

# Lecture 3: Functions and modules

FIE463: Numerical Methods in Macroeconomics and Finance using Python

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See GitHub repository for notebooks and data:

<https://github.com/richardfoltyn/FIE463-V25>

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## 1 Reusing code: Functions and modules

In this unit, we learn how to build reusable code with functions. We also briefly discuss modules and packages.

### 1.1 Functions

Functions are used to implement code that performs a narrowly defined task. We use functions for two reasons:

1. A function can be called repeatedly without having to write code again and again.
2. Even if a function is not called frequently, functions allow us to write code that is “shielded” from other code we write and is called via a clean interface. This helps to write more robust and error-free code.

So far, we only used functions written by others, e.g., `len()` and `sum()` which are part of the [built-in functions](#) available in core Python. However, for any program of even modest complexity, we want to define our own functions.

Functions are defined using the `def` keyword, and the function body needs to be an indented block:

```
[1]: def func():  
      print('func called')  
  
      # invoke func without arguments  
      func()
```

func called

### 1.1.1 Arguments

Functions can have an arbitrary number of positional arguments (also called parameters).

```
[2]: # Define func to accept argument x  
      def func(x):  
          print(f'func called with argument {x}')  
      # call function with various arguments.  
      func(1)  
      func('foo')
```

func called with argument 1  
func called with argument foo

### 1.1.2 Return values

Functions can return values to their caller using the `return` statement.

```
[3]: def func(x):  
      return x * 2.0  
  
      result = func(1.0)  
      print(result)      # prints 2.0
```

2.0

A `return` statement without any argument immediately exits the functions. The default return value is the special type `None`.

A function can return multiple values which are then automatically collected into a tuple:

```
[4]: def func():  
      return 1, 2, 3  
  
      values = func()      # call func(), get tuple of values  
      type(values)
```

[4]: tuple

Python supports “unpacking” of tuples, lists, etc. We can use this to directly assign names to multiple return values:

```
[5]: def func():
      return 'a', 'b', 'c'

value1, value2, value3 = func()    # call func(), unpack return values
print(f'Value 1: {value1}, Value 2: {value2}, Value 3: {value3}')
```

Value 1: a, Value 2: b, Value 3: c

### 1.1.3 Documenting functions

It is possible to use so-called *doc-strings* to comment functions (and other Python constructs). These doc-strings use triple quotes `"""` or `'''` and can span multiple lines. They need to be placed right after the function header and can contain various types of markup syntax. While these doc-strings are completely ignored by the Python interpreter, they are picked up by editors such as Visual Studio Code and used to display helpful documentation while editing files.

For example, we could use the following doc-strings to comment a function that squares its argument:

```
[6]: def square(x):
      '''
      Return the square of x.

      Parameters
      -----
      x : float
          The number to square.

      Returns
      -----
      float
          The square of x.
      '''
      x2 = x ** 2
      return x2
```

You'll see such doc-strings frequently in later parts of the course as our code gets more complicated.

#### Your turn.

1. Write a function `power()` which takes a single argument and returns the argument taken to the power of 2.
2. Modify the function such that it returns the original argument and its square.

### 1.1.4 Accessing data from the outer scope

A function need not have arguments or a return value, but that limits its usefulness somewhat. However, a function can access outside data which is defined in the so-called *outer scope*:

```
[7]: x = 1.0
      def func():
          # Read x from outer scope
          print(f'func accessing x from outer scope: x = {x}')

      # prints value of x from within func()
      func()
```

func accessing x from outer scope: x = 1.0

We can write functions without any arguments that only operate on outside data. However, this is terrible programming practice and should be avoided in most cases.

*Note:* Because functions can operate on external data, they are not analogous to mathematical functions. In math, whenever we write  $f(x)$  we usually mean that  $f$  is a function of  $x$  only (and possibly some constant parameters). By definition we must have

$$x_1 = x_2 \implies f(x_1) = f(x_2),$$

i.e., a function always returns the same value when called with the same parameters. However, this is not the case in Python or most other programming languages:

```
[8]: a = 1.0
def func(x):
    return a*x

x = 1.0
print(func(x))      # prints 1.0

a = 2.0
print(func(x))      # x unchanged, but prints 2.0
```

```
1.0
2.0
```

### 1.1.5 More on arguments

#### Default arguments

Python offers an extremely convenient way to specify default values for arguments using the syntax `name=value`, so these need not be passed when the function is called:

```
[9]: # define function with a default value of 1.0 for argument alpha
def func(x, alpha=1.0):
    return x * alpha

print(func(2.0))      # uses default value for alpha
print(func(2.0, 3.0)) # use some other value for alpha
```

```
2.0
6.0
```

