Python Introduction IMCBio

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2025-05-16

Table of contents

1 Python introduction

2 Lesson 1 - Introduction, representing and manipulating data

3 Introduction

3.1 Aim of the class

At the end of this class, you will:

- Be familiar with the Python environment
- Understand the major data types in Python
- Manipulate variables with operators and built-in functions

Figure 3.1: Python logo

3.2 Requirements

You need to have a computer, and either:

- install Python 3.0.0 (or above) and install a text editor (Word is not a text editor!).

> **Note**
>
> An IDE (integrated development environment) is an improved text editor. It is a software that provides functionalities like syntax highlighting, auto completion, help, debugger… For example Visual Studio Code (install and learn how to use it with Python), but any other IDE will work.

- have a github account, create a new codespace, and select the Repository `vgilbart/python-intro` to copy from. This is a free solution up to 60 hours of computing and 15 GB per month.

3.3 What is Python?

Figure 3.2: Guido van Rossum

Python is a programming language first released in 1991 and implemented by Guido van Rossum.

It is widely used, with various applications, such as:

- software development
- web development
- data analysis
- ...

It supports different types of programming paradigms (i.e. way of thinking) including the procedural programming paradigm. In this approach, the program moves through a linear series of instructions.

```
# Create a string seq
seq = 'ATGAAGGGTCC'
# Call the function len() to retrieve the length of the string
size = len(seq)
# Call the function print() to print a text
print('The sequence has', size, 'bases.')
```

```
The sequence has 11 bases.
```

3.4 Why use Python?

- Easy-to-use and easy-to-read syntax
- Large standard library for many applications (`pandas` for tables, `matplotlib` for graphs, `scikit-learn` for machine learning...)
- Interactive mode making it easy to test short snippets of code
- Large community (stackoverflow)

Figure 3.3: Just google (or ChatGPT/Copilot) it!

3.5 How can I program in Python?

Python is an interpreted language, this means that all scripts written in Python need a software to be run. This software is called an interpreter, which "translate" each line of the code, into instructions that the computer can understand. By extension, the interpreter that is able to read Python scripts is also called Python. So, whenever you want your Python code to run, you give it to the Python interpreter.

3.5.1 Interactive mode

One way to launch the Python interpreter is to type the following, on the command line of a terminal:

```
python3
```

> **Note**
>
> You can also try `python`, `/usr/bin/env python3`, `/usr/bin/python3`... There are many ways to call python! You can see where your current python is located by running `which python3`.

From this, you can start using python interactively, e.g. run:

```
print("Hello world")
```

```
Hello world
```

To get out of the Python interpreter, type `quit()`or `exit()`, followed by `enter`. Alternatively, on Linux/Mac press `[ctrl + d]`, on Windows press `[ctrl + z]`.

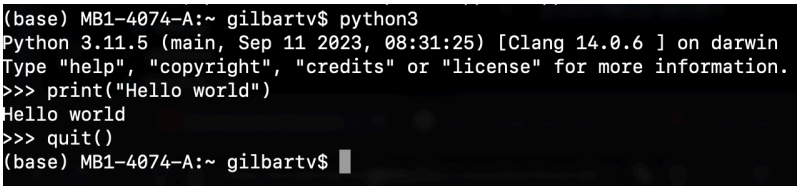


Figure 3.4: Interactive mode

3.5.2 Script mode

To run a script, create a folder named `script`, in which a file named `intro.py` contains:

```
#!/usr/bin/env python3
# -*- coding: UTF-8 -*-

print("Hello world")
```

and run

```
./script/intro.py
```

You should get the same output as before, that is:

```
Hello world
```

The shebang `#!` followed by the interpreter `/usr/bin/env python3` can be put at the beginning of the script in order to ommit calling `python3` in command-line. If you don't put it, you will have to run `python3 script/intro.py` instead of simply `./script/intro.py`.

The `-*- coding: UTF-8 -*-` specify the type of encoding to use. UTF-8 is used by default (which means that this line in the script is not necessary). This accepts characters from all languages. Other valid encoding are available, such as ascii (English characters only).

Warning

Some common errors can occur at this step:

- `bash: script/intro.py: No such file or directory` i.e. you are not in the right directory to run the file.

  Solution: run `ls */` and make sure you can find `script/: intro.py`, if not go to the correct directory by running `cd <insert directory name here>`

- `bash: script/intro.py: Permission denied` i.e. you don't have the right to execute your script.

