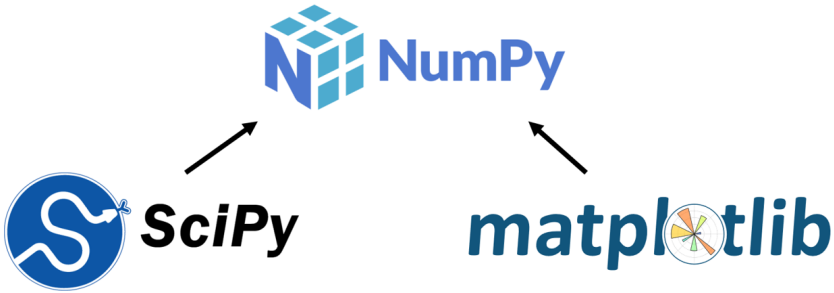
Programming for Essential Digital Skills, Part 2

Pieter Kleer

2025

Chapter 9 - Mathematics and plotting

Data science with Python



Mathematical tasks:
- Root finding
- Optimization
- Integration
- Linear algebra

Visualization and plotting:
- Function plotting
- Data visualization
- 3D-plotting

SciPy: Scientific Computing with Python

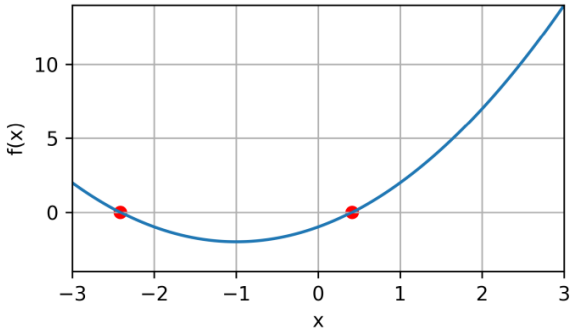
Subpackages

SciPy is organized into subpackages covering different scientific computing domains. These are summarized in the following table:

Subpackage	Description
`cluster`	Clustering algorithms
`constants`	Physical and mathematical constants
`fft`	Discrete Fourier transforms
`fftpack`	Fast Fourier Transform routines (legacy)
`integrate`	Integration and ordinary differential equation solvers
`interpolate`	Interpolation and smoothing splines
`io`	Input and Output
`linalg`	Linear algebra
`ndimage`	N-dimensional image processing
`odr`	Orthogonal distance regression
`optimize`	Optimization and root-finding routines

Root finding

Consider $f(x) = x^2 + 2x - 1$. A root x of the function f is a point that satisfies $f(x) = 0$.



Solving the equation $f(x) = 0$ using `fsolve()`

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```
# Import optimize package from SciPy

# Define f as Python function

# Use fsolve() to solve f(x) = 0 with initial guess

# Print the found root
```

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```
import scipy.optimize as optimize

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

guess = 3
f_zero = optimize.fsolve(f,guess)[0]

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

```
A root of the function f is given by 0.41421356237309503
```

Solving the equation $f(x) = 3$

Suppose we want to solve $f(x) = 3$. **Question:** How to do this with root finding?

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- If we define $g(x) = f(x) - 3$, then $g(x) = 0$ if and only if $f(x) = 3$.

```
def g(x):
    return f(x) - 3

guess = 4
f_zero = optimize.fsolve(g,guess)[0]

print("A number x satisfying f(x) = 3, is given by", f_zero)
```

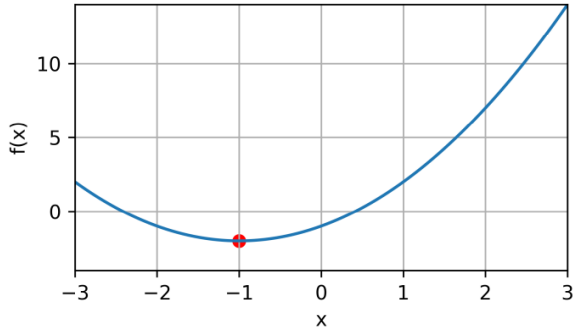
```
A number x satisfying f(x) = 3, is given by 1.2360679774998171
```

Solving the equation $f(x) = c$