#### Keyword (or named) arguments

Arguments don't need to be provided in the same order as specified in the function signature. We can use argument names to explicitly assign values to the corresponding argument.

```
[10]: def func(arg1, arg2):
    print(f'arg1: {arg1}, arg2: {arg2}')

func(1, 2)          # Call using purely positional arguments
func(arg1=1, arg2=2) # Use argument names to explicitly assign values
func(arg2=2, arg1=1) # With keyword arguments, the order does not matter!
```

```
arg1: 1, arg2: 2
arg1: 1, arg2: 2
arg1: 1, arg2: 2
```

### Your turn.

1. Modify the `power()` function you wrote earlier to take an additional optional argument `xp` (for “exponent”) with a default value of 2. The first argument should now be taken to the power of `xp`.
2. Call the function in three different ways: (1) without the optional argument `xp`; (2) with the optional argument passed as a positional argument; and (3) with the optional argument passed as a keyword argument.

### Arbitrary number of optional arguments

Python supports functions which accept an arbitrary number of positional and keyword arguments. This is accomplished via two special tokens:

- `*args`: collects any number of “excess” *positional arguments* and packs them into a tuple.
- `**kwargs`: collects any number of “excess” *keyword arguments* and packs them into a dictionary. It needs to be placed at the end of the argument list!

*Example: Function with unnamed positional arguments*

```
[11]: # Define function unlimited unnamed positional arguments
def func(*args):
    for i, arg in enumerate(args):
        print(f'Positional argument {i}: {arg}')

# Call with positional arguments
func(1.0, 'abc')
```

Positional argument 0: 1.0  
Positional argument 1: abc

Note that it is not possible to call this function with *named* keyword arguments since it was defined to only accept *unnamed* positional arguments:

```
[12]: func(arg='value')
```

```
TypeError: func() got an unexpected keyword argument 'arg'
```

*Example: Function with unlimited keyword arguments*

```
[13]: # Define function to accept arbitrary keyword arguments
def func(**kwargs):
    for name, value in kwargs.items():
        print(f'Argument {name}: {value}')

# Call function with several keyword arguments
func(arg1='value1', arg2=2)
```

Argument arg1: value1  
Argument arg2: 2

Note that it is not possible to call this function with positional (unnamed) arguments:

```
[14]: func('value1', 2)
```

```
TypeError: func() takes 0 positional arguments but 2 were given
```

*Example: Function with multiple types of arguments*

Lastly, we can define a function which includes all the types of arguments we have discussed so far (including arguments with default values):

```
[15]: # Define function with mandatory, optional, optional positional
      # and optional keyword arguments

      def func(x, opt='default', *args, **kwargs):
          print(f'Required argument x: {x}')
          print(f'Optional argument opt: {opt}')
          if args:
              # if the tuple 'args' is non-empty, print its contents
              print('Optional positional arguments:')
              for i, arg in enumerate(args):
                  print(f' Position {i}: {arg}')
          if kwargs:
              # if the dictionary 'kwargs' is non-empty, print its contents
              print('Optional keyword arguments:')
              for key, value in kwargs.items():
                  print(f' {key}: {value}')
```

```
[16]: # Call only with required argument
      func(0)
```

```
Required argument x: 0
Optional argument opt: default
```

```
[17]: # Call with required and optional arguments
      func(0, 'optional')
```

```
Required argument x: 0
Optional argument opt: optional
```

```
[18]: # Call with required and optional arguments, and
      # optional positional arguments
      func(0, 'optional', 1, 2, 3)
```

```
Required argument x: 0
Optional argument opt: optional
Optional positional arguments:
  Position 0: 1
  Position 1: 2
  Position 2: 3
```

```
[19]: # Call with required and optional arguments, and
      # optional positional and keyword arguments
      func(0, 'optional', 1, 2, 3, arg1='value1', arg2='value2')
```

```
Required argument x: 0
Optional argument opt: optional
Optional positional arguments:
  Position 0: 1
  Position 1: 2
  Position 2: 3
Optional keyword arguments:
  arg1: value1
  arg2: value2
```

We don't even need to specify arguments in the order they are defined in the function, except for optional positional arguments, since these have no argument names. We can just use the name=value syntax:

```
[20]: # call func() with interchanged argument order
      func(opt='optional value', x=1)
```

Required argument x: 1  
Optional argument opt: optional value

Note, however, that in a function call any positional arguments must come first and those passed as name=value pairs last:

```
[21]: x = 1

      # this will not work, cannot specify positional arguments last
      func(opt='optional value', x)
```

```
Cell In[21], line 4
      func(opt='optional value', x)
                                ^
SyntaxError: positional argument follows keyword argument
```