  Solution: run `ls -l script/intro.py` and make sure you have at least `-rwx` (read, write, exectute rights) as the first 4 characters, if not run `chmod 744 script/intro.py` to change your rights.

4 Basic concepts

4.1 Values and variables

You will manipulate values such as integers, characters or dictionaries. These values can be stored in memory using variables. To assign a value to a variable, use the = operator as follow:

```
seq = 'ATGAAGGGTCC'
```

To output the variable value, either type the variable name or use a function like `print()`:

```
seq
```

```
'ATGAAGGGTCC'
```

```
print(seq)
```

```
ATGAAGGGTCC
```

We can change a variable value by assigning it a new one:

```
seq = seq + 'AAAA' # The + operator can be used to concatenate strings
seq
```

```
'ATGAAGGGTCCAAAA'
```

A variable can have a short name (like x and y) or a more descriptive name (seq, motif, genome_file). Rules for Python variable names:

- must start with a letter or the underscore character
- cannot start with a number
- can only contain alpha-numeric characters and underscores (A-z, 0-9, and _)
- are case-sensitive (seq, Seq and SEQ are three different variables)
- cannot be any of the Python keywords (run `help('keywords')` to find the list of keywords).

> ! Exercise
>
> Are the following variables names legal?
>
> - `2_sequences`
> - `_sequence`
> - `seq-2`
> - `seq 2`
>
> You can try to assign a value to these variable names to be sure of your answer!

4.2 Function calls

A function stores a piece of code that performs a certain task, and that gets run when called. It takes some data as input (parameters that are required or optional), and returns an output (that can be of any type). Some functions are predefined (but we will also learn how to create our own later on).

To run a function, write its name followed by parenthesis. Parameters are added inside the parenthesis as follow:

```
# round(number, ndigits=None)
x = round(number = 5.76543, ndigits = 2)
print(x)
```

```
5.77
```

Here the function `round()` needs as input a numerical value. As an option, one can add the number of decimal places to be used with digits. If an option is not provided, a default value is given. In the case of the option ndigits, `None` is the default. The function returns a numerical value, that corresponds to the rounded value. This value, just like any other, can be stored in a variable.

To get more information about a function, use the `help()` function.

> **Note**
>
> If you provide the parameters in the exact same order as they are defined, you don't have to name them. If you name the parameters you can switch their order. As good practice, put all required parameters first.

```
round(5.76543, 2)
```

```
5.77
```

```
round(ndigits = 2, number = 5.76543)
```

```
5.77
```

In Table 16.1 you will find some basic but useful python functions:

Table 4.1: List of useful Python functions.

Function	Description
`print()`	Print into the screen the values given in argument.
`help()`	Execute the built-in help system
`quit()` or `exit()`	Exit from Python
`len()`	Return the length of an object
`round()`	Round a numbers

4.3 Getting help

To get more information about a function or an operator, you can use the `help()` function. For example, in interactive mode, run `help(print)` to display the help of the `print()` function, giving you information about the input and output of this function. If you need information about an operator, you will have to put it into quotes, e.g. `help('+')`

> Browse the help
>
> If the help is long, press `[enter]` to get the next line or `[space]` to get the next 'page' of information.
> To quit the help, press `q`.

4.4 Comment your code

Except for the shebang and coding specifications seen before, all things after a hashtag `#` character will be ignored by the interpreter until the end of the line. This is used to add comments in your code.

Comments are used to:

- explain assumptions
- justify decisions in the code
- expose the problem being solved
- inactivate a line to help debug
- …

5 How can I represent data?

Each programming language has its own set of data types, from the most basics (`bool`, `int`, `string`) to more complex structures (`list`, `tuple`, `set`…).

5.1 Simple data types

5.1.1 Boolean

Booleans represent one of two values: `True` or `False`.

