also works for two-dimensional arrays. For example, determining the relative order of the elements in every column can be done by adding `axis=0` (and similarly in every row by using `axis=1`).

```
A = np.array([
 [0.89, 0.5, 0.57, 0.34],
 [0.61, 0.12, 0.04, 1. ],
 [0.27, 0.26, 0.28, 0.25],
 [0.9, 0.84, 0.15, 1. ]])

# Determine relative order in every column
N = np.argsort(A, axis=0)
print(N)
```

```
[[2 1 1 2]
 [1 2 3 0]
```

```
[0 0 2 1]
[3 3 0 3]]
```

### 4.3.2 Summary statistics

There are various other mathematical functions that can perform operations along axes by adding the `axis` keyword argument. Here we list some common ones from NumPy, that yield so-called summary statistics of a (one-dimensional) array:

- Sum and product: `sum()`, `prod()`,
- Mean, standard deviation, median: `mean()`, `std()`, `median()`
- Maximum and minimum: `max()`, `min()`.

We will illustrate the use of these six functions using `max()`, but the same code applies to all other functions (if the task at hand is mathematically well-defined).

```
A = np.array([
    [2,3,6],
    [4,2,3]
])
```

If we apply the `max()` function directly to a (two-dimensional) array, it will give the maximum value in the whole array.

```
# Gives maximum of all elements in A
A_max = np.max(A)

print(A_max)
```

6

If we add the `axis` keyword argument, we can either obtain the maximum of every row, or every column.

```
# Gives maximum of every column
A_column_max = np.max(A, axis=0)

print(A_column_max)
```

[4 3 6]

```
# Gives max of every row
A_row_max = np.max(A, axis=1)

print(A_row_max)
```

[6 4]

Another useful function is `argmax()` than can return the index (position) at which the maximum in an array is attained.

```
# Gives position of maximum in every column
A_col_argmax = np.argmax(A, axis=0)

print(A_col_argmax)
```

```
[1 0 0]
```

```
# Gives position of maximum in every row
A_row_argmax = np.argmax(A, axis=1)

print(A_row_argmax)
```

```
[2 0]
```

Note that the array containing the positions of the maxima is given as a row array. If you want to turn this into a column array (because the rows are ordered vertically in a two-dimensional array), recall you can do this as follows.

```
A_row_argmax = A_row_argmax[:, None]

print(A_row_argmax)
```

```
[[2]
 [0]]
```

If we try `np.argmax(A)` without using the `axis` keyword argument, then Python first flattens the matrix into a one-dimensional array, after which it returns the position of the maximum in the flattened array. Note that this flattening happens according to the largest index changing fastest principle (so it places all the rows after each other, and not all the columns under each other).

Also note that if the maximum is attained in multiple places, then Python only returns the position of the first element that attains the maximum.

```
# Gives position of maximum
N = np.array([
 [2, 3, 4],
 [4, 4, 3]
])

N_argmax = np.argmax(N) # Turns N into [2,3,4,4,3];
# returns first position with maximum

print(N_argmax)
```

```
2
```

There are also more advance functions that give some summative information about an array:

- Cumulative sum: `cumsum()`,
- Cumulative product: `cumprod()`.

The function `cumsum()` return the cumulative sum of a one-dimensional array. As an example, if  $x = [1, 4, 2, 5]$ , then the cumulative sums will be given by

$$x_{\text{cumsum}} = [1, 1 + 4, 1 + 4 + 2, 1 + 4 + 2 + 5] = [1, 5, 7, 12].$$

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

# Cumulative sum of x
x_cumsum = np.cumsum(x)
```

```
print('x_cumsum =', x_cumsum)

x_cumsum = [ 1  5  7 12]
```

The function can also be vectorized using the `axis` keyword argument.

The function `cumprod()` returns the cumulative product. Again, if  $x = [1, 4, 2, 5]$ , then the cumulative products will be given by

$$x_{\text{cumprod}} = [1, 1 \cdot 4, 1 \cdot 4 \cdot 2, 1 \cdot 4 \cdot 2 \cdot 5] = [1, 4, 8, 40].$$

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

# Cumulative product of x
x_cumprod = np.cumprod(x)
print('x_cumprod =', x_cumprod)

x_cumprod = [ 1  4  8 40]
```

This function can also be vectorized using the `axis` keyword argument.

# Chapter 5

## Linear algebra and optimization

In this chapter we will see how Python can be used for performing linear algebra tasks, like solving systems of linear equations, and (integer) linear optimization.

Linear algebra forms the basis of many statistical tasks like principle component analysis (PCA), which can be used to identify important properties/dimensions of large data sets. This typically makes, e.g., machine learning algorithms more efficient as this avoid the so-called curse of dimensionality.

Applications of (integer) linear optimization range from scheduling, routing, transportation and food aid problems to solving Sudoku puzzles.

Let us first again import NumPy. Later on we will also use its linear algebra package (or module) `linalg`.

```
import numpy as np
```

### 5.1 Linear algebra

In this section we will often refer to one-dimensional arrays as row or column vectors, and to two-dimensional arrays as matrices.

#### 5.1.1 Matrix multiplications

Recall from Section 4.1.1 that for an  $m \times n$  matrix  $A$  and  $m \times 1$  column vector  $x$ , the command `A*x` gives a matrix in which every column of  $A$  gets pointwise multiplied by the column vector  $x$ , that is,

$$\begin{aligned} A * x &= \begin{bmatrix} a_{00} & a_{01} & \dots & a_{0(n-1)} \\ a_{10} & a_{11} & \dots & a_{1(n-1)} \\ \vdots & \vdots & \ddots & \vdots \\ a_{(m-1)0} & a_{(m-1)1} & \dots & a_{(m-1)(n-1)} \end{bmatrix} * \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_{(m-1)} \end{bmatrix} \\ &= \begin{bmatrix} a_{00} \cdot x_0 & a_{01} \cdot x_0 & \dots & a_{0(n-1)} \cdot x_0 \\ a_{10} \cdot x_1 & a_{11} \cdot x_1 & \dots & a_{1(n-1)} \cdot x_1 \\ \vdots & \vdots & \ddots & \vdots \\ a_{(m-1)0} \cdot x_{m-1} & a_{(m-1)1} \cdot x_{m-1} & \dots & a_{(m-1)(n-1)} \cdot x_{m-1} \end{bmatrix} \end{aligned}$$

```
A = np.array([  
    [1, 2],
```

```
[3,4]])

x = np.array([1,5])
x = x[:,None] # Turn x into (2,1) shaped column vector

print('A = \n', A)
print('x = \n', x)
print('A*x = \n', A*x)
```

```
A =
[[1 2]
[3 4]]
x =
[[1]
[5]]
A*x =
[[ 1  2]
[15 20]]
```

In the linear algebra sense, the multiplication  $Ax$  gives an  $m \times 1$  column vector defined by

$$\begin{aligned} Ax &= \begin{bmatrix} a_{00} & a_{01} & \dots & a_{0(n-1)} \\ a_{10} & a_{11} & \dots & a_{1(n-1)} \\ \vdots & \vdots & \ddots & \vdots \\ a_{(m-1)0} & a_{(m-1)1} & \dots & a_{(m-1)(n-1)} \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_{(m-1)} \end{bmatrix} \\ &= \begin{bmatrix} a_{00}x_0 + a_{01}x_1 + \dots + a_{0(n-1)}x_{n-1} \\ a_{10}x_0 + a_{11}x_1 + \dots + a_{1(n-1)}x_{n-1} \\ \vdots \\ a_{(m-1)0}x_0 + a_{(m-1)1}x_1 + \dots + a_{(m-1)(n-1)}x_{n-1} \end{bmatrix} \end{aligned}$$

This can be achieved in Python with the `@` ('at') operator, that is, by writing `A @ x` (the white spaces are not needed; they are included here for readability).

```
print('A = \n', A)
print('x = \n', x)

print('Ax = \n', A @ x)

A =
[[1 2]
[3 4]]
x =
[[1]
[5]]
Ax =
[[11]
[23]]
```

If we talk about matrix multiplication, it will always be clear from context whether we mean `A*x` or `A @ x`.

We can also use `@` to multiply a  $k \times m$  and  $m \times n$  matrix with each other in the linear algebra sense.

```

A = np.array([
[1,2],
[3,4],
[3,7]])

B = np.array([
[2,5,1,7],
[3,4,-1,8]])

# Note that k = 3, m = 2, n = 4
print('AB = \n',A @ B)

```

```

AB =
[[ 8 13 -1 23]
 [18 31 -1 53]
 [27 43 -4 77]]

```

A special case of this is if we multiple a column vector

$$x = \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_{n-1} \end{bmatrix}$$

with its transpose (being a row vector) resulting in a matrix that contains  $x_i x_j$  on position  $(i,j)$ .

```

x = np.array([
[1],
[2],
[4]])

print('xx^T = \n', x @ x.T)

xx^T =
[[ 1  2  4]
 [ 2  4  8]
 [ 4  8 16]]

```

### 5.1.2 Matrix properties

Using the `linalg` subpackage from NumPy, we can compute various well-known properties of a matrix (that you should recall from your Linear Algebra course).

- `linalg.matrix_rank(A)`: Computes rank of matrix  $A$ .
- `linalg.det(A)`: Computes determinant of square  $A$ .
- `linalg.eig(A)`: Computes eigenvalues and (right) eigenvectors of matrix  $A$ , i.e., values  $\lambda$  that satisfy  $Av = \lambda v$  for some (eigen)vector  $v$ .
- `linalg.inv(A)`: Computes the inverse matrix  $A^{-1}$  of  $A$ , that is, the matrix that satisfies  $A^{-1}A = AA^{-1} = I$ , where  $I$  is the identity matrix.
- `linalg.norm(A)`: Computes the norm of matrix (or vector).

We can access these function with the syntax `np.linalg.function_name(A)`.

Finally, there is also the trace function `trace(A)` in NumPy that computes the trace of  $A$ , i.e., the sum of the elements on the diagonal. This function is implemented directly in NumPy, so you don't have to go to

the subpackage `linalg` first.

Let us look at some examples of these commands.

```
A = np.array([
    [1, 2],
    [3, 4]])

# Rank of A
print('Rank of A: ', np.linalg.matrix_rank(A))
```

Rank of A: 2

```
# Determinant of A
print('Determinant of A: ', np.linalg.det(A))
```

Determinant of A: -2.0000000000000004

```
# Trace of A
print('Trace of A: ', np.trace(A))
```

Trace of A: 5

```
# Inverse of A
print('Inverse of A: \n', np.linalg.inv(A))
```

Inverse of A:  
[[ -2. 1. ]  
 [ 1.5 -0.5]]

The function `linalg.eig()` is special in that it does not output one, but two arrays.

The first array is one-dimensional and contains the eigenvalues  $[\lambda_0, \dots, \lambda_{n-1}]$  of  $A$ ; the second array is two-dimensional, and contains the corresponding eigenvectors  $v^0, \dots, v^{n-1}$  as columns of the matrix. The eigenvalues and eigenvectors are paired in the sense that  $Av^i = \lambda_i v^i$  for  $i = 0, \dots, n-1$ .

```
# Eigenvalues and eigenvectors of A
lambdas, V = np.linalg.eig(A)

print('Eigenvalues of A: \n', lambdas)
print('Matrix with eigenvectors of A: \n', V)
```

Eigenvalues of A:  
[-0.37228132 5.37228132]  
Matrix with eigenvectors of A:  
[[ -0.82456484 -0.41597356]
 [ 0.56576746 -0.90937671]]

You can output only the eigenvalues or the eigenvectors by suppressing the other output argument with `_`.

```
# Only eigenvalues of A
lambdas, _ = np.linalg.eig(A)

# Only eigenvectors of A
```

```
_ , V = np.linalg.eig(A)
```

If you want to recall how you can handle multiple outputs, and suppress the ones that you are not interested, have a look at Appendix B.

Let us check that the eigenvalues and eigenvectors indeed satisfy  $Av^i = \lambda_i v^i$  for  $i = 0, 1$ .

```
v0 = V[:,0]
v1 = V[:,1]

print('Verify first eigenvector:', A @ v0 - lambdas[0]*v0)
print('Verify second eigenvector:', A @ v1 - lambdas[1]*v1)
```

```
Verify first eigenvector: [0.0000000e+00 5.55111512e-17]
```

```
Verify second eigenvector: [0. 0.]
```

The function `linalg.norm(A)` computes the  $L^2$ -norm of a matrix  $A = (a_{ij})_{i=1,\dots,m, j=1,\dots,n}$ , also known as the Frobenius norm. It is defined as

$$\|A\|_F = \sqrt{\sum_{i=0}^{m-1} \sum_{j=0}^{n-1} a_{ij}^2}.$$

If you apply the function to a row or column vector  $x = [x_0, \dots, x_{n-1}]$ , you get the usual  $L^2$ -norm defined as

$$\|x\|_2 = \sqrt{\sum_{i=0}^{n-1} x_i^2}.$$

You can also use this function in a vectorized manner. For example, if you want to compute the  $L^2$ -norm of every row in a matrix, you can use the `axis` keyword argument.

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

row_norms = np.linalg.norm(A, axis=1)

print(row_norms)
```

```
[2.23606798 5.           7.81024968]
```

### 5.1.3 Equation solving

For a given  $m \times n$  matrix  $A = (a_{ij})$  and  $m \times 1$  column vector  $b = [b_0, \dots, b_{m-1}]^T$ , perhaps the most important question in linear algebra is to compute an  $x = [x_0, \dots, x_{n-1}]^T$  that satisfies  $Ax = b$ , i.e., the linear systems of equalities

$$\begin{array}{ccccccccc} a_{00}x_0 & + & a_{01}x_1 & + & \dots & + & a_{0(n-1)}x_{n-1} & = & b_0 \\ a_{10}x_0 & + & a_{11}x_1 & + & \dots & + & a_{1(n-1)}x_{n-1} & = & b_1 \\ & & & & & & \vdots & & \\ a_{(m-1)0}x_0 & + & a_{(m-1)1}x_1 & + & \dots & + & a_{(m-1)(n-1)}x_{n-1} & = & b_{m-1} \end{array}.$$

If  $A$  is a square, invertible matrix then this can be done with `linalg.solve(A,b)`. This gives the unique solution  $x = A^{-1}b$ .

```
A = np.array([
[1,2],
[3,4]])

b = np.array([[1],[4]])

print('Solution to Ax = b: \n', np.linalg.solve(A,b))
```

```
Solution to Ax = b:
[[ 2. ]
 [-0.5]]
```

In fact, you can compute  $x$  directly as  $x = A^{-1}b$  using the inverse of  $A$  that we have seen earlier.

```
print('Solution to Ax = b: \n', np.linalg.inv(A) @ b)
```

```
Solution to Ax = b:
[[ 2. ]
 [-0.5]]
```

If the system is overdetermined, then there is not necessarily a unique solution. This can happen when there are more constraints than variables, i.e., when  $m > n$ . In this case, we can find a solution  $x$  that is approximately optimal with the least squares method. It finds a solution  $x$  that solves the (non-linear) problem

$$\min_x \|Ax - b\|_2.$$

The least squares method can be executed with `linalg.lstsq(A,b)`; we will see this method in the next chapter, when we consider non-linear optimization problems. This function can also be used to solve under-determined systems, where  $n > m$ .

## 5.2 Linear optimization

Recall that in a linear optimization problem the goal is to compute a vector  $x = [x_0, \dots, x_{n-1}]$  of decision variables that maximizes, or minimizes, a linear objective function subject to a collection of linear constraints, which can either be a  $\leq$ ,  $\geq$  or  $=$  constraint.

In this section we will consider a general linear optimization problem of the form

$$\begin{aligned} \min_x \quad & c^T x \\ \text{s.t.} \quad & Ax = b \\ & Wx \leq z \\ & \ell \leq x \leq u \end{aligned}$$

where  $c, \ell, u \in \mathbb{R}^n$ ,  $A \in \mathbb{R}^{m \times n}$ ,  $b \in \mathbb{R}^m$ ,  $U \in \mathbb{R}^{k \times n}$ , and  $z \in \mathbb{R}^k$  are the input data, or input parameters.

Written out this means we have a system with  $m$  equality constraints,  $k$  inequality constraints and upper and lower bounds on the decision variables.

$$\begin{array}{llllll}
\min & c_1 x_1 & + & \cdots & + & c_n x_n \\
\text{s.t.} & a_{01} x_0 & + & \cdots & + & a_{0(n-1)} x_{n-1} = b_0 \\
& & & & \vdots & \\
& a_{(m-1)1} x_0 & + & \cdots & + & a_{(m-1)(n-1)} x_{n-1} = b_{m-1} \\
& w_{01} x_0 & + & \cdots & + & w_{0(n-1)} x_{n-1} \leq z_0 \\
& & & & \vdots & \\
& w_{(k-1)1} x_0 & + & \cdots & + & w_{(k-1)(n-1)} x_{n-1} \leq z_{k-1} \\
\ell_0 \leq & x_0 & & & & \leq u_0 \\
& & & & \ddots & \\
& & & & & \\
\ell_{n-1} \leq & & & & & x_{n-1} \leq u_{n-1}
\end{array}$$

You can model a  $\geq$  constraint by multiplying it with  $-1$ , so that it turns into a  $\leq$  constraint.

If, in addition, we require that  $x_i \in \mathbb{N}$  for  $i = 1, \dots, n$ , i.e., that the variables are integral, then we call the above problem an integer linear optimization problem.

We will look at two packages that can be used to solve (integer) linear optimization problems. The difference is that the first function `linprog` allows us to explicitly input the data  $c, A, B, \ell$  and  $u$ , whereas the second package `pulp` allows us to define constraints one-by-one. The latter is more convenient if the input data his not given explicitly.

### 5.2.1 Explicit input data

If the input data is given explicitly, we can solve linear optimization problems quickly with the `linprog` function, which is part of the `optimize` package of SciPy. We will see more functionality of SciPy in later chapters of this book.

We can import `linprog` as follows:

```
from scipy.optimize import linprog
```

This package is suitable for solving problem of the general form above. We will implement the following example:

$$\begin{array}{llll}
\max & z = & 15x_1 & + 20x_2 \\
\text{s.t.} & 2x_1 & + 2x_2 & \leq 8\frac{1}{2} \\
& x_1 & + 2x_2 & \leq 6 \\
& 12x_1 & + 17x_2 & = 51 \\
& x_1 & & \geq 0 \\
& & x_2 & \geq 0
\end{array}$$

Because `linprog` works with explicitly input data, we first define these. We define all the input data as NumPy arrays, but you can actually also use plain lists for this.

Note that we multiply the objective function  $c$  with  $-1$ , so that our maximization problem turns into a minimization problem.

```
## Define input data

# Coefficients of the objective function
c = np.array([-15, -20]) # Minimize -15x1 - 20x2

# Coefficients of the equality constraints (Ax = b)
A = np.array([[12, 17]]) # 12x1 + 17x2 = 51
```

```

b = np.array([51])

# Coefficients of the inequality constraints (Ux <= z)
U = np.array([
[2, 2], # 2x1 + 2x2 <= 8.5
[1, 2]]) # x1 + 2x2 <= 6

z = np.array([[8.5], [6]])

```

The bounds on  $x_i$  have to be inputted as tuple  $(\ell_i, u_i)$ . If the lower or upper bound is not present, meaning either  $\ell_i = -\infty$  or  $u_i = +\infty$ , you can replace the entry with `None`.

```

# Bounds for the variables x1 and x2 (l = 0, u = infinity)
x1_bounds = (0, None) # x1 >= 0
x2_bounds = (0, None) # x2 >= 0

```

We can solve the problem with `linprogr()`. It takes input arguments

- `c` : The vector with objective function coefficients
- `A_eq` : The constraint matrix for the equality constraints
- `b_eq` : The right hand side vector of the equality constraints
- `A_ub` : The constraint matrix for the inequality constraints
- `b_ub` : The right hand side vector of the inequality constraints
- `bounds` : List of tuples with each tuple having the upper and lower bound for the corresponding variable

Note that `A_eq` and `b_eq` can be left out as input arguments if there are no equality constraints; the same holds for `A_ub` and `b_ub`.

```

# Solve the linear programming problem
# (You can use \ to continue command on next line)
result = linprog(c, A_eq=A, b_eq=b, \
                  A_ub=U, b_ub=z, \
                  bounds=[x1_bounds, x2_bounds])

```

The `result` variable contains various aspects of the solution. The two most important for us are

- `result.x` : The optimal solution  $x$
- `result.fun` : The function value attained by the the optimal solution.

```

# Output the results
print('The problem is solved by', result.x, \
      'with objective function value', result.fun)

```

`The problem is solved by [4.25 0. ] with objective function value -63.75`

If we want to solution to be integral, we add the input argument `integrity=1`. See the documentation to read about this and to find more options.

```

# Solve the integer linear optimization problem
# (You can use \ to continue command on next line)
result_integral = linprog(c, A_eq=A, b_eq=b, \
                           A_ub=U, b_ub=z, \
                           bounds=[x1_bounds, x2_bounds], \
                           integrity=1)

```

```

        integrality=1)

# Output the results
print('The problem is solved by', result_integral.x, \
      'with objective function value', result_integral.fun)

```

The problem is solved by [0. 3.] with objective function value -60.0

The complete code of this section can be found below.

```

import numpy as np
from scipy.optimize import linprog

## Define input data

# Coefficients of the objective function
c = np.array([-15, -20]) # Minimize -15x1 - 20x2

# Coefficients of the equality constraints (Ax = b)
A = np.array([[12, 17]]) # 12x1 + 17x2 = 51

b = np.array([51])

# Coefficients of the inequality constraints (Ux <= z)
U = np.array([
[2, 2], # 2x1 + 2x2 <= 8.5
[1, 2]]) # x1 + 2x2 <= 6

z = np.array([[8.5], [6]])

## Bounds for the variables x1 and x2 (l = 0, u = infinity)
x1_bounds = (0, None) # x1 >= 0
x2_bounds = (0, None) # x2 >= 0

## Solve the linear optimization problem
## (You can use \ to continue command on next line)
result = linprog(c, A_eq=A, b_eq=b, \
                  A_ub=U, b_ub=z, \
                  bounds=[x1_bounds, x2_bounds])

# Output the results
print('The linear optimization problem is solved by', result.x, \
      'with objective function value', result.fun)

#####
## With integrality constraints ##
#####

# Solve the problem
result_integral = linprog(c, A_eq=A, b_eq=b, \
                          A_ub=U, b_ub=z, \
                          bounds=[x1_bounds, x2_bounds], \
                          integrality=1)

```

```
# Output the results
print('The integer linear optimization problem is solved by', result_integral.x, \
      'with objective function value', result_integral.fun)
```

### 5.2.2 Implicit input data

If the constraints are not given explicitly, creating the input data matrices like  $A$  and  $U$  can be quite tedious. In this case, it works better to define the constraints directly, based on the given problem description.

In this section we will consider the maximum weight bipartite matching problem. We are given a (complete) bipartite graph  $G = (V, W, E)$  with node sets  $V = \{0, \dots, n - 1\}$  and  $W = \{0, \dots, n - 1\}$  and edges  $ij \in E = \{ab : a \in V, b \in W\}$  connecting the nodes  $i \in V$  with  $j \in W$ . Every such edge has a weight  $w_{ij}$ . We want to match up every node in  $V$  with a node in  $W$  so that the total summed weight of the selected edges is maximal.

We introduce (binary) decision variables  $x_{ij}$  with the interpretation that  $x_{ij} = 1$  if  $i$  and  $j$  get matched, and  $x_{ij} = 0$  otherwise. The constraints then mean that every node  $i \in V$  should get matched up with precisely one  $j \in W$  and vice versa.

$$\begin{aligned} \max \quad & \sum_{i=0}^{n-1} \sum_{j=0}^{n-1} w_{ij} x_{ij} \\ \text{s.t.} \quad & \sum_{i=0}^{n-1} x_{ij} = 1 \quad \text{for } j = 0, \dots, n-1 \\ & \sum_{j=0}^{n-1} x_{ij} = 1 \quad \text{for } i = 0, \dots, n-1 \\ & x_{ij} \geq 0 \quad \text{for all } i, j = 0, \dots, n-1 \\ & x_{ij} \in \{0, 1\} \quad \text{for all } i, j = 0, \dots, n-1 \end{aligned}$$

In fact, the last conditions defining the decisions variables to be binary, are redundant: If we leave them out then the optimal solution that is found will satisfy them regardless (you might have seen this in a Combinatorial Optimization course). For now, we will ignore this mathematical fact, and define the decision variables as binary variables.

Defining the constraint matrix explicitly is quite a hassle, and given that many of its entries are zero, it is not very efficient for Python to store it explicitly, so using `linprog` here is not very convenient.

Instead, in this section we will use the `pulp` package to solve this problem.

```
import pulp
```

We create some input data (weights) for the problem that we are going to build.

```
# Size of the node sets
n = 4

# Weights of the edges ij
w = np.arange(1,n**2+1).reshape(n,n)

print(w)
```

```
[[ 1  2  3  4]
 [ 5  6  7  8]]
```

```
[ 9 10 11 12]
[13 14 15 16]]
```

Problem instantiation. We first initialize the problem object that we want to solve with `LpProblem()` that takes as input:

- Problem name: String variable
- Problem type: Maximization (`pulp.LpMaximize`), or minimization (`pulp.LpMinimize`).

```
prob = pulp.LpProblem("Weighted_Bipartite_Matching", pulp.LpMaximize)
```

As opposed to `linprog` we need to explicitly instantiate the decision variables, so that we can use them later to add constraints to our problem.

Decision variables. A decision variable  $y$  can be instantiated with `LpVariable()` that takes as input

- Variable name: String being name of variable
- Variable category: Keyword argument `cat` being Binary, Integer or Continuous (default if `cat` is not specified).

```
pulp.LpVariable('y', cat='Binary')
```

To initiate our decision variables we need to loop over the indices  $i$  and  $j$ , which can be done as follows. Note that the syntax `f"y_{i}_{j}"` allows us to incorporate/format the loop indices  $i$  and  $j$  into the variable name (which is a string).

```
x = np.zeros((n,n), dtype=object) # Data type of variable is 'object'
for i in range(n):
    for j in range(n):
        x[i,j] = pulp.LpVariable(f"x_{i}_{j}", cat='Binary')
```

This can be done more compactly using list comprehension, which is a quick alternative for doing the for-loops explicitly. Avoiding for-loops altogether here is not possible, because variables cannot be generated in a vectorized manner if we want to give them all a separate name.

```
# With list comprehension
x = np.array([[pulp.LpVariable(f"x_{i}_{j}", cat='Binary') \
               for j in range(n)] for i in range(n)])
```

In both cases we have created an  $n \times n$  NumPy array whose elements are decision variables  $x_{ij}$ .

```
# Print names of decision variables
print(x)
```

```
[[x_0_0 x_0_1 x_0_2 x_0_3]
 [x_1_0 x_1_1 x_1_2 x_1_3]
 [x_2_0 x_2_1 x_2_2 x_2_3]
 [x_3_0 x_3_1 x_3_2 x_3_3]]
```

We will use these variables to define the objective function and constraints.

Objective function. We next construct the objective function

$$\max \sum_{i=0}^{n-1} \sum_{j=0}^{n-1} w_{ij} x_{ij}$$

Because both the weight matrix  $w$  and the decision variables  $x$  are stored in NumPy arrays, we can do a pointwise multiplication of these arrays, and sum up the elements of the resulting array, to get the objective.

Summing up decision variables in arrays, in our case the array  $w*x$ , can be done using `lpSum()` within PuLP. To add the objective to the problem, and later constraints, we use the syntax `prob += [objective]` where `[objective]` contains the objective function expression in terms of the decision variables that we instantiated. You should think of the syntax `+=` as adding something to the instantiated problem `prob`.

```
prob += pulp.lpSum(w*x)
```

Note that we write `lpSum()` and not `LpSum()` with a capital L. This has to do with the fact that `lpSum()` is a function, whereas `LpProblem` and `LpVariable` are classes (that have different naming conventions in Python modules).

```
# Print objective function
print(prob.objective)
```

```
x_0_0 + 2*x_0_1 + 3*x_0_2 + 4*x_0_3 + 5*x_1_0 + 6*x_1_1 + 7*x_1_2 + 8*x_1_3 + 9*x_2_0 + 10*x_2_1 + 11*x_2_2 + 12*x_2_3
```

Constraints. Finally, we add the constraints

$$\begin{aligned} \sum_{i=0}^{n-1} x_{ij} &= 1 \quad \text{for } j = 0, \dots, n-1 \\ \sum_{j=0}^{n-1} x_{ij} &= 1 \quad \text{for } i = 0, \dots, n-1 \end{aligned}$$

to the problem, which can also be done with the `prob += [constraint]` syntax, where `[constraint]` is the constraint we want to add. We can add our constraints as follows.

```
for j in range(n):
    prob += pulp.lpSum([x[i,j] for i in range(n)]) == 1

for i in range(n):
    prob += pulp.lpSum([x[i,j] for j in range(n)]) == 1
```

To print the constraints, we need to realize that they are stored in an (ordered) dictionary. We can print the keys and values of this dictionary as follows.

```
# Print constraints
for key, value in prob.constraints.items():
    print(f"{key}: {value}")
```

```
_C1: x_0_0 + x_1_0 + x_2_0 + x_3_0 = 1
_C2: x_0_1 + x_1_1 + x_2_1 + x_3_1 = 1
_C3: x_0_2 + x_1_2 + x_2_2 + x_3_2 = 1
_C4: x_0_3 + x_1_3 + x_2_3 + x_3_3 = 1
_C5: x_0_0 + x_0_1 + x_0_2 + x_0_3 = 1
_C6: x_1_0 + x_1_1 + x_1_2 + x_1_3 = 1
_C7: x_2_0 + x_2_1 + x_2_2 + x_2_3 = 1
_C8: x_3_0 + x_3_1 + x_3_2 + x_3_3 = 1
```

Solving the problem. We solve the problem with the `solve()` function.

We can access the values of the objective function and the variables using `pulp.value()`. The objective function of the problem is stored in `prob.objective`, and so its value in the optimized model can be

accessed with `pulp.value(prob.objective)`.

We want to represent the optimal matching nicely in a binary matrix. Unfortunately, printing the values of the optimized model is difficult to do without for-loops since the function `pulp.value(x[i,j])` that returns the value of variable  $x_{ij}$  only works for numbers and not lists or arrays.

```
# Solve the problem
prob.solve()

# Store the results in matrix 'matching'
matching = np.zeros((n,n), dtype=int)
for i in range(n):
    for j in range(n):
        matching[i,j] = pulp.value(x[i,j])

# Print solution
print("The optimal matching is: \n", matching)
print(f"Optimal value of the objective function: {pulp.value(prob.objective)}")
```

The optimal matching is:

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

Optimal value of the objective function: 34.0

The complete code of this section can be found below.

```
import pulp

# Size of the node sets (input data)
n = 4

# Weights of the edges ij (input data)
w = np.arange(1,n**2+1).reshape(n,n)

# Instantiate problem
prob = pulp.LpProblem("Weighted_Bipartite_Matching", pulp.LpMaximize)

# Instantiate decision variables and store in NumPy array
x = np.array([[pulp.LpVariable(f"x_{i}_{j}", cat='Binary') \
               for i in range(n)] for j in range(n)])

# Set objective function
prob += pulp.lpSum(w*x)

# Set constraints
for j in range(n):
    prob += pulp.lpSum([x[i,j] for i in range(n)]) == 1

for i in range(n):
    prob += pulp.lpSum([x[i,j] for j in range(n)]) == 1

# Store the results in matrix 'matching'
```

```

matching = np.zeros((n,n), dtype=int)
for i in range(n):
    for j in range(n):
        matching[i,j] = pulp.value(x[i,j])

# Print solution and objective value
print("The optimal matching is: \n", matching)
print(f"Optimal value of the objective function: {pulp.value(prob.objective)}")

```

### 5.2.3 Remarks

The `linprog` function is typically convenient for small linear optimization problems, especially for problems whose input data (such as the constraint matrices) you can define explicitly.

The `pulp` package is more useful when the input data is defined implicitly, e.g., using different sets of inequalities defined through indices. Furthermore, when problems become of larger scale, as you will typically encounter in practice, it is better to use state-of-the-art solvers such as [CPLEX](#), [GUROBI](#), or [MOSEK](#). PuLP is able to be coupled to such solvers, that is, you can define a problem in PuLP and then have it solved with the external solver software.

Many of these solvers can also handle other problems such as mixed integer linear optimization problems, in which there is a mixture of continuous, integer and binary variables, and various non-linear optimization problems. We will see more of those in the next chapter.

# Chapter 6

## Nonlinear algebra and optimization

In this chapter we will see functions for solving systems of nonlinear equations and how to optimize a nonlinear function.

For equation solving, the main goal is to compute an  $x \in \mathbb{R}^n$  that satisfies the system

$$\begin{cases} f_0(x) = 0 \\ f_1(x) = 0 \\ \vdots \\ f_{n-1}(x) = 0 \end{cases}$$

where  $f_0, \dots, f_{n-1} : \mathbb{R}^n \rightarrow \mathbb{R}$  are continuous,  $n$ -variate functions. That is, we have a systems of  $n$  equations and  $n$  variables. We will also see the least squares method for problems in which the number of equations is not equal to the number of variables (i.e., the system is under- or overdetermined).

For optimizing a function, we have a single continuous,  $n$ -variate function  $f : \mathbb{R}^n \rightarrow \mathbb{R}$ , and the goal is to compute an  $x \in \mathbb{R}^n$ , that attains

$$\min_{x \in \mathbb{R}^n} f(x).$$

When there is only one (nonlinear) equation in one variable, we will also see ways to specify the interval in which the solution to the respective problems should be searched for.

The Python package SciPy contains all the functions we will need to achieve these goals, in particular, the `optimize` submodule. We import it under the alias `optimize` for convenience, and also import NumPy.