The same applies for optional arguments passed in via \*args and \*\*kwargs:

```
[22]: # fails because arguments collected in *args must
      # be specified before arguments collected in **kwargs!
      func(1.0, 'opt', arg1='value1', arg2='value2', 1, 2, 3)
```

```
Cell In[22], line 3
      func(1.0, 'opt', arg1='value1', arg2='value2', 1, 2, 3)
                                                ^
SyntaxError: positional argument follows keyword argument
```

### Your turn.

1. Write a function `my_sum()` which accepts an arbitrary number of positional arguments and returns their sum (you can assume that arguments are numeric).
2. Test your function with zero, one, and multiple arguments. When called without any arguments, your function should return 0.

## 1.1.6 Modifying data in the outer scope

So far, we covered read-only access to data defined outside of a function and relied on return values to pass results back to the caller. However, it is possible to directly *modify* data in the outer scope, even though this should usually be avoided:

- Using arguments and return values clearly defines a function's interface, there are no unpleasant surprises.
- Conversely, if a function starts modifying values in the caller's environment, there is no way to be sure what the function is changing in the outer scope other than by examining its source code.

Consider first the following attempt to modify a value defined outside of the function:

```
[22]: var = 'outer scope'

# Create function, assign value to var
def modify_var():
    var = 'inner scope'

print(var)
modify_var()
print(var)
```

```
outer scope
outer scope
```

This code prints 'outer scope' twice. What happened? Without any further instructions, the assignment inside the function creates a *local* variable `var` that is completely disconnected from `var` in the outer scope!

We need to use the `global` statement to tell Python to instead assign to a variable in the global (outer) scope:

```
[23]: var = 'outer scope'

def modify_var():
    global var
    var = 'inner scope'

print(var)
modify_var()
print(var)
```

```
outer scope
inner scope
```

The second output now reads 'inner scope'.

Note that `global` in Python actually means global to a module, i.e., a symbol that is defined at the top level within a module (we discuss modules below). There are no truly global variables in Python unlike in languages such as C or Matlab.

The requirement that the name in the `global` statement refers to a global variable has subtle implications. Consider the following example of two *nested* functions:

```
[24]: def outer():
    var = 'outer function'

    def inner():
        # Bind var to global name var
        global var
        var = 'inner function'

    print(var)
    inner()
    print(var)

outer()
```

```
outer function
outer function
```

Surprisingly, the code above prints 'outer function' twice. The reason is that `var` defined in `outer()` is *not* a global variable as it was not defined at the top level within a module. Instead, it is a *local* variable in `outer()`.



For such scenarios, Python has the `nonlocal` statement which works similarly to `global` except that it operates on a name in the immediate outer scope, irrespective of whether this outer scope is another function or the module itself.

We can use `nonlocal` to get the desired behaviour:

```
[25]: def outer():
      # var is in outer's local scope
      var = 'outer function'

      def inner():
          # bind var to name in immediate outer scope,
          # which is the local scope of outer()
          nonlocal var
          var = 'inner function'

      print(var)
      inner()
      print(var)

outer()
```

```
outer function
inner function
```

### 1.1.7 Pass by value or pass by reference?

Can functions modify their arguments? This questions usually comes down to whether a function call uses *pass by value* or *pass by reference*:

- *pass by value* means that a copy of every argument is created before it is passed into the function. A function therefore cannot modify a value in the caller's environment.
- *pass by reference* means that only a reference to a value is passed to the function, so the function can directly modify values at the call site.

This programming model is used in languages such as C (pass by value) or Fortran (pass by reference), but not in Python. Sloppily speaking, we can say that in Python a reference ("variable name") is passed by value. This means that assigning a different value to an argument ("the reference") within a function has no effect outside of the function:

```
[26]: def func(x):
      # x now points to something else
      x = 1.0

x = 123
func(x)

x      # prints 123, x in the outer scope is unchanged
```

[26]: 123

However, if a variable is a mutable object (such as a list or a dict), the function can use its own copy of the reference to that object to modify the object even in the outer scope:

```
[27]: def func(x):
      # uses reference x to modify list object outside of func()
      x.append(4)

lst = [1,2,3]
func(lst)
lst      # prints [1,2,3,4]
```

```
[27]: [1, 2, 3, 4]
```