```
def solve_eq(f,c,guess):
    # This function returns the solution to f(x) = c using
    # fsolve() on the function g(x) = f(x) - c

    def g(x):
        return f(x) - c

    x = optimize.fsolve(g,guess)[0]
    return x
```

Minimizing a function f

Consider $f(x) = x^2 + 2x - 1$. Minimum of f is a point x for which $f(x)$ is smallest.



Computing a minimum of f using `fmin()`

```
import scipy.optimize as optimize

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

guess = 1
minimum = optimize.fmin(f,guess)

print('The minimum of the function f is attained at x = ', minimum)
```

```
Optimization terminated successfully.
         Current function value: -2.000000
         Iterations: 19
         Function evaluations: 38
The minimum of the function f is attained at x =  [-1.]
```

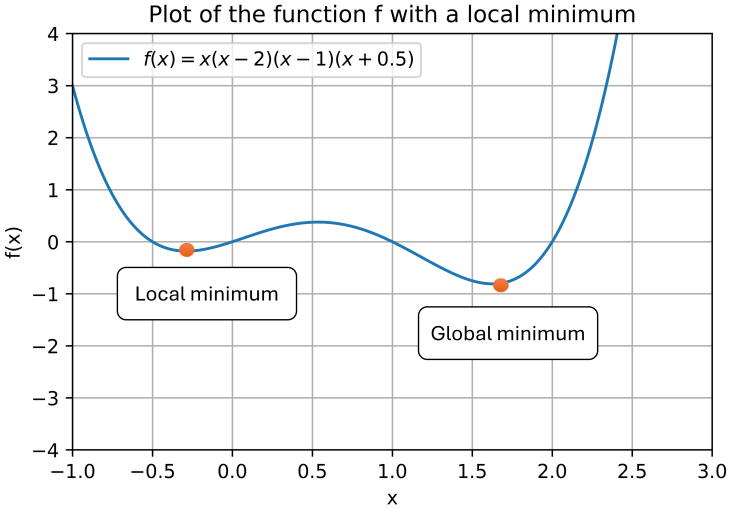
Computing a minimum of f using `fmin()`

```
import scipy.optimize as optimize

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

guess = 1
minimum = optimize.fmin(f,guess,disp=False)[0]