When you compare two values, the expression is evaluated and Python returns the Boolean answer:

```
print(10 > 9)
```

```
True
```

5.1.2 Numeric

Python provides three kinds of numerical type:

- `int` ($\mathbb{Z}$), integers
- `float` ($\mathbb{R}$), real numbers
- `complex` ($\mathbb{C}$), complex numbers

Python will assign a numerical type automatically.

```
x = 1
y = 2.8
z = 1j + 2 # j is the convention in electrical engineering
```

```
type(x)
```

```
int
```

```
type(y)
```

```
float
```

```
type(z)
```

```
complex
```

5.1.3 Text

String type represents textual data composed of letters, numbers, and symbols. The character string must be expressed between quotes.

```
"""my string"""
'''my string'''
"my string"
'my string'
```

are all the same thing. The difference with triple quotes is that it allows a string to extend over multiple lines. You can also use single quotes and double quotes freely within the triple quotes.

```
# A multi-line string
my_str = '''This is a multi-line string. This is the first line.
This is the second line.
"What's your name?," I asked.
He said "Bond, James Bond."
'''

print(my_str)
```

```
This is a multi-line string. This is the first line.
This is the second line.
"What's your name?," I asked.
He said "Bond, James Bond."
```

You can get the number of characters inside a string with `len()`.

```
print(seq)
len(seq)
```

```
ATGAAGGGTCCAAAA
```

```
15
```

Strings have specific methods (i.e. functions specific to this class of object). Here are a few:

Method	Description
`.count()`	Returns the number of times a specified value occurs in a string
`.startswith()`	Returns true if the string starts with the specified value
`.endswith()`	Returns true if the string ends with the specified value
`.find()`	Searches the string for a specified value and returns the position of where it was found
`.replace()`	Returns a string where a specified value is replaced with a specified value

They are called like this:

```
seq.count('A')
```

```
7
```

> **Tip**
>
> To get the `help()` of the `.count()` method, you need to run `help(str.count)`.

> **Exercise**
>
> 1. Check if the sequence `seq` starts with the codon `ATG`
> 2. Replace all `T` into `U` in `seq`

5.2 Data structures

Data structures are a collection of data types and/or data structures, organized in some way.

5.2.1 List

List is a collection which is ordered and changeable. It allows duplicate members. They are created using square brackets `[]`.

```
seq = ['ATGAAGGGTCCAAAA', 'AGTCCCCGTATGAT', 'ACCT', 'ACCT']
```

List items are indexed, the first item has index `[0]`, the second item has index `[1]` etc.

```
seq[1]
```

```
'AGTCCCCGTATGAT'
```

> **Tip**
>
> You can count backwards, with the index `[-1]` that retrieves the last item.

As a list is changeable, we can change, add, and remove items in a list after it has been created.

```
seq[1] = 'ATG'
seq
```

```
['ATGAAGGGTCCAAAA', 'ATG', 'ACCT', 'ACCT']
```

You can specify a range of indexes by specifying the start (included) and the end (not included) of the range.

```
seq[0:2]
```

```
['ATGAAGGGTCCAAAA', 'ATG']
```

> **Tip**
>
> By leaving out the start value, the range will start at the first item:
>
> ```
> seq[:2]
> ```
>
> ```
> ['ATGAAGGGTCCAAAA', 'ATG']
> ```
>
> Similarly, by leaving out the end value, the range will end at the last item.

> **Note**
>
> Indexes also conveniently work on `str` types.

```
print(seq[0])
print(seq[0][0:5])
print(seq[0][2])
print(seq[0][-1])
```

```
ATGAAGGGTCCAAAA
ATGAA
G
A
```

You can get how many items are in a list with `len()`.

```
len(seq)
```

```
4
```

Lists have specific methods. Here are a few:

Method	Description
`.append()`	Inserts an item at the end
`.insert()`	Inserts an item at the specified index
`.extend()`	Append elements from another list to the current list
`.remove()`	Removes the first occurance of a specified item
`.pop()`	Removes the specified (by default last) index

! Exercise

1. Create a list `l = ['AAA', 'AAT', 'AAC']`, and add `AAG` at the end, using `.append()`.
2. Replace all `T` into `U` in the element `AAT`, using `.replace()`.

5.2.2 Tuple

Tuple is a collection which is ordered and unchangeable. It allows duplicate members. Tuples are written with round brackets `()`.

```
my_favorite_amino_acid = ('Y', 'Tyr', 'Tyrosine')
```

Just like for the list, you can get items with their index. The only difference is that you cannot change a tuple that has been created.

Tuples have specific methods. Here are a few:

Method	Description
`.count()`	Returns the number of times a specified value occurs
`.index()`	Searches for a specified value and returns the position of where it was found

> ! Exercise
>
> Try to change the value of the first element of `my_favorite_amino_acid` and see what happens.

5.2.3 Set

Set is a collection which is unordered and unindexed. It does not allow duplicate members (they will be ignored). Sets are written with curly brackets `{}`.

```
seq = {'BRCA1', 'TP53', 'EGFR', 'MYC'}
```

Once a set is created, you cannot change its items directly (as they don't have index), but you modify the set by removing and adding items.