Nevertheless, even for mutable objects the rule from above applies: when a new value is *assigned* to a named argument, that name then references a different object, leaving the original object unmodified:

```
[28]: def func(x):  
      # this does not modify object in outer scope,  
      # x now references a new (local) object.  
      x = ['a', 'b', 'c']  
  
      lst = [1,2,3]  
      # pass list, which is mutable and can thus be changed in func()  
      func(x)  
  
      lst      # prints [1,2,3]
```

```
[28]: [1, 2, 3]
```

For immutable objects such as tuples, the reference passed to the function of course cannot be used to modify the object inside the function:

```
[29]: def func(x):  
      x[0] = 'modified in func'  
  
      items = (1, 2, 3)      # create tuple of integers  
      func(items)
```

```
TypeError: 'tuple' object does not support item assignment
```

Passing in a mutable collection such as a list, however, works as expected:

```
[30]: items = [1, 2, 3]  
  
      func(items)  
  
      items
```

```
[30]: ['modified in func', 2, 3]
```

### 1.1.8 Methods

Methods are simply functions that perform an action on a particular object which they are bound to. We will not write methods in this course ourselves (they are part of what's called object-oriented programming), but we frequently use them when we invoke actions on objects such as lists:

```
[31]: # Create a list  
      lst = [1,2,3]  
  
      # append() is a method of the list class and can be invoked  
      # on list objects.  
      lst.append(4)  
      lst
```

```
[31]: [1, 2, 3, 4]
```

### 1.1.9 Functions as objects

Functions are objects in their own right, which means that you can perform various operations with them:

- Assign a function to a variable.
- Store functions in collections.
- Pass function as an argument to other functions.

Examples:

```
[32]: def func1(x):
      print(f'func1 called with argument {x}')

      def func2(x):
          print(f'func2 called with argument {x}')

      # List of functions
      funcs = [func1, func2]

      # Assign functions to variable f
      for f in funcs:
          # call function referenced by f
          f('foo')
```

```
func1 called with argument foo
func2 called with argument foo
```

```
[33]: # Pass one function as argument to another function
      func1(func2)
```

```
func1 called with argument <function func2 at 0x7fd235d9e020>
```

### 1.1.10 lambda expressions

You can think of lambda expressions as light-weight functions. The syntax is

**lambda** x: <do something with x>

The return value of a lambda expression is whatever its body evaluates to. There is no need (or possibility) to explicitly add a return statement.

One big difference to regular functions is that lambda expressions are *expressions*, not statements.

- At this point we gain little from a technical discussion on *statements* vs *expressions*. Loosely speaking, statements are one level above expressions in the Python syntax hierarchy, and the language puts restrictions on where statements can appear. Function definitions, for and while loops, and if/elif/else blocks are statements, among others.
- Conversely, *expressions* are more flexible and can appear basically anywhere. They usually evaluate to some object that can be assigned, passed to a function, etc., whereas statements can't.

The take-away is that we can fiddle in lambda expressions almost anywhere, even as arguments in function calls!

For example, we might have a function that applies some algebraic operation to its arguments, and the operation can be flexibly defined by the caller.

```
[34]: def func(items, operation=lambda z: z + 1):
      # default operation: increment value by 1
```

```

    result = [operation(i) for i in items]
    return result

numbers = [1.0, 2.0, 3.0]
# call with default operation
func(numbers)           # prints [2.0, 3.0, 4.0]

```

[34]: [2.0, 3.0, 4.0]

```

[35]: # We can also use lambda expressions to specify
      # an alternative operation directly in the call!

      func(numbers, lambda x: x**2.0)    # prints [1.0, 4.0, 9.0]

```

[35]: [1.0, 4.0, 9.0]

While we could have defined the operation using a “regular” function statement, this is shorter.

**Your turn.** Consider the tuple (1, 2, 3).

1. Find the minimum of this tuple using the built-in `min()` function.
2. Now imagine you want to find the maximum but don’t have a `max()` function at hand. While this seems far-fetched, in fact all of the optimization routines we will encounter later in the SciPy package are minimizers.

Any minimizer can be repurposed to be a maximizer by flipping the sign. This can be achieved using key argument of `min()`. Write a lambda expression that takes a single argument `x` and returns `-x`, and pass this lambda expression to `min()` using the key argument to find the maximum of the above tuple.

## 1.2 Modules and packages

### 1.2.1 Modules

Modules allow us to further encapsulate code that implements some particular functionality.

- Each Python file (with the extension `.py`) automatically corresponds to a module of the same name.
- This implies that you should only use file names that are valid Python names as otherwise a module cannot be imported. In particular, this means avoiding any spaces in file names!
- Objects defined within such a module are by default not visible outside of the module, thus helping to avoid naming conflicts.