print('The minimum of the function f is attained at x = ', minimum)
```

```
The minimum of the function f is attained at x =  -1.0000000000000018
```

Local vs. global minima

`fmin()` might return a "local" minimum, which is not the true minimum of the function.



Matplotlib: Data visualization

Matplotlib is a package that can be used for data visualization

- For this we use the `matplotlib.pyplot` (sub)package ...
- ... which we usually import under the name `plt`

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

How are functions plotted in Python?

1. Create a vector of x-values, e.g.,

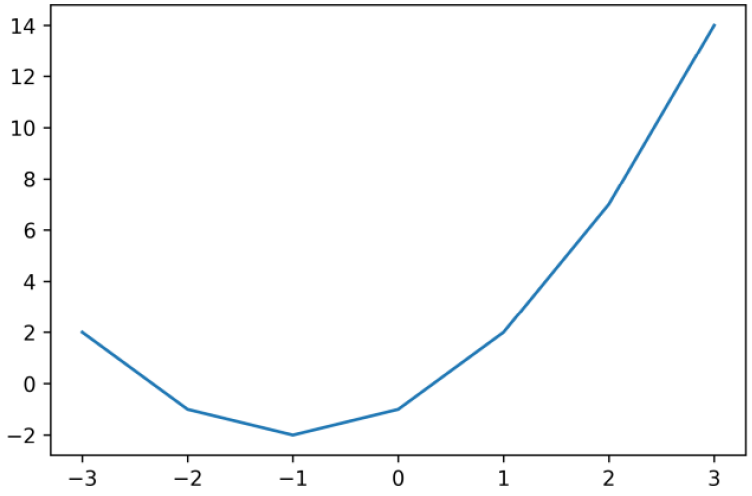
$$x = [-3, -, 2, -1, 0, 1, 2, 3].$$

2. Compute the function values

$$[f(-3), f(-2), f(-1), f(0), f(1), f(2), f(3)] = [2, -1, -2, -1, 2, 7, 14].$$

3. Draw the points $(x_i, f(x_i))$ and connect them with line segments.

Resulting Python plot



Plotting a "smooth" line

Increase the number of points in x to get a smoother line using `np.linspace()`.

- Command `np.linspace(a,b,k)` gives array with k evenly spaced points in interval $[a, b]$; first point is a and last point b.
- **Question:** Which points does `np.linspace(0,1,11)` create?

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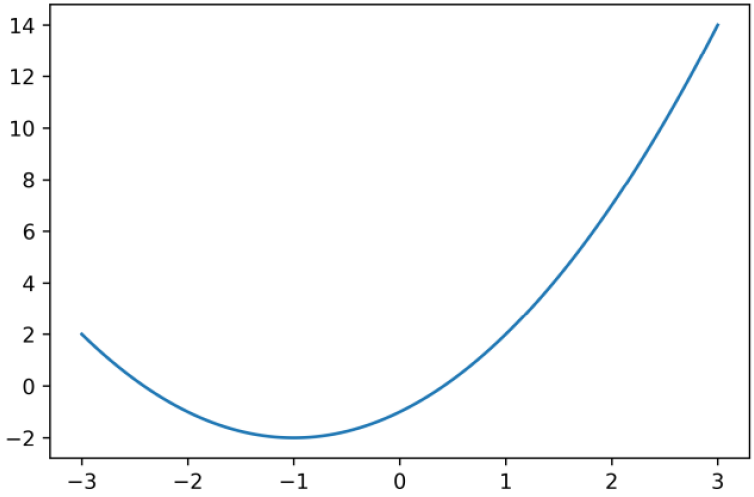
```
import numpy as np