Sets have specific methods. Here are a few:

Method	Description
`.add()`	Adds an element to the set

Method	Description
`.difference()`	Returns a set containing the difference between two sets
`.intersection()`	Returns a set containing the intersection between two sets
`.union()`	Returns a set containing the union of two sets
`.remove()`	Remove the specified item
`.pop()`	Removes a random element

! Exercise

Get the common genes between the following sets:

```
organism1_genes = {'BRCA1', 'TP53', 'EGFR', 'MYC'}
organism2_genes = {'TP53', 'MYC', 'KRAS', 'BRAF'}
```

5.2.4 Dictionary

Dictionaries are used to store data values in `key: value` pairs. A dictionary is a collection which is ordered (as of Python >= 3.7), changeable and does not allow duplicates keys. Dictionaries are written with curly brackets `{}`, with keys and values.

```
organism1_genes = {
  #key: value;
  'BRCA1': 'DNA repair',
  'TP53': 'Tumor suppressor',
  'EGFR': 'Cell growth',
  'MYC': 'Regulation of gene expression'
}
```

Dictionary items can be referred to by using the key name.

```
organism1_genes["BRCA1"]
```

```
'DNA repair'
```

Dictionaries have specific methods. Here are a few:

Method	Description
`.items()`	Returns a list containing a tuple for each key value pair
`.keys()`	Returns a list containing the dictionary's keys
`.values()`	Returns a list of all the values in the dictionary
`.pop()`	Removes the element with the specified key
`.get()`	Returns the value of the specified key

> ! Exercise
>
> From the dictionary `organism1_genes` created as example, get the value of the key `BRCA1`. If the key does not exist, return `Unknown` by default. Try your code before **and after** removing the `BRCA1` key:value pair.
> Check the help of `get` by running `help(dict.get)`.

5.3 Conversion between types

You can get the data type of any object by using the function `type()`. You can (more or less easily) convert between data types.

Function	Description
`bool()`	Convert to boolean type
`int()`, `float()`	Convert between integer or float types
`complex()`	Convert to complex type
`str()`	Convert to string type
`list()`, `tuple()`, `set()`	Convert between list, tuple, and set types

Function	Description
`dict()`	Convert a tuple of order (key, value) into a dictionary type

```
bool(1)
```

```
True
```

```
int(5.8)
```

```
5
```

```
str(1)
```

```
'1'
```

```
list({1, 2, 3})
```

```
[1, 2, 3]
```

```
set([1, 2, 3, 3])
```

```
{1, 2, 3}
```

```
dict((('a', 1),
      ('f', 2),
      ('g', 3)))
```

```
{'a': 1, 'f': 2, 'g': 3}
```

6 How can I manipulate data?

In the previous section we have learned how data can be represented in different types and gathered in various data structures. In this section we will see how we can manipulate data in order to do more complex tasks.

6.1 Operators

Operators are used to perform operations on variables and values. We will present a few common ones here.

6.1.1 Arithmetic operators

Arithmetic operators are used with numeric values to perform common mathematical operations:

Operator	Name
`+`	Addition
`-`	Substraction
`*`	Multiplication
`/`	Division
`**`	Power

> **Warning**
>
> Do not use the `^` operator to raise to a power. That is actually the operator for bitwise XOR, which we will not cover.

Python will convert data type according to what is necessary. Thus, when you divide two `int` you will obtain a `float` number, if you add a `float` to an `int`, you will get a `float`, …

```
# Example
2/10
```

```
0.2
```

> **Note**
>
> `+` also conveniently work on `str` types.
>
> ```
> 'AC' + 'AT'
> ```
>
> ```
> 'ACAT'
> ```

6.1.2 Assignment operators

Assignment operators are used to assign values to variables:

Operator	Example as	Same as
`=`	`x = 5`	`x = 5`
`+=`	`x += 5`	`x = x + 5`
`-=`	`x -= 5`	`x = x - 5`

> **Note**
>
> The same principle applies to multiplication, division and power, but are less commonly used.