```
import numpy as np
import scipy.optimize as optimize
```

### 6.1 Root finding

In this section we will discuss various root finding methods. We start by introducing various methods for finding the root of a univariate function, and then show similar methods for the multivariate case. We end with the least squares method, that finds an approximately optimal solution when a solution might not exist.

#### 6.1.1 Univariate function

We present three type of methods and information that can be used to find roots of a function. We emphasize that none of these methods guarantee that a root will always be found if it exists, but in many cases they do.

## Using `fsolve()`

The easiest-to-use function for finding the root of a univariate function  $f : \mathbb{R} \rightarrow \mathbb{R}$  is `fsolve()` from the `optimize` module. It takes two mandatory input arguments:

- The function we want to find the root of, and
- an initial guess for the root.

As an example, suppose we want to find the root of the equation

$$f(x) = x^2 + 2 \cdot x - 1,$$

that is plotted below. You do not have to look at the code generating this figure (but it is included for completeness).

```
import numpy as np
import matplotlib.pyplot as plt

# Define the x range
x = np.linspace(-3, 3, 600)

# Define the function f
def f(x):
    return x**2 + 2*x - 1

# Create the plot
plt.figure(figsize=(6, 4))
plt.plot(x, f(x), label='$f(x) = x^2 + 2x - 1$')

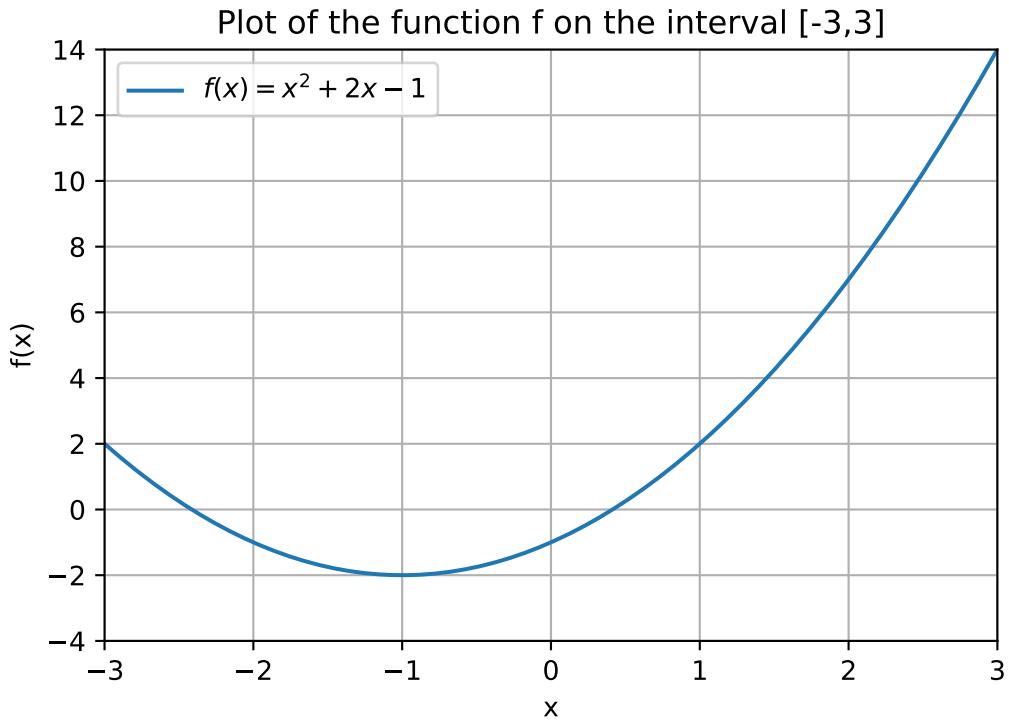
# Add labels and title
plt.title('Plot of the function f on the interval [-3,3]')
plt.xlabel('x')
plt.ylabel('f(x)')

# Add a grid
plt.grid(True)

# Set range
plt.xlim(-3,3)
plt.ylim(-4,14)

# Add a legend
plt.legend()

# Show the plot
plt.show()
```



Our initial guess will be `guess = 3`. There are various ways in which you can input the function and initial guess. Either as

- Keyword arguments: Use `func` for the function and `x0` for the initial guess.
- Positional arguments: Input function followed by initial guess, without keywords.

```
def f(x):
    return x**2 + 2*x - 1

guess = 3
x_root = optimize.fsolve(f,x0=guess)

# Also works:
# x_root = optimize.fsolve(func=f,x0=guess)
# x_root = optimize.fsolve(x0=guess, func=f)
# x_root = optimize.fsolve(f,guess), here the order matters!

# Does not work
# x_root = optimize.fsolve(x0=guess,f), f is positional, order matters!
# x_root = optimize.fsolve(guess,f), order matters!

print("A root of the function f is given by", x_root)

# x_root is an array one element;
# can access index 0 to only get value
print("A root of the function f is given by", x_root[0])
```

A root of the function  $f$  is given by [0.41421356]  
A root of the function  $f$  is given by 0.41421356237309503

For any function, in SciPy and beyond, you should look at the order of the required arguments of a function in its documentation.

Because different root finding and optimization methods use a different keyword argument for the function of interest (e.g., `func`, `fun`, `f`), we will introduce the convention in this chapter that the first input argument of any SciPy function that we use is the function we want to find the root of, or optimize over, and all other input arguments will have a keyword (such as `x0`). The order of the keyword input arguments is not relevant, as long as they come after the function, which is the first input argument.

The choice of initial guess can determine which root we end up in. The function  $f$  has two roots as can be seen from the figure. If we start with another initial guess, such as `guess=4`, we find the other root of  $f$ .

```
def f(x):
    return x**2 + 2*x - 1

guess = -4
x_root = optimize.fsolve(f,x0=guess)

print("Another root of the function f is given by", x_root)
```

Another root of the function f is given by [-2.41421356]

If the function  $f$  would have had multiple input arguments, than `fsolve()` interprets the first argument of  $f$  as being the unknown variable that it needs to compute. Any remaining arguments of  $f$  should be specified in the `args` keyword argument.

For example, suppose that we would have defined  $g(x, a, b, c) = a \cdot x^2 + b \cdot x + c$ . Then executing `x_root = optimize.fsolve(g,x0=guess)` will result in an error because `fsolve()` cannot determine a root  $x$  if it does not know the values of  $a, b$  and  $c$ . Therefore, we need to specify these additional inputs in the `args` keyword argument of `fsolve()`.

```
def g(x,a,b,c):
    return a*x**2 + b*x + c

a, b, c = 1, 2, -1

guess = -4
x_root = optimize.fsolve(g,x0=guess,args=(a,b,c))

print("A root of the function g is given by", x_root)
```

A root of the function g is given by [-2.41421356]

We could have also stored the parameters  $a, b, c$  in an array so that  $g$  would have only had one additional input argument. This is illustrated below.

```
def g(x,coeff):
    return coeff[0]*x**2 + coeff[1]*x + coeff[2]

coeff = np.array([1,2,-1])

guess = -4
x_root = optimize.fsolve(g, x0=guess, args=(coeff))
```

```
print("A root of the function g is given by", x_root)
```

```
A root of the function g is given by [-2.41421356]
```

### Bracket information

Another function that can find the root of a univariate function is `root_scalar()` from the `optimize` module.

Whereas `fsolve()` uses one fixed method in the background to find a root, `root_scalar()` allows the user to choose from a collection of methods. Some methods might perform better than others, depending on the type of function you are trying to find a root of. You can specify which method you want to use with the `method` keyword argument. Some methods require additional keyword arguments to be specified; see the documentation.

One such additional keyword argument is `bracket`, that allows you to specify the interval, or bracket,  $[a, b]$  in which the root should be searched for. This does, however, come with the requirement that the function values in the points  $a$  and  $b$  should have a different sign: Either  $f(a) < 0 < f(b)$  or  $f(b) < 0 < f(a)$ . The reason is that this guarantees, by the Intermediate Value Theorem, that there is at least one root in the interval  $[a, b]$ . If the bracket does not satisfy this condition, then Python will raise an error (try this yourself).

Let us look at an example where we use the Bisection method, called '`bisect`' in SciPy, with interval  $[0, 4]$ . The order in which you place the keyword argument `bracket` and `method` does not matter.

```
def f(x):
    return x**2 + 2*x - 1

interval = [0,4]

result = optimize.root_scalar(f, bracket=interval, method='bisect')
print(result)
```

```
converged: True
flag: 'converged'
function_calls: 43
iterations: 41
root: 0.41421356237151485
```

Note that Python returns a lot of information regarding the root finding process. For example, it tells us whether the process has converged, meaning it found a point that satisfies  $f(x) = 0$  up to a default precision. You can access these properties with the syntax `result.property_name` where `property_name` is the property of interest.

```
print("The root finding process converged:", result.converged)
```

```
The root finding process converged: True
```

For us, the most important property is `root`, which gives the value of the root.

```
print("A root of the function f is given by", result.root)
```

```
A root of the function f is given by 0.41421356237151485
```

### Derivative information

If a function is differentiable, it is also possible to specify its derivative in some methods. This typically results in much faster root finding methods.

Recall, for example, Newton's method from Section Section 2.4 that finds a root by iteratively computing better approximations using the formula

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

starting from some initial guess  $x_0$ . The formula to compute the next iterate relies on

- The derivative  $f'(x)$ , and
- an initial guess  $x_0$ .

Let us look at an example of using Newton's method. The derivative  $f'$  should be defined as a function and can be entered in the `fprime` keyword argument. The initial guess is inputted in the `x0` keyword argument.

For our function  $f(x) = x^2 + 2x - 1$  we have  $f'(x) = 2(x + 1)$ .

```
def f(x):
    return x**2 + 2*x - 1

def f_deriv(x):
    return 2*(x+1)

guess = 4
result = optimize.root_scalar(f, method='newton', \
                             fprime=f_deriv, x0 = guess)
print(result)

converged: True
flag: 'converged'
function_calls: 14
iterations: 7
root: 0.41421356237309503
```

Although it is a little bit like comparing apples and pears, the number of function calls and iterations (determining how long a method needs to converge) of Newton's method is much lower than that of the Bisection method.

Finally, we remark that the `args` keyword argument to specify additional input parameters can also be used in combination with methods that use bracket or derivative information.

### 6.1.2 Multivariate functions

#### Using `fsolve()`

The `fsolve()` function can also be used to compute a root of a system of  $n$  functions with  $n$  unknown variables. It again takes two input arguments:

- The system of function equations to be solved, and
- an initial guess for the (unknown) root.

The system of equations should be modelled as a Python function, i.e., we need a function that takes as input an array  $x = [x_0, \dots, x_{n-1}]$  and outputs the array  $f(x) = [f_0(x), \dots, f_{n-1}(x)]$ . This function will then be the input for `fsolve()`.

As an example for  $n = 2$ , suppose we want to solve the system

$$\begin{cases} x_0^2 + x_1^2 &= 4 \\ x_0 + x_1 &= 1 \end{cases} .$$

That is, we have  $f_0(x_0, x_1) = x_0^2 + x_1^2 - 4$  and  $f_1(x_0, x_1) = x_0 + x_1 - 1$ , and want to solve  $f_0(x) = 0, f_1(x) = 0$ . The array  $[f_0(x), f_1(x)]$  can be defined as a function in the following way.

```
def f(x):
    # Input  : Array x = [x_0, x_1]
    # Output : Array f = [f_0(x), f_1(x)]

    f = np.array([x[0]**2 + x[1]**2 - 4, x[0] + x[1] - 1])
    return f
```

We emphasize that here the array  $x = [x_0, x_1]$  is the input of the function, and not  $x_0$  and  $x_1$  separately. If we would define  $f$  as a function of two inputs, i.e.,  $f(x_0, x_1)$ , then `fsolve()` would want to find a root with respect to its first argument  $x_0$  only, which is not what we want.

Using `fsolve()` to do the root finding gives us the following solution.

```
guess = np.array([1,1]) # Our initial guess
root = optimize.fsolve(f, x0=guess)

print(root)
```

[ 1.82287566 -0.82287566]

Note that the initial guess is an array in  $\mathbb{R}^2$  this time, as we are considering a function with two variables.

Also here we can use the `args` keyword argument to specify additional input parameters. Suppose we want to solve, for  $a = 2$  and  $b = 4$ , the system

$$\begin{cases} a \cdot x_0^2 + x_1^2 = 4 \\ x_0 + b \cdot x_1 = 1 \end{cases}.$$

```
def f(x,a,b):
    return np.array([a*x[0]**2 + x[1]**2 - 4, x[0] + b*x[1] - 1])

guess = np.array([1,1]) # Our initial guess
a, b = 2, 4
x_root = optimize.fsolve(f, x0=guess, args=(a,b))

print(x_root)
```

[ 1.41233385 -0.10308346]

You can double-check that the root  $x^*$  you found is indeed a root by plugging the solution into the system of equations, i.e., checking if it satisfies

$$f(x^*) = [f_0(x^*), \dots, f_{n-1}(x^*)] = [0, \dots, 0].$$

```
print(f(x_root,a,b)) # Both coordinates approximately equal to zero
```

[9.59232693e-14 0.0000000e+00]

## Derivative information

Just as in the univariate case, it is also possible to use other function for finding a root. The analogue of `root_scalar()` is the function `root()`. Although it is not possible to input bracket information for

this function, it does have methods that use derivative information. These methods are typically faster than `fsolve()`.

Consider again the system

$$\begin{cases} x_0^2 + x_1^2 - 4 = 0 \\ x_0 + x_1 - 1 = 0 \end{cases}.$$

The “derivative” of the function  $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$  given by  $f(x) = [f_0(x), \dots, f_{n-1}(x)]$  is the Jacobian matrix

$$J(f) = \frac{\partial(f_0, \dots, f_{n-1})}{\partial(x_0, \dots, x_{n-1})} = \begin{bmatrix} \frac{\partial f_0}{\partial x_0} & \frac{\partial f_0}{\partial x_1} & \cdots & \frac{\partial f_0}{\partial x_n} \\ \frac{\partial f_1}{\partial x_0} & \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_{n-1}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_{n-1}}{\partial x_0} & \frac{\partial f_{n-1}}{\partial x_1} & \cdots & \frac{\partial f_{n-1}}{\partial x_{n-1}} \end{bmatrix}.$$

For the two equations at hand, we have

$$J(f) = \begin{bmatrix} 2x_0 & 2x_1 \\ 1 & 1 \end{bmatrix}.$$

Just as in the univariate case when using Newton’s method, we need to input an initial guess and the Jacobian matrix, where the latter should be defined as a function. The Jacobian is inputted in the `jac` keyword argument; the initial guess in `x0`.

```
def f(x):
    return np.array([x[0]**2 + x[1]**2 - 4, x[0] + x[1] - 1])
```

```
def jac_f(x):
    J = np.array([[2*x[0], 2*x[1]], [1, 1]])
    return J
```

```
guess = np.array([1, 1]) # Our initial guess
result = optimize.root(f, jac=jac_f, x0=guess)
```

```
print(result)
```

```
message: The solution converged.
success: True
status: 1
fun: [ 0.000e+00  0.000e+00]
x: [ 1.823e+00 -8.229e-01]
nfev: 27
njev: 2
fjac: [[-9.745e-01 -2.243e-01]
        [-2.243e-01  9.745e-01]]
r: [-4.458e+00  6.983e-01  1.187e+00]
qtf: [ 1.848e-10  4.255e-11]
```

We can access the properties of the result of the root finding procedure with the syntax `result.property_name` where `property_name` is the property of interest. Here the root is given by the property `x`.

```
print("A root of the function f is given by", result.x)
```

A root of the function  $f$  is given by [ 1.82287566 -0.82287566]

Note that this is the same root that we found with `fsolve()`.

### 6.1.3 Least squares method

If the number of functions is not equal to the number of variables, or if the system does not have a solution, the least squares method `optimize.least_squares` is your best pick to find a root.

The function (when using the default settings) tries to compute a point  $x$  that attains the minimum of the residual function

$$R(f_0, \dots, f_{n-1}) = \min_{x \in \mathbb{R}^n} \sum_{i=1}^{n-1} f_i(x)^2,$$

It should be observed that  $R(f_0, \dots, f_{n-1}) \geq 0$  and  $R(f_0, \dots, f_{n-1}) = 0$  if and only if the system  $f_0(x) = 0, \dots, f_{n-1}(x) = 0$  has a root.

The function `optimize.least_squares` takes just like `fsolve()` two input arguments: The system of equations and an initial guess.

Let's look at an example. Consider the system

$$\begin{cases} f_0(x) = \sin(x) = 0 \\ f_1(x) = (x - \pi + 0.1)^2 = 0 \\ f_2(x) = (x - \pi) = 0 \end{cases}.$$

Without the 0.1-term, this system would have the unique solution  $x = \pi$ , but this small perturbation causes it to become infeasible. We can still find an approximately optimal solution with the least squares method. The number  $\pi$  can be accessed in NumPy using `np.pi`.

```
def system(x):
    return np.array([np.sin(x[0]), (x[0]-np.pi + 0.1)**2, x[0] - np.pi])

guess = 1
result = optimize.least_squares(system, x0=guess)

print("Least squares solution found is x = ", result.x) # Close to pi
```

Least squares solution found is x = [3.1406215]

Although `optimize.least_squares` often works well, it does not necessarily compute a root of the function even if one exists. What it actually does, is compute a local minimum of the residual function.

Let us illustrate this with an example. Consider the function  $f(x) = x^4 + 0.3x^3 - 2.5x^2 + 1.5$ , which has two (real) roots as can be seen from the figure below.

```
import numpy as np
import matplotlib.pyplot as plt

# Define the x range
x = np.linspace(-2, 2, 600)

# Define the function f
def f(x):
    return x**4 + 0.3*x**3 - 2.5*x**2 + 1.5

# Create the plot
plt.figure(figsize=(6, 4))
```

```

plt.plot(x, f(x), label='$f(x) = x^4 + 0.3x^3 - 2.5x^2 + 1.5$')

# Add labels and title
plt.title('Plot of the function f on the interval [-2,2]')
plt.xlabel('x')
plt.ylabel('f(x)')

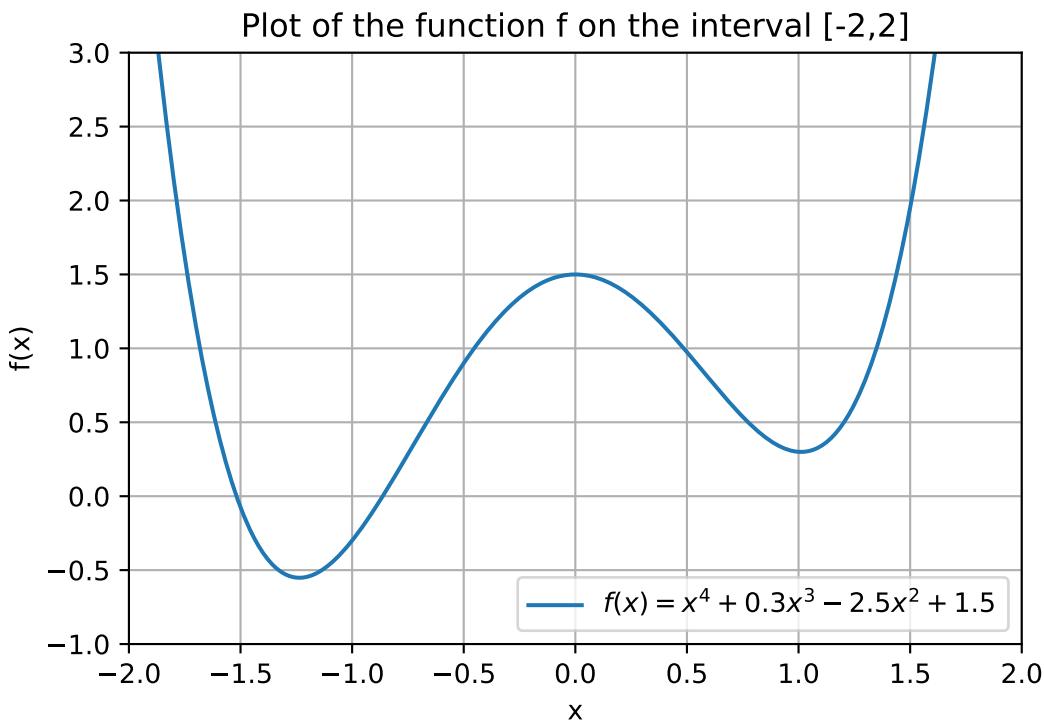
# Add a grid
plt.grid(True)

# Set range
plt.xlim(-2,2)
plt.ylim(-1,3)

# Add a legend
plt.legend()

# Show the plot
plt.show()

```



We execute both Newton's and the least squares method with the same initial guess.

```

# Function f
def f(x):
    return (x**4 + 0.3*x**3 - 2.5*x**2 + 1.5)

# Derivative of f
def f_deriv(x):

```

```

    return 4*x***3 + 0.9*x***2 -5*x

guess = 1.5

# Newton's method
result = optimize.root_scalar(f, method='newton', \
                               fprime=f_deriv, x0 = guess)
print("Root found by Newton's method: \n x =", result.root,
      f"with f(x) =", f(result.root))

# Least squares method
result_ls = optimize.least_squares(f, x0=guess)
print("Root found by least squares method: \n x =", result_ls.x,
      f"with f(x) =", f(result_ls.x))

```

Root found by Newton's method:  
 $x = -1.5180670079327394$  with  $f(x) = -8.881784197001252e-16$   
Root found by least squares method:  
 $x = [1.01118148]$  with  $f(x) = [0.29943799]$

As you can see, the least squares method does not find a root, because the function value in the computed point is almost 0.3. What goes wrong here? Consider the residual problem

$$R(f) = \min_x (x^4 + 0.3x^3 - 2.5x^2 + 1.5)^2.$$

The function  $g(x) = f(x)^2 = (x^4 + 0.3x^3 - 2.5x^2 + 1.5)^2$  is plotted below. As you can see, it has a local minimum around 1. Because we started out with the initial guess 1.5, the least squares method gets stuck in this local minimum.

```

import numpy as np
import matplotlib.pyplot as plt

# Define the x range
x = np.linspace(-2, 2, 600)

# Define the function f
def f(x):
    return (x**4 + 0.3*x***3 - 2.5*x***2 + 1.5)**2

# Create the plot
plt.figure(figsize=(6, 4))
plt.plot(x, f(x), label='$f(x)^2 = (x^4 + 0.3x^3 - 2.5x^2 + 1.5)^2$')

# Add labels and title
plt.title('Plot of the function f on the interval [-2,2]')
plt.xlabel('x')
plt.ylabel('f(x)')

# Add a grid
plt.grid(True)

# Set range
plt.xlim(-2,2)

```

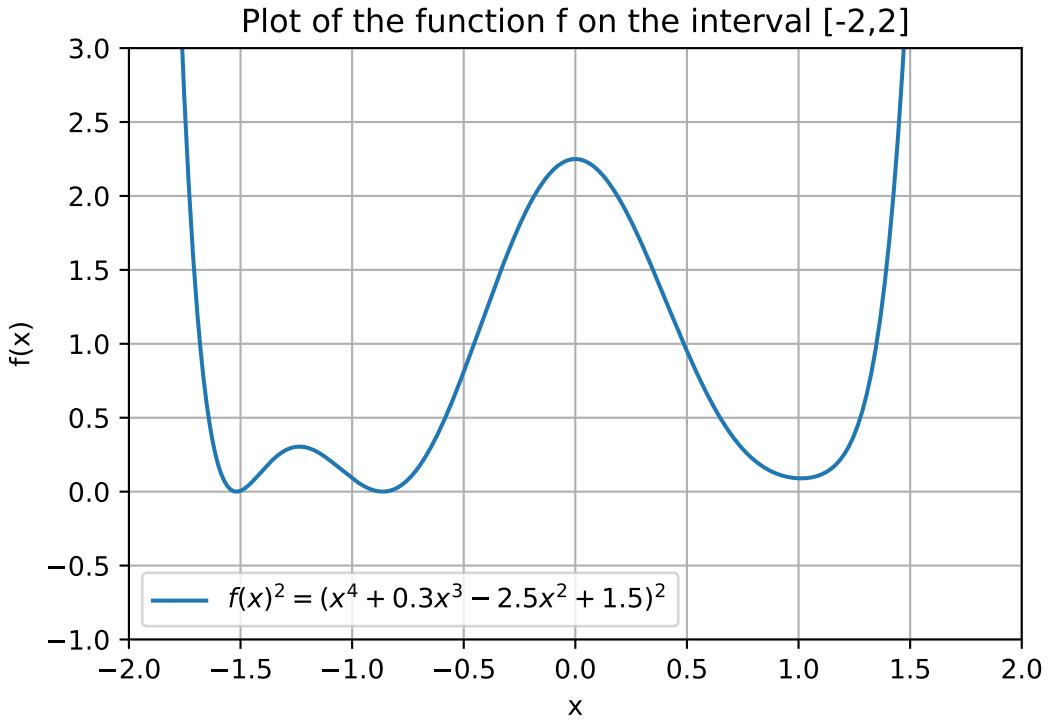
```

plt.ylim(-1,3)

# Add a legend
plt.legend()

# Show the plot
plt.show()

```



To close this section, we again emphasize that no method is guaranteed to always find a root for every function. For example, `fsolve()` is also not able to find a root of the function  $f$  in this section (try this yourself).

Therefore, always check whether a found solution is actually a root by evaluating the function in the solution found and checking if the resulting value is (almost) zero.

## 6.2 Nonlinear optimization

In this section we consider the minimization problem

$$\min_{x \in \mathbb{R}^n} f(x).$$

for a function  $f : \mathbb{R}^n \rightarrow \mathbb{R}$ . Note that maximization can be done by considering the function  $-f$ .

We again start with univariate functions and then switch to multivariate functions later on. In the last section we will also see some examples of constrained optimization, where the domain of  $f$  is a subset of  $\mathbb{R}^n$ . The syntax for using minimization functions from SciPy will be similar to the syntax we saw for root finding methods.

In particular, also here we can use the `args` keyword argument to specify any additional input arguments of the function we want to minimize over, so that the optimization can happen with respect to the unknown first input argument of the function.

### 6.2.1 Univariate function

If  $f : \mathbb{R} \rightarrow \mathbb{R}$  is a univariate function then the easiest-to-use functions for minimization are `fmin()` and `minimize_scalar()` from the `optimize` module. We emphasize that these functions find a local minimum of the function  $f$ , which might or might not be a global minimum.

The function `fmin()` works similar as `fsolve()` in that it requires an initial guess.

```
def f(x):
    return x**4 + 0.3*x**3 - 2.5*x**2 + 1.5

guess=1.5
x_min = optimize.fmin(f,x0=guess)

print("The minimum found is x =", x_min) # Local minimum
```

```
Optimization terminated successfully.
      Current function value: 0.299438
      Iterations: 15
      Function evaluations: 30
The minimum found is x = [1.01118164]
```

With a different initial guess the method is able to find the global minimum; see the figure in the previous section. Furthermore, you can suppress the output message of `fmin()` by setting the keyword argument `disp=False`; see the documentation of `fmin()`.

```
guess=-1.5
x_min = optimize.fmin(f,x0=guess,disp=False)

print("The minimum found is x =", x_min) # Local minimum
```

```
The minimum found is x = [-1.23618164]
```

The function `minimize_scalar()` gives more flexibility in terms of input arguments. First of all, we can execute it without any additional arguments, but then it more easily gets stuck in a local minimum.

```
result = optimize.minimize_scalar(f)
print(result)

# We access root with result.x
print("The minimum found is x =", result.x)

message:
    Optimization terminated successfully;
    The returned value satisfies the termination criteria
    (using xtol = 1.48e-08 )
success: True
fun: 0.29943799106751934
x: 1.011179780213775
nit: 11
nfev: 14
The minimum found is x = 1.011179780213775
```

We can also set an interval in which we want to find a minimum using the `bounds` keyword argument. Note that in the example below, the function `minimize_scalar()` does not get stuck in the local minimum around 1.

```

interval = [-2,2]
result = optimize.minimize_scalar(f,bounds=interval)

print("The minimum found is x =", result.x)

```

The minimum found is x = -1.2361799028533706

For more options and different methods that can be used with the `method` keyword argument, see the documentation of `minimize_scalar`.

### 6.2.2 Multivariate function

For multivariate functions, we can use the `minimize()` function from `optimize`, being the analogue of `root()` for root finding. This function can take into account derivative, or gradient, information with certain methods. The gradient of  $f$  is given by

$$\nabla f(x) = \left[ \frac{\partial f}{\partial x_0}, \dots, \frac{\partial f}{\partial x_{n-1}} \right].$$

We can input the gradient again with the keyword argument `jac`. The default method that `minimize()` uses is 'BFGS' and this method can use gradient information. You can choose your own method with the `method` keyword argument; see the documentation.

```

# Define the function
def f(x):
    return (x[0] - 3)**2 + (x[1] + 4)**2 - 1

# Define the gradient
def grad_f(x):
    return np.array([2 * (x[0] - 3), 2 * (x[1] + 4)])

# Initial guess
guess = np.array([0.0, 0.0])

# Minimization with gradient information
result = optimize.minimize(f, x0=guess, jac=grad_f)

# Print the result
print("The minimum found is:", result.x)
print("Function value at minimum:", result.fun)

```

The minimum found is: [ 3. -4.]  
Function value at minimum: -1.0

### 6.2.3 Constrained optimization

Just as with `minimize_scalar()` the function `minimize()` can also include interval information using the `bounds` keyword argument. The syntax for this argument is a list of tuples that for every variable in  $x = [x_0, \dots, x_{n-1}]$  contains the lower and upper bound value for the variable. Recall that this is the same way how variable bounds were specified in the `linprog` package for solving (integer) linear optimization problems.

That is, if we have the constraints  $\ell_i \leq x_i \leq u_i$  for  $i = 0, \dots, n - 1$ , then the input for `bounds` is  $[(l_0, u_0), (l_1, u_1), \dots, (l_{n-1}, u_{n-1})]$ . Just as in `linprog` you can set an upper or lower bound equal to `None` to model that the lower bound is  $-\infty$ , or that the upper bound is  $+\infty$ .