a = 0
b = 1
k = 11

x = np.linspace(a,b,k)
print(x)
```

```
[0.  0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1. ]
```

Resulting “smoothed” Python plot

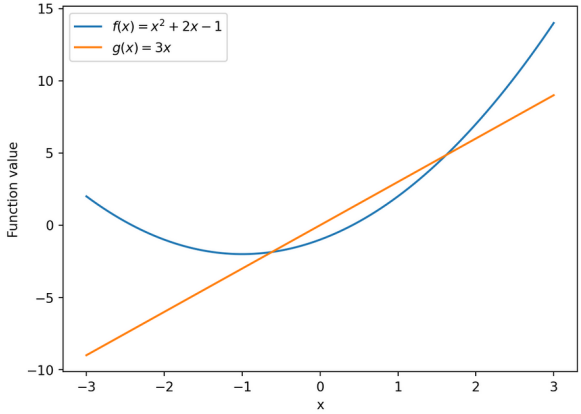
Using `x = np.linspace(-3,3,600)`



Adding legend to plot

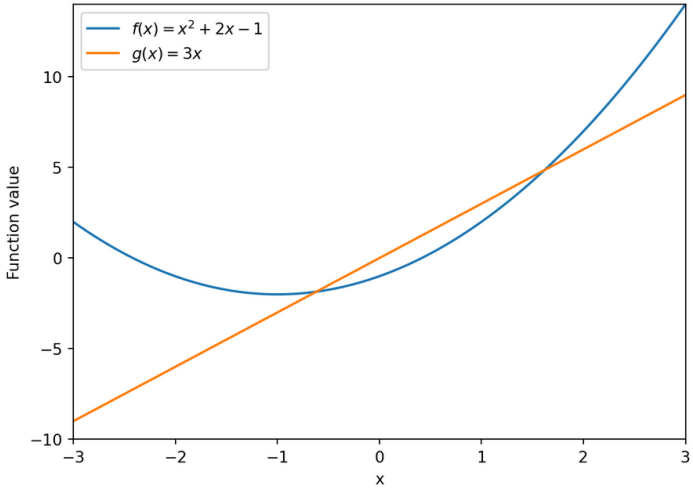
Use label-argument in `plt.plot()` in combination with `plt.legend()` at the end …

- … and `plt.xlabel('x')` and `plt.ylabel('Function value')` for axis labels.



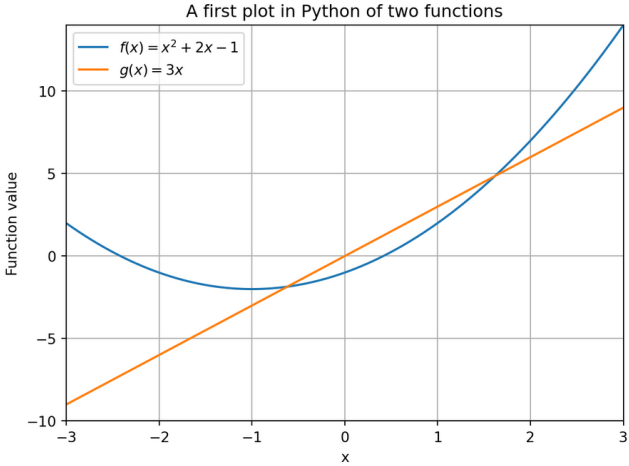
Fixing axes ranges

Use `plt.xlim(-3,3)` and `plt.ylim(-10,14)` to fix range of horizontal/vertical axis, resp.



Adding title and grid

- Use `plt.title('A first plot of two functions')` to add title
- Use `plt.grid()` to add grid.



Classroom Exercise 1

Consider the function $f(x) = \frac{9}{10}x^4 - 3x^3 - \frac{7}{2}x^2 + 12x + 3$.

- Plot this function with horizontal axis range $[-6, 6]$, and vertical axis range $[-15, 15]$.
- Find four roots of this function with `fsolve()` by trying out different initial guesses.
- Find a minimum of this function with `fmin()` by using initial guesses -1 and 2. Are both solutions actual minima of the function?

Chapter 10 - Object oriented programming

Object oriented programming

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- Personal information
- Course registrations
- Study progress

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In programming terms, every student is considered an object in the administration.

- Creating an object is done with a `Class` in Python.

Attributes and methods

When a students joins the university, an object is initialized for them containing their personal information, for example,

- Name
- Age
- Student number (or student ID)

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When a students joins the university, an object is initialized for them containing their personal information, for example,

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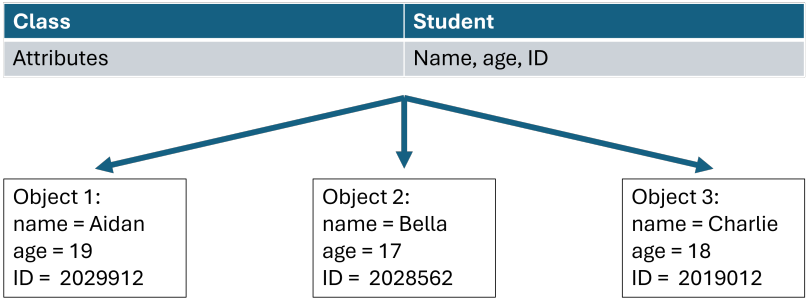
These pieces of information are called the attributes of the object.

Student example

We will create a class `Student` whose objects are students with attributes: name, age, (student) ID.



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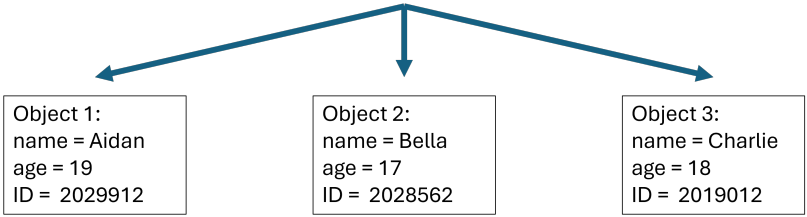
Further (self-defined) methods could be:

- Checking if a student is an adult based on their age (for legal reasons)
- Checking if a student is registered for an exam
- Keeping track of list of registered courses

Student example: overview

Class	Student
Attributes	Name, age, ID
Methods	Initialize object, check if adult, check exam registration, keep track of registered courses



A class in Python creates objects with attributes, and can use methods to investigate and modify these objects.

Initializing objects

Initialization is always done with `__init__()` function.