To actually demonstrate the usage of modules, we need to use files outside of this notebook. To this end, there is an additional Python file in the current directory:

```

lecture03/
    lecture03_mod.py

```

The module `lecture03_mod.py` contains the following definitions:

```

# Contents of lecture03_mod.py

# global variable in this module
var = 'Variable defined in lecture03_mod'

# global function in this module
def func():
    print(f'func in module lecture03_mod called')

```

## Automatic reloading of module contents

Jupyter notebooks have a special `%autoreload` cell magic which instructs the Python interpreter to automatically reload any changes in modules applied outside of the notebook. This is only supported in Jupyter notebooks as it only makes sense for interactive documents. It does not work (and is not needed) for traditional `.py` files.

This cell magic needs to be inserted only once per Jupyter notebook.

```
[36]: %load_ext autoreload
      %autoreload 2
```

## Module search path

Before getting into the details, we first need to verify that we can import the module `lecture03_mod` using the import statement:

```
[37]: import lecture03_mod
```

Depending on where exactly you are running this code, the above import statement might fail with a `ModuleNotFoundError` (if no error was raised you can skip the rest of this section). This happens whenever the directory in which the module resides is not in the *module search path* used by Python.

To fix this, check the module search path as follows:

```
[38]: import sys
      sys.path
```

```
[38]: ['/home/richard/.conda/envs/FIE463/lib/python3.12.zip',
      '/home/richard/.conda/envs/FIE463/lib/python3.12',
      '/home/richard/.conda/envs/FIE463/lib/python3.12/lib-dynload',
      '',
      '/home/richard/.local/lib/python3.12/site-packages',
      '/home/richard/.local/lib/python3.12/site-packages/opt_einsum-3.4.0-py3.12.egg',
      '/home/richard/build/rocm/jax',
      '/home/richard/.local/lib/python3.12/site-packages/ml_dtypes-0.5.0-py3.12-linux-x86_64.egg',
      '/home/richard/.conda/envs/FIE463/lib/python3.12/site-packages',
      '/home/richard/.conda/envs/FIE463/lib/python3.12/site-packages/setuptools/_vendor']
```

If the `lecture03/` directory is not included in this list, you can add it manually. For example, this notebook is executed in the git repository's root directory, you need to execute

```
[39]: import sys
      # add lectures/ directory using a relative path
      sys.path.append('./lectures/lecture03')
```

## Importing symbols

We now want to use `func` and `var` from `lecture03_mod` in our notebook. However, by default these symbols are not visible and first need to be imported. We can do this in several ways:

1. We can import the module and use fully qualified names to reference objects from `lecture03_mod`.
2. We can select which names from `lecture03_mod` should be directly accessible.

The first variant looks like this:

```
[40]: import lecture03_mod

# Access variable defined in lecture03_mod
print(lecture03_mod.var)

# Call function defined in lecture03_mod
lecture03_mod.func()
```

Variable defined in lecture03\_mod  
func in module lecture03\_mod called

If a symbol from lecture03\_mod is used frequently, we might want to make it accessible without the lecture03\_mod prefix. This is the second variant:

```
[41]: from lecture03_mod import var, func

# Access variable defined in lecture03_mod
print(var)

# Call function defined in lecture03_mod
func()
```

Variable defined in lecture03\_mod  
func in module lecture03\_mod called

What if our notebook itself defines a function func() which would overwrite the reference to the one imported from lecture03\_mod, as in the following example?

```
[42]: from lecture03_mod import func

# Calls func() defined in lecture03_mod
func()

# overwrites definition from lecture03_mod with local version
def func():
    print('func in notebook called')

# Calls func() defined in notebook
func()
```

func in module lecture03\_mod called  
func in notebook called

In such a scenario, we can assign aliases to imported symbols using as:

```
[43]: from lecture03_mod import func as imported_func    # The function formerly known
                                                    # as func is now imported_func

def func():
    print('func in notebook called')

# call our own func
func()

# call func from module lecture03_mod
imported_func()
```

func in notebook called  
func in module lecture03\_mod called

We can even alias the module name itself, as we frequently do with widely used modules such as numpy:

```
[44]: # Import module, assign it short-hand name l4
import lecture03_mod as l4

l4.func()    # call function from module lecture03_mod
```

func in module lecture03\_mod called

```
[45]: # Import NumPy, using standard convention to assign it the alias 'np'
import numpy as np
```

**Your turn.** Recall the `power()` function you wrote earlier in this unit.

1. Create a module `mymath.py` and place it in the same directory as this notebook.
2. Add a print statement to `power()` so it reports the module where it is located:  
`print(f'Called from {__name__}')`
3. Import the `power()` function from this module and call it.