6.1.3 Comparison operators

Comparison operators are used to compare two values:

Operator	Name
==	Equal
!=	Not equal
>	Greater than
>=	Greater than or equal to
<	Less than
<=	Less than or equal to

```
# Example
2 == 1 + 1
```

```
True
```

> **Warning**
>
> You should never use equalty operators (==or !=) with floats or complex values.
>
> ```
> # Example
> 2.1 + 3.2 == 5.3
> ```
>
> ```
> False
> ```
>
> This is a floating point arithmetic problem seen in other programming languages. It is due to the difficulty of having a fixed number of binary digits (bits) to accurately represent some decimal number. This leads to small rounding errors in calculations.
>
> ```
> 2.1 + 3.2
> ```
>
> ```
> 5.300000000000001
> ```
>
> If you need to use equalty operators, do it with a degree of freedom:
>
> ```
> tol = 1e-6 ; abs((2.1 + 3.2) - 5.3) < tol
> ```
>
> ```
> True
> ```

6.1.4 Logical operators

Logical operators are used to combine conditional statements:

Operator	Description
`and`	Returns True if both statements are true
`or`	Returns True if one of the statements is true
`not`	Reverse the result, returns False if the result is true

```
# Example
False and False, False and True, True and False, True and True
```

```
(False, False, False, True)
```

```
# Example
False or False, False or True, True or False, True or True
```

```
(False, True, True, True)
```

```
# Example
True or not True
```

```
True
```

6.1.5 Membership operators

Operator	Description
`in`	Returns True if a sequence with the specified value is present in the object
`not in`	Returns True if a sequence with the specified value is not present in the object

```
# Example
'ACCT' in seq
```

```
False
```

6.1.6 Operator precedence

Operator precedence describes the order in which operations are performed.

The precedence order is described in the table below, starting with the highest precedence at the top:

Operator	Description
`()`	Parenthesis
`**`	Power
`* /`	Multiplication, division
`+ -`	Addition, substraction
`==,!=,>,>=,<,<=,is,is not in, not`	Comparisons, identity, and membership operators
`not`	Logical NOT
`and`	AND
`or`	OR

If two operators have the same precedence, the expression is evaluated from left to right.

> **!** Exercise
>
> Try to guess what will output the following expressions:
>
> - `1+1 == 2 and "actg" == "ACTG"`
> - `True or False and True and False`
> - `"Homo sapiens" == "Homo" + "sapiens"`
> - `'Tumor suppressor' in organism1_genes`
>
> Verify with Python.

6.2 Conditionals

Conditionals allows you to make decisions in your code based on certain conditions.

```
if something is true:
    do task a
otherwise:
    do task b
```

The comparison (`==`, `!=`, `>`, `>=`, `<`, `<=`), logical (`and`, `or`, `not`) and membership (`in`, `not in`) operators can be used as conditions.

In Python, this is written with an `if ... elif ... else` statement like so:

```
# Define gene expression levels
gene1_expression = 100
gene2_expression = 50

# Analyze gene expression levels
if gene1_expression > gene2_expression:
  print("Gene 1 has higher expression level.")
elif gene1_expression < gene2_expression:
  print("Gene 2 has higher expression level.")
else:
  print("Gene 1 and Gene 2 have the same expression level.")
```

```
Gene 1 has higher expression level.
```

The `elif` keyword is Python's way of saying "if the previous conditions were not true, then try this condition". The following code is equivalent to the one before:

```
# Analyze gene expression levels
if gene1_expression > gene2_expression:
  print("Gene 1 has higher expression level.")
else:
```

```
  if gene1_expression < gene2_expression:
    print("Gene 2 has higher expression level.")
  else:
    print("Gene 1 and Gene 2 have the same expression level.")
```

```
Gene 1 has higher expression level.
```

! Exercise

Are these two codes equivalent?

```
# Code A
if "ATG" in dna_sequence:
  print("Start codon found.")
elif "TAG" in dna_sequence:
  print("Stop codon found.")
else:
  print("No interesting codon not found.")
```

```
# Code B
if "ATG" in dna_sequence:
  print("Start codon found.")
  if "TAG" in dna_sequence:
    print("Stop codon found.")
else:
  print("No interesting codon not found.")
```

6.3 Notes on indentation

i Note

Python relies on **indentation** (the spaces at the beginning of the lines).

Indentation is not just for readability. In Python, you use spaces or tabs to indent code blocks. Python uses it to determine the scope of functions, loops, conditional statements, and classes.

Any code that is at the same level of indentation is considered part of the same block. Blocks of code are typically defined by starting a line with a colon (`:`) and then indenting the following lines.

When you have nested structures like a conditional statement inside another conditional statement, you must further to show the hierarchy. Each level of indentation represents a deeper level of nesting.