```

# Define the function
def f(x):
    return (x[0] - 3)**2 + (x[1] + 4)**2 - 1

# Define the gradient
def grad_f(x):
    return np.array([2 * (x[0] - 3), 2 * (x[1] + 4)])

# Initial guess
guess = np.array([0.0, 0.0])
intervals = [(None, 2), (-2, None)] # x_0 <= 2, x_1 >= -2

# Minimization with gradient information
result = optimize.minimize(f, x0=guess, bounds=intervals)

# Print the result
print("The minimum found is:", result.x)
print("Function value at minimum:", result.fun)

```

The minimum found is: [ 2. -2.]  
 Function value at minimum: 4.0

Next to specifying variable bounds, `minimize()` can also take into account more complex constraints that restrict the domain of  $f$ , i.e., the search space of `minimize()`, using the `constraints` keyword argument.

That is, we can solve the problem

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \quad & f(x) \\ \text{s.t.} \quad & g_j(x) \geq 0 \quad \text{for } j = 1, \dots, q-1 \\ & h_k(x) = 0 \quad \text{for } k = 0, \dots, r-1 \end{aligned}$$

The syntax for adding constraints is to use a tuple containing dictionaries, where each dictionary models a constraints with keys

- 'type': Use 'ineq' for a  $\geq$ -constraint and 'eq' for an  $=$ - constraint;
- 'fun': Python function that describes  $g_j$  or  $h_k$ .

There is also the optional keyword argument 'args' that allows you to specify additional parameters that appear in the function  $g_j$  or  $h_k$ .

As an example, suppose we want to solve the problem

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \quad & x_0^2 + 5x_1^2 \\ \text{s.t.} \quad & x_0 + x_1 \geq 5 \\ & x_0 - 2x_1 = 3 \end{aligned}$$

Then we have  $g_0(x) = x_0 + x_1 - 5$  and  $h_0(x) = x_0 - 2x_1 - 3$ .

```

# Define functions of constraints
def g(x):
    return x[0] + x[1] - 5

def h(x):
    return x[0] - 2*x[1] - 3

```

```
# Define tuple containing constraints as dictionaries
cons = ({'type' : 'ineq', 'fun' : g},
         {'type' : 'eq', 'fun' : h})
```

Let us now do the optimization using these constraints.

```
def f(x):
    return x[0]**2 + x[1]**2

guess = np.array([0,0]) # minimize() always needs guess

result = optimize.minimize(f, x0=guess, constraints=cons)

print("The minimum found is:", result.x)
print("Function value at minimum:", result.fun)
```

The minimum found is: [4.3333333 0.66666667]

Function value at minimum: 19.222222222229

This allows us, for example, to optimize a nonlinear function subject to linear constraints.

#### 6.2.4 Remarks

Just as in the previous chapter, we remark here that there are various other packages in Python to perform optimization tasks with. For example, there is `cvxpy` for convex optimization, and you can also couple external solvers with Python, as explained in the last chapter.

# Chapter 7

## Visualization

In this chapter we will explain the basics for plotting functions and data, for which we will use the `matplotlib.pyplot` (sub)package. We import it under the alias `plt`. You might wonder why we use the name `plt` and not the perhaps more obvious choice `plot`. This is because `plot()` is a command that we will be using, so we do not want to create any conflicts with this function when executing a Python script.

### 7.1 Basic plotting

In this section we will explain step-by-step how to generate a nice looking figure containing a visualization of a one-dimensional function. We start with plotting the function  $f(x) = x^2 + 2x - 1$  for some values of  $x$  in a two-dimensional figure.

```
import numpy as np
import matplotlib.pyplot as plt

# Define the function f
def f(x):
    return x**2 + 2*x - 1

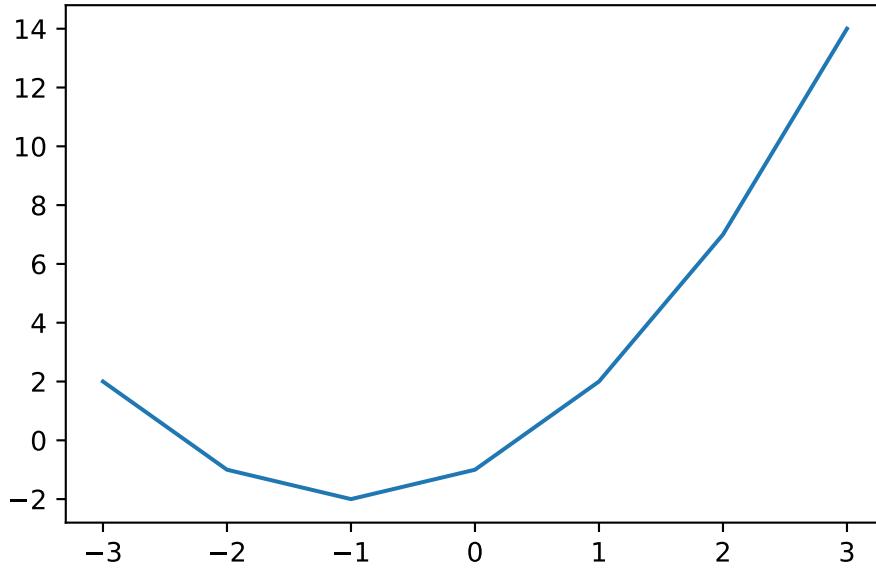
# Define the x range of x-values
x = np.array([-3,-2,-1,0,1,2,3])

# Compute the function values f(x[i]) of the elements x[i]
# and store them in the array y
y = f(x)

#Create the figure
plt.figure()

# Create the plot
plt.plot(x, y)

# Show the plot
plt.show()
```



You can view the figure in the Plots pane (or tab) in Spyder.

If the resolution of the plots in the Plots pane does not seem good enough, you can increase it by going to “Tools > Preferences > IPython console > Graphics > Inline backend > Resolution” and set the resolution to, for example, 300 dpi.

You can get the Plots pane in fullscreen by going to the button with the three horizontal lines in the top right corner and choose “Undock”. You can “Dock” the pane again as well if you want to leave the fullscreen mode.

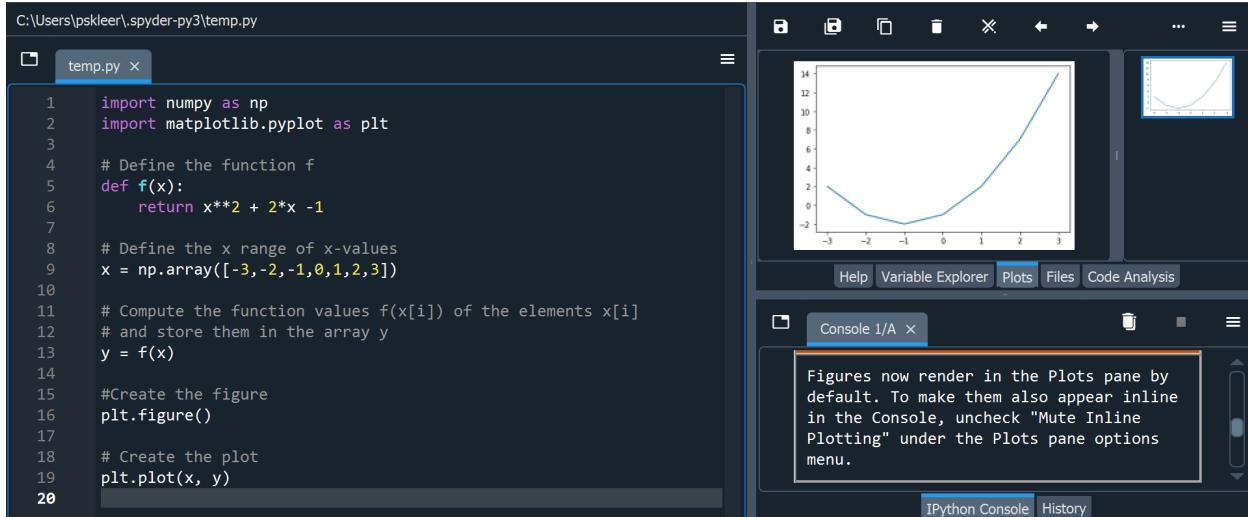


Figure 7.1: IPython Console

We will next explain what the code above is doing. After defining the function  $f$ , we create the vector (i.e., Numpy array)

$$x = [x_1, x_2, x_3, x_4, x_5, x_6, x_7] = [-3, -2, -1, 0, 1, 2, 3].$$

Because the function  $f$  is vectorized, we can right away compute all the function values in these points. We store them in the array  $y = f(x)$ , that is,

$$\begin{aligned}y = f(x) &= [f(x_1), f(x_2), f(x_3), f(x_4), f(x_5), f(x_6), f(x_7)] \\&= [2, -1, -2, -1, 2, 7, 14].\end{aligned}$$

Next, we create an (empty) figure using the command `plt.figure()`. Then comes the most important command, `plt.plot(x,y)`, that plots the elements in the vector  $x$  against the elements in the vector  $y = f(x)$ , and connects consecutive combinations  $(x_i, y_i)$  and  $(x_{i+1}, y_{i+1})$  with a line segment. For example, we have  $(x_1, y_1) = (-3, 2)$  and  $(x_2, y_2) = (-2, -1)$ . The left most line segment is formed by connecting these points.

If you only want to plot the points  $(x_i, y_i)$ , and not the line segments, you can use `plt.scatter(x,y)` instead of `plt.plot(x,y)`.

```
import numpy as np
import matplotlib.pyplot as plt

# Define the function f
def f(x):
    return x**2 + 2*x - 1

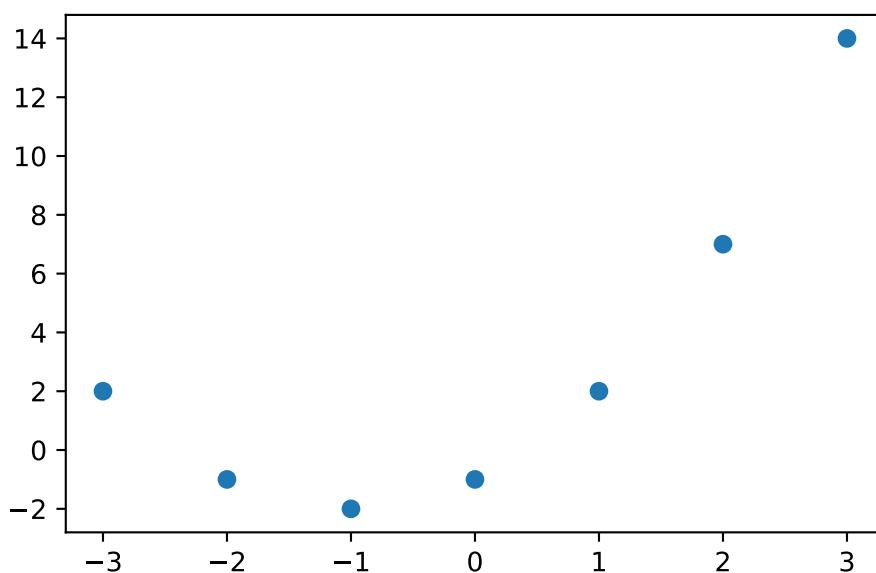
# Define the x range of x-values
x = np.array([-3,-2,-1,0,1,2,3])

# Compute the function values f(x[i]) of the elements x[i]
# and store them in the array y
y = f(x)

#Create the figure
plt.figure()

# Create the plot
plt.scatter(x, y)

# Show the plot
plt.show()
```



Observe that the (blue) line in the figure that was generated using `plt.plot(x,y)` is not very “smooth”, i.e., the function visibly is connected by line segments. To get a smoother function line, we can include more points in the vector  $x$ . This can be done, for example, with the `linspace()` function that we have seen in Chapter 3.

Let us plot again the function  $f$ , but this time with 600 elements in  $x$  in the interval  $[-3,3]$ . We use `plt.plot()` again, instead of `plt.scatter()`. We now obtain a much smoother function line.

```
import numpy as np
import matplotlib.pyplot as plt

# Define the function f
def f(x):
    return x**2 + 2*x - 1

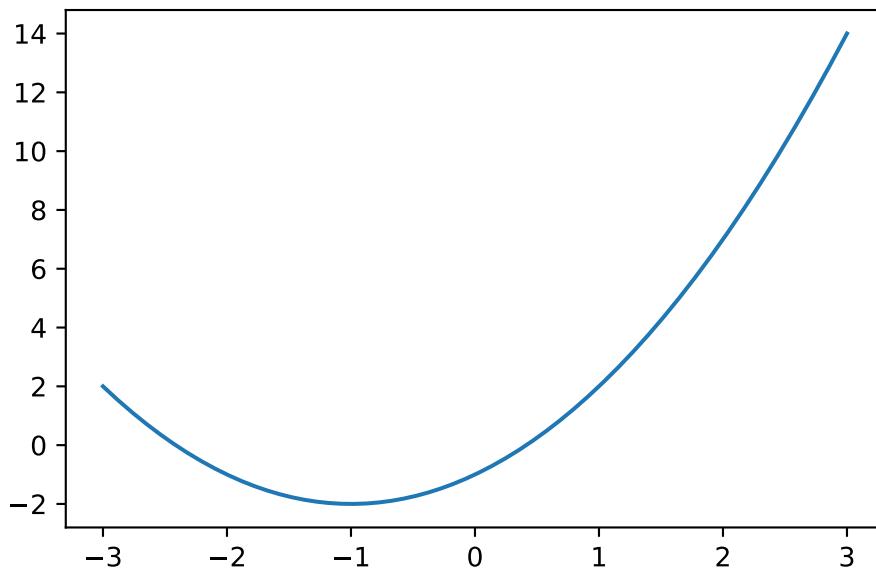
# Define the x range of x-values
x = np.linspace(-3,3,600)

# Compute the function values f(x[i]) of the elements x[i]
# and store them in the array y
y = f(x)

# Create the figure
plt.figure()

# Create the plot
plt.plot(x, y)

# Show the plot
plt.show()
```



You can add a legend for the line/points that you plot by using the `label` argument of `plt.plot()`. For example we can add the function description using `plt.plot(x,y,label='$f(x) = x^2 + 2x - 1$')`. This is in particular useful if you plot multiple functions in one figure, as the example below illustrates. There we plot the functions  $f$  and  $g$ , with  $g(x) = 3x$  a new function. To have the labels appear in the legend of

the figure, you need to add a legend to the figure with `plt.legend()`.

If you want to add labels to the horizontal and vertical axis, you can use the commands `plt.xlabel()` and `plt.ylabel()`.

```
import numpy as np
import matplotlib.pyplot as plt

# Define the function f
def f(x):
    return x**2 + 2*x - 1

# Define the function g
def g(x):
    return 3*x

# Define the x range of x-values
x = np.linspace(-3,3,600)

# Compute the function values f(x[i]) of the elements x[i]
# and store them in the array y
y = f(x)
z = g(x)

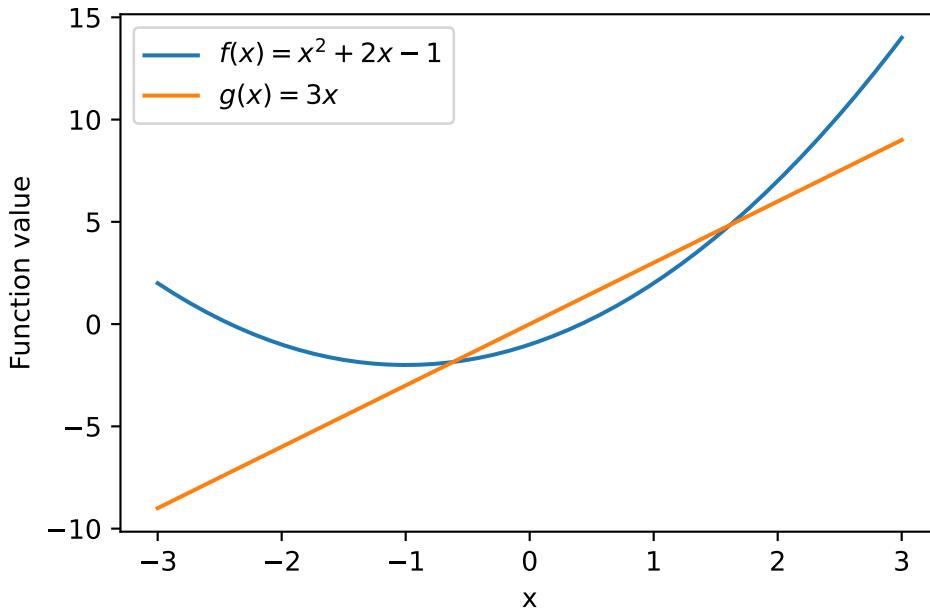
#Create the figure
plt.figure()

# Create the plot
plt.plot(x, y, label='$f(x) = x^2 + 2x - 1$')
plt.plot(x, z, label='$g(x) = 3x$')

# Create labels for axes
plt.xlabel('x')
plt.ylabel('Function value')

# Create the legend with the specified labels
plt.legend()

# Show the plot
plt.show()
```



You might observe that the range on the vertical axis changed now that we added a second function to the plot. When we only plotted the function  $f$ , the vertical axis ranged from  $-2$  to  $14$ , but now with the function  $g$  added to it, it ranges from  $-10$  to  $15$ .

You can fix the range  $[c, d]$  on the vertical axis using the command `plt.ylim(c,d)`, and to fix the range of the horizontal axis to  $[a, b]$ , you can use `plt.xlim(a,b)`. In the figure below, we fix the vertical range to  $[c, d] = [-10, 14]$  and the horizontal axis to  $[a, b] = [-3, 3]$ .

```

import numpy as np
import matplotlib.pyplot as plt

# Define the function f
def f(x):
    return x**2 + 2*x - 1

# Define the function g
def g(x):
    return 3*x

# Define the x range of x-values
x = np.linspace(-3,3,600)

# Compute the function values f(x[i]) of the elements x[i]
# and store them in the array y
y = f(x)
z = g(x)

#Create the figure object
plt.figure()

# Create the plot within the figure
plt.plot(x, y, label='$f(x) = x^2 + 2x - 1$')
plt.plot(x, z, label='$g(x) = 3x$')

```

```

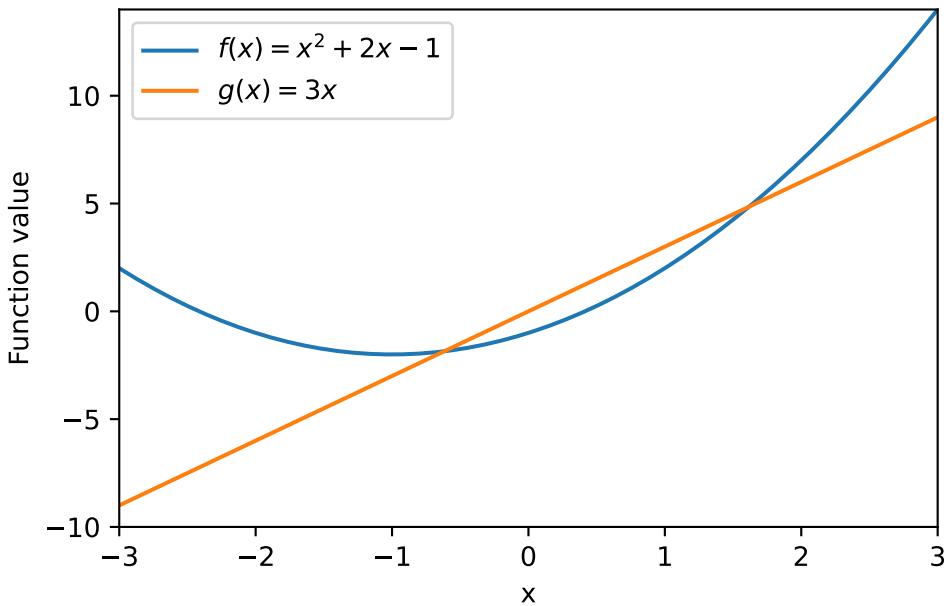
# Create labels for axes
plt.xlabel('x')
plt.ylabel('Function value')

# Create the legend with the specified labels
plt.legend()

# Fix the range of the axes
plt.xlim(-3,3)
plt.ylim(-10,14)

# Show the plot
plt.show()

```



Finally, you can also add a title to the plot using the command `plt.title()` as well as a grid in the background of the figure using `plt.grid()`. These are illustrated in the figure below.

```

import numpy as np
import matplotlib.pyplot as plt

# Define the function f
def f(x):
    return x**2 + 2*x - 1

# Define the function g
def g(x):
    return 3*x

# Define the x range of x-values
x = np.linspace(-3,3,600)

```

```

# Compute the function values f(x[i]) of the elements x[i]
# and store them in the array y
y = f(x)
z = g(x)

#Create the figure
plt.figure()

# Create the plot
plt.plot(x, y, label='f(x) = x^2 + 2x - 1')
plt.plot(x, z, label='g(x) = 3x')

# Create labels for axes
plt.xlabel('x')
plt.ylabel('Function value')

# Create the legend with the specified labels
plt.legend()

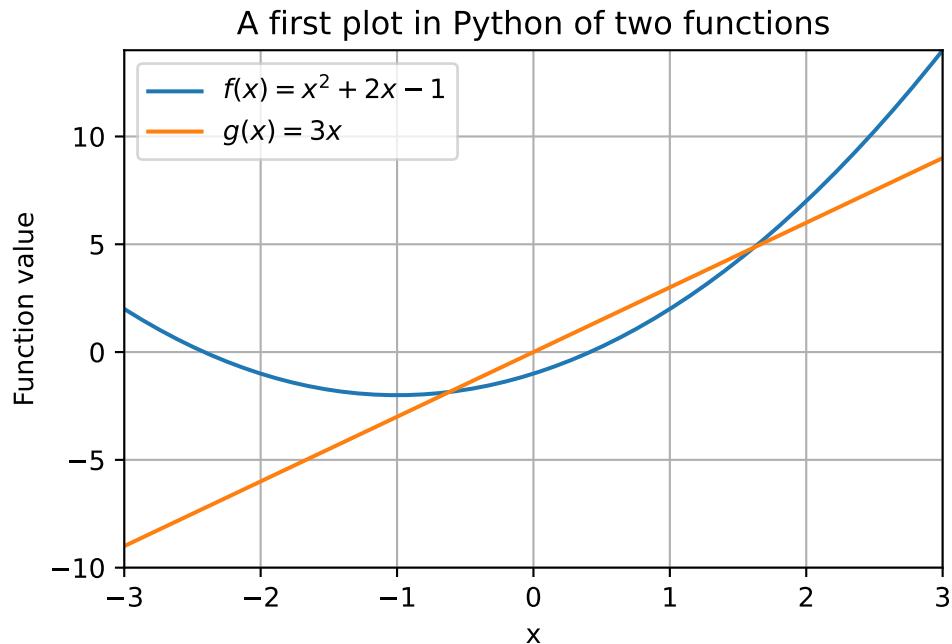
# Fix the range of the axes
plt.xlim(-3,3)
plt.ylim(-10,14)

# Add title to the plot
plt.title('A first plot in Python of two functions')

# Add grid to the background
plt.grid()

# Show the plot
plt.show()

```



This completes the description of the basics of plotting a figure. As a final remark, there are many more plotting options that we do not cover here, but which can be found in the documentation. For example, with the `plt.xticks()` and `plt.yticks()` commands you can specify the numbers you want to have displayed on the horizontal and vertical axis, respectively. Also, there are commands to specify line color, width, type (e.g., dashed) and much more!

## 7.2 Subplots

In this section we will describe how you can create multiple subplots in one figure. There are various ways to do this, e.g., in a predefined grid or on a plot-by-plot basis.

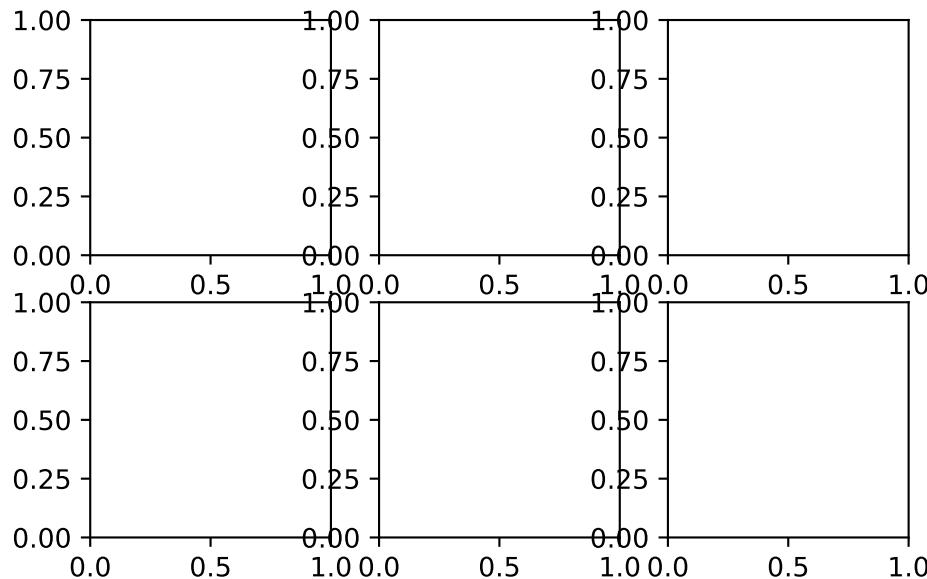
### 7.2.1 Fixed grid

We start with explaining the basics of the `subplots()` function. The syntax for creating a figure with a predefined grid on which plots can be placed is as follows.

```
m, n = 2, 3

# Create figure with six subplots in an n x m grid
fig, ax = plt.subplots(m,n)

plt.show()
```



This creates a figure object, with name `fig` in this case, and a  $2 \times 3$  array `ax` with so-called Axes objects that is place inside the figure. We are going to place the plots on the positions of the `ax` array.

```
# Shape of array
print(np.shape(ax))
```

(2, 3)

The fact that arrays can also store other objects besided numbers, is something we also already saw when using the `pulp` package for linear optimization in Chapter 5.

One might argue that the figure above is visually not very appealing, especially because the horizontally adjacent plots are very close to each other. You can get more control over the size of the figure (in which the plots are placed) by using the `figsize` keyword whose argument should be a tuple  $(w, h)$  indicating the width  $w$  and the height  $h$  of the figure.

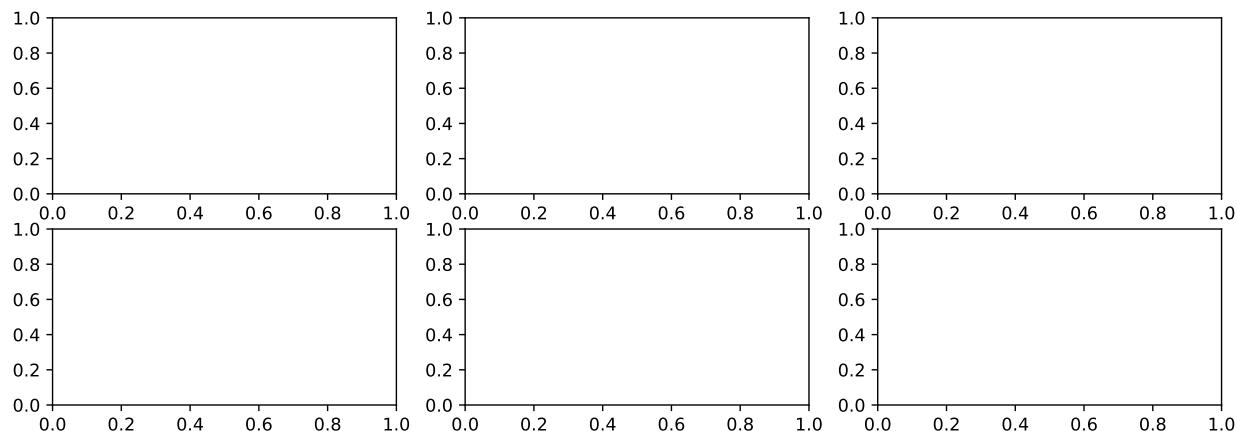
Note that the input arguments of `figsize` are perhaps a bit counterintuitive, as for the shape of a NumPy array (like the command above) the first number is always the “height” of the matrix, and the second number the “width”, but this is the other way around for the measurements of a figure.

```
# Parameters for figure with n x m subplots
m, n = 2, 3

# Parameters w (width) and h (height) for figure size
w, h = 12, 4

# Create figure with six subplots in a 2 x 3 fashion
fig, ax = plt.subplots(m,n, figsize=(w,h))

# Show the plot
plt.show()
```



It usually also helps to put in the command `plt.tight_layout()` that prevents plots within a figure from overlapping by adding some spacing between them.

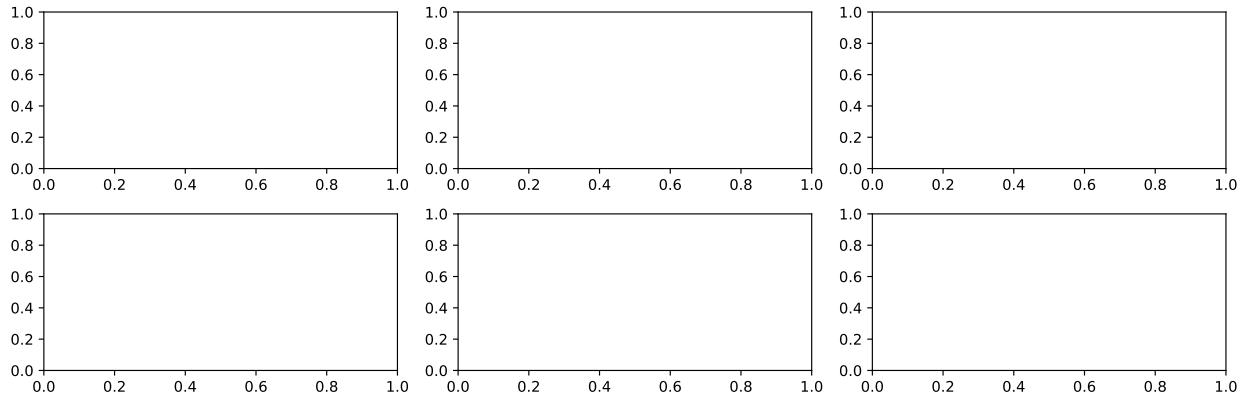
```
# Parameters for figure with n x m subplots
m, n = 2, 3

# Parameters w (width) and h (height) for figure size
w, h = 12, 4

# Create figure with six subplots in a 2 x 3 fashion
fig, ax = plt.subplots(m,n, figsize=(w,h))

# Tighten layout
plt.tight_layout()

# Show the plot
plt.show()
```



We continue by explaining how you can add information to the individual plots in the figure. For this, we will switch to a figure with a  $2 \times 2$  array for in total four subplots.

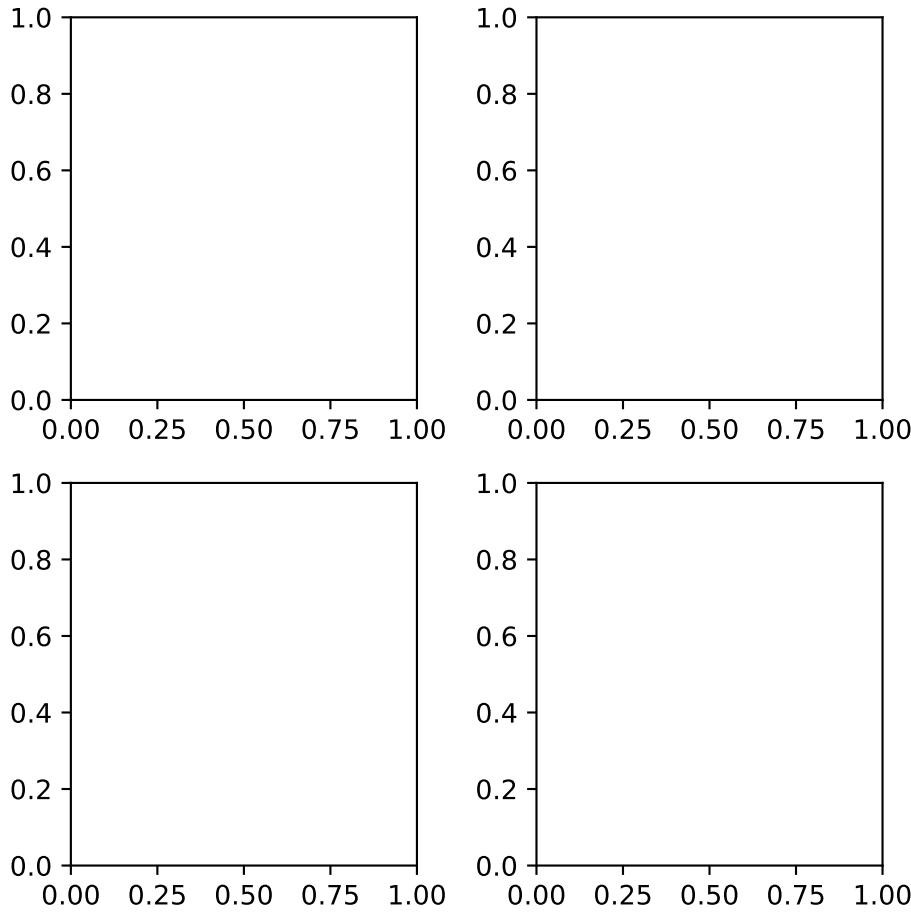
```
# Parameters for figure with n x m subplots
n = 2

# Parameters w (width) and h (height) for figure size
w = 5

# Create figure with six subplots in a 2 x 2 fashion
fig, ax = plt.subplots(n,n, figsize=(w,w))

# Tighten layout
plt.tight_layout()

# Show plot
plt.show()
```



You can access the individual plot at position  $(i,j)$  of the array `ax` using `ax[i,j]`, and set properties of it using `ax[i,j].plot_option` where `plot_option` is a plotting command.

Sometimes you need to use a slightly different command than when you plot a single plot in a figure. For many commands, you need to add `set_` to it. For example, instead of `plt.xlim(a,b)` you need to use `ax[i,j].set_xlim(a,b)`.

To set the title of the whole figure, when named `fig`, you can use `fig.suptitle()` instead of `plt.title()`.