```
class Student:
    # This function initializes an object of the class Student
    # by setting the attributes (name, age and ID) of an object.
    def __init__(self,name,age,student_number):
        self.name = name
        self.age = age
        self.ID = student_number
```

The argument `self` should be thought of as the object that we want to create.

- The use of `self` as a variable name for this is standard in Python

Methods

Methods are Python functions in a class. `__init__()` is also a method of the class.

```
class Student:
    def __init__(self,name,age,student_number):
        self.name = name
        self.age = age
        self.ID = student_number

    # Check if student is adult
    def adult(self):
        if self.age >= 18:
            return print(self.name," is an adult")
        else:
            return print(self.name,"is not an adult")
```

- Every method has first input argument `self`.
- Attribute `attribute_name` can be accessed in method using `self.attribute_name`.

Additional inputs and changing attributes

Methods can require additional input arguments beside `self`.

- See `reg_check()` example in course document.

Methods can be used to manipulate attributes.

- See `addCourse()`/`delCourse` example in course document.

Adding course to course list

We add a new attribute `courses` that is an (initially empty) list.

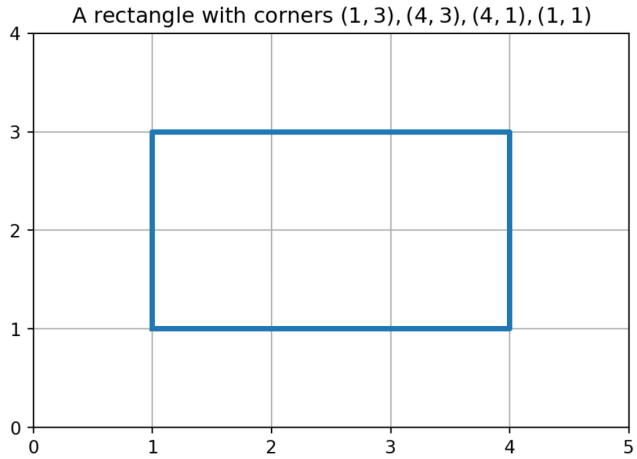
```
class Student:
    def __init__(self,name,age,student_number):
        self.name = name
        self.age = age
        self.ID = student_number
        self.courses = []
```

Write method `addCourse()` that can add (append) course names to this list.

```
    def addCourse(self, course_name):
        return self.courses.append(course_name)
```

Mathematical example: Rectangles

We create a class `Rectangle` whose objects are rectangles in a two-dimensional plane.



How to model a rectangle? What should the attributes be?

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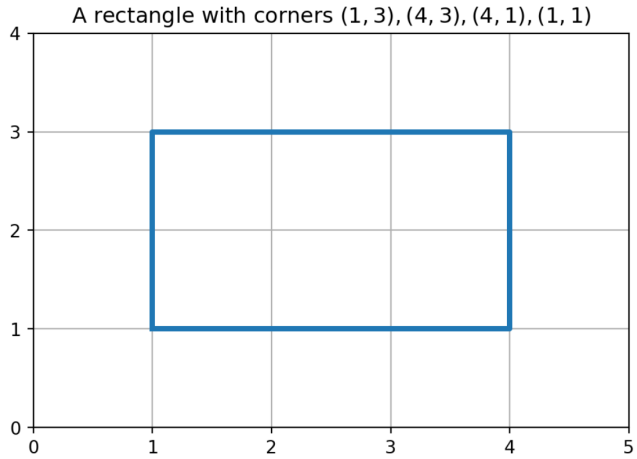
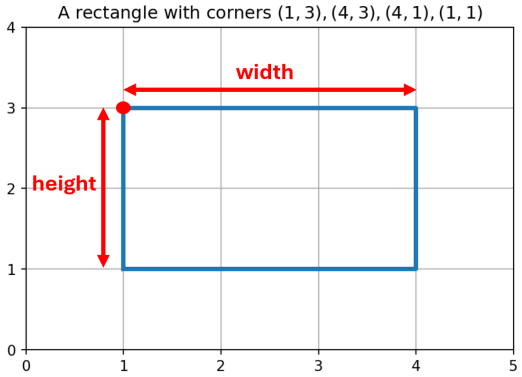


How to model a rectangle? What should the attributes be? Depends on desired methods...

Rectangle attributes

To uniquely determine a rectangle, it suffices to know: Upper-left corner point, width and height.



Rectangle __init__() method