It's essential to be consistent with your indentation throughout your code. The styling guide of Python PEP8 recommands 4 spaces as indentation.

! Exercise

Here are three codes, they all are incorrect, can you tell why?
Of course, you can run them and read the error that Python gives!

```
amino_acid_list = ["MET", "ARG", "THR", "GLY"]

if "MET" in amino_acid_list:
  print("Start codon found.")
  if "GLY" in amino_acid_list:
    print("Glycine found.")
else:
print("Start codon not found.")
```

```
dna_sequence = "ATGCTAGCTAGCTAG"

if "ATG" in dna_sequence:
  print("Start codon found.")
if "TAG" in dna_sequence
  print("Stop codon found.")
```

```
x = 7

if x > 5:
  print("x is greater than 5")
  if x > 10:
    print("x is greater than 10")
  elif x = 10:
    print("x equals 10")
  else:
    print("x is less than 10")
```

6.4 Iterations

Iteration involves repeating a set of instructions or a block of code multiple times.

There are two types of loops in python, `for` and `while`.

Iterating through data structures like lists allows you to access each element individually, making it easier to perform operations on them.

6.4.1 For loops

When using a for loop, you iterate over a sequence of elements, such as a list, tuple, or dictionary.

```
for item in data_structure:
    do task a
```

The loop will execute the indented block of code for each element in the sequence until all elements have been processed. This is particularly useful when you know the number of times you need to iterate.

```
all_codons = [
    'AAA', 'AAC', 'AAG', 'AAT',
    'ACA', 'ACC', 'ACG', 'ACT',
    'AGA', 'AGC', 'AGG', 'AGT',
    'ATA', 'ATC', 'ATG', 'ATT',
    'CAA', 'CAC', 'CAG', 'CAT',
    'CCA', 'CCC', 'CCG', 'CCT',
    'CGA', 'CGC', 'CGG', 'CGT',
    'CTA', 'CTC', 'CTG', 'CTT',
    'GAA', 'GAC', 'GAG', 'GAT',
    'GCA', 'GCC', 'GCG', 'GCT',
    'GGA', 'GGC', 'GGG', 'GGT',
    'GTA', 'GTC', 'GTG', 'GTT',
    'TAA', 'TAC', 'TAG', 'TAT',
    'TCA', 'TCC', 'TCG', 'TCT',
    'TGA', 'TGC', 'TGG', 'TGT',
    'TTA', 'TTC', 'TTG', 'TTT'
]

count = 0
for codon in all_codons:
  if codon[1] == 'T':
    count += 1

print(count, 'codons have a T as a second nucleotide.')
```

```
16 codons have a T as a second nucleotide.
```

What it does is the following: it processes each element in the list `all_codons`, called in the following code `codon`. If the `codon` has as a second character a `T`, it adds 1 to a counter (the variable called `count`).

> **Warning**
>
> You cannot modify an element of a list that way.

```
for codon in all_codons:
  if 'T' in codon :
    codon = codon.replace('T', 'U')

print(all_codons)
```

```
['AAA', 'AAC', 'AAG', 'AAT', 'ACA', 'ACC', 'ACG', 'ACT', 'AGA', 'AGC', 'AGG', 'AGT', 'ATA',
```

This is because `all_codons` was converted to an iterator in the `for` statement.

6.4.2 Iterators

An iterator is a special object that gives values in succession.

In the previous example, the iterator returns a copy of the item in a list, not a reference to it. Therefore, the `codon` inside the `for` block is not a view into the original list, and changing it does not do anything to the original list.

A way to modify the list would be to use an iterable to access the original data. The `range(start, stop)` function creates an iterable to count from one integer to another.

```
for i in range(2, 10):
    print(i, end='  ')
```

```
2  3  4  5  6  7  8  9
```

We could count from 0 to the size of the list, loop though every element of the list by calling them by their index, and modify them if necessary. That's what the following code does:

```
for i in range(0, len(all_codons)):
  if 'T' in all_codons[i] :
    all_codons[i] = all_codons[i].replace('T', 'U')

print(all_codons)
```

```
['AAA', 'AAC', 'AAG', 'AAU', 'ACA', 'ACC', 'ACG', 'ACU', 'AGA', 'AGC', 'AGG', 'AGU', 'AUA', 'AU
```