```
# Define function to plot
def f(x):
    return x**2

a = -3
b = 3

# Define x-range
x = np.linspace(a,b,600)

# Create figure with six subplots in a 2 x 2 fashion
fig, ax = plt.subplots(2,2, figsize=(w,w))

# Title of whole figure
fig.suptitle("Four plots in one figure")
```

```

# Tighten layout
plt.tight_layout()

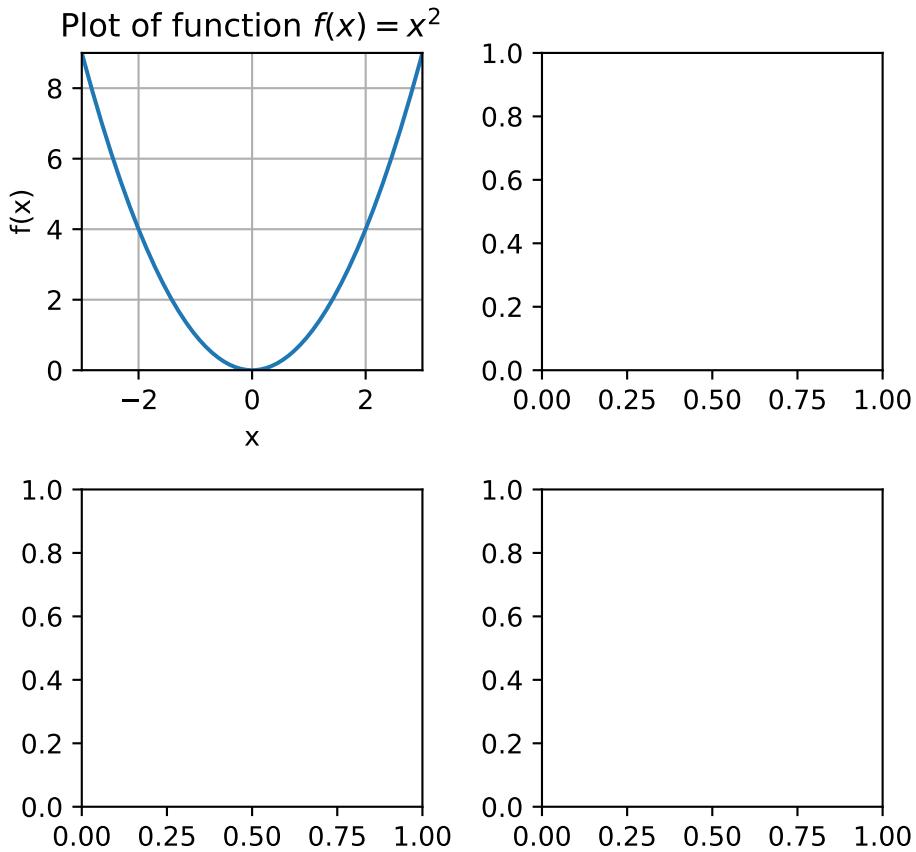
# Create plot on top-left position
ax[0,0].plot(x,f(x))
ax[0,0].set_xlim(a,b)
ax[0,0].set_ylim(0,9)
ax[0,0].set_xlabel("x")
ax[0,0].set_ylabel("f(x)")
ax[0,0].set_title("Plot of function $f(x) = x^2$")
ax[0,0].grid()

# Tighten layout
plt.tight_layout()

# Show plot
plt.show()

```

Four plots in one figure



### 7.2.2 Iterative adding

Instead of predefining a grid in which the subplots will appear, it is also possible to add subplots in a more dynamic, iterative fashion to a grid using `add_subplot()`. The function typically gives you a bit more

flexibility.

For example, we can create four plots of which one spans the whole first “row” and that has three smaller plots underneath it. The numbering of the subplots follows the largest axis changing fastest principle, so the subplots are placed first along the first row, then the second row, etc.

If we would have a  $2 \times 3$  grid, then the numbering of the subplots would be as follows:

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}$$

Note that the counting start at 1 instead of 0, as is more common in Python.

After having created a figure, we can add subplots to an  $m \times n$  grid using `fig.add_subplot(m,n,(p,q))`. The tuple `(p,q)` indicates that we want to place the subplot on positions  $p$  through  $q$  in the figure. If there is only one position  $p$  at which you want to place the subplot, you can use `(p)`, or simply `p`, as the third argument of `add_subplot()`.

To avoid unnecessary repetition, it can often help to plot subplots using a for-loop. We will illustrate this for the figure below, in which we plot the function  $f(x) = \sin(x)$  on the first row of our grid, and its first three derivatives in smaller subplots under it.

You can make the plot look nicer by adding labels, legends, different line colors, a grid, etc.

```
# Define x-range
x = np.linspace(-5,5,600)

# Function values
y = np.sin(x)

# Values of 1st, 2nd and 3rd derivative
deriv = np.vstack((np.cos(x),-np.sin(x),-np.cos(x)))

# Store function names in list
function_names = ["Function f", "First derivative",
                  "Second derivative",
                  "Third derivative"]

# Create figure
fig = plt.figure(figsize=(7,5))

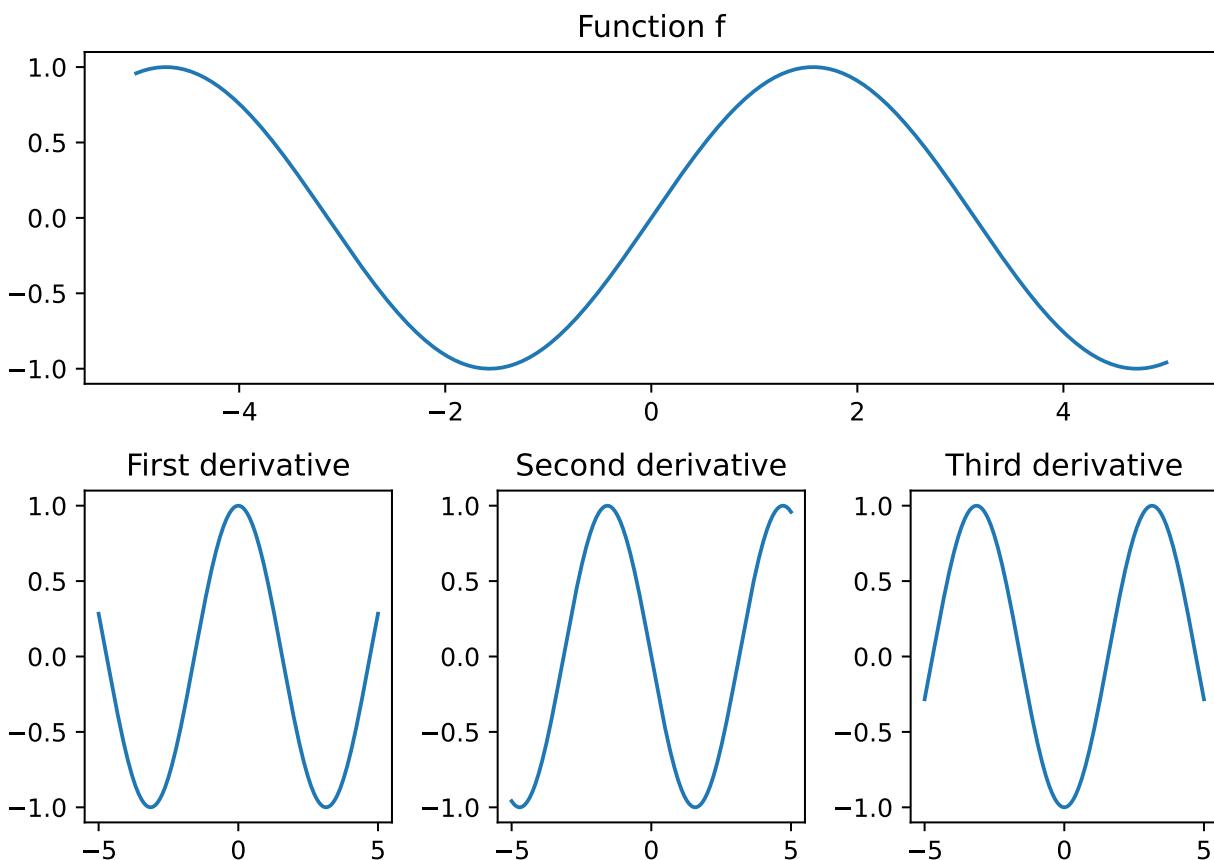
# Will create an m x n grid with subplots
m, n = 2, 3

# Add first subplot
ax_f = fig.add_subplot(m,n,(1,n))
ax_f.plot(x,y)
ax_f.set_title(function_names[0])

# Add derivatives
for i in range(n):
    ax_deriv = fig.add_subplot(m,n,n+1+i)
    ax_deriv.plot(x,deriv[i])
    ax_deriv.set_title(function_names[1+i])
```

```
# Tighten layout
plt.tight_layout()

# Show plot
plt.show()
```



## 7.3 Bivariate functions

In Python it is also possible to plot a function with two variables, a so-called bivariate function. For example, consider  $z = f(x, y) = x^2 + y^2$  that we would like to visualize on the  $(x, y)$ -domain  $[0, 4] \times [3, 8]$ .

Before going into the plotting commands we discuss in more detail how to efficiently compute the function values on the specified domain.

Just as with two-dimensional plotting, the idea is that we want compute the function values on a fine-grained discretization of the desired domain. In two dimensions, we can create such a discretization easily using the `mgrid` function from NumPy.

Suppose we discretize  $[0, 4] \times [3, 8]$  by considering all the integer combinations. We can do this with `mgrid` by specifying for both dimensions the range that we are interested in using index slicing.

```
# Note that the end index is not included
X, Y = np.mgrid[0:5, 3:9]
```

If you input two ranges then the output are two matrices. You could also use this function for higher-dimensional problems.

```

print("X = \n", X)

X =
[[0 0 0 0 0 0]
 [1 1 1 1 1 1]
 [2 2 2 2 2 2]
 [3 3 3 3 3 3]
 [4 4 4 4 4 4]]


print("Y = \n", Y)

Y =
[[3 4 5 6 7 8]
 [3 4 5 6 7 8]
 [3 4 5 6 7 8]
 [3 4 5 6 7 8]
 [3 4 5 6 7 8]]
```

The matrices  $X$  and  $Y$  together form a representation of all the integer points in the domain  $[0, 4] \times [3, 8]$ , namely

$$\begin{array}{ccccccc} (0,3) & (0,4) & (0,5) & (0,6) & (0,7) & (0,8) \\ (1,3) & (1,4) & (1,5) & (1,6) & (1,7) & (1,8) \\ (2,3) & (2,4) & (2,5) & (2,6) & (2,7) & (2,8) \\ (3,3) & (3,4) & (3,5) & (3,6) & (3,7) & (3,8) \\ (4,3) & (4,4) & (4,5) & (4,6) & (4,7) & (4,8) \end{array}$$

To be precise, the matrix  $X$  contains the first element of every coordinate  $(i, j) \in [a, b] \times [c, d]$ , that is, the value  $i$ , and  $Y$  contains the second element, that is, the value  $j$ .

The same can be achieved with the function `meshgrid()` that takes as input the discretized ranges of  $x$  and  $y$ . Here the matrix  $X$  and  $Y$  are tranposed compared to the output of `mgrid`.

```

x = np.arange(0,5)
y = np.arange(3,9)

X, Y = np.meshgrid(x,y)

print("X = \n", X)
print("Y = \n", Y)

X =
[[0 1 2 3 4]
 [0 1 2 3 4]
 [0 1 2 3 4]
 [0 1 2 3 4]
 [0 1 2 3 4]]
Y =
[[3 3 3 3 3]
 [4 4 4 4 4]]
```

```
[5 5 5 5 5]
[6 6 6 6 6]
[7 7 7 7 7]
[8 8 8 8 8]
```

If we now want to compute the function values in the points  $(i, j)$ , we can simply use  $Z = X^{**2} + Y^{**2}$ . Note that  $**$  is a vectorized operation that is pointwise applied when executed on a two-dimensional array. So  $X^{**2}$  gives the squares of all the  $x$ -coordinate of all the grid points, and  $Y^{**2}$  the squares of all the  $y$ -coordinates. In other words, for a grid point  $(i, j)$  we get  $Z[i, j] = X[i, j] * * 2 + Y[i, j] * * 2$ .

```
# Compute function values of f(x,y) = x^2 + y^2
Z = X**2 + Y**2 # For every (i,j), computes i**2 + j**2

print("Z = \n", Z)
```

```
Z =
[[ 9 10 13 18 25]
 [16 17 20 25 32]
 [25 26 29 34 41]
 [36 37 40 45 52]
 [49 50 53 58 65]
 [64 65 68 73 80]]
```

We can also do this by defining the function  $f$ .

```
# Define function
def f(x,y):
    return x**2 + y**2

# Define grid
X, Y = np.mgrid[0:5, 3:9]

# f(X,Y) gives all function values of the grid points.
print("f(x,y) = \n", f(X,Y))
```

```
f(x,y) =
[[ 9 16 25 36 49 64]
 [10 17 26 37 50 65]
 [13 20 29 40 53 68]
 [18 25 34 45 58 73]
 [25 32 41 52 65 80]]
```

We can create a more fine-grained plot by including more points in the ranges of the  $x$ - and  $y$ -values. Again, this can be done using slicing notation.

```
# Define function
def f(x,y):
    return x**2 + y**2

# Define grid with step size of 0.2 in x,y-coordinates
step = 0.2
X, Y = np.mgrid[0:2.1:step, 3:4.1:step]

# Print x-values of grid points
```

```
print("X = \n", X)

# Print y-values of grid points
print("Y = \n", Y)

# f(X,Y) gives all function values of the grid points.
print("f(X,Y) = \n", f(X,Y))
```

```

X =
[[0.  0.  0.  0.  0.  0.  ]
 [0.2 0.2 0.2 0.2 0.2 0.2]
 [0.4 0.4 0.4 0.4 0.4 0.4]
 [0.6 0.6 0.6 0.6 0.6 0.6]
 [0.8 0.8 0.8 0.8 0.8 0.8]
 [1.  1.  1.  1.  1.  1.  ]
 [1.2 1.2 1.2 1.2 1.2 1.2]
 [1.4 1.4 1.4 1.4 1.4 1.4]
 [1.6 1.6 1.6 1.6 1.6 1.6]
 [1.8 1.8 1.8 1.8 1.8 1.8]
 [2.  2.  2.  2.  2.  2.  ]]

Y =
[[3.  3.2 3.4 3.6 3.8 4.  ]
 [3.  3.2 3.4 3.6 3.8 4.  ]
 [3.  3.2 3.4 3.6 3.8 4.  ]
 [3.  3.2 3.4 3.6 3.8 4.  ]
 [3.  3.2 3.4 3.6 3.8 4.  ]
 [3.  3.2 3.4 3.6 3.8 4.  ]
 [3.  3.2 3.4 3.6 3.8 4.  ]
 [3.  3.2 3.4 3.6 3.8 4.  ]
 [3.  3.2 3.4 3.6 3.8 4.  ]
 [3.  3.2 3.4 3.6 3.8 4.  ]
 [3.  3.2 3.4 3.6 3.8 4.  ]
 [3.  3.2 3.4 3.6 3.8 4.  ]
 [3.  3.2 3.4 3.6 3.8 4.  ]
 [3.  3.2 3.4 3.6 3.8 4.  ]
 [3.  3.2 3.4 3.6 3.8 4.  ]]
f(X,Y) =
[[ 9.    10.24 11.56 12.96 14.44 16.   ]
 [ 9.04 10.28 11.6   13.    14.48 16.04]
 [ 9.16 10.4   11.72 13.12 14.6   16.16]
 [ 9.36 10.6   11.92 13.32 14.8   16.36]
 [ 9.64 10.88 12.2   13.6   15.08 16.64]
 [10.    11.24 12.56 13.96 15.44 17.   ]
 [10.44 11.68 13.    14.4   15.88 17.44]
 [10.96 12.2   13.52 14.92 16.4   17.96]
 [11.56 12.8   14.12 15.52 17.    18.56]
 [12.24 13.48 14.8   16.2   17.68 19.24]
 [13.    14.24 15.56 16.96 18.44 20.   ]]

```

### 7.3.1 Contour plot

One way to visualize a function  $f : \mathbb{R}^2 \rightarrow \mathbb{R}$  is by using a contour plot with `plt.contour()`. What such a plot does is that it creates a two-dimensional plot where for given values  $z_0 \in \mathbb{R}$  it plots all points  $(x, y) \in \mathbb{R}^2$  for which  $f(x, y) = z_0$  with the same color.

The function `plt.contour()` takes as input the arrays  $X$ ,  $Y$  and  $Z$ . The input order is important here. Python plots the point  $(X[i, i], Y[i, j])$  and assigns a common color to all such points with the same function value (i.e., the same  $Z[i, j]$ -value).

The `levels` keyword argument determines how many different colors, i.e.,  $z_0$ -values, are plotted. For this Python uses a so-called colormap that has a shifting scale indicating a shift in the value of  $z_0$ . You can plot a color legend with `plt.colorbar()`.

```
# Define function
def f(x,y):
    return x**2 + y**2

# Grid parameters
b = 4
step = 0.001

# Define grid [0,b]^2 with given step size
X, Y = np.mgrid[0:b:step, 0:b:step]

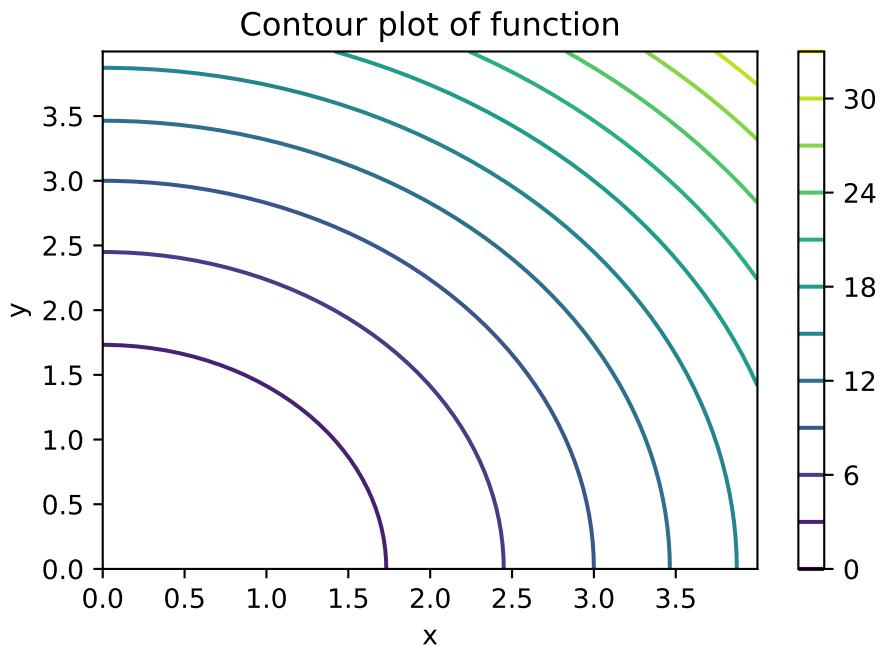
# Create figure
plt.figure()

# Create contour plot
plt.contour(X, Y, f(X,Y), levels=10)

# Add labels and title
plt.xlabel("x")
plt.ylabel("y")
plt.title("Contour plot of function")

# Show the plot
plt.colorbar() # Add a color bar for reference

# Show plot
plt.show()
```



The same plot as above with 50 color levels is given below.

```
# Define function
def f(x,y):
    return x**2 + y**2

# Grid parameters
b = 4
step = 0.001

# Define grid [0,b]^2 with given step size
X, Y = np.mgrid[0:b:step, 0:b:step]

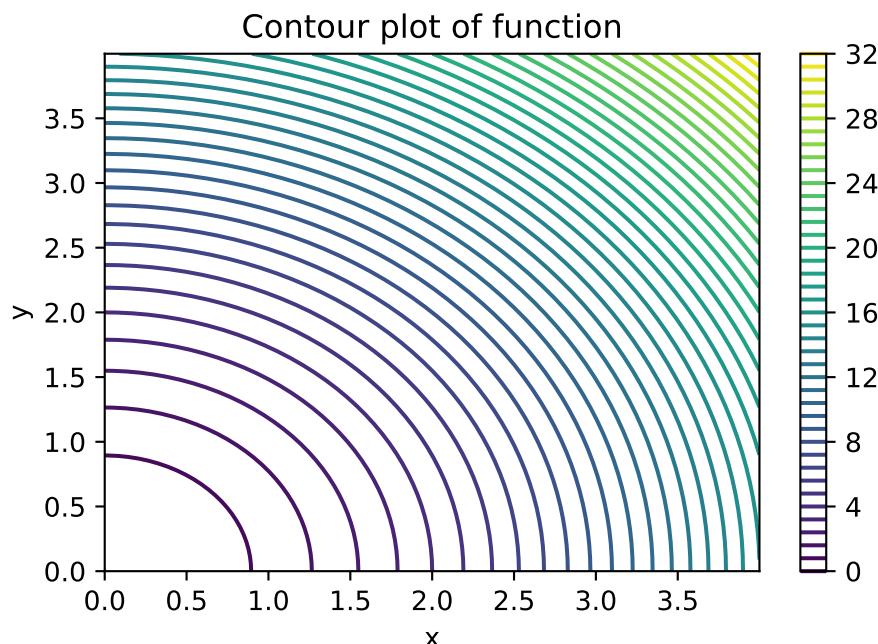
# Create figure
plt.figure()

# Create contour plot
plt.contour(X, Y, f(X,Y), levels=50)

# Add labels and title
plt.xlabel("x")
plt.ylabel("y")
plt.title("Contour plot of function")

# Show the plot
plt.colorbar() # Add a color bar for reference

# Show plot
plt.show()
```



You can also choose to fill up the white space between the different contour lines. Then you should use `plt.contourf()` instead of `plt.contour()`. The same plot with 50 color levels and `plt.contourf()` is

given below.

```
# Define function
def f(x,y):
    return x**2 + y**2

# Grid parameters
b = 4
step = 0.001

# Define grid [0,b]^2 with given step size
X, Y = np.mgrid[0:b:step, 0:b:step]

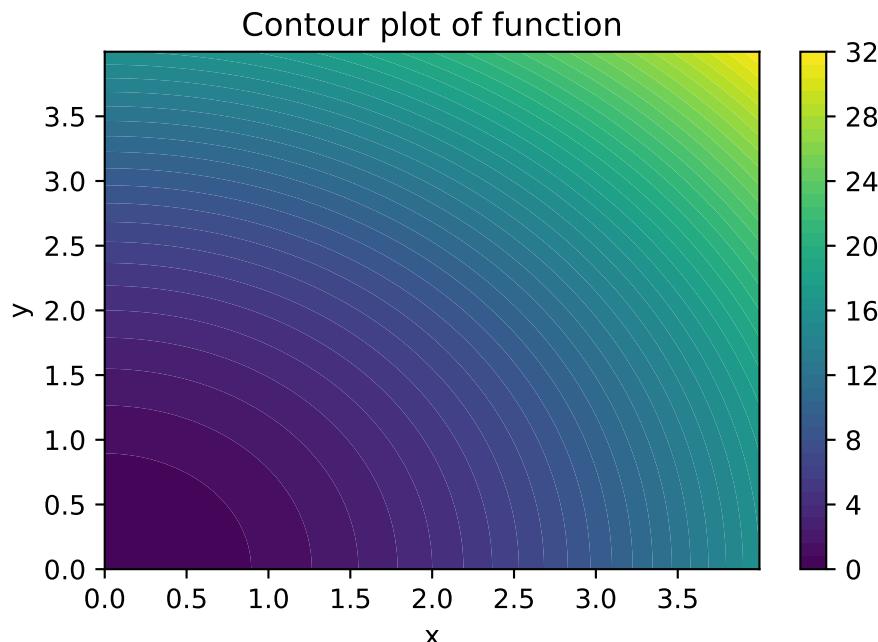
# Create figure
plt.figure()

# Create contour plot with 50 levels
plt.contourf(X, Y, f(X,Y), levels=50)

# Add labels and title
plt.xlabel("x")
plt.ylabel("y")
plt.title("Contour plot of function")

# Show the plot
plt.colorbar() # Add a color bar for reference

# Show plot
plt.show()
```



Finally, you can change the color chosen by Python using the `cmap` keyword argument. There are various color maps available; see the documentation.

Below we have plotted the figure above with the inferno colormap.

```
# Define function
def f(x,y):
    return x**2 + y**2

# Grid parameters
b = 4
step = 0.001

# Define grid [0,b]^2 with given step size
X, Y = np.mgrid[0:b:step, 0:b:step]

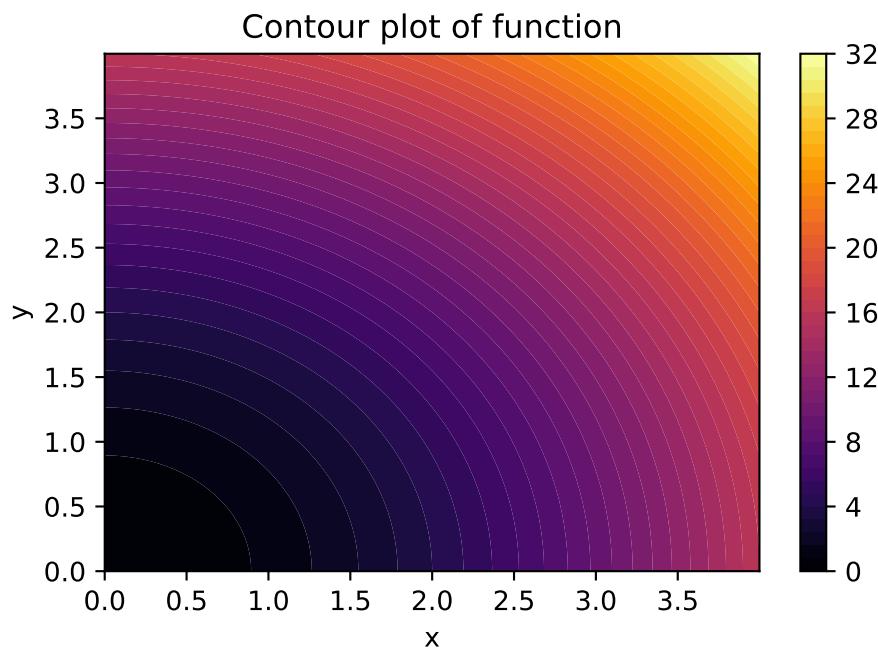
# Create figure
plt.figure()

# Create contour plot with 50 levels
plt.contourf(X, Y, f(X,Y), levels=50, cmap="inferno")

# Add labels and title
plt.xlabel("x")
plt.ylabel("y")
plt.title("Contour plot of function")

# Show the plot
plt.colorbar() # Add a color bar for reference

# Show plot
plt.show()
```



### 7.3.2 3D plot

Another way of visualizing a bivariate function is using a 3D plot, in which we have an  $x$ -,  $y$ - and  $z$ -axis. This you can do, e.g., with the `plot_surface()` function. To use this function we have to explicitly create an Axes object (plot), which we call `ax`, with three axes using `ax = plt.axes(projection='3d')`.

```
# Define function
def f(x,y):
    return x**2 + y**2

# Grid parameters
b = 4
step = 0.001

# Define grid [0,b]^2 with given step size
X, Y = np.mgrid[0:b:step, 0:b:step]

# Create figure
fig = plt.figure(figsize=(7,5))

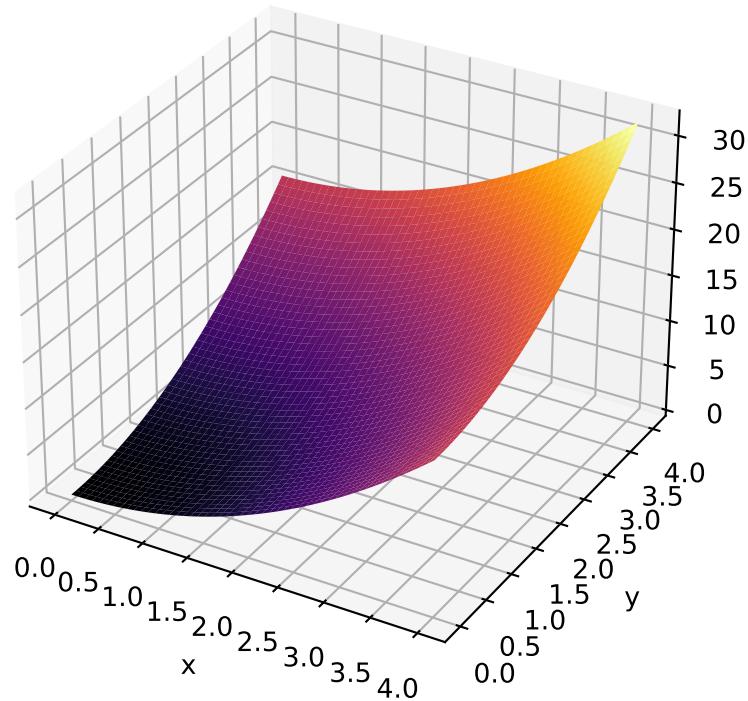
# Create Axes object with three axes
ax = plt.axes(projection='3d')

# Create surface plot
ax.plot_surface(X, Y, f(X,Y), cmap="inferno")

# Add labels and title
ax.set_xlabel("x")
ax.set_ylabel("y")
ax.set_title("Surface plot of function")

# Show plot
plt.show()
```

## Surface plot of function



We close this chapter by remarking that we have only shown a small fraction of the plotting functionality that Python has to offer. There are many more options to create nice looking plots.

# Chapter 8

## Probability theory

### 8.1 Randomness

There are various ways to generate random variables and sets in Python. Throughout this chapter we will rely on basic concepts from probability theory such as probability density function (pdf) and cumulative density function (cdf).

Furthermore, we will be working with the normal, uniform and other distributions. Familiarity with those is assumed. Whenever you run into a mathematical or probabilistic aspect you do not understand, please look it up and otherwise ask the teacher about it.

We will use functionality from the `random` subpackage of NumPy. This subpackage is not to be confused with the `random` package of Python, which has a lot of similar functionality.

```
import numpy as np
```

#### 8.1.1 Samples

The `random` subpackage has functions that can generate so-called pseudo-random numbers. Informally speaking, these numbers “behave” as random numbers when performing numerical experiments with them, but they are not truly random (which can be an issue, e.g., if you would use such numbers of cryptographic purposes).

We next discuss some functions to generate random numbers from well-known distributions.

`np.random.rand(m,n)`: Generate an  $m \times n$  two-dimensional array with numbers uniformly drawn from the interval  $[0, 1]$  (i.e., every number is equally likely).

```
m,n = 2, 4
```

```
M = np.random.rand(m,n)
print(M)
```

```
[[0.4499988  0.07503895  0.31377349  0.76124686]
 [0.72888496  0.93489974  0.94289126  0.77049604]]
```

When  $m$  and  $n$  are not inputted, a single random number is returned.

```
x = np.random.rand()
print(x)
```

```
0.8173915547569017
```

`np.random.randn(m,n)`: Generates an  $m \times n$  two-dimensional array with numbers drawn from the normal distribution with mean  $\mu = 0$  and standard deviation  $\sigma = 1$ .