### 1.2.2 Packages

Packages are roughly speaking collections of modules and a little magic on top. We will not be creating packages, but we have already been using them: basically everything besides the built-in functions is defined in some package. For example, the NumPy library is a collection of packages.

## 1.3 Optional exercises

### Exercise 1: Sign function

Implement a function `sign` which returns the following values:

$$\text{sign}(x) = \begin{cases} -1 & \text{if } x < 0 \\ 0 & \text{if } x = 0 \\ 1 & \text{if } x > 0 \end{cases}$$

Test your function on a negative, zero and positive argument.

### Exercise 2: Sum of arbitrary number of elements

Create a function called `my_sum` which accepts an arbitrary number of arguments (possibly zero) and returns their sum. Assume that all arguments are numeric.

Test your function with the following arguments:

```
my_sum(10.0)    # one argument
my_sum(1,2,3)   # multiple arguments
my_sum()        # no arguments
```

Make sure that in the last case your function returns zero, which is the sum over an empty set.

### Exercise 3: Fibonacci sequence

A classical introductory exercise to programming is to write a function that returns the first  $n$  terms of the Fibonacci sequence. The  $i$ -th element of this sequence is the integer  $x_i$  defined as

$$x_i = \begin{cases} 0 & \text{if } i = 0 \\ 1 & \text{if } i = 1 \\ x_{i-1} + x_{i-2} & \text{else} \end{cases}$$

Write a function `fibonacci(i)`,

```
def fibonacci(i):  
    ...
```

which returns the  $i$ -th item in the sequence using recursion. A recursive function is a function that calls itself to perform (part of) its task, i.e., you should compute  $x_i$  like this:

```
xi = fibonacci(i-1) + fibonacci(i-2)
```

Use this function to compute the first 10 elements of this sequence with a list comprehension.

### Exercise 4: Factorials

1. Implement a function that computes the factorial of a non-negative integer  $n$  defined as  $n! = \prod_{i=1}^n i$ . Keep in mind that this definition implies that  $0! = 1$ . Use the list comprehension syntax to create a tuple that contains the factorials for the integers  $n = 1, \dots, 10$ .

*Hint:* The factorial can be written as a recurrence relation  $n! = n \cdot (n-1)!$ , which you can use to implement the recursive function.

2. Provide an alternative implementation that does not rely on recursion, but instead uses NumPy's `prod()` function to compute the product of a sequence of numbers. Again, create a tuple that contains the factorials for the integers  $n = 1, \dots, 10$  using a list comprehension.

*Hint 1:* To compute the product of the integers  $i, i+1, \dots, j$ , you can use `np.prod(range(i, j+1))`.

*Hint 2:* The product of an empty set is 1, which is what `np.prod()` returns.

### Exercise 5: Bisection root-finding algorithm (advanced)

We revisit the binary search algorithm from the previous lecture, this time applied to finding the root of a continuous function. This is called the [bisection method](#).

Implement a function `bisection(f, a, b, tol, xtol)` which finds the root of the function  $f(x)$ , i.e., the value  $x_0$  where  $f(x_0) = 0$  on the interval  $[a, b]$ . Assume that  $a < b$  and that the function values  $f(a)$  and  $f(b)$  have opposite signs.

Test your implementation using the function  $f(x) = x^2 - 4$  on the interval  $[-3, 0]$ , which has a (unique) root at  $x_0 = -2$ .

The bisection algorithm proceeds as follows, which you need to convert to Python code:

1. Define tolerance levels  $\epsilon > 0$  and  $\epsilon_x > 0$ . The algorithm completes successfully whenever we have either  $|f(x_0)| < \epsilon$  or  $|b - a| < \epsilon_x$ .
2. Main loop of the algorithm:
  1. Compute the midpoint  $x_m = (a + b)/2$
  2. Compute function value  $f_m = f(x_m)$
  3. If either  $|f_m| < \epsilon$  or  $|b - a| < \epsilon_x$ , accept  $x_m$  as the solution and exit.



4. Otherwise, update either  $a$  or  $b$ :

1. If  $\text{sign}(f(b)) = \text{sign}(f_m)$ , set  $b = x_m$

*Hint:* One way to check whether two non-zero values have the same sign is to check if  $f(b) \cdot f_m > 0$ .