Another useful function that returns an iterator is `enumerate()`. It is an iterator that generates pairs of index and value. It is commonly used when you need to access both the index and value of items simultaneously.

```
seq = 'ATGCATGC'

# Print index and identity of bases
for i, base in enumerate(seq):
    print(i, base)
```

```
0 A
1 T
2 G
3 C
4 A
5 T
6 G
7 C
```

```
# Loop through sequence and print index of G's
for i, base in enumerate(seq):
    if base in 'G':
        print(i, end='  ')
```

```
2  6
```

6.4.3 While loops

A while loop continues executing a set of statement as long as a condition is true.

```
while condition is true:
    do task a
```

This type of loop is handy when you're not sure how many iterations you'll need to perform or when you need to repeat a block of code until a certain condition is met.

```
seq = 'TACTCTGTCGATCGTACGTATGCAAGCTGATGCATGATTGACTTCAGTATCGAGCGCAGCA'
start_codon = 'ATG'

# Initialize sequence index
i = 0
# Scan sequence until we hit the start codon
while seq[i:i+3] != start_codon:
  i += 1

# Show the result
print('The start codon begins at index', i)
```

```
The start codon begins at index 19
```

Figure 6.1: Hopefully not you!

> **Warning**
>
> Remember to increment i, or you'll get stuck in a loop.

Actually, the previous code is quite dangerous. You can also get stuck in a loop… if the `start_codon` does not appear in `seq` at all.

Indeed, even when you go above the given length of `seq`, the condition `seq[i:i+3] != start_codon` will still be true because `seq[i:i+3]` will output an empty string.

```
seq[9999:9999+3]
```

```
''
```

So, once the end of the sequence is reached, the condition `seq[i:i+3] != start_codon` will always be true, and you'll get stuck in an infinite loop.

> **Note**
>
> To interrupt a process, press `[ctrl + c]`.

6.4.4 Break statement

Iteration stops in a `for` loop when the iterator is exhausted. It stops in a `while` loop when the conditional evaluates to `False`. There is another way to stop iteration: the `break` keyword. Whenever `break` is encountered in a `for` or `while` loop, the iteration stops and execution continues outside the loop.

```
seq = 'ACCATTTTTTGGGGGGGCGGGGGGAGGGGGGG'
start_codon = 'ATG'

# Initialize sequence index
i = 0
# Scan sequence until we hit the start codon
while seq[i:i+3] != start_codon:
  i += 1
  if i+3 > len(seq): # Get out of the loop if we parsed the full seq
    print('Codon not found in sequence.')
    break
else:
  print('The start codon starts at index', i)
```

```
Codon not found in sequence.
```

> **Note**
>
> Also, note that the `else` statement can be used in `for` and `while` loops. In `for` loops it is executed when the **loop is finished**. In `while` loops, it is executed when the condition is **no longer true**. In both case, the loops need to **not** encounter a `break` to enter in the `else` block.

6.4.5 Continue statement

In addition to the break statement, there is also the continue statement in Python that can be used to alter the flow of iteration in loops. When continue is encountered within a loop, it skips the remaining code inside the loop for the current iteration and moves on to the next iteration.

Here's an example showcasing the continue statement in a loop:

```
# List of DNA sequences
dna_sequences = ['ATGCTAGCTAG', 'ATCGATCGATC', 'ATGGCTAGCTA', 'ATGTAGCTAGC']

# Find sequences starting with a start codon
for sequence in dna_sequences:
    if sequence[:3] != 'ATG':  # Check if the sequence does not start with a start codon
        print(f"Sequence '{sequence}' does not start with a start codon. Skipping analysis.")
        continue  # Skip further analysis for this sequence
    print(f"Analyzing sequence '{sequence}' for protein coding regions...")
    # Additional analysis code here
else:
  print('All sequences were processed.')
```

```
Analyzing sequence 'ATGCTAGCTAG' for protein coding regions...
Sequence 'ATCGATCGATC' does not start with a start codon. Skipping analysis.
Analyzing sequence 'ATGGCTAGCTA' for protein coding regions...
Analyzing sequence 'ATGTAGCTAGC' for protein coding regions...
All sequences were processed.
```

The continue statement in this example skips the analysis code for sequence that does not start with a start codon.

> **Note**
>
> The annotation `f"Some text followed by a {variable}"` is a straight-forward and clear way to format strings called F-Strings. `{variable}` will be interpreted so that its value is output.