```
m,n = 3, 5

M = np.random.randn(m,n)
print(M)
```

```
[[ 0.68246742  1.06378492  0.50720193  0.47033812 -1.09764858]
 [-0.86551221 -0.48160594  0.27322299  0.43560834  0.95792075]
 [ 1.81748017  0.18965122 -0.41809564 -0.1867069   1.70123015]]
```

We conclude with sampling numbers from the discrete uniform distribution over a set  $\{a, a + 1, \dots, b - 1\}$ . Here every number  $i$  in this discrete interval is generated with equal probability  $1/(b - a)$ .

`np.random.randint(a,b,(m,n))`: Generates an  $m \times n$  two-dimensional array with numbers drawn from the discrete uniform distribution on  $\{a, a + 1, \dots, b - 1\}$ .

```
a, b = 4, 10
m,n = 3, 15

M = np.random.randint(a,b,(m,n))
print(M)
```

```
[[7 9 5 7 7 4 5 8 4 5 5 6 7 4 4]
 [6 6 8 4 9 4 6 5 5 5 5 6 8 7 7]
 [7 9 9 5 8 9 9 5 9 4 8 5 9 5 8]]
```

For almost every well-known probability distribution we can get samples from its distribution. See the documentation for a list of all the distributions.

Finally, we remark that it is also possible to generate samples from different distributions from the same family. As an example, consider a normal distribution with mean  $\mu$  and standard deviations  $\sigma$ . We can generate samples from this distribution with `np.random.normal()`.

As input it takes two keyword arguments: `loc` for the mean  $\mu$  and `scale` for the standard deviation  $\sigma$ . You can figure this out by inspecting the documentation.

Most distributions have a `loc` and or `scale` keyword input argument, that takes a default value if none is inputted; `loc=0` and `scale=1` are the defaults for `np.random.normal`.

# numpy.random.normal

`random.normal(loc=0.0, scale=1.0, size=None)`

Draw random samples from a normal (Gaussian) distribution.

The probability density function of the normal distribution, first derived by De Moivre and 200 years later by both Gauss and Laplace independently [2], is often called the bell curve because of its characteristic shape (see the example below).

The normal distributions occurs often in nature. For example, it describes the commonly occurring distribution of samples influenced by a large number of tiny, random disturbances, each with its own unique distribution [2].

## Note

New code should use the `normal` method of a `Generator` instance instead; please see the [Quick start](#).

### Parameters:

`loc : float or array_like of floats`

Mean ("centre") of the distribution.

`scale : float or array_like of floats`

Standard deviation (spread or "width") of the distribution. Must be non-negative.

Figure 8.1: Documentation for generating normally distributed samples

```
mu = 1
sigma = 2

samples = np.random.normal(loc=mu, scale=sigma)

print(samples)
```

-0.259229489194871

This function also allows vectorized inputs: If we input an array of means and standard deviations, then a sample for every combination is generated.

```
mu = np.array([0,1,2,2])
sigma = np.array([1,2,4,2])

samples = np.random.normal(loc=mu, scale=sigma)

print(samples)
```

```
[1.29281253 0.49668017 3.93026623 1.16257678]
```

Finally, if you want to have  $m$  samples from all combinations of location and scale parameters, you can specify this in the `size` keyword argument by setting it to `(m,n)` where  $n$  is the common length of the location and scale array. For every scale-location combination, the  $m$  samples of this combination can be found in a column of the output.

```
mu = np.array([0,1,2,2])
sigma = np.array([1,2,4,2])

m = 3
n = np.size(mu)

samples = np.random.normal(loc=mu, scale=sigma, size=(m,n))

print(samples)
```

```
[[ 1.86300853  1.07396318  9.92470774  1.05585534]
 [-0.89835638 -0.93775266 -0.56682232  3.15777827]
 [ 1.99631585  0.25785768  5.097944   0.67468006]]
```

## 8.1.2 Subsets

Next to the generation of random numbers, it is also possible to generate random subsets of elements of a given array using the `choice()` function. It takes as input an array from which we want to obtain a subset and we can set the size of the subset that we want to have using the `size` keyword argument.

```
k = 15
x = np.arange(0,11,1)

subset = np.random.choice(x,size=k)

print(subset)
```

```
[3 7 4 7 7 5 3 8 2 0 7 3 5 9 5]
```

As can be seen from the output above, some numbers appear twice in the subset, meaning that `choice()` samples a subset with replacement. If you want to sample without replacement, you can set the keyword `replace` to `False`.

```
k = 8
x = np.arange(0,11,1)

subset = np.random.choice(x,size=k,replace=False)

print(subset)
```

```
[ 5 10  4  7  1  3  6  8]
```

Finally, you can also specify the probability with which every element should be sampled using the keyword argument `p`.

```
k = 8
```

```

# Set {0,1,2,...,9}
x = np.arange(0,10,1)

# Probabilities for elements in set
prob = np.array([1/3,1/3,0,0,0,0,0,0,0,1/3])

# Generating random subset
subset = np.random.choice(x,size=k,p=prob)

# Only 0, 1, 9 have positive probabilities
print(subset)

```

[0 1 1 1 9 0 9 1]

There is also the `permutation()` function that returns the elements in an array in a random order. That is, it creates a so-called random permutation of the elements in the array.

```

x_perm = np.random.permutation(x)

print(x_perm)

```

[8 7 1 3 2 6 9 5 0 4]

If you would apply this function on a two-dimensional array, it returns the same array in which the rows are randomly permuted (i.e., the inner lists are randomly permuted).

```

X = np.arange(0,18,1).reshape(3,6)

x_perm = np.random.permutation(X)

print(x_perm)

```

[[ 0 1 2 3 4 5]  
 [12 13 14 15 16 17]  
 [ 6 7 8 9 10 11]]

### 8.1.3 Seed

When writing code that involves random numbers or objects, it can sometimes be useful to “fix” the randomness in the script, e.g., when debugging. This can be done by setting a so-called random seed using the `seed()` function.

For sake of comparison, let us first generate two random numbers from [0, 1].

```

a = np.random.rand()
b = np.random.rand()

print(a,b)

```

0.2701427666898114 0.11471228107750131

If you rerun the code above it will give different outputs every time. Try this yourself by copying the code into Spyder.

We next do the same, but with a fixed seed  $s$  using `seed(s)`. Different choices of  $s$  fix the randomness in a different way. If you copy the code below into Spyder and rerun it a couple of times, the output will always be the same.

```
#Set seed to be s = 3
np.random.seed(3)

a = np.random.rand()
b = np.random.rand()

print(a,b)
```

```
0.5507979025745755 0.7081478226181048
```

## 8.2 Probability distributions

The `stats` module of SciPy has many built-in probability distributions. Each distribution can be seen as an object on which various methods can be performed (such accessing its probability density function or summary statistics like the mean and median). You should think of an ‘object’ in the context of object oriented programming, see, e.g., here to recall the basics of this paradigm.

```
import scipy
```

In this section we will focus on continuous probability distributions. SciPy also has many built-in discrete probability distributions.

A list of all continuous distributions that are present in the `stats` module can be found here; they are so-called `stats.rv_continuous` objects. We can instantiate a distributional object by using `scipy.stats.dist_name` where `dist_name` is the name of a built-in (continuous) probability distribution in the mentioned list.

Many distributions have input parameters `scale` and `loc` that model the scale and location of the distribution, respectively. Depending on the distribution that is considered, these parameters have different meanings.

As an example, the normal distribution has probability density function

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

which is parameterized by  $\mu$  and  $\sigma$ .

In Python  $\mu$  is the `loc` parameter, and  $\sigma$  the `scale` parameter. To figure out the function of the `scale` and `loc` parameter, you can check the documentation (which can be found here for the Normal distribution).

# scipy.stats.norm

**norm = <scipy.stats.\_continuous\_distns.norm\_gen object>** [\[source\]](#)

A normal continuous random variable.

The location (`loc`) keyword specifies the mean. The scale (`scale`) keyword specifies the standard deviation.

As an instance of the [rv\\_continuous](#) class, `norm` object inherits from it a collection of generic methods (see below for the full list), and completes them with details specific for this particular distribution.

Figure 8.2: Documentation of the normal distribution

All distributions have default values for these parameters, which are typically `loc=0` and `scale = 1`.

```
# Create normal distribution object with mu=0, sigma=1
dist_norm = scipy.stats.norm(loc=0, scale=1)
```

Once a distribution object has been instantiated, we can use methods (i.e., functions) to obtain various properties of the distribution, such as its probability density function (pdf), cumulative density function (cdf) and summary statistics such as the mean, variance and median (or, more general, quantiles).

We give a list of some common methods for a distribution object named `dist_name`. We start with common functions associated with a probability distribution.

- `dist_name.pdf(x)`: Value  $f(x)$  where  $f$  is the pdf of the distribution.
- `dist_name.cdf(x)`: Value  $F(x)$  where  $F$  is the cdf of the distribution.
- `dist_name.sf(x)`: Value  $S(x)$  where  $S$  is the survival function ( $1 - F$ ) of the distribution.
- `dist_name.ppf(alpha)`: Returns  $x$  so that  $F^{-1}(x) = \alpha$  where  $\alpha \in (0, 1)$ .

```
x = 1
print(dist_norm.pdf(x))
```

0.24197072451914337

```
alpha = 1/2
print(dist_norm.ppf(alpha))
```

0.0

All the above functions are vectorized, in the sense that they can also handle higher-dimensional arrays as input. This is convenient, e.g., for visualizing these functions as the example below illustrates.

```

import matplotlib.pyplot as plt

# Define the x range of x-values
x = np.linspace(-10,10,600)

# Function values of pdf
y = dist_norm.pdf(x) # Computes pdf values of all elements in x

#Create the figure
plt.figure()

# Create the plot
plt.plot(x, y)

# Create labels for axes
plt.xlabel('x')
plt.ylabel('Function value')

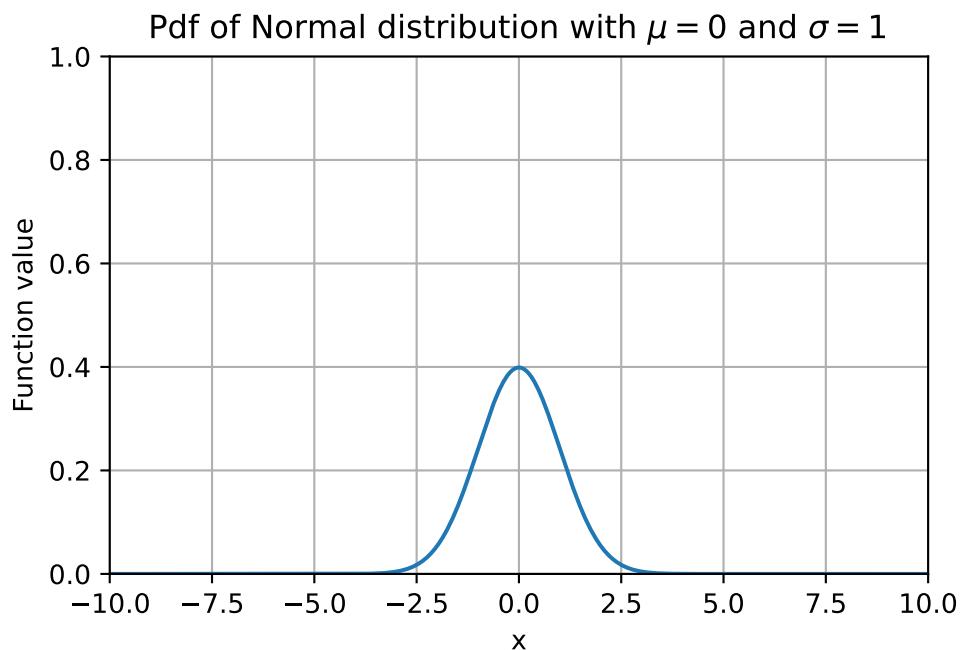
# Fix the range of the axes
plt.xlim(-10,10)
plt.ylim(0,1)

# Add title to the plot
plt.title('Pdf of Normal distribution with  $\mu=0$  and  $\sigma=1$ ')

# Add grid to the background
plt.grid()

# Show the plot
plt.show()

```



We can also access various summary statistics:

- `dist_name.mean()`: Returns mean of the distribution
- `dist_name.var()`: Returns variance of the distribution
- `dist_name.median()`: Returns median of the distribution

```
dist_norm = scipy.stats.norm(loc=0,scale=2)

mean = dist_norm.mean()
variance = dist_norm.var()
median = dist_norm.median()

print("Mean of the distribution is", mean)
print("Variance of the distribution is", variance)
print("Median of the distribution is", median)
```

```
Mean of the distribution is 0.0
Variance of the distribution is 4.0
Median of the distribution is 0.0
```

Note that in the example above the standard deviation equals  $\sigma = 2$ ; the variance is then  $\sigma^2 = 4$ .

Finally it is also possible to access the support upper and lower bound of a distribution.

- `dist_name.support()` : Returns values  $a, b$  of (smallest) interval  $[a, b]$  for which all probability mass is contained in it.

Let us first consider the uniform distribution.

[Home](#) > [SciPy API](#) > [Statistical functions \(`scipy.stats`\)](#) > [scipy.stats.uniform](#)

## scipy.stats.uniform

`uniform` = `<scipy.stats._continuous_distns.uniform_gen object>`

A uniform continuous random variable.

[\[source\]](#)

In the standard form, the distribution is uniform on `[0, 1]`. Using the parameters `loc` and `scale`, one obtains the uniform distribution on `[loc, loc + scale]`.

As an instance of the `rv_continuous` class, `uniform` object inherits from it a collection of generic methods (see below for the full list), and completes them with details specific for this particular distribution.

Figure 8.3: Documentation of the uniform distribution

Here the `scale` and `loc` parameters result in a uniform distribution on the interval `[loc, loc + scale]`.

```
#Uniform distribution on [3,3+4] = [3,7]
dist_unif = scipy.stats.uniform(3,4)

a,b = dist_unif.support()

print(f"The distribution is supported on the interval [{a},{b}]")
```

The distribution is supported on the interval [3.0,7.0]

Some distributions have an unbounded support. In the case of the Normal distribution, we have  $a = -\infty$  and  $b = \infty$ . For the Exponential Distribution, we have  $a = 0$  and  $b = \infty$ .

```
dist_norm = scipy.stats.norm(loc=0, scale=1)

a,b = dist_norm.support()

print(f"The Normal distribution is \
supported on the interval [{a},{b}]")
```

The Normal distribution is supported on the interval [-inf,inf]

```
dist_exp = scipy.stats.expon(loc=0,scale=1)

a,b = dist_exp.support()

print(f"The Exponential distribution is \
supported on the interval [{a},{b}]")
```

The Exponential distribution is supported on the interval [0.0,inf]

The value `inf` that  $b$  has in the example above is in fact a number within NumPy, namely `np.inf`. Let us check that the upper bound of the exponential distribution is indeed `np.inf`.

```
statement = (b == np.inf)

print(statement)
```

True

### 8.2.1 Distributions as input arguments

Distributional objects can also serve as input arguments of a function. In that case, you can access the methods of the object inside the function.

Suppose we want to write a function that outputs a message saying whether or not the mean or the median of a distribution is larger. We can do this as follows for an arbitrary distribution.

```
def mean_median(dist):
    if dist.mean() < dist.median():
        return "The mean is smaller than the median"
    elif dist.mean() == dist.median():
        return "The mean and median are equal."
    elif dist.mean() > dist.median():
```

```
    return "The mean is larger than the median."
```

In the function above, the input argument `dist` is a distribution object whose methods `mean()` and `median()` we access within the function.

```
dist_norm = scipy.stats.norm(loc=1,scale=2)  
  
comparison = mean_median(dist_norm)  
print(comparison)
```

The mean and median are equal.

# Chapter 9

## Statistics and data fitting

In this chapter we will study some data analysis techniques that are often used in statistics and data science. We first consider statistical coefficients that can determine whether two or more data arrays exhibit correlation or not. Afterwards, we look at various fitting techniques to fit a function to given data: Regression, interpolation and distributional fitting.

### 9.1 Correlation coefficients

Suppose we have collected two features of a group of  $n$  people, their weight (kg) and height (cm), in arrays  $x = [x_0, \dots, x_{n-1}]$  and  $y = [y_0, \dots, y_{n-1}]$ , respectively. One might expect some correlation between these two features, as taller people typically weigh a bit more than shorter people. One way to quantify such relations is to compute a correlation coefficient of the data.

#### 9.1.1 Pearson coefficient

The Pearson correlation coefficient for these arrays is defined as

$$P(x, y) = \frac{\sum_{i=0}^{n-1} (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=0}^{n-1} (x_i - \bar{x})^2 \sum_{i=0}^{n-1} (y_i - \bar{y})^2}}$$

where  $\bar{x}$  and  $\bar{y}$  are the means (or averages) of the vectors  $x$  and  $y$ , respectively. It holds that  $P(x, y) \in [-1, 1]$  with the interpretation that the larger  $|P(x, y)|$  is, the more correlation (positive or negative) the arrays have.

NumPy has a built-in function `corrcoef()` to compute the Pearson coefficient of the arrays  $x$  and  $y$ . In fact, this function works in a vectorized way. If we input a two-dimensional array, then this function computes the Pearson coefficient for every pair of rows of the array.

```
import numpy as np
import scipy.stats

# Heights
x = np.array([187, 174, 179, 192, 188, 160, 179, 168, 168, 174])
```

```

# Weights
y = np.array([94, 88, 91, 96, 95, 80, 91, 84, 85, 86])

data = np.vstack((x,y)) # Store data in two-dimensional array

P = np.corrcoef(data)

print(P)

```

```
[[1.          0.98888612]
 [0.98888612 1.          ]]
```

Note that there will always be ones on the diagonal as the first row is perfectly correlated with itself, and that this matrix is symmetric since  $P(X, Y) = P(Y, X)$ . Let us also add a feature (age) which is not really correlated with the other two features and recompute the Pearson coefficients.

```

# Heights
x = np.array([187, 174, 179, 192, 188, 160, 179, 168, 168, 174])

# Weights
y = np.array([94, 88, 91, 96, 95, 80, 91, 84, 85, 86])

# Age
a = np.array([23, 23, 23, 24, 25, 24, 24, 23, 24, 23])

data = np.vstack((x,y,a))

P = np.corrcoef(data)

print(P)

```

```
[[1.          0.98888612  0.21342006]
 [0.98888612 1.          0.24120908]
 [0.21342006 0.24120908 1.          ]]
```

As you can see, the correlation coefficients of the height-age ( $\approx 0.21$ ) and height-weight ( $\approx 0.24$ ) combinations is rather low.

The `stats` module of SciPy also has a built-in function `pearsonr()` to compute the Pearson coefficient of two arrays of feature data. This function also performs some additional hypothesis testing on the data, but can unfortunately not handle two-dimensional arrays as input.

If you only want to compute the coefficient for two features, then this function is also suitable, but if you want to compute a correlation coefficient matrix like above, `corrcoef()` is the better choice.

### 9.1.2 Spearman rank coefficient

Another famous correlation coefficient is the Spearman rank coefficient. Whereas the Pearson correlation is useful when you expect a linear relation between the two features under consideration, the Spearman coefficient is more useful when you expect only a monotone, but non necessarily linear, relation. Monotone here means that when the value of the first feature becomes larger, the value of the second feature also becomes larger.

There are other factors that determine whether the Pearson or Spearman coefficient is more suitable, but we omit those here.

Suppose we have collected data about the number of hours that students study for an exam and their grade. One might expect that students who have studied more hours also have obtained a higher grade, but it is not to be expected that this relation is linear. For example, studying a double number of hours is not always guaranteed to double your grade.

We have collected some data in the arrays `hours` and `grade` with `hours[i]` denoting the number of hours that student  $i$  studied, and `grade[i]` the grade this student obtained. That data is visualized below as well. Note that in the figure one can see a monotone relation between the features (study hours and grade), but this relation is not linear.

```
# Study hours
hours = np.array([1, 2, 2, 4, 3, 5, 7, 8, 6, 10, 14, 12, 15, 18, 20])
```

```
# Grades
grade = np.array([1.3, 3, 2.4, 3, 3.5, 3.8, 5, 7, 7, 8, 8.3, 8, 9, 8.4, 9.5])
```

```
import matplotlib.pyplot as plt

# Create figure
plt.figure()

# Create scatter plot of data points
plt.scatter(hours,grade)

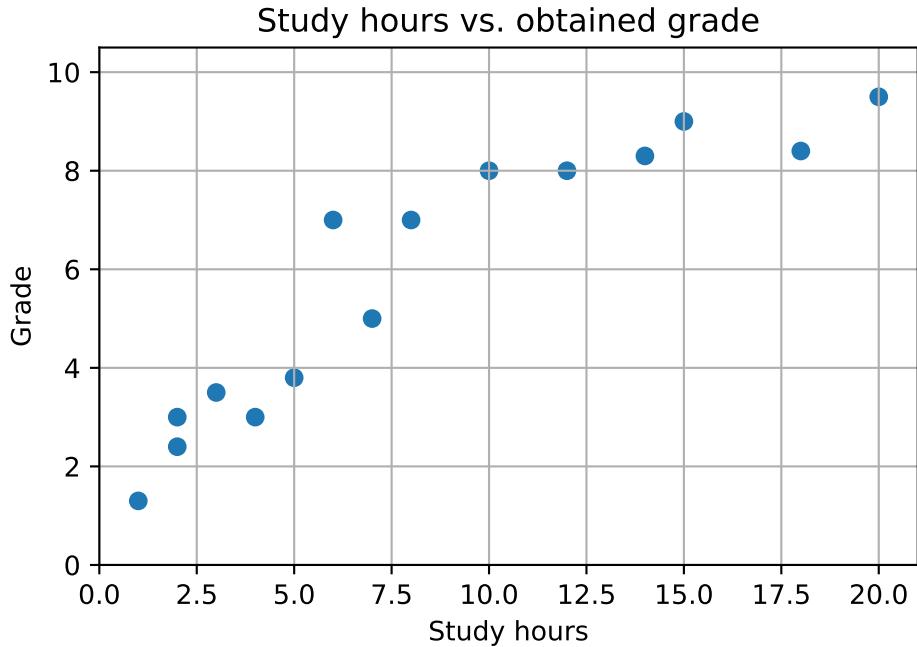
# Set axes limits
plt.xlim(0,np.max(hours)+1)
plt.ylim(0,np.max(grade)+1)

# Set axes labels
plt.xlabel("Study hours")
plt.ylabel("Grade")

# Set title
plt.title("Study hours vs. obtained grade")

# Create grid
plt.grid()

# Show plot
plt.show()
```



To determine the Spearman rank coefficient, we first compute the ranks of the data of the features. The smallest value in a feature array gets rank 1, the second smallest rank 2, etc. This can be done with the `rankdata()` function from the `stats` module.

```
# Ranks of study hours values
ranks_hours = scipy.stats.rankdata(hours)

print(ranks_hours)

[ 1.  2.5  2.5  5.   4.   6.   8.   9.   7.   10.  12.  11.  13.  14.
 15. ]
```

Note that when a number appears multiple times in the array, then an average rank is computed.

```
# Ranks of grade values
ranks_grades = scipy.stats.rankdata(grade)

print(ranks_grades)

[ 1.   3.5  2.   3.5  5.   6.   7.   8.5  8.5  10.5 12.  10.5 14.  13.
 15. ]
```

After having computed the ranks, the Spearman rank coefficient is obtained by computing the Pearson correlation coefficients of the rank arrays.

```
rank_data = np.vstack((ranks_hours, ranks_grades))

S = np.corrcoef(rank_data)

print(S)

[[1.          0.98118437]
 [0.98118437 1.          ]]
```

There is a built-in function `spearmanr()` that carries out the two steps mentioned above. This function is vectorized in the sense that if we put in a two-dimensional array, then every column is interpreted as the data corresponding to a feature, and the correlation between different columns is computed. If the data of a feature is given as a row, we can set the `axis` keyword argument to `axis=1`.

```
# Study hours
hours = np.array([1, 2, 2, 4, 3, 5, 7, 8, 6, 10, 14, 12, 15, 18, 20])

# Grades
grade = np.array([1.3, 3, 2.4, 3, 3.5, 3.8, 5, 7, 7, 8, 8.3, 8, 9, 8.4, 9.5])

data = np.vstack((hours, grade))

S = scipy.stats.spearmanr(data, axis=1)

print(S)
```

`SignificanceResult(statistic=0.9811843713228874, pvalue=1.1432541280704027e-10)`

This function `spearmanr()` outputs the Spearman rank coefficient and a  $p$ -value. You can read about the latter in the documentation. The rank coefficient is stored in the `statistic` attribute.

```
print(S.statistic)
```

0.9811843713228874

Alternatively, you can suppress the  $p$ -value output argument to only get the rank coefficient.

```
S, _ = scipy.stats.spearmanr(data, axis=1)

print(S)
```

0.9811843713228874

### 9.1.3 Other coefficients

There are many other correlation coefficients that can be computed with Python, see here for a list. A large collection of statistical tests has also been implemented in the `stats` module.

## 9.2 Data fitting

In this section we will see various ways in which you can compute a function that fits given data best, using regression, (polynomial) interpolation, or distributional fitting.

### 9.2.1 Regression

In a regression model, we are given a relation of the form

$$y_i = f(x_i, \beta) + \epsilon_i$$

where  $f : \mathbb{R}^{n+k} \rightarrow \mathbb{R}$  is a known function,  $(x_i, y_i)$  known data points for  $i = 0, \dots, m - 1$ , with  $x_i = [x_{i0}, \dots, x_{(n-1)i}] \in \mathbb{R}^n$  and  $y_i \in \mathbb{R}$ . The term  $\epsilon_i$  is an unknown error term that is often assumed to be normally distributed. Its exact distribution is not relevant at this point, because we assume it is unknown.

The goal is to determine a vector  $\beta = [\beta_0, \dots, \beta_{k-1}] \in \mathbb{R}^k$  that minimizes a given error function. The most well-known choice here is to minimize the sum of the squared errors, i.e., to find a solution to the problem

$$\min_{\beta} \sum_{i=0}^{m-1} \epsilon_i^2 = \min_{\beta} \sum_{i=0}^{m-1} (y_i - f(x_i, \beta))^2.$$

Note that  $\beta = [\beta_0, \dots, \beta_{k-1}]$  is the only unknown in the right hand side expression above. In other words, this problem tries to find the least squares solution to the system of  $m$  equations given by

$$y_i - f(x_i, \beta) = 0$$

for  $i = 0, \dots, m-1$ . An exact solution does not exist because of the (unknown) error terms  $\epsilon_i$ .

Let us look at a simple form of linear regression where  $n = 1$  and  $k = 2$ . That is, we have  $f : \mathbb{R} \rightarrow \mathbb{R}$  defined by  $f(x) = \beta_0 + \beta_1 x$ . Suppose we are given data points  $(x_i, y_i) \in \mathbb{R}^2$  for  $i = 0, \dots, m-1$ . Note that  $x_i$  is a scalar and not an array in this case, because  $n = 1$ . We are looking for a  $\beta = [\beta_0, \beta_1]$  that solves the system

$$\begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \\ 1 & x_m \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}.$$

Because of the error term in the regression model (and the fact that this system is overdetermined), we compute a least squares solution. We have already seen various functions that can do this for us, in particular `least_squares` from SciPy's `optimize` module.

Recall from Chapter 6 that `least_squares` takes as input an array of functions  $g_0(\beta), \dots, g_{m-1}(\beta)$  and then minimizes over  $\beta$  the expression  $\sum_i g_i(\beta)^2$ . In our case we have  $g_i(\beta) = y_i - f(x_i, \beta) = y_i - (\beta_0 + \beta_1 x_i)$ .

Below we create the function `model()` whose output is the array

$$\begin{pmatrix} y_0 - f(x_0, \beta) \\ y_1 - f(x_1, \beta) \\ \vdots \\ y_{m-1} - f(x_{m-1}, \beta) \end{pmatrix}.$$

This function will serve as the input for `least_squares()`. To keep the code clean, we create a separate Python function for  $f$ .

```
import scipy.optimize as optimize

# Function f
def f(x,beta):
    return (beta[0] + beta[1]*x)

# System of error terms
def model(beta,x,y): # beta is first input here; later optimized over
    return y - f(x,beta)
```

It is important that  $\beta$  is the first input argument of `model()` as this will be the array that we optimize over when looking for a least squares solution. For the function  $f$ , we could have also reversed the input arguments.

We next generate some synthetic  $(x_i, y_i)$  data points.

```

# Fix random seed
np.random.seed(42)

# Number of data points
m = 10

# Create points (1,1), (2,2), ..., (m,m) with some random noise.
x = np.arange(1,m+1) + 0.25*np.random.randn(m)
y = np.arange(1,m+1) + 0.25*np.random.randn(m)

```

Next, we perform `least_squares` on the linear model define above. Recall that this function needs an initial guess for the parameters in  $\beta$  to be fitted. Also, we need to use the `args` keyword argument to specify  $x$  and  $y$ , which are the additional input arguments of our `model()` function that are fixed (i.e., are not optimized over).

```

# Set initial guess
guess = np.array([2,2])

# Perform least squares method
result = optimize.least_squares(model,x0=guess,args=(x,y))

# Print fitted parameters
print(result)

```

```

message: `gtol` termination condition is satisfied.
success: True
status: 1
fun: [ 9.163e-03  1.787e-01  1.752e-01 -5.660e-01 -7.205e-02
       2.321e-01 -3.143e-01  2.312e-01  2.441e-01 -1.181e-01]
x: [-2.340e-01  9.865e-01]
cost: 0.3339323530848278
jac: [[-1.000e+00 -1.124e+00]
      [-1.000e+00 -1.965e+00]
      ...
      [-1.000e+00 -8.883e+00]
      [-1.000e+00 -1.014e+01]]
grad: [ 2.220e-16  8.122e-09]
optimality: 8.121683325867934e-09
active_mask: [ 0.000e+00  0.000e+00]
nfev: 3
njev: 3

```

The values in  $\beta$  can be found in the `x` attribute

```

beta = result.x

print(beta)

```

```
[ -0.23404544  0.98652277]
```

Finally, we plot the  $(x_i, y_i)$  data points together with the fitted line  $f(x) = \beta_0 + \beta_1 x$  to visually inspect our fitting procedure.

```
# Determine x- and y-values for the fitted line
x_line = np.linspace(0,11,100)
y_line = f(x_line,beta)

# Create figure
plt.figure()

# Scatter plot of data points
plt.scatter(x,y,label="Data points")

# Plot fitted line
plt.plot(x_line,y_line,c='r',label="Fitted model")

# Set axes limits
plt.xlim(0,m+1)
plt.ylim(0,m+1)

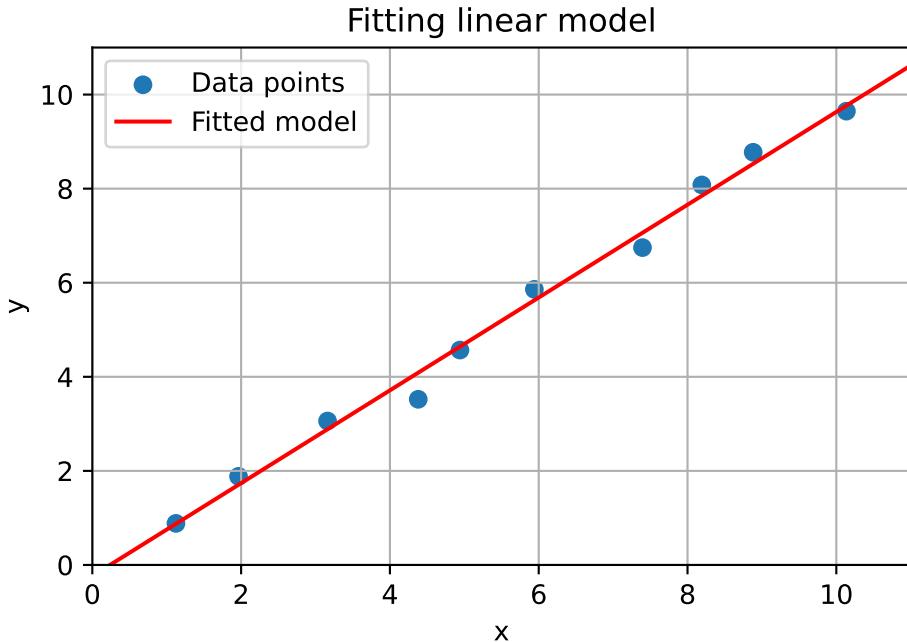
# Set axes labels
plt.xlabel("x")
plt.ylabel("y")

# Set title
plt.title("Fitting linear model")

# Create grid
plt.grid()

# Create legend
plt.legend()

# Show plot
plt.show()
```



One should recall that because of the fact that  $f$  is linear in the parameters in  $\beta$ , we could have also used the `linalg.lstsq()` function from Numpy. Although you do not need to fully understand the code below, we include it here for sake of reference.