```
class Rectangle:
    # Here corner is the upper-left corner point which
    # should be a list containing the x- and y-coordinate.
    def __init__(self, corner, height, width):
        self.corner= corner
        self.height = height
        self.width = width

rectangle1 = Rectangle([1,3],2,3)

# Print upper left corner of the rectangle
print(rectangle1.corner)
```

```
[1, 3]
```

Rectangle methods: Area and circumference

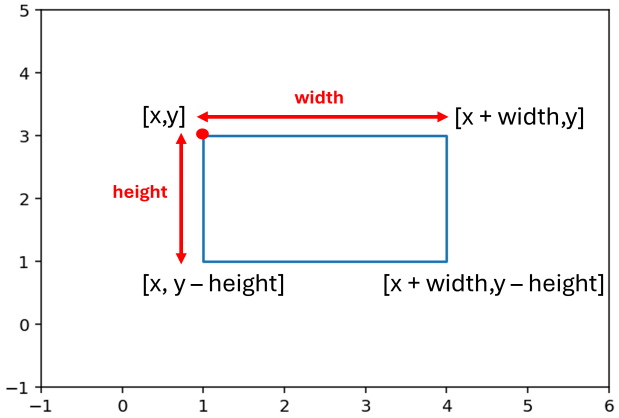
```
class Rectangle:
    # Initialize rectangle by providing upper-left corner, width and height
    def __init__(self,corner,width,height):
        self.corner = corner
        self.height = height
        self.width = width

    # Compute area = width*height of rectangle
    def area(self):
        return self.height*self.width

    # Compute circumference = 2*width + 2*height of rectangle
    def circumference(self):
        return 2*self.width + 2*self.height
```

Rectangle methods: Compute all corner points

Given upper left corner $[x, y]$, width and height, we can compute the coordinates of the remaining corner points.



Rectangle methods: Compute all corner points (cont'd)

```
class Rectangle:
    # Initialize rectangle by providing upper-left corner, width and height
    def __init__(self, corner, height, width):
        self.corner= corner
        self.height = height
        self.width = width

    # Compute corner points: the output has the points in the
    # order [upper-left, upper-right, lower-right, lower-left]
    def corners(self):
        up_right = [self.corner[0] + self.width, self.corner[1]]
        low_right=[self.corner[0]+self.width,self.corner[1]-self.height]
        low_left = [self.corner[0],  self.corner[1] - self.height]
        return [self.corner, up_right, low_right, low_left]
```

Rectangle methods: Plotting

You can find the `plotting()` method in the course document. The idea is as follows:

- Determine all corner points using the `corners()` method.
- Plot the points in order: upper-left, upper-right, lower-right, lower-left, upper-left.

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- Determine all corner points using the `corners()` method.
- Plot the points in order: upper-left, upper-right, lower-right, lower-left, upper-left.

The `plot()` function plots these five points and connects them with a line segment (resulting in a rectangle shape).

- Plot list with all x-coordinates against list with all y-coordinates of the five points.