6.4.6 Exercises

! Exercise 1

Given a list of DNA sequences, find the first sequence that contains a specific motif `'TATA'`, print the sequence, and stop the process. If no sequence contains the motif, print a message accordingly. You must use only one `for` loop. With the input given below, the output should look like this:

```
# List of DNA sequences with a TATA
dna_sequences = [
'ATGCTACAGCTAG',
'ATCGATATAATC', # TATA
'ATGGCTAGCTA',
'ATGTAGCTAGC',
'ATGTAGCTATA'   # TATA
]

for ...
  # Your code here
```

```
Sequence 'ATCGATATAATC' contains the 'TATA' motif.
```

```
# List of DNA sequences without a TATA
dna_sequences = [
'ATGCTACAGCTAG',
'ATCGATACAATC',
'ATGGCTAGCTA',
'ATGTAGCTAGC'
]

for ...
  # Your code here
```

```
No sequence contains the 'TATA' motif.
```

! Exercise 2

Analyze a DNA sequence to count the number of consecutive `'A'` nucleotides. You must use only one `while` loop. With the input given below, the output should look like this:

```
# DNA sequence to analyze
dna_sequence = 'ATGATAAGAGAAAGTAAAAGCGATCGAAAAAA'

while ...
  # Your code here
```

```
Number of consecutive 'A's: 6
```

7 Conclusion

Congrats! You now know the (very) basics of Python programming.

If you want to keep on practising with simple exercises, you can check out w3schools.

For more biology-related exercises check out pythonforbiologist.org, they have exercises availables in each chapters.

For french speakers, the AFPy (Association Francophone Python) has a learning tool called HackInScience.

Or keep on googling for more python exercises!

References

Here are some references and ressources that (greatly) inspired this class:

- Python doc
- w3schools
- pythonforbiologists
- justinbois's Bootcamp

8 Lesson 2 - Functions, file handling, dataframe and plots

9 Introduction

9.1 Aim of the class

At the end of this class, you will be able to:

- Create simple functions
- Upload, modify and download files into Python
- Install and import packages
- Basic use of pandas (manipulate data)
- Basic use of matplotlib.pyplot (visualize data)

10 Function

A function stores a piece of code that performs a certain task, and that gets run when called. It takes some data as input (parameters that are required or optional), and returns an output (that can be of any type).

> Tip
>
> We already learned how to run a predefined function in the last lesson. You need to write its name followed by parenthesis. Parameters are added inside the parenthesis as follow:
>
> ```
> # round(number, ndigits=None)
> x = round(number = 5.76543, ndigits = 2)
> print(x)
> ```
>
> ```
> 5.77
> ```
>
> To get more information about a function, use the `help()` function.

We will now learn how to create our own function.

10.1 Syntax

In python, a function is declared with the keyword `def` followed by its name, and the arguments inside parenthesis. The next block of code, corresponding to the content of the function, must be indented. The output is defined by the `return` keyword.

```
def hello(name):
  """Presenting myself.

  Parameters:
  name (str): My name.
  """

  presentation = f"Hello, my name is {name}."
  return presentation
```

```
text = hello(name = "Valentine")
print(text)
```

```
Hello, my name is Valentine.
```

10.2 Documentation

As you may have noticed, you can also add a description of the function directly after the function definition. It is the message that will be shown when running `help()`. As it can be along text over multiple lines, it is common to put it inside triple quotes `"""`.

```
help(hello)
```

```
Help on function hello in module __main__:

hello(name)
    Presenting myself.

    Parameters:
    name (str): My name.
```

10.3 Arguments

You can have several arguments. They can be mandatory or optional. To make them optional, they need to have a default value assigned inside the function definition, like so:

```
def hello(name, french = True):
  """Presenting myself.

  Parameters:
  name (str): My name.
  french (bool, optional): Whether to greet in french (True) or not (False).
  """

  if french:
    presentation = f"Bonjour, je m'appelle {name}."
  else:
    presentation = f"Hello, my name is {name}."
  return presentation
```

The parameter `name`is mandatory, but `french` is optional.

```
hello("Valentine")
```

```
"Bonjour, je m'appelle Valentine."
```

```
hello(french = False)
```

```
TypeError: hello() missing 1 required positional argument: 'name'
---------------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)
Cell In[7], line 1
----> 1 hello(french = False)
TypeError: hello() missing 1 required positional argument: 'name'
```

> **Note**
>
> Reminder: if you provide the parameters in the exact same order as they are defined, you don't have to name

them. If you name the parameters you can switch their order. As good practice, put all required parameters first.

```
hello(french