```
# Create left hand side matrix of system above
A = np.vstack((np.ones(m),x)).T

# Right hand side vector of system
b = y

# We add rcond=None to avoid a warning raised by Python
result = np.linalg.lstsq(A,b,rcond=None)[0] # First output is our beta

print(result)
```

`[-0.23404544 0.98652277]`

Most importantly, `least_squares` is also able to handle non-linear function  $f$  in our regression framework, for example

$$y_i = \left( \frac{\beta_0 + \sqrt{x_i}}{\beta_1 \sqrt{x_i}} \right)^2 + \epsilon_i$$

for  $i = 0, \dots, m - 1$ . Note that also here  $n = 1$  and  $k = 2$ .

Carrying out the same steps as above we obtain the following code to fit this function on given synthetic  $(x_i, y_i)$  data points.

```
# Fix random seed
np.random.seed(42)

# Function f
def f(x,beta):
```

```

    return ((beta[0] + np.sqrt(x))/(beta[1]*np.sqrt(x)))**2

# Define the non-linear model
def model(beta,x,y):
    return y - f(x,beta)

# Number of data points
m = 10

# These will be the choice of beta for which we generate the data
beta_true = np.array([4,2])

#Generate synthetic data points with some random noise.
x = np.arange(1,m+1)
y = f(x,beta_true) + 0.25*np.random.randn(m)

# Set initial guess
guess = np.array([1,1])

# Perform least squares method on x,y data
result = optimize.least_squares(model,x0=guess,args=(x,y))

# Fitted parameters
beta_fit = result.x

print(beta_fit)

```

[3.49914009 1.78657584]

```

# Determine x- and y-values for the fitted line
x_line = np.linspace(0.01,11,100)
y_line = f(x_line,beta_fit)

# Create figure
plt.figure()

# Scatter plot of data points
plt.scatter(x,y,label="Data points")

# Plot fitted line
plt.plot(x_line,y_line,c='r',label="Fitted model")

# Set axes limits
plt.xlim(0,m+1)
plt.ylim(0,m+1)

# Set axes labels
plt.xlabel("x")
plt.ylabel("y")

# Set title
plt.title("Fitting nonlinear model")

```

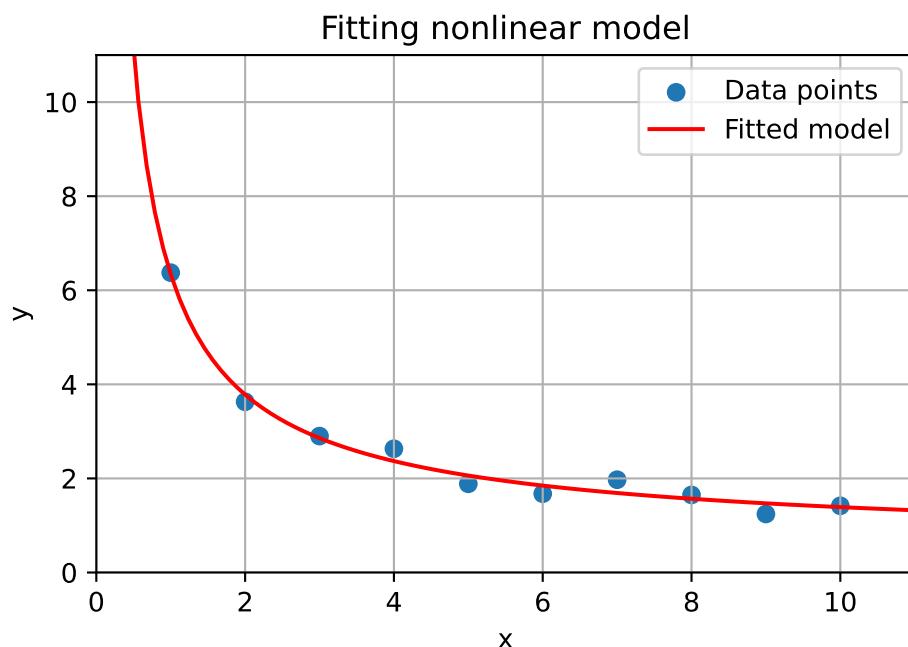
```

# Create grid
plt.grid()

# Create legend
plt.legend()

# Show plot
plt.show()

```



### 9.2.2 Interpolation

If we want to create a function that goes exactly through given data points, we can do this with interpolation. Suppose we have some data points from the function  $f(x) = \sin(x)$  given below.

```

def f(x):
    return np.sin(x)

# Data points
x = np.array([0, 1, 3, 5, 6, 8, 10])
y = f(x)

```

Let us plot the sine function and the data points that we created.

```

# x-range for plotting
x_plot = np.linspace(np.min(x), np.max(x), 1000) # Define range based on data points

# Plotting sine function
plt.plot(x_plot, f(x_plot), label='Sine function')

# Plotting data points

```

```

plt.scatter(x, y, label='Data points')

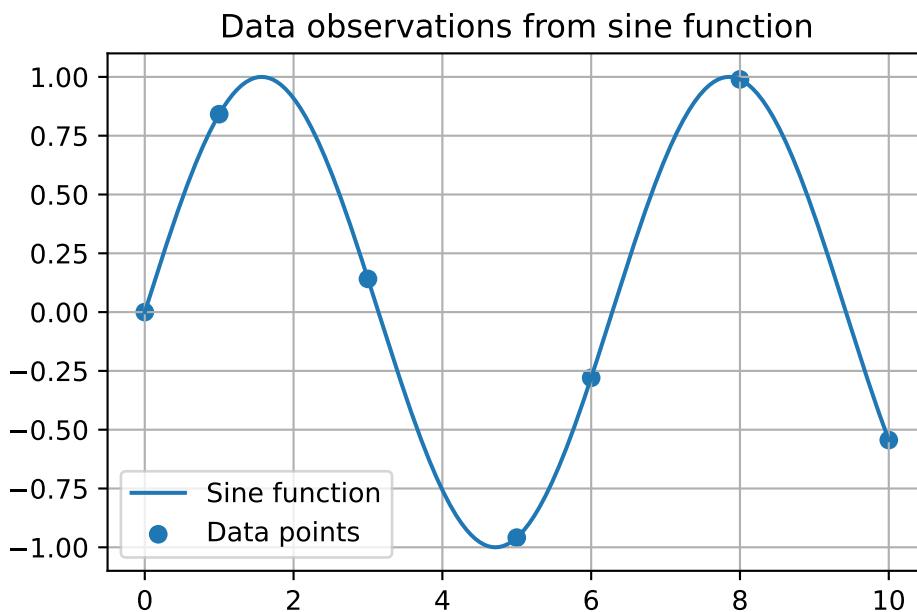
# Set title
plt.title('Data observations from sine function')

# Set legend
plt.legend()

# Create grid
plt.grid()

# Show figure
plt.show()

```



Suppose now that we would only know the data points. Polynomial interpolation asks for a piecewise polynomial that passes through all the data points, i.e., a function that is a polynomial between any two consecutive data points. This is also often referred to as spline interpolation.

SciPy has a built-in function `make_interp_spline()` in its `interpolate` module that can yield such a polynomial. It takes as first two inputs arrays the  $x$ - and  $y$ -coordinates it should pass through.

Furthermore, the keyword argument `k` allows you to choose the degree of the polynomial on every segment formed by two consecutive data points.

Below we create an interpolation that is a linear between any two data point, i.e., we have  $k = 1$ . In other words, this form of interpolation simply connects consecutive data points with a straight line segment.

The `make_interp_spline()` function creates an object that acts as a function, i.e., we can input a scalar or array into it and get back the function values at inputted points.

```

import scipy.interpolate as interpolate

# Creates a so-called BSpline object

```

```
linear_spline = interpolate.make_interp_spline(x,y,k=1)

# Object can be evaluated in vectorized fashion
a = np.array([1,2,3])
print(linear_spline(a))
```

```
[0.84147098  0.4912955  0.14112001]
```

Let us compare the interpolation polynomial with the original sine function in a figure.

```
# x-range for plotting
x_plot = np.linspace(0, 10, 1000)

# Plotting sine function
plt.plot(x_plot, f(x_plot), label='Sine function')

# Plotting first degree interpolation polynomial
plt.plot(x_plot, linear_spline(x_plot), label='Piecewise linear spline')

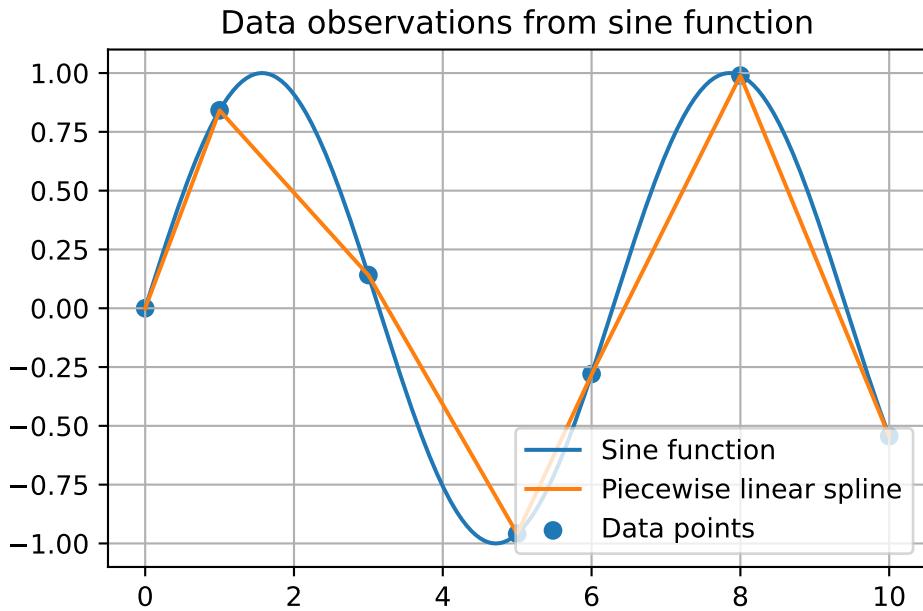
# Plotting data points
plt.scatter(x, y, label='Data points')

# Set title
plt.title('Data observations from sine function')

# Set legend
plt.legend()

# Create grid
plt.grid()

# Show figure
plt.show()
```



### 9.2.3 Distributional fitting

It is possible to fit the parameters of a known distribution to given data samples using the `fit()` function of a distribution object. For example, suppose you suspect your data comes from a normal distribution, but do not know its mean and standard deviation.

Below we generate some data from a normal distribution.

```
# Fix randomness
np.random.seed(3)

# Samples from normal distribution with given mean and standard dev.
n = 1000
samples = np.random.normal(loc=5,scale=3,size=n)
```

Now pretend we are given `x` but do not know the `loc` and `scale` parameters that were used to create this array. We can fit the data in `x` on a normal distribution with the `fit()` function from the `stats` module. The output of this function is a tuple with the fitted parameters of the distribution, typically the first one being the location and the second one the scale parameter.

The syntax for the `fit()` function is `scipy.stats.distribution_name.fit()` where `distribution_name` is the name of the distribution that we want to fit the data on; see here all the available options.

Let us fit the data on a normal distribution, with `norm` as choice for `distribution_name`.

```
parameters = scipy.stats.norm.fit(samples)

print(parameters)

(5.051852998942502, 3.0252056971538166)

print("Estimated mean is", parameters[0])
print("Estimated standard deviation is", parameters[1])
```

```
Estimated mean is 5.051852998942502
Estimated standard deviation is 3.0252056971538166
```

If you know one of the scale or location parameters, you can fix these using the `floc` or `fscale` keyword arguments. For example, suppose we know that the mean of the data that the distribution was generated from is equal to 5, then we can set `floc=5`.

```
mu, sigma = scipy.stats.norm.fit(x, floc=5)

print("Estimated mean is", mu)
print("Estimated standard deviation is", sigma)
```

```
Estimated mean is 5
Estimated standard deviation is 3.3806170189140663
```

The fit function uses (as default) the maximum likelihood estimation method to determine the distributional parameters that fit the data best.

To inspect whether the returned fitted parameters accurately represents the data, we can visualize the data samples and the fitted distribution in a histogram. We plot the samples using `plt.hist()`. We have seen this function before in one of the exercises.

The first input argument of the `hist()` function is the list of samples for which we want to create the histogram. The `bins` keyword argument specifies the number of bars in the histogram, and `density=True` rescales the histogram so that the total area of the bars equal 1 (which is the same value you get by integrating the area under the probability density function of a distribution).

```
# Fit data
mu, sigma = scipy.stats.norm.fit(samples)

# Round coefficients
mu = np.around(mu, decimals=2)
sigma = np.around(sigma, decimals=2)

# Create an array of x values for plotting the PDF
x = np.linspace(np.min(samples), np.max(samples), 100)

# Create figure
plt.figure()

# Compute PDF-values of elements in x for fitted normal distribution
pdf_norm_fit = scipy.stats.norm.pdf(x, mu, sigma)

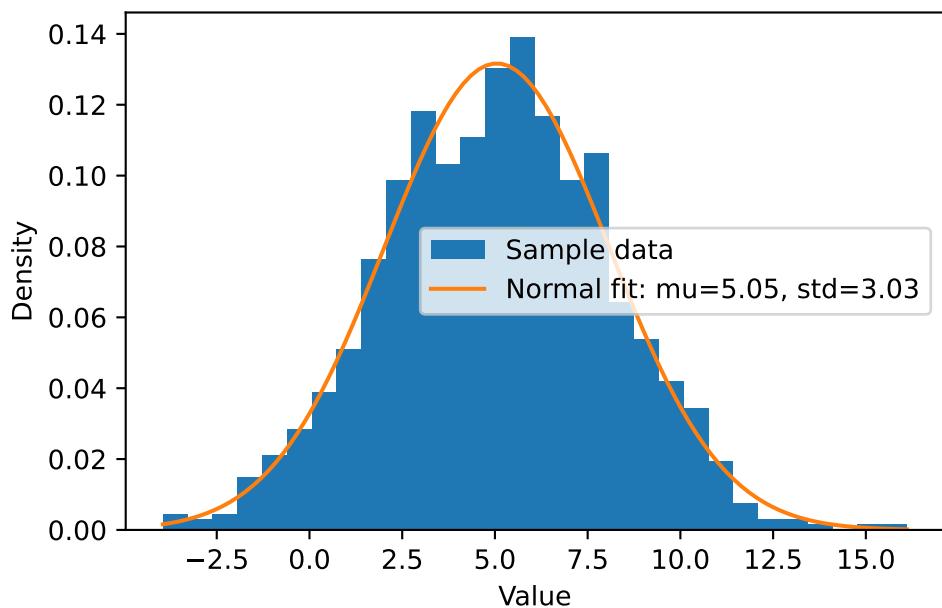
# Plot the histogram of the data
plt.hist(samples, bins=30, density=True, label='Sample data')

# Plot the fitted normal distribution
plt.plot(x, pdf_norm_fit, label=f'Normal fit: mu={mu}, std={sigma}')

# Add labels and legend
plt.xlabel('Value')
plt.ylabel('Density')
plt.legend()

# Show plot
```

```
plt.show()
```



# Chapter 10

## Learning problems

In this chapter, we will see some algorithms for learning problems such as classification and clustering, which are fundamental tasks in machine learning for the analysis of large data sets. We remark that some of the problems we have seen in earlier chapters, such as regression, can also be seen as learning problems.

Classification is concerned with deciding for every data point (or observation) what label or category, from a pre-determined list, it belongs to. Think of (binary) tasks like determining whether an e-mail is spam or not, or deciding whether an employee should get a promotion. Classification is an example of a supervised learning problem.

Clustering is concerned with grouping similar data points in clusters. Here there is not (necessarily) an underlying “ground truth” label for every cluster. The goal is merely to group similar points together. Clustering is an example of an unsupervised learning problem.

One very useful package for machine learning in Python is the Scikit-learn package `sklearn` that builds on NumPy, SciPy and Matplotlib. If you will be doing machine learning with Python in the future, this package is a good starting point. In this chapter, we will illustrate some functionality `sklearn`.

### 10.1 Binary logistic regression

Consider the problem of deciding whether an employee should get promoted, based on an overall grade  $x \in [1, 10]$  representing their performance. The high-level idea is to come up with a non-decreasing function  $f : [1, 10] \rightarrow [0, 1]$  indicating whether, given a grade  $x$ , an employee should get a promotion. You may interpret  $f(x)$  as the probability that, given grade  $x$ , an employee gets promoted.

We promote an employee with grade  $x$  if and only if  $f(x) > 0.5$ . More formally, we define the classifier function  $g : [1, 10] \rightarrow \{0, 1\}$  by

$$g(x) = \begin{cases} 1 & f(x) > 0.5 \\ 0 & f(x) \leq 0.5 \end{cases}.$$

We say that an employee with grade  $x_i$  has label 1, or is in class 1, if  $g(x_i) = 1$ , and label/class 0 if  $g(x_i) = 0$ .

#### 10.1.1 Input data

The idea will be to fit a function  $f$  on (historical) data, and thereby indirectly also the function  $g$ . The historical data points are given as  $(x_i, y_i)$  for  $i = 0, \dots, m - 1$ , where  $x_i \in [1, 10]$  is the grade of person  $i$  for  $i = 0, \dots, m - 1$  together with the decision  $y_i \in \{0, 1\}$  whether a person with that grade got promoted (label 1) or not (label 0).

The purpose of fitting such a function is that we can use it to make promotion decision in the future, i.e., if a new employee  $x_m$  is up for promotion, we use the fitted function  $g$  to decide whether this person gets promoted or not.

```
import numpy as np
import matplotlib.pyplot as plt

# Grades
x_data = np.array([2.7, 3.7, 4.8, 5.7, 6.1, 6.8, 6.9,
                   7.0, 7.4, 7.5, 8, 8.2, 8.7, 8.9, 9.6])

# Promotion decisions (binary label)
y_data = np.array([0, 0, 0, 0, 1, 1, 1, 0,
                   0, 1, 1, 1, 1, 1, 1, 1])

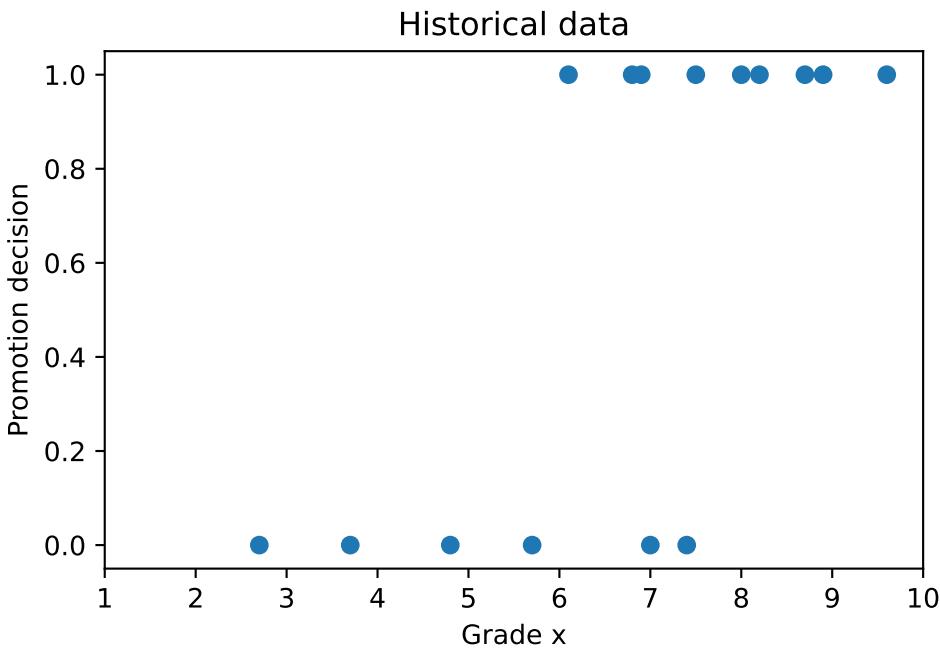
# Create figure
plt.figure()

# Scatter data points
plt.scatter(x_data,y_data)

# Add labels and axis information
plt.xlim(1,10)
plt.xlabel('Grade x')
plt.ylabel('Promotion decision');

# Add title
plt.title("Historical data")

# Show plot
plt.show()
```



### 10.1.2 Classification model

The idea of logistic regression is to look for a sigmoid function  $f$  that is of the form

$$f(x) = \frac{1}{1 + e^{-p(x)}}$$

with  $p(x) = \alpha + \beta \cdot x$  an affine function. The goal is to fit, or “learn” in machine learning terminology, the weights  $\alpha$  and  $\beta$  based on the historical data. Such a function  $f$  is more appropriate than, for example, an affine function  $f$ , when solving this type of classification problem.

Below we plot an example of such a function for  $\alpha = -5, \beta = 1$ .

```
# An example of a sigmoid function
def sigmoid(x,alpha,beta):
    return 1/(1 + np.exp(-(alpha + beta*x)))

# Choice of beta for plot
alpha, beta = -5, 1

# Arrays to plot
x = np.linspace(1,10)
y = sigmoid(x,alpha,beta)

# Create figure
plt.figure()

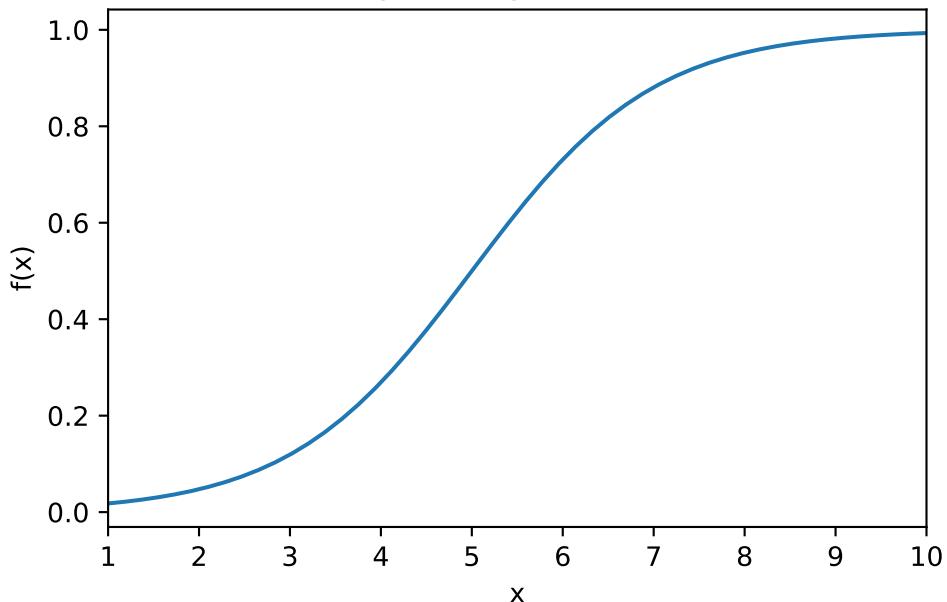
# Plot function
plt.plot(x,y)

# Add labels and axis information
plt.xlim(1,10)
plt.xlabel('x')
plt.ylabel('f(x)');

# Add title
plt.title("Example of sigmoid function")

# Show plot
plt.show()
```

Example of sigmoid function



We next import the logistic regression class `LogisticRegression` from the `sklearn.linear_model` module to do the fitting with, and create an instance of this class.

```
from sklearn.linear_model import LogisticRegression

# Create instance/object of class
promotion = LogisticRegression(penalty=None)
```

When creating the instance, we add the keyword argument `penalty` which we set to `None`. As a default, `LogisticRegression` uses a regularization term (as we saw in the exercises corresponding to the previous chapter) in the minimization problem to find the best fit.

By setting `penalty=None`, this regularization term will be set to zero when we do the fitting later on. There are also other conditions you can impose on the fitting procedure; have a look at the documentation for these.

We continue with the `fit()` method that is used to do the fitting. As can be seen in the documentation (figure below), the input data of the  $x$ -array should be a two-dimensional array where every column represents one feature of the data. In our setting, there is only one feature, the grade of an employee. Another feature could for example be the number of years that someone has been working for the company already.

## `fit(x, y, sample_weight=None)`

[\[source\]](#)

Fit the model according to the given training data.

### Parameters:

#### **X** : {array-like, sparse matrix} of shape (n\_samples, n\_features)

Training vector, where `n_samples` is the number of samples and `n_features` is the number of features.

#### **y** : array-like of shape (n\_samples,)

Target vector relative to X.

#### **sample\_weight** : array-like of shape (n\_samples,) default=None

Array of weights that are assigned to individual samples. If not provided, then each sample is given unit weight.

Figure 10.1: Documentation of `fit()` function for LogisticRegression instance

```
# Historical data (with x_data as n x 1 column array)
x_data = np.array([2.7, 3.7, 4.8, 5.7, 6.1, 6.8, 6.9,
                  7.0, 7.4, 7.5, 8, 8.2, 8.7, 8.9, 9.6])[:,None]

y_data = np.array([0, 0, 0, 0, 1, 1, 1, 0,
                  0, 1, 1, 1, 1, 1, 1])

# Fit the instance with historical data
promotion = promotion.fit(x_data,y_data)
```

The fitted model has various attributes with information about the fitted model.

- `classes_`: Distinct labels that appear in label array `y_data`.

```
# Distinct labels in y-data
print("Classes = ", promotion.classes_)
```

Classes = [0 1]

```
# Fitted parameters
print("alpha = ", promotion.intercept_[0])
print("beta = ", promotion.coef_[0,0])
```

alpha = -9.403012405877018  
beta = 1.4505735782392242

- `intercept_`: Fitted coefficient  $\alpha$  (in one-dimensional array)
- `coef_`: Fitted coefficient  $\beta$  (in two-dimensional array)

Note that `intercept_` and `coef_` return a one- and two-dimensional array, respectively. This is because, in general, we can also fit models with  $c \geq 2$  classes and  $n$  data features, meaning  $x_i \in \mathbb{R}^n$ . Then `intercept_` is an array of length  $c - 1$  and `coef_` a  $(c - 1) \times n$  array.

Next to the attributes, there are also various function that we can execute on the fitted model.

- `predict_proba()`: Returns array  $P$  whose rows correspond to the observations, and whose columns to the classes. Entry  $P_{ij}$  is the probability that observation  $x_i$  is in class  $j$ . In our example, the first column is the value  $1 - f(x_i)$ , i.e., the probability of being in class 0, and the second column is the value  $f(x_i)$ , i.e., the probability of being in class 1.

```
# Class prediction probabilities
P = promotion.predict_proba(x_data)

print(P)
```

```
[[0.99587462 0.00412538]
 [0.98263686 0.01736314]
 [0.9198462  0.0801538 ]
 [0.75671314 0.24328686]
 [0.63518214 0.36481786]
 [0.3867752  0.6132248 ]
 [0.35298469 0.64701531]
 [0.32060287 0.67939713]
 [0.20895564 0.79104436]
 [0.18598853 0.81401147]
 [0.09960903 0.90039097]
 [0.07644273 0.92355727]
 [0.0385318  0.9614682 ]
 [0.0291111  0.9708889 ]
 [0.01074519 0.98925481]]
```

- `predict()`: Gives predicted class of every observation. For us it returns 1 if the predicted probability  $> 0.5$ , and 0 otherwise. This is the implementation of the function  $g$  that we introduced earlier.

```
# Class predictions
y_pred = promotion.predict(x_data)

print("Predicted classes are",y_pred)
print("Original classes are ",y_data)
```

```
Predicted classes are [0 0 0 0 1 1 1 1 1 1 1 1]
Original classes are [0 0 0 0 1 1 1 0 0 1 1 1 1]
```

- `score()`: Computes the fraction of correctly classified data points, i.e, the points  $(x_i, y_i)$  for which their predicted label is the same as their true label  $y_i$ .

```
# Model score
score = promotion.score(x_data,y_data)

print(score)
```

0.8

### 10.1.3 Visualization

We can plot the fitted sigmoid function with the observations. We have added a dashed red line at the  $x$  for which  $f(x) = 0.5$ . This is the boundary between values of  $x$  whose predicted label is 0 (left of the line) and whose predicted label is 1 (right of the line).

As you can see, three points are misclassified: One points receives predicted label 0 although its true label is 1, and two points receive predicted label 1 although their true label is 0.

```
import scipy.optimize as optimize

# An example of a sigmoid function
def sigmoid(x,alpha,beta):
    return 1/(1 + np.exp(-(alpha + beta*x)))

# Choice of beta for plot
alpha, beta = promotion.intercept_, promotion.coef_[0]

# Determine x where f(x) = 0.5
def g(x,alpha,beta):
    return sigmoid(x,alpha,beta) - 0.5

x_b = optimize.fsolve(g,x0=5.5,args=(alpha,beta))

# Arrays to plot
x = np.linspace(1,10)
y = sigmoid(x,alpha,beta)

# Create figure
plt.figure()

# Plot fitted sigmoid function
plt.plot(x,y,label="Fitted function f")

# Plot vertical line at x_b
plt.axvline(x_b,linestyle='--',color='red',label="Point x where f(x) = 0.5")

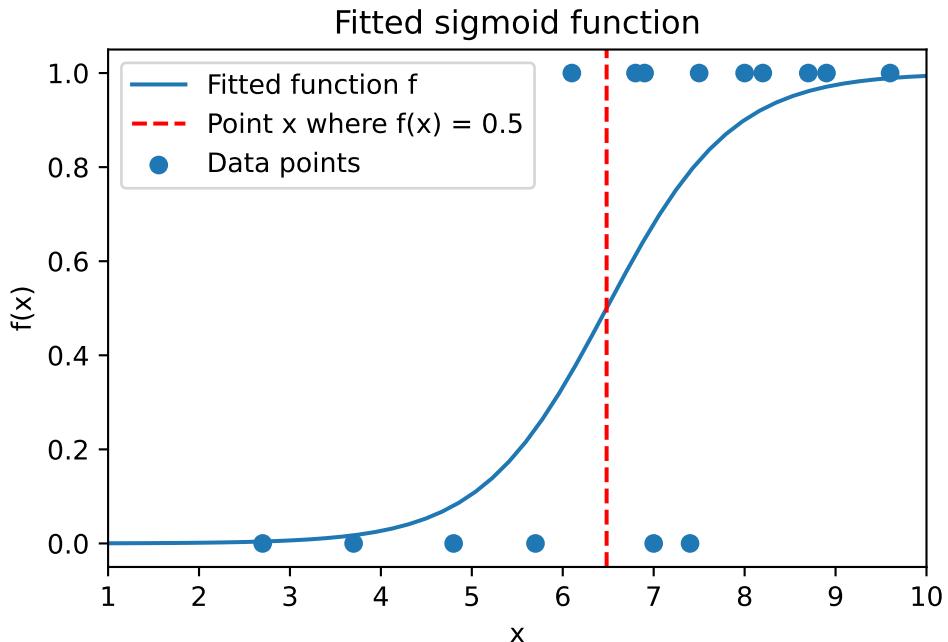
# Scatter data points
plt.scatter(x_data,y_data,label="Data points")

# Add labels and axis information
plt.xlim(1,10)
plt.xlabel('x')
plt.ylabel('f(x)');

# Add title
plt.title("Fitted sigmoid function")

# Add legend
plt.legend()

# Show plot
plt.show()
```



It is also possible to visualize the number of correctly and wrongly classified points using the `confusion_matrix()` function from the `sklearn.metrics` package. If the first input argument of this function is the array with the true labels, and the second input argument the array with the predicted labels, then `heatmap()` returns a matrix  $C$  where entry  $C_{ij}$  is the number of observations whose true label is  $i$ , but was predicted to have label  $j$ .

This means that the sum of the diagonal entries of this matrix is the correctly classified observations.