2. Otherwise,  $a = x_m$

5. Proceed to next iteration of main loop.

## 1.4 Solutions

### Solution for exercise 1

```
[46]: import numpy as np

def sign(x):
    if x < 0.0:
        return -1.0
    elif x == 0.0:
        return 0.0
    elif x > 0.0:
        return 1.0
    else:
        # Argument is not a proper numerical value, return NaN
        # (NaN = Not a Number)
        return np.nan

# Test on a few values
print(sign(-123))
print(sign(0))
print(sign(12345))
```

```
-1.0
0.0
1.0
```

Note that NumPy has a “proper” sign function, `np.sign()`, which implements the same logic but is more robust, accepts array arguments, etc.

### Solution for exercise 2

For a function to accept an arbitrary number of arguments, we need to declare an `*args` argument.

One possible implementation of `my_sum()` looks as follows:

```
[47]: def my_sum(*args):
    # Initialise sum to 0
    s = 0
    for x in args:
        s += x
    return s

# Test with sequences of arguments
print(my_sum(10.0))
print(my_sum(1, 2, 3))
print(my_sum())
```

```
10.0
6
0
```

Of course in real code we would use the built-in function `sum()`, or preferably the NumPy variant `np.sum()`:

```
[48]: import numpy as np

print(np.sum(10.0))

# Need to pass argument as collection
print(np.sum((1, 2, 3)))

# np.sum() cannot be invoked without arguments, but we can
# call it with an empty tuple ()
np.sum(())
```

```
10.0
6
```

```
[48]: np.float64(0.0)
```

### Solution for exercise 3

The recursive definition of `fibonacci(i)` could look like this:

```
[49]: def fibonacci(i):
    if i == 0:
        # No recursion needed
        xi = 0
    elif i == 1:
        # No recursion needed
        xi = 1
    else:
        # Assume that i > 1. We will learn later how to
        # return an error if this is not the case.
        # Use recursion to compute the two preceding values
        # of the sequence.
        xi = fibonacci(i-1) + fibonacci(i-2)
    return xi

# Compute the first 10 elements of the sequence using a list comprehension
first10 = [fibonacci(i) for i in range(10)]
first10
```

```
[49]: [0, 1, 1, 2, 3, 5, 8, 13, 21, 34]
```

Note that this is a terribly inefficient way to compute things, as the same elements of the sequence will needlessly be calculated over and over again.

### Solution for exercise 4

The following code implements a function to compute the factorial  $n!$  using recursion:

```
[50]: def factorial(n):
    if n == 0:
        return 1
    else:
        # Use recursion to compute factorial
        return n * factorial(n-1)
```

```
fact10 = tuple(factorial(n) for n in range(10))
fact10
```

[50]: (1, 1, 2, 6, 24, 120, 720, 5040, 40320, 362880)

An implementation without recursion can be created using NumPy's `prod()` function which computes the product of a sequence of numbers:

```
[51]: import numpy as np
fact10 = tuple(np.prod(range(1,n+1)) for n in range(10))
fact10
```

```
[51]: (np.float64(1.0),
      np.int64(1),
      np.int64(2),
      np.int64(6),
      np.int64(24),
      np.int64(120),
      np.int64(720),
      np.int64(5040),
      np.int64(40320),
      np.int64(362880))
```

Notice that the first element of this sequence is a floating-point value 1.0, while the remaining elements are integers. Why is that? Examine the argument passed to `np.prod()` for `n=0`:

```
[52]: n = 0
      # We have to embed range() in an expression that forces the Python
      # interpreter to actually expand the range object, such as a tuple().
      tuple(range(1,n+1))
```

[52]: ()

As you see, for `n=0` this is an empty container without elements. The mathematical convention is that the product over an empty set is  $\prod_{i \in \emptyset} = 1$ , and this is exactly what `np.prod()` returns. However, by default NumPy creates floating-point values, and so the return value is 1.0, not 1.

You can get around this by explicitly specifying the data type using the `dtype` argument, which is accepted by many NumPy functions.

```
[53]: import numpy as np
      # Force result to be of integer type
fact10 = tuple(np.prod(range(1,n+1), dtype=int) for n in range(10))
fact10
```

```
[53]: (np.int64(1),
      np.int64(1),
      np.int64(2),
      np.int64(6),
      np.int64(24),
      np.int64(120),
      np.int64(720),
      np.int64(5040),
      np.int64(40320),
      np.int64(362880))
```

Alternatively, we can use `np.arange()` instead of `range()` as the former by default returns integer arrays, even if they are empty:

```
[54]: import numpy as np
      # Force result to be of integer type
fact10 = tuple(np.prod(np.arange(1,n+1)) for n in range(10))
```

```
fact10
```

```
[54]: (np.int64(1),  
      np.int64(1),  
      np.int64(2),  
      np.int64(6),  
      np.int64(24),  
      np.int64(120),  
      np.int64(720),  
      np.int64(5040),  
      np.int64(40320),  
      np.int64(362880))
```

Finally, you of course would not need to implement the factorial function yourself, as there is one in the `math` module shipped with Python:

```
[55]: import math  
fact10 = tuple(math.factorial(n) for n in range(10))  
fact10
```

```
[55]: (1, 1, 2, 6, 24, 120, 720, 5040, 40320, 362880)
```

### Solution for exercise 5

Below you find a simple implementation of a bisection algorithm. This function does not perform any error checking and assumes that the initial bracket  $[a, b]$  actually contains a root, and that the values  $f(a)$  and  $f(b)$  have opposite signs.