```
from sklearn.metrics import confusion_matrix

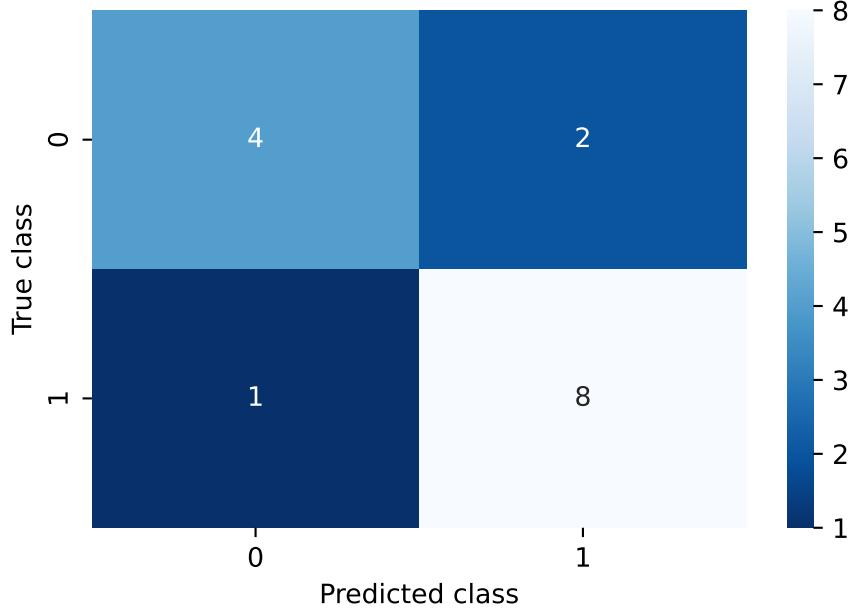
# Inputs are true labels and predicted labels
C = confusion_matrix(y_data,y_pred)
print(C)
```

```
[[4 2]
 [1 8]]
```

You can also represent this matrix visually using the `heatmap()` function from the Seaborn package. You do not need to know this package, but we include it here for completeness. It contains functionality for visualization of statistical data.

```
import seaborn

seaborn.heatmap(C,annot=True,cmap='Blues_r')
plt.xlabel('Predicted class')
plt.ylabel('True class');
```



## 10.2 Clustering

Another fundamental problem in the area of machine learning and computer science is that of clustering. Here the task is to divide (unlabelled) data points  $x_0, \dots, x_{n-1} \in \mathbb{R}^d$  with  $x_i = [x_{i0}, \dots, x_{i(d-1)}]$  having  $d$  features, into groups/clusters that are ‘similar’ in a certain sense. An example is customer segmentation, where you want to have a similar advertisement policy for similar customers, and so you need to decide how to segment the customers (although a priori it is not clear what makes customers similar).

The high-level idea of many clustering algorithms is to come up with  $K$  centers  $c_0, \dots, c_{K-1} \in \mathbb{R}^d$  with  $c_k = [c_{k0}, \dots, c_{k(d-1)}]$  for  $k = 0, \dots, K - 1$ , and assign every point  $x_i$  to a center. All the points assigned to the same center are called a cluster. The index of the cluster that a data point  $x_i$  is assigned to, is called its label. The goal is to find the appropriate centers and an assignment from points to clusters.

The quality of a clustering  $C = \{c_0, \dots, c_{K-1}\}$  is often measured in terms of the sum of squared errors (SSE)

$$\begin{aligned} \text{SSE}_{x_0, \dots, x_{n-1}}(c_1, \dots, c_k) &= \sum_{i=0}^{n-1} \min_{k=0, \dots, K-1} \|x_i - c_k\|_2^2 \\ &= \sum_{i=1}^{n-1} \min_{k=0, \dots, K-1} \sum_{j=0}^{d-1} (x_{ij} - c_{kj})^2 \end{aligned}$$

which aggregates the squared  $L^2$ -norm distances of all data points to their closest center.

### 10.2.1 Input data

Below we generate some data that we will cluster later on in this section. The data is generated using a built-in data generation function from the `sklearn.datasets` module. This module contains many functions to generate so-called synthetic data. You do not need to know the function `make_blobs`, but we include it here for completeness. Have a look at its documentation if you are interested.

The function `make_blobs` can take as input specified centers, and then randomly generate data points around every center (based on normally distributed randomness). Those data points have as “true” label the index of the corresponding center they were generated around.

Most importantly, using `make_blobs` we create an

- $n \times d$  array `x_data` where every row is a data point  $x_i \in \mathbb{R}^d$  with  $d = 2$ ;
- $n$ -dimensional array `x_cluster` with the cluster every data point was generated in.

```
from sklearn.datasets import make_blobs

# Define K = 4 centers
r = 5
chosen_centers = np.array([[-r,-r],[-r,r],[r,r],[r,-r]])

# Creates n = 200 data points with four clusters of size n/K = 50
x_data, x_cluster = make_blobs(
    n_samples=200, # n = 200
    n_features=2, # d = 2
    centers=chosen_centers,
    cluster_std=2.5, # Set std of generated cluster points
    random_state=32, # Fix randomness
)

# First three rows of x_data
print("First three data points: \n", x_data[0:3], "\n")

# Clusters of first three data points
print("Labels of first three data points: \n", x_cluster[0:3], "\n")
```

First three data points:

```
[ [ 6.25214191 -1.46808492]
  [-9.46978032 -7.12935057]
  [-6.31577839 -6.69882724] ]
```

Labels of first three data points:

```
[3 0 0]
```

We can also visualize the data in a scatter plot using indexing. This plot will be explained later on.

```
import matplotlib.pyplot as plt

# Define parameters based on data arrays
K, d = np.shape(chosen_centers)

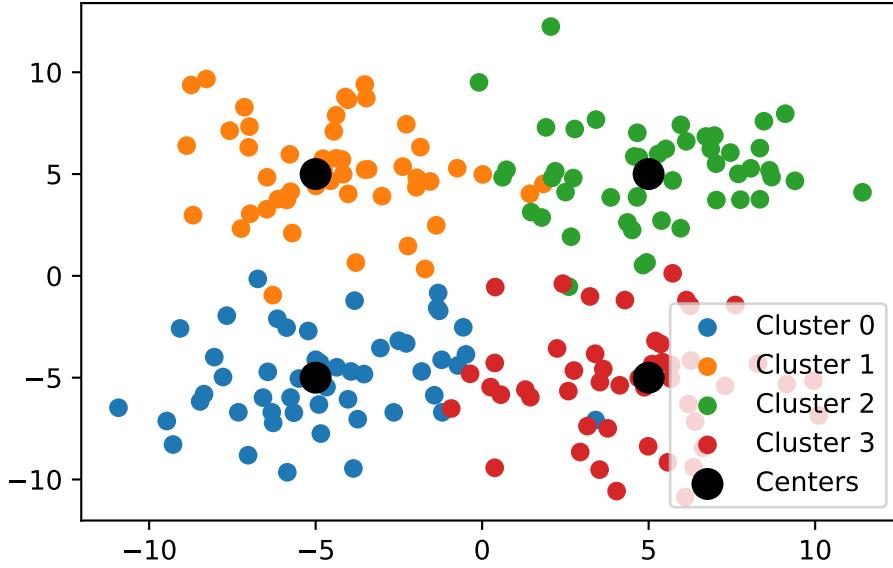
# Create figure()
plt.figure()

# Scatter points per cluster
for k in range(K):
    mask = (x_cluster == k) # Determine rows with label k
    # Plot x- against y-coordinate of points in R^2
    plt.scatter(x_data[mask,0],x_data[mask,1],label=f"Cluster {k}")

# Plot chosen centers
plt.scatter(chosen_centers[:,0], chosen_centers[:,1],
           linewidth=6, label="Centers", color='black')
```

```
# Create legend
plt.legend()

# Show plot
plt.show()
```



### 10.2.2 Clustering algorithm

Next assume that only the data points  $x_0, \dots, x_{n-1} \in \mathbb{R}^d$  are given to us, and our goal will be to compute centers and assign every data point to a cluster. We will do this using the K-means algorithm.

The  $K$ -means algorithm starts with initially chosen centers  $c_0, \dots, c_{K-1}$  and carries out the following two steps for  $T \in \mathbb{N}$  iterations:

1. Assign every data point  $x_i$  to its closest (in Euclidean distance) center from the set  $\{c_0, \dots, c_{K-1}\}$ , i.e., give  $x_i$  label

$$L_i = \operatorname{argmin}_{k=0, \dots, K-1} \|x_i - c_k\|_2$$

2. For  $k = 0, \dots, K-1$ , let  $G_k = \{i : L_i = k\}$  and compute new centers  $\hat{c}_k$  by the formula

$$\hat{c}_k = \frac{1}{|G_k|} \sum_{i \in G_k} x_i.$$

That is, the new center is the average of all points that are assigned the same label in Step 1. Set  $c_j \leftarrow \hat{c}_j$  and go back to Step 1.

This procedure has been implemented in Python in the `KMeans` class of the `sklearn.cluster` module. We first import and create an instance of this class. Below we explain the input keyword arguments.

```
from sklearn.cluster import KMeans

kmeans = KMeans(
    n_clusters=4, # Our parameter K
    init="random", # Choose initial clusters randomly from data points
    random_state=42, # Fix randomness
```

```

        n_init=5, # Number of runs of algorithm with initial clusters
        max_iter=300, # Our parameter T
    )

```

When creating an instance, we specify

- **n\_clusters**: Number of clusters/centers; this is our value  $K$ .
- **init**: Decides how initial cluster centers are chosen. Option '**random**' chooses them randomly from the list of data points.
- **random\_state**: Fixes the randomness used in the algorithm (comparable to setting a random seed).
- **n\_init**: Number of times algorithm is run with different initial centers (that are chosen according to the option specified in **init**). Clustering with lowest SSE (see above) is returned.
- **max\_iter**: Maximum number  $T$  of iterations performed by the  $K$ -means algorithm.

There are other input keyword arguments, and other options for the ones above; see the documentation. We remark that the algorithm implemented in the **KMeans** class actually stops prematurely before having done  $T$  iterations if no significant improvements are achieved in consecutive iterations.

We also note that the choice of  $K$  above is a modelling choice. We set it equal to  $K = 4$  because we know that our synthetic data is generated based on four centers, but in general, an appropriate choice of  $K$  might be less clear.

We next run the  $K$ -means algorithm on our data points using the **fit()** method. Executing this code will raise a **UserWarning** in Python, but you can ignore that for now. The method still executes correctly.

```
kmeans = kmeans.fit(x_data)
```

```
C:\Users\pskleer\AppData\Local\anaconda3\lib\site-packages\sklearn\cluster\_kmeans.py:1382: UserWarning:
```

```
KMeans is known to have a memory leak on Windows with MKL, when there are less chunks than available th
```

After fitting there are various attributes providing information about the clustering that was found, such as

- **cluster\_centers\_**: Gives the final cluster centers  $c_1, \dots, c_k$  at the end of the execution of the  $K$ -means algorithm

```

# Predicted clusters
pred_centers = kmeans.cluster_centers_

print(pred_centers)

```

```
[[ 4.50206784 -5.28714729]
 [ 5.18662428  4.92215083]
 [-4.52665943  5.36762011]
 [-4.74671502 -4.87353381]]
```

- **labels\_**: Specifies for every point the label/index of the center it is assigned to.

```

# Predicted clusters
pred_labels = kmeans.labels_

print(pred_labels)

```

```
[0 3 3 1 2 3 3 0 0 3 0 0 1 2 3 3 3 3 2 3 2 1 1 0 0 0 1 3 2 1 3 0 2 0 1
 1 3 3 0 1 2 3 0 0 0 3 1 0 1 0 0 0 2 3 0 0 1 0 1 2 3 1 2 0 1 1 2 3 2 3 1
 2 1 2 0 3 1 1 2 1 1 3 2 0 2 2 3 3 2 1 0 3 3 2 0 1 1 1 2 3 2 3 3 0 3 1
 3 2 2 0 0 0 2 3 1 2 0 3 0 2 0 0 1 1 2 2 0 0 2 0 1 1 1 1 2 2 3 3 1 1 1 2]
```

```
0 3 3 3 2 3 3 1 1 3 2 1 0 0 0 3 3 3 1 1 2 0 3 2 1 2 1 2 0 3 2 0 0 1 1 1 2  
2 2 3 2 3 0 2 3 2 1 3 1 0 1 2]
```

- `inertia_`: This gives the SSE of the run of the algorithm with lowest SSE (remember that we used `n_init` to specify how often to run the algorithm with random initial clusters).

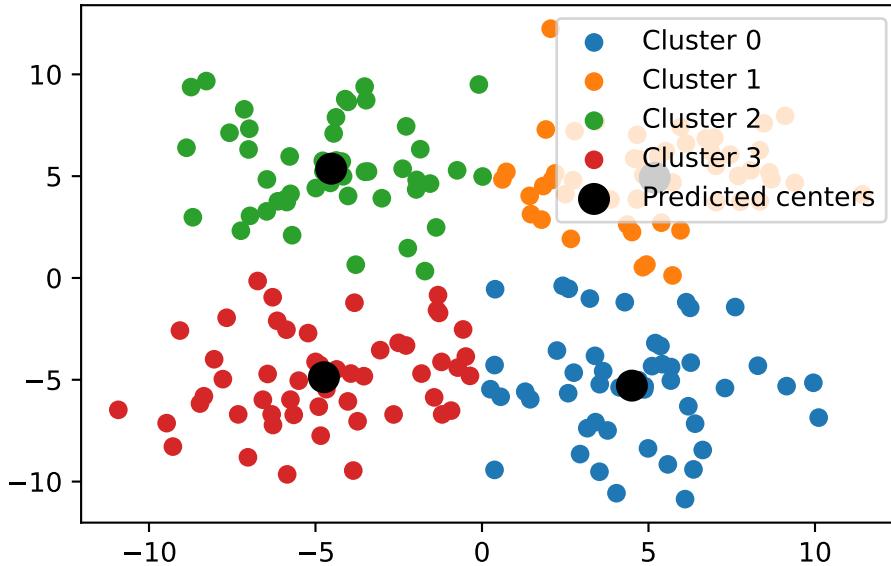
```
# SSE for best run of algorithm  
sse = kmeans.inertia_  
  
print("Sum of squared errors equals", sse)
```

```
Sum of squared errors equals 2349.1338559122655
```

### 10.2.3 Visualization

We can visualize the data as before using the following code. Below we plot all the data points that are clustered together with the same color.

```
import matplotlib.pyplot as plt  
  
# Define parameters based on data arrays  
K, d = np.shape(chosen_centers)  
  
# Create figure()  
plt.figure()  
  
# Scatter points per cluster  
for k in range(K):  
    mask = (pred_labels == k) # Determine rows with label k  
    # Plot x- against y-coordinate of two-dimensional points  
    plt.scatter(x_data[mask,0],x_data[mask,1],label=f"Cluster {k}")  
  
# Plot predicted centers  
plt.scatter(pred_centers[:,0], pred_centers[:,1],  
            linewidth=6, label="Predicted centers", color='black')  
  
# Create legend  
plt.legend()  
  
# Show plot  
plt.show()
```



The figure above is created by looping over the  $K = 4$  label choices that we have. Within the `for`-loop over  $k$ , we first create a Boolean array that indicates for every  $i = 0, \dots, n - 1$  whether its predicted label  $L_i$  equals  $k$  at the end of the  $K$ -means algorithm (`True`) or not (`False`).

We then index the rows of  $x$  where the Boolean array is `True`, i.e., we access the data points that have label  $k$ . We scatter plot the first coordinates of these data points, found in the column `x_data[:, 0]`, against the second coordinates of these data points, found in the column `x_data[:, 1]`. Recall that the data points were stored as rows in `x_data`.

Finally, we plot the centers in a similar fashion (but no Boolean indexing is needed for that). We use the `color` keyword argument to color the dots of the centers black, and the `linewidth` keyword argument to create dots that are bigger than those of the data points.

We can also compare the locations of the cluster centers that were used for the data generation to the cluster centers found by the  $K$ -means algorithm. As you can see from the figure, the  $K$ -means algorithm was able to relatively well find the clusters that were used to generate the data.

```

import matplotlib.pyplot as plt

# Create figure()
plt.figure()

# Plot chosen centers
plt.scatter(chosen_centers[:,0], chosen_centers[:,1],
           linewidth=6, label="Chosen centers", color='black')

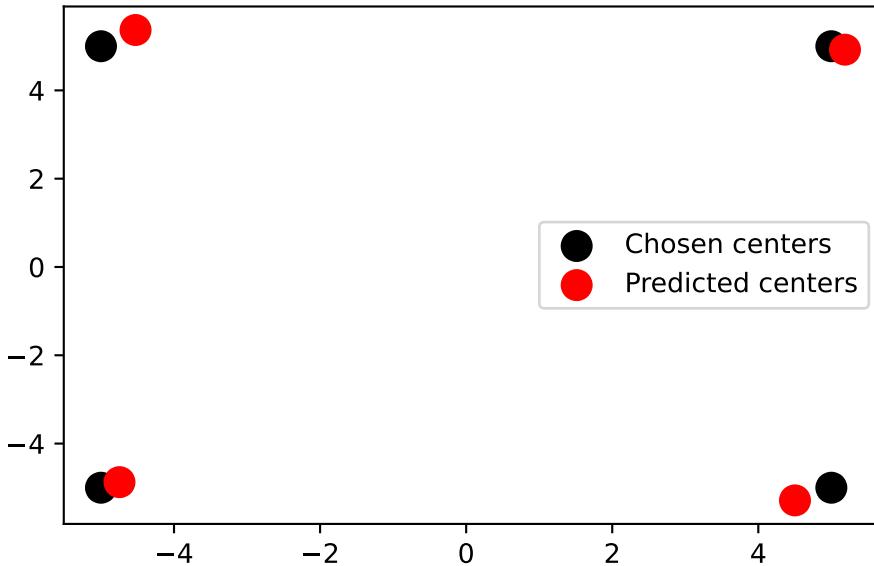
# Plot predicted centers
plt.scatter(pred_centers[:,0], pred_centers[:,1],
           linewidth=6, label="Predicted centers", color='red')

# Create legend
plt.legend()

# Show plot

```

```
plt.show()
```



We emphasize that, in general, clustering is typically classified as an unsupervised learning problem, meaning that it is not assumed that for every data point there is some “ground truth” label that is assigned to it. Instead, the goal is merely to group similar data points together without an underlying prior assumption about what makes them similar (although you might identify such criteria after having run a clustering algorithm).

Furthermore, we assumed that there were going to be  $K = 4$  clusters based on the data generation that we did using `make_blobs`. In general, however, if you are not aware of where the data comes from, it might not even be clear how many clusters  $K$  you should aim for.

### 10.3 Support vector machine (SVM)

Another learning problem, which has some flavours of the two problems in the previous sections, is that of linear classification in higher dimensions. We are given historical data  $(x_i, y_i)$  for  $i = 0, \dots, m - 1$  where each tuple consists of a data point  $x_i \in \mathbb{R}^d$  and label  $y_i \in \{-1, 1\}$ . The goal is to come up with a classification algorithm that for a new data point  $z \in \mathbb{R}^d$  decides for us whether the point should get label  $y = -1$  or  $y = 1$ .

The idea of support vector machines is to compute a vector  $w \in \mathbb{R}^d$  and  $b \in \mathbb{R}$ , and use the hyperplane  $w^T z + b = 0$  as a boundary for deciding what label a new data point gets. The point  $z$  gets label  $y = -1$  if  $w^T z + b \leq 0$  and label  $y = 1$  if  $w^T z + b > 0$ .

Among all the separating hyperlanes that can serve as such a boundary, we look for one that maximizes the “margin” between data points with different labels in the historical data. This idea will be made rigorous below.

#### 10.3.1 Input data

We consider the following historical data, which is also plotted below.

```
# Historical data
x_data = np.array([[3,3],[1.5,2.5],[1,2],[0.5,1.5],[2,2],[2,4],
```

```

[4,4],[2,6],[5,5.5],[7,6]]) # Data points

y_data = np.array([-1,-1,-1,-1,-1,
                   1,1,1,1]) # Labels

labels = [-1,1] # Distinct labels
colors = ['red','blue']

# Create figure()
plt.figure()

# Plot data points with given colors
for i in range(len(labels)):
    mask = (y_data == labels[i])
    plt.scatter(x_data[mask,0],x_data[mask,1],
                color=colors[i],
                label=f"Data points with label {labels[i]}")

# Set axes ranges
plt.xlim(0,8)
plt.ylim(0,7)

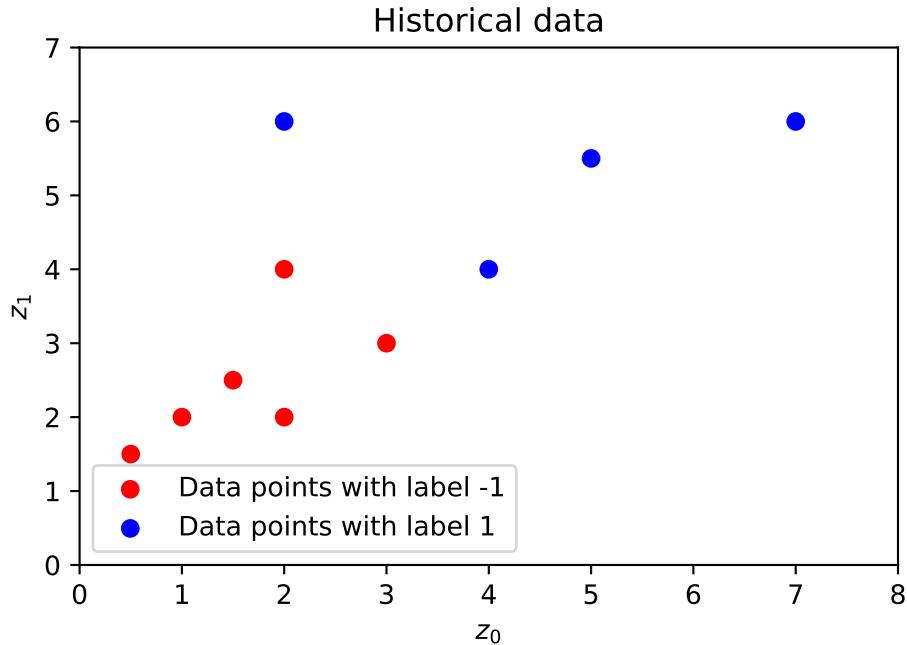
# Set axes labels
plt.xlabel('$z_0$')
plt.ylabel('$z_1$')

# Create legend
plt.legend()

# Create title
plt.title("Historical data")

# Show plot
plt.show()

```



Using the notation  $z = (z_0, z_1)$  for a general two-dimensional point in  $\mathbb{R}^2$ , a hyperplane separating the data would, for example, be  $0.9z_0 + 1.1z_1 - 7.5 = 0$ . We can write this hyperplane as  $w^T z + b = 0$  by defining  $w = [w_0, w_1] = [0.9, 1.1]$  and  $b = -7.5$ .

In the figure below, all the red points with label  $-1$  appear under the line, i.e., satisfy  $w^T z + b < 0$ , and all the points with label  $1$  satisfy  $w^T z + b > 0$ .

```

labels = [-1,1] # Distinct labels
colors = ['red','blue']

# Create figure()
plt.figure()

# Plot data points with given colors
for i in range(len(labels)):
    mask = (y_data == labels[i])
    plt.scatter(x_data[mask,0],x_data[mask,1],
                color=colors[i],
                label=f"Data points with label {labels[i]}")

# Plot hyperplane 0.9z_0 + 1.1z_1 - 7.5 = 0
w = np.array([0.9,1.1])
b = -7.5

z0 = np.linspace(0,8,100)
z1 = (-b-w[0]*z0)/w[1] # Rewrite z1 in terms of z0

plt.plot(z0,z1,label=f'${w[0]}z_0 + {w[1]}z_1 {b} = 0$')

# Set axes ranges
plt.xlim(0,8)

```

```

plt.ylim(0,7)

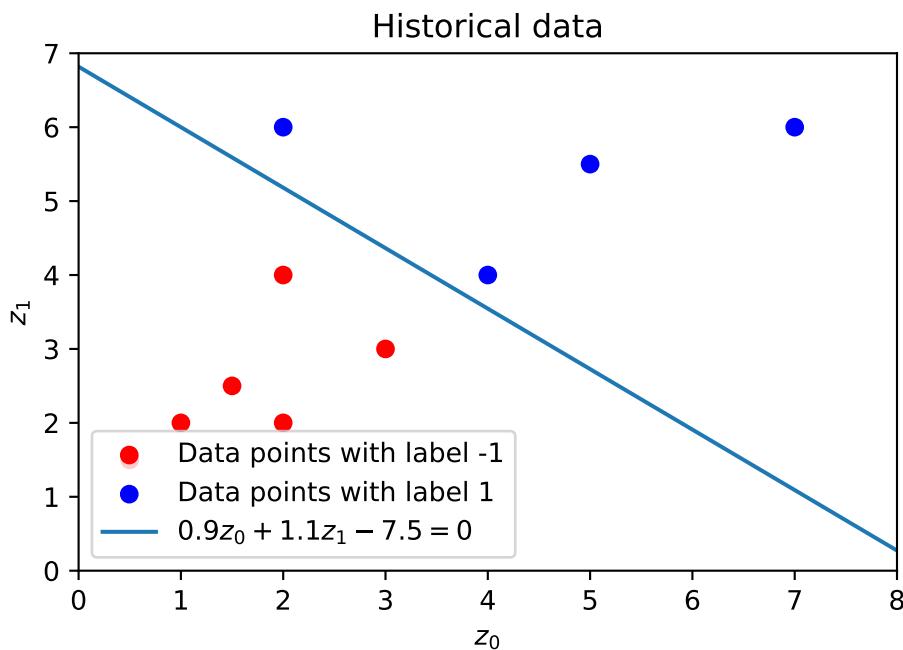
# Set axes labels
plt.xlabel('$z_0$')
plt.ylabel('$z_1$')

# Create legend
plt.legend()

# Create title
plt.title("Historical data")

# Show plot
plt.show()

```



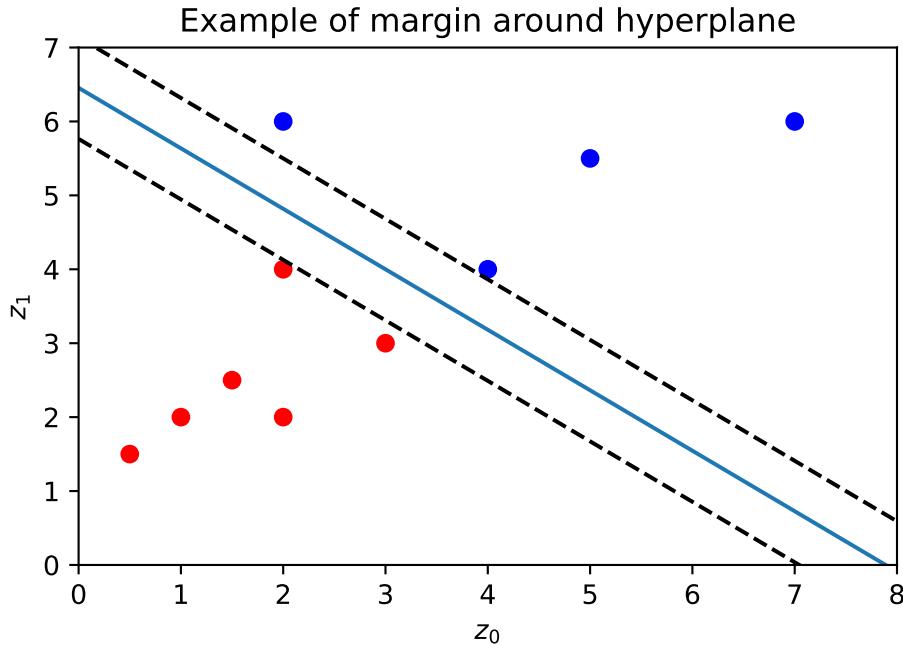
We remark at this point that a hyperplane  $w^T z + b = 0$  separating the historical data points with different labels might not exist. In that case we say that the data is non-separable. If a separating hyperplane exists, we call the data separable.

### 10.3.2 Classification model

You might have noticed that there exist multiple hyperplanes that separate the red point with label  $-1$  from the blue points with label  $1$ .

The goal of the support vector machine algorithm is to find the hyperplane that creates the largest margin between the hyperplane and the (perpendicular) closest data points on either side of the hyperplane. The points that are closest to the hyperplane are called the support vectors of the data.

The below figure illustrates this margin, which is the perpendicular distance between the two dashed lines, i.e., the width of the strip created by the two dashed lines.



It turns out that finding a separating hyperplane  $w^T z + b = 0$ , with  $w = [w_1, \dots, w_{d-1}] \in \mathbb{R}^d$  and  $b \in \mathbb{R}$  that maximizes the margin can be done by solving the minimization problem

$$\begin{aligned} & \min_{w_0, \dots, w_{d-1}, b} \sum_{i=0}^{d-1} w_i^2 \\ \text{s.t. } & y_i(w^T x_i + b) \geq 1 \quad \forall i \in \{0, \dots, m-1\} \end{aligned} .$$

Note that this optimization problem has an objective function that is quadratic in the  $w_i$ , and has constraints that are linear constraints in  $w_0, \dots, w_{d-1}$  and  $b$ . Recall that the tuples  $(x_i, y_i)$  are given input data. We will not give the derivation of this formulation here. You can look this up yourself if you are interested.

Solving the problem above can be done with the `LinearSVC` (linear support vector classification) class from the `sklearn.svm` module.

```
from sklearn.svm import LinearSVC
```

The algorithm implemented in the `LinearSVC` class actually solves a slightly different optimization problem. For a given parameters  $C > 0$ , and historical data  $\{(x_i, y_i)\}_{i=0}^{m-1}$ , it finds a solution to the unconstrained problem

$$\min_{w_0, \dots, w_{d-1}, b} \frac{1}{2} \sum_{i=0}^{d-1} w_i^2 + C \sum_{i=0}^{m-1} \max(0, 1 - y_i(w^T x_i + b)).$$

Comparing the two minimization problems, the constrained problem above strictly enforces the historical data points to be on the correct side of the hyperplane (i.e., they should be classified correctly). The unconstrained problem allows historical data points to be on the wrong side of the hyperplane (i.e., they might be misclassified), but penalizes these points in the objective function. The unconstrained problem can therefore also be used for instances with non-separable data, i.e., data for which a separating hyperplane does not exist.

For separable data, with guaranteed existence of a separating hyperplane, the two minimization problems become more or less equivalent as  $C \rightarrow \infty$ .

To solve the unconstrained optimization problem, we can apply the `fit()` function on an instance of the class `LinearSVC` (similar to how this was done to solve the clustering problem in the previous section).

We first create an instance, for which we set two properties. For other properties you can fix, see the documentation. We fix the value of  $C$  in the keyword argument `C`, and we fix the randomness using `random_state`. The randomness arises in the algorithm that is used by Python to solve the minimization problem.

```
# Create instance of linear support vector classification
separator = LinearSVC(C=30,random_state=42)
```

We next apply the `fit()` method on our instance.

```
# Historical data
x_data = np.array([[3,3],[1.5,2.5],[1,2],[0.5,1.5],[2,2],[2,4],
                  [4,4],[2,6],[5,5.5],[7,6]]) # Data points

y_data = np.array([-1,-1,-1,-1,-1,
                  1,1,1,1]) # Labels

separator = separator.fit(x_data,y_data)
```

```
C:\Users\pskleer\AppData\Local\anaconda3\lib\site-packages\sklearn\svm\_base.py:1244: ConvergenceWarning:
```

```
Liblinear failed to converge, increase the number of iterations.
```

As you see above, this did not work as the algorithm did not converge under the default settings.

Python suggests to increase the number of iterations of the underlying algorithm. We can do this with the `max_iter` keyword argument, whose default value is 1000 (see documentation).

```
# Increase iterations to ten thousand
separator = LinearSVC(C=30,random_state=42,max_iter=10000)

# Historical data
x_data = np.array([[3,3],[1.5,2.5],[1,2],[0.5,1.5],[2,2],[2,4],
                  [4,4],[2,6],[5,5.5],[7,6]]) # Data points

y_data = np.array([-1,-1,-1,-1,-1,
                  1,1,1,1]) # Labels

separator = separator.fit(x_data,y_data)
```

This time the algorithm converged.

The values of  $w = [w_0, \dots, w_{d-1}]$  and  $b$  can be accessed in the `coef_` and `intercept_` attributes, respectively, of the fitted instance. The reason we index these attributes at 0 is because of how they are returned by the `fit()` method. This is illustrated in the documentation below.

#### Attributes:

**coef\_** : ndarray of shape (1, n\_features) if n\_classes == 2 else (n\_classes, n\_features)

Weights assigned to the features (coefficients in the primal problem).

**coef\_** is a readonly property derived from `raw_coef_` that follows the internal memory layout of liblinear.

**intercept\_** : ndarray of shape (1,) if n\_classes == 2 else (n\_classes,)

Constants in decision function.

Figure 10.2: Attributes of fitted LinearSVC instance

```
# Obtain array w
w = separator.coef_[0]
print("Array w of hyperplane is", w)

# Obtain scalar b
b = separator.intercept_[0]
print("Scalar b of hyperplane is", b)
```

```
Array w of hyperplane is [0.79584228 0.83654119]
Scalar b of hyperplane is -5.719991167349982
```

### 10.3.3 Visualization

We can plot the fitted separating hyperplane using the code below. This code uses similar ideas as that we have seen in earlier sections in this chapter.