We impose two termination criteria, and the algorithm will end successfully whenever one of them is satisfied:

1. The function value is sufficiently close to zero, i.e.,  $|f(x_0)| < \epsilon$  for some small  $\epsilon > 0$ .
2. The bracket is sufficiently small, i.e.,  $|b - a| < \epsilon_x$ , again for some small  $\epsilon_x > 0$

This is standard practice in numerical optimisation since we don't want the algorithm to continue unnecessarily if the desired degree of precision was achieved.

We specify the termination tolerance as optional arguments `tol` and `xtol` with sensible defaults. We also add the maximum permissible number of iterations as an optional argument `maxiter`.

```
[56]: def bisect(f, a, b, tol=1.0e-6, xtol=1.0e-6, maxiter=100):  
  
    for iteration in range(maxiter):  
        # Compute candidate value as midpoint between a and b  
        mid = (a + b) / 2.0  
        if abs(b-a) < xtol:  
            # Remaining interval is too small  
            break  
  
        fmid = f(mid)  
  
        if abs(fmid) < tol:  
            # function value is close enough to zero  
            break  
  
        print(f'Iteration {iteration}: f(mid) = {fmid:.4e}')  
        if fmid*f(b) > 0.0:  
            # f(mid) and f(b) have the same sign, update upper bound b  
            print(f'  Updating upper bound to {mid:.8f}')  
            b = mid  
        else:  
            # f(mid) and f(a) have the same sign, or at least one of
```

```

        # them is zero.
        print(f' Updating lower bound to {mid:.8f}')
        a = mid

    return mid

# Compute root of  $f(x) = x^2 - 4$  on the interval  $[-3, 0]$ 
# We pass the function  $f$  as the first argument, and use a lambda expression
# to define the function directly in the call.
x0 = bisect(lambda x: x**2.0 - 4.0, -3.0, 0.0)

# Print root. The true value is -2.0
x0

```

```

Iteration 0: f(mid) = -1.7500e+00
    Updating upper bound to -1.50000000
Iteration 1: f(mid) = 1.0625e+00
    Updating lower bound to -2.25000000
Iteration 2: f(mid) = -4.8438e-01
    Updating upper bound to -1.87500000
Iteration 3: f(mid) = 2.5391e-01
    Updating lower bound to -2.06250000
Iteration 4: f(mid) = -1.2402e-01
    Updating upper bound to -1.96875000
Iteration 5: f(mid) = 6.2744e-02
    Updating lower bound to -2.01562500
Iteration 6: f(mid) = -3.1189e-02
    Updating upper bound to -1.99218750
Iteration 7: f(mid) = 1.5640e-02
    Updating lower bound to -2.00390625
Iteration 8: f(mid) = -7.8087e-03
    Updating upper bound to -1.99804688
Iteration 9: f(mid) = 3.9072e-03
    Updating lower bound to -2.00097656
Iteration 10: f(mid) = -1.9529e-03
    Updating upper bound to -1.99951172
Iteration 11: f(mid) = 9.7662e-04
    Updating lower bound to -2.00024414
Iteration 12: f(mid) = -4.8827e-04
    Updating upper bound to -1.99987793
Iteration 13: f(mid) = 2.4414e-04
    Updating lower bound to -2.00006104
Iteration 14: f(mid) = -1.2207e-04
    Updating upper bound to -1.99996948
Iteration 15: f(mid) = 6.1035e-05
    Updating lower bound to -2.00001526
Iteration 16: f(mid) = -3.0518e-05
    Updating upper bound to -1.99999237
Iteration 17: f(mid) = 1.5259e-05
    Updating lower bound to -2.00000381
Iteration 18: f(mid) = -7.6294e-06
    Updating upper bound to -1.99999809
Iteration 19: f(mid) = 3.8147e-06
    Updating lower bound to -2.00000095
Iteration 20: f(mid) = -1.9073e-06
    Updating upper bound to -1.99999952

```

[56]: -2.000000238418579