```
labels = [-1,1] # Distinct labels
colors = ['red','blue'] # Color names (strings) for plotting data points

# Create figure()
plt.figure()

# Plot data points with given colors
for i in range(len(labels)):
    mask = (y_data == labels[i])
    plt.scatter(x_data[mask,0], x_data[mask,1], color=colors[i])

# Rounded hyperplane coefficients
w = np.around(separator.coef_[0], decimals=2)
b = np.around(separator.intercept_[0], decimals=2)

# Arrays for plotting line
z0 = np.linspace(0,8,100)
z1 = (-b-w[0]*z0)/w[1] # Rewrite z1 in terms of z0

# Plotting hyperplane
plt.plot(z0,z1,label=f"${w[0]}z_0 + {w[1]}z_1 - {b} = 0$")

# Set axes ranges
plt.xlim(0,8)
```

```

plt.ylim(0,7)

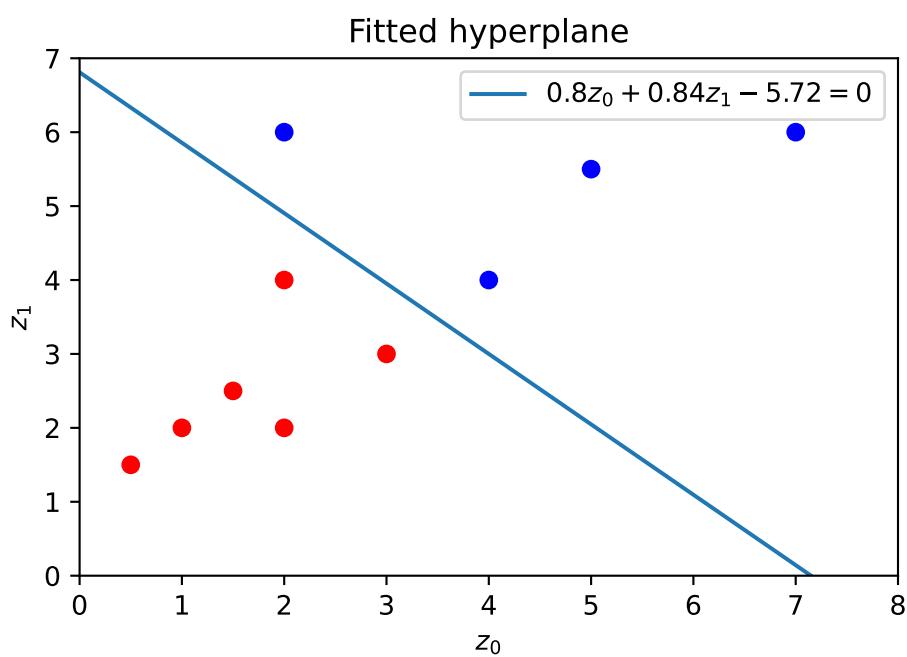
# Set axes labels
plt.xlabel('$z_0$')
plt.ylabel('$z_1$')

# Create legend()
plt.legend()

# Create title
plt.title("Fitted hyperplane")

# Show plot
plt.show()

```



# Chapter 11

## Higher-dimensional arrays

In this chapter we will look at arrays whose dimension is three or higher, as opposed to the one- and two-dimensional arrays we have seen so far. Many Python functions that we have seen also can be used on higher dimensional arrays.

```
import numpy as np
```

### 11.1 Creating arrays

Recall that a two-dimensional array is a list of one-dimensional lists. In the same way a three-dimensional array is a list of two-dimensional arrays (which in turn are lists of one-dimensional arrays). A four-dimensional array is a list of three-dimensional arrays, etc.

Let us create a three-dimensional array.

```
A = np.array([
    [[10, 5, 2, 5],
     [19, 3, 16, 1],
     [9, 5, 2, 4]],
    [[11, 2, 9, 2],
     [29, 2, 89, 9],
     [7, 7, 3, 8]]
])

print(A)
```

```
[[[10  5  2  5]
  [19  3  16  1]
  [ 9  5  2  4]]

 [[11  2  9  2]
  [29  2  89  9]
  [ 7  7  3  8]]]
```

Note that the shape of  $A$  is  $2 \times 3 \times 4$ . This is because the outer list consists of two lists (the two-dimensional arrays), and every one of those lists contains again three lists (the one-dimensional arrays), and these in turn all have 4 elements.

```
print("The shape of A is ", np.shape(A))
```

The shape of A is (2, 3, 4)

Below we have given a visual representation of the array above, with the idea that the white boxes represent the first two-dimensional array, and the shaded boxes the second two-dimensional array.

We have also indicated the axes corresponding to the dimensions of the array in the figure below. The outer list corresponds to the 0-axis, the first inner list to the 1-axis, etc. We will come back to those later in this chapter.

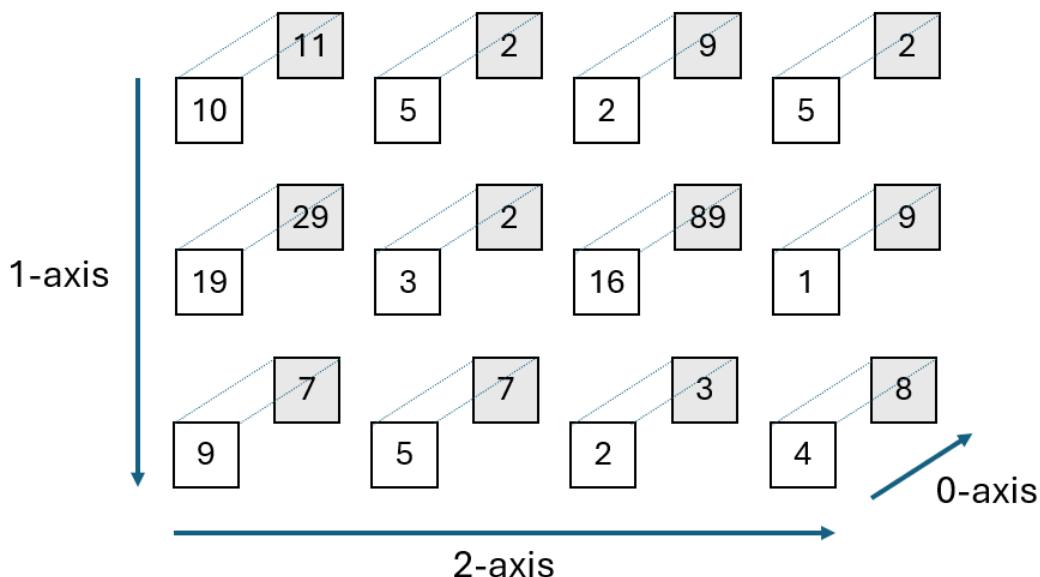


Figure 11.1: Three-dimensional  $2 \times 3 \times 4$  array.

We can index three-dimensional arrays in a similar way as we do two-dimensional arrays.

```
# Print two-dimensional array at index 0
print(A[0])
```

```
[[10  5  2  5]
 [19  3  16  1]
 [ 9  5  2  4]]
```

```
# Print row at index 2 of two-dimensional array at index 1
print(A[1,2,:])
```

```
[7 7 3 8]
```

```
# Print element at index 0 of row A[1,2]
print(A[0,2,3])
```

4

An overview of all the indices of a  $2 \times 3 \times 4$  array is given in the figure below.

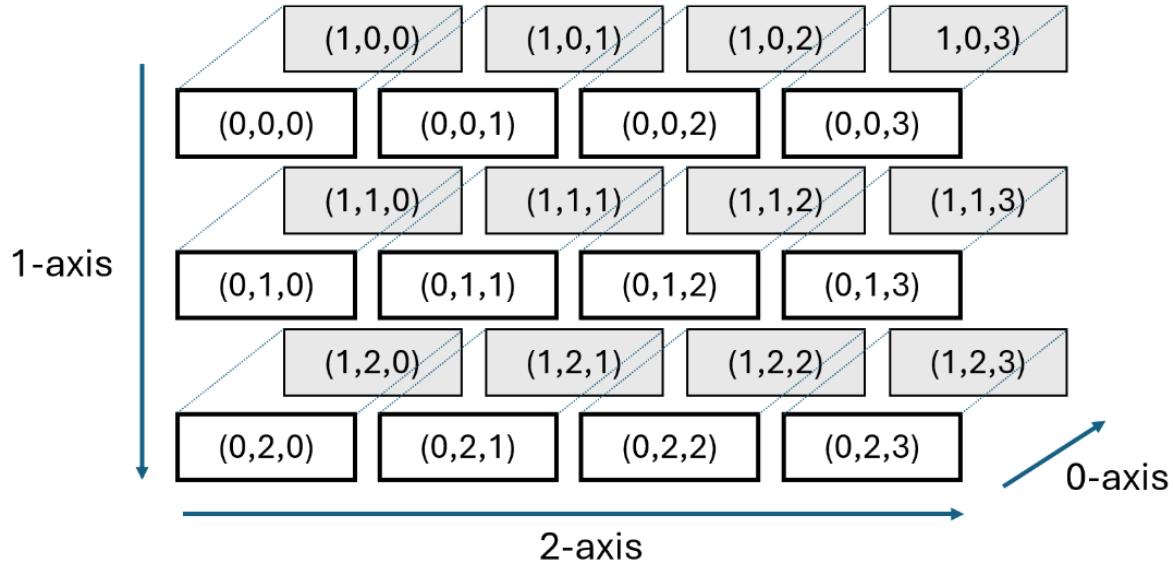


Figure 11.2: Visualization of indices of  $2 \times 3 \times 4$  array.

We can also use index slicing.

```
# Print from both two-dimensional arrays
# the rows at indices 0 and 1
# and columns at indices 1 and 2
print(A[:,0:2,1:3])
```

```
[[[ 5  2]
 [ 3 16]]

 [[ 2  9]
 [ 2 89]]]
```

We can also create special arrays in higher dimensions, like the all-ones array.

```
# Create 3 x 4 x 2 array with ones (works with np.zeros() as well)
B = np.ones((3,4,2))

print(B)
```

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

 [[1. 1.]
 [1. 1.]
 [1. 1.]
 [1. 1.]]

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

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

Also, concepts like broadcasting work in higher dimensions. Below we add a two-dimensional array to a three-dimensional array, in which case the two-dimensional array gets added to each of the three inner two-dimensional arrays.

```
C = np.array([
    [0, 0],
    [2, 2],
    [3, 3],
    [1, 1]])

print(B + C) # Add two- to three-dimensional array
```

```
[[[1. 1.]
  [3. 3.]
  [4. 4.]
  [2. 2.]]

 [[1. 1.]
  [3. 3.]
  [4. 4.]
  [2. 2.]]

 [[1. 1.]
  [3. 3.]
  [4. 4.]
  [2. 2.]]]
```

Functions like `mgrid` also work in higher dimensions. For example, we can create a three-dimensional grid of all points in  $\{1, 2\} \times \{2, 3, 4\} \times \{4, 5, 6\}$  as follows.

```
# Recall that the end index of a slice is not included
X, Y, Z = np.mgrid[1:3,2:5,4:7]

print("X =\n",X)
print("Y =\n",Y)
print("Z =\n",Z)
```

```
X =
[[[1 1 1]
  [1 1 1]
  [1 1 1]]
```

```
  [[2 2 2]
  [2 2 2]
  [2 2 2]]]
```

```
Y =
[[[2 2 2]
  [3 3 3]
  [4 4 4]]
```

```
  [[2 2 2]
  [3 3 3]
  [4 4 4]]]
```

```

Z =
[[[4 5 6]
 [4 5 6]
 [4 5 6]]

 [[4 5 6]
 [4 5 6]
 [4 5 6]]]

```

For every (feasible) combination of indices  $(i, j, k)$ , the point  $(X_{ijk}, Y_{ijk}, Z_{ijk})$  now corresponds to a grid point in  $\{1, 2\} \times \{2, 3, 4\} \times \{4, 5, 6\}$ . You can also create a more fine-grained grid, by including more points in every slice using a step size.

## 11.2 Itertools

A tool that is useful for enumerating all points in a higher-dimensional set is the `itertools` package.

```
import itertools
```

Let's consider again the set of points in  $\{1, 2\} \times \{2, 3, 4\} \times \{4, 5, 6\}$ . We can enumerate over all such points using the `product` function, that takes as input the ranges of the individual coordinates and outputs all possible combinations as tuples.

```

x = np.array([1,2])
y = np.array([2,3,4])
z = np.array([4,6])

for point in itertools.product(x,y,z):
    print(point)

```

```

(1, 2, 4)
(1, 2, 6)
(1, 3, 4)
(1, 3, 6)
(1, 4, 4)
(1, 4, 6)
(2, 2, 4)
(2, 2, 6)
(2, 3, 4)
(2, 3, 6)
(2, 4, 4)
(2, 4, 6)

```

You can also have the combinations be returned as arrays.

```

x = np.array([1,2])
y = np.array([2,3,4])
z = np.array([4,6])

for point in itertools.product(x,y,z):
    print(np.array(point))

```

```

[1 2 4]
[1 2 6]

```

```
[1 3 4]
[1 3 6]
[1 4 4]
[1 4 6]
[2 2 4]
[2 2 6]
[2 3 4]
[2 3 6]
[2 4 4]
[2 4 6]
```

If the sets of all coordinates are the same, you can also use the `repeat` keyword argument. Suppose we want to enumerate all points in the set  $\{1, 3, 5\}^4$ . Then we can do the following.

```
a = np.array([1,3,5])
k = 4

for point in itertools.product(a, repeat=k):
    print(point)
```

```
(1, 1, 1, 1)
(1, 1, 1, 3)
(1, 1, 1, 5)
(1, 1, 3, 1)
(1, 1, 3, 3)
(1, 1, 3, 5)
(1, 1, 5, 1)
(1, 1, 5, 3)
(1, 1, 5, 5)
(1, 3, 1, 1)
(1, 3, 1, 3)
(1, 3, 1, 5)
(1, 3, 3, 1)
(1, 3, 3, 3)
(1, 3, 3, 5)
(1, 3, 5, 1)
(1, 3, 5, 3)
(1, 3, 5, 5)
(1, 5, 1, 1)
(1, 5, 1, 3)
(1, 5, 1, 5)
(1, 5, 3, 1)
(1, 5, 3, 3)
(1, 5, 3, 5)
(1, 5, 5, 1)
(1, 5, 5, 3)
(1, 5, 5, 5)
(3, 1, 1, 1)
(3, 1, 1, 3)
(3, 1, 1, 5)
(3, 1, 3, 1)
(3, 1, 3, 3)
(3, 1, 3, 5)
(3, 1, 5, 1)
```

```
(3, 1, 5, 3)
(3, 1, 5, 5)
(3, 3, 1, 1)
(3, 3, 1, 3)
(3, 3, 1, 5)
(3, 3, 3, 1)
(3, 3, 3, 3)
(3, 3, 3, 5)
(3, 3, 5, 1)
(3, 3, 5, 3)
(3, 3, 5, 5)
(3, 5, 1, 1)
(3, 5, 1, 3)
(3, 5, 1, 5)
(3, 5, 3, 1)
(3, 5, 3, 3)
(3, 5, 3, 5)
(3, 5, 5, 1)
(3, 5, 5, 3)
(3, 5, 5, 5)
(5, 1, 1, 1)
(5, 1, 1, 3)
(5, 1, 1, 5)
(5, 1, 3, 1)
(5, 1, 3, 3)
(5, 1, 3, 5)
(5, 1, 5, 1)
(5, 1, 5, 3)
(5, 1, 5, 5)
(5, 3, 1, 1)
(5, 3, 1, 3)
(5, 3, 1, 5)
(5, 3, 3, 1)
(5, 3, 3, 3)
(5, 3, 3, 5)
(5, 3, 5, 1)
(5, 3, 5, 3)
(5, 3, 5, 5)
(5, 5, 1, 1)
(5, 5, 1, 3)
(5, 5, 1, 5)
(5, 5, 3, 1)
(5, 5, 3, 3)
(5, 5, 3, 5)
(5, 5, 5, 1)
(5, 5, 5, 3)
(5, 5, 5, 5)
```

Note that the `product` function gives a convenient way to enumerate over all entries in a  $k$ -dimensional array that has size  $n$  in all dimensions.

```
A = np.array([
    [[10, 5, 4],
```

```

[19,3,1],
[9,5,7]
],
[[11,2,3],
[29,2,1],
[7,7,0]
],
[[11,2,3],
[29,12,1],
[17,70,0]
]])

```

```

k = np.ndim(A) # Number of dimensions

n, *_ = np.shape(A) # Common size of every dimension

for point in itertools.product(range(n),repeat=k):
    print(A[point]) # Print entry as position 'point'

```

```

10
5
4
19
3
1
9
5
7
11
2
3
29
2
1
7
7
0
11
2
3
29
12
1
17
70
0

```

### 11.3 Axis operations

We can also perform operations along axes in higher dimensional arrays. The outer list of an array corresponds to the 0-axis, the second outer list to the 1-axis, etc.

Below we again give the visualization of the axes of a three-dimensional array, where the coordinates in the

boxes represent the position of an element in the array.

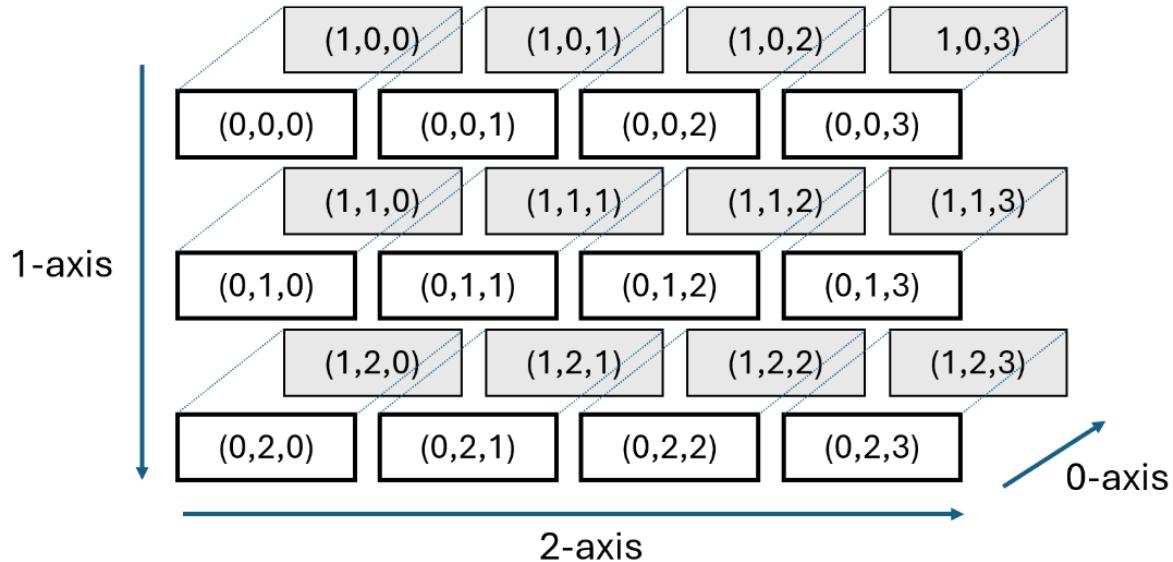


Figure 11.3: Visualization of indices of  $2 \times 3 \times 4$  array.

### 11.3.1 Arithmetic operations

If you perform an operation like summing elements along an axis of a  $k$ -dimensional array, you end up with a  $(k - 1)$ -dimensional array.

```
A = np.array([
    [[10, 5, 2, 5],
     [19, 3, 16, 1],
     [9, 5, 2, 4]],
    [[11, 2, 9, 2],
     [29, 2, 89, 9],
     [7, 7, 3, 8]]
])

print("A = \n", A)
```

```
A =
[[[10  5  2  5]
 [19  3 16  1]
 [ 9  5  2  4]]

 [[11  2  9  2]
 [29  2 89  9]
 [ 7  7  3  8]]]

print("Summing along 0-axis: \n", np.sum(A, axis=0))
```

```
Summing along 0-axis:
[[ 21   7  11   7]
 [ 48   5 105  10]
 [ 16  12   5  12]]
```

```
print("Summing along 1-axis: \n", np.sum(A, axis=1))
```

```
Summing along 1-axis:  
[[ 38  13  20  10]  
 [ 47  11  101  19]]
```

```
print("Summing along 2-axis: \n", np.sum(A, axis=2))
```

```
Summing along 2-axis:  
[[ 22  39  20]  
 [ 24 129  25]]
```

Note that in the last command, Python sums along the second axis, reducing the original  $2 \times 3 \times 4$  array to a  $2 \times 3$  array.

You can also fix the dimensions, so that the new array after summing remains a  $k$ -dimensional array. You can achieve this by setting the keyword argument `keepdims` to `True` (the default is `False`).

```
print("Summing along 2-axis fixing dimension: \n",  
      np.sum(A, axis=2, keepdims=True))
```

```
Summing along 2-axis fixing dimension:  
[[[ 22]  
 [ 39]  
 [ 20]]  
  
 [[ 24]  
 [129]  
 [ 25]]]
```

### 11.3.2 Reshaping

We can also shape higher dimensional arrays into other higher dimensional arrays. In earlier chapters, we have seen how to reshape a two-dimensional array into a two-dimensional array of a different shape, or into a one-dimensional array.

```
A = np.array([[5,1,3,2,3,2],[5,2,9,3,8,5]])  
print("A = \n",A)
```

```
A =  
[[5 1 3 2 3 2]  
 [5 2 9 3 8 5]]
```

```
x = A.flatten() # Turn A into one-dimensional array of shape (12,)  
print("x = \n",x)
```

```
x =  
[5 1 3 2 3 2 5 2 9 3 8 5]
```

```
y = A.reshape(1,12) # Turn A into two-dimensional array of shape (1,12)  
print("y = \n",y)
```

```
y =  
[[5 1 3 2 3 2 5 2 9 3 8 5]]
```

```
B = A.reshape(4,3) # Reshape A to 4 x 3 array
print("B = \n",B)
```

```
B =
[[5 1 3]
 [2 3 2]
 [5 2 9]
 [3 8 5]]
```

Recall that reshaping happens according to the largest axis (index) changing fastest principle. This means that when reshaping  $A$  into  $B$ , the matrix  $B$  gets filled in a row-by-row fashion (starting with the lowest row index) by placing in it the elements from  $A$  taken row-by-row.

That is, we fill the entries in  $B$  in the order

$$(0,0), (0,1), (0,2), (1,0), (1,1), (1,2), (2,0), (2,1), (2,2), (3,0), (3,1), (3,2)$$

with the elements of  $A$  taken in the order

$$(0,0), (0,1), (0,2), (0,3), (0,4), (0,5), (1,0), (1,1), (1,2), (1,3), (1,4), (1,5).$$

We can also reshape, e.g., a three-dimensional array  $A$  into a two-dimensional array  $B$ . Because of the largest axis (index) changing fastest principle, this means the matrix  $B$  is again filled in a row-by-row fashion (i.e., along the 1-axis first; note that  $B$  has a 0- and 1-axis only).

The largest axis (index) changing fastest principle also applies to  $A$ , meaning that we start taking the entries from  $A$  first along its 2-axis, with index 0 for both the 0- and 1-axis. In other words, we start by taking entries from row  $A[0,0,:]$ .

More concrete, we first take the entries 10, 5, 2 from the row  $A[0,0,:]$  and place them on the first row of  $B$ . Then we take the last element from this row, 5, and move up one index on the 1-axis (to the second row of the first two-dimensional array), and take the entries 19 and 3. Together with the 5 from the first row, these entries are placed on the second row of  $B$ . Once we have exhausted all the entries of the first two-dimensional array of  $A$ , we switch to the second two-dimensional array, i.e., we increase the index along the 0-axis by one.

```
A = np.array([
 [[10,5,2,5],
 [19,3,16,1],
 [9,5,2,4]],
 [[11,2,9,2],
 [29,2,89,9],
 [7,7,3,8]
 ]])
```

```
print("A = \n",A)
```

```
A =
[[[10  5  2  5]
 [19  3 16  1]
 [ 9  5  2  4]]

 [[11  2  9  2]
 [29  2 89  9]
 [ 7  7  3  8]]]
```

```
B = A.reshape((8,3))
print("Reshaping A into 8 x 3 array B = \n",B)
```

```
Reshaping A into 8 x 3 array B =
[[10  5  2]
 [ 5 19  3]
 [16  1  9]
 [ 5  2  4]
 [11  2  9]
 [ 2 29  2]
 [89  9  7]
 [ 7  3  8]]
```

We can also reshape a three-dimensional array into another three-dimensional array (with the same number of elements). Make sure you understand how, in the example below, the entries of  $A$  are used to fill the array  $B$ .

```
C = A.reshape((2,2,6))
print("Reshaping A into 2 x 2 x 6 array C = \n",C)
```

```
Reshaping A into 2 x 2 x 6 array C =
[[[10  5  2  5 19  3]
 [16  1  9  5  2  4]]
 [[11  2  9  2 29  2]
 [89  9  7  7  3  8]]]
```

## 11.4 Unpacking

Sometimes the number of input arguments of a function only becomes clear after a user has set some input data.

For example, suppose we want to generate a  $k$ -dimensional grid, i.e., the points in

$$\prod_{i=0}^{k-1} \{a_i, a_i + 1, \dots, b_i - 1, b_i\}$$

for given values of  $a_0, \dots, a_{k-1}, b_0, \dots, b_{k-1}$  with the `meshgrid()` function from NumPy. The `meshgrid()` function takes as input  $k$  ranges, and then generates a  $k$ -dimensional grid with those ranges. We have already seen the function `mgird()` in an earlier chapter that achieves the same, but whose syntax is different.

Below all the points in the set

$$\{1, 2, 3\} \times \{9, 10\} = \{(1, 9), (1, 10), (2, 9), (2, 10), (3, 9), (3, 10)\}$$

are generated. The first coordinate  $i$  of every point  $(i, j) \in \{1, 2, 3\} \times \{9, 10\}$  is stored in the first two-dimensional array, and the second coordinate  $j$  in the second two-dimensional array. The sampe principle applies for higher-dimensional grids.

```
# a_0 = 1, b_0 = 3, a_1 = 9, b_1 = 10
range1 = np.array([1,2,3]) # np.arange(1,3+1)
range2 = np.array([9,10]) # np.arange(9,10+1)

x = np.meshgrid(range1,range2)
```

```

print(x)

[array([[1, 2, 3],
       [1, 2, 3]], array([[ 9,  9,  9],
       [10, 10, 10]]])

```

Suppose now we want to generate a three-dimensional grid  $\{1, 2, 3\} \times \{9, 10\} \times \{5, 6\}$ , then we need to add another range variable `range3`, but also adjust the variable `x` by adding the new range to it as input argument.

```

range1 = np.array([1,2,3])
range2 = np.array([9,10])
range3 = np.array([5,6])

x = np.meshgrid(range1,range2,range3)

print(x)

[array([[[1, 1],
         [2, 2],
         [3, 3]],

        [[[1, 1],
          [2, 2],
          [3, 3]]], array([[[[ 9,  9],
          [ 9,  9],
          [ 9,  9]],

         [[[10, 10],
           [10, 10],
           [10, 10]]], array([[[[5, 6],
           [5, 6],
           [5, 6]]])])

```

We can avoid having to adjust `x`, if we instead store the ranges in a list (or array). We name this list `ranges` here. We can unpack the elements in the list `ranges` as input arguments of the `meshgrid()` function using `*ranges`.

Unpacking the elements of a list or array, done with the `*`, means that the first element in the list, in our case the array with the first range, becomes the first input argument of `meshgrid()`, the second element of the list becomes the second input argument, etc.

We show this in the code below, which gives the same output as the code above.

```

ranges = [np.array([1,2,3]),np.array([9,10]),np.array([5,6])]

x = np.meshgrid(*ranges)

print(x)

[array([[[1, 1],
         [2, 2],
         [3, 3]],

        [[[1, 1],
          [2, 2],
          [3, 3]]], array([[[[ 9,  9],
          [ 9,  9],
          [ 9,  9]],

         [[[10, 10],
           [10, 10],
           [10, 10]]], array([[[[5, 6],
           [5, 6],
           [5, 6]]])])

```

[array([[[1, 1],

```

[2, 2],
[3, 3]],

[[1, 1],
 [2, 2],
 [3, 3]]], array([[[ 9,  9],
 [ 9,  9],
 [ 9,  9]],

[[10, 10],
 [10, 10],
 [10, 10]]]), array([[[5, 6],
 [5, 6],
 [5, 6]]])

```

The use of unpacking is especially useful if the number of ranges only becomes clear after some input parameter has been chosen. For example, suppose we want to generate the  $k$ -dimensional binary grid  $\{0,1\}^k$ .

In the code below we only have to adjust the value of  $k$  if we want to increase the dimension of the grid. This you can not achieve without the use of unpacking, in general.

We first generate a two-dimensional array (recall this is a list of lists) `ranges`, where each of the  $k$  rows of this array is the two-element list  $[0,1]$ . We then unpack these ranges as input arguments of `meshgrid()` using `*ranges`.

```

k = 3
ranges = np.hstack((np.zeros((k,1)),np.ones((k,1)))) 

x = np.meshgrid(*ranges)

print(x)

[array([[0., 0.],
       [1., 1.]],

[[0., 0.],
 [1., 1.]]], array([[[0., 0.],
 [0., 0.]],

[[1., 1.],
 [1., 1.]]], array([[[0., 1.],
 [0., 1.]],

[[0., 1.],
 [0., 1.]]])

```

# Appendix A

## Corrections and changes

This chapter contains a list of corrections and changes that were made during the teaching of the Python II module. If you spot a spelling error or mistake, feel free to let the teacher know! This will improve the quality of the book in the future significantly.

### A.1 Chapter 11

- The Itertools-section is now Section 11.2 (was Section 11.3 before).

### A.2 Section 8.2.1

- Added explanation of how to generate vectorized samples when multiple location-scale combinations are inputted.

### A.3 Section 3.2.2

- `mgrid()` explanation is moved to Chapter 5.

### A.4 Section 4.3.1

- Corrected the explanation of `np.argsort()`.

### A.5 Section 3.5

- Corrected `M_repeat = np.tile(M,3)` by `M_repeat = np.repeat(M,3)`
- Corrected `vstack(a,b)` to `vstack((a,b))`.
- Corrected `hstack(a,b)` to `hstack((a,b))`.

# Appendix B

## Function basics

In this chapter we will explain some basic commands for Python functions defined using `def`.

### B.1 Output arguments

Suppose we have a function that takes two inputs, and yields four outputs.

```
def f(a,b):
    return a + b, a - b, a*b, a/b

a = 5
b = 3
```

There are various ways to get one or more specific outputs from Python.

```
# Returns all output variables in tuple
output = f(a,b)

print(output)
```

(8, 2, 15, 1.6666666666666667)

```
# Store outputs in variables w, x, y and z
w, x, y, z = f(a,b)

print(w, x, y, z)
```

8 2 15 1.6666666666666667

We can suppress one or more output arguments using `_`.

```
# Only store first and last output
w, _, _, z = f(a,b)

print(w, z)
```

8 1.6666666666666667

If we only want the first output, and suppress the other ones, we can use `*_`

```
# Only store first output
x, *_ = f(a,b) # This is the same as x, _, _, _ = f(a,b)

print(x)
```

8

If we only want the first two outputs, and suppress the remaining ones, we can do something similar.

```
# Only store first output
w, x, *_ = f(a,b) # This is the same as w, x, _, _ = f(a,b)

print(w,x)
```

8 2

If we only want the last output, we can do the following.

```
# Only store last output
*_ , z = f(a,b) # This is the same as _, _, _, z = f(a,b)

print(z)
```

1.6666666666666667

Also here, if we would like the last two outputs, we can do the following.

```
# Only store last output
*_ , y, z = f(a,b) # This is the same as _, _, y, z = f(a,b)

print(y,z)
```

15 1.6666666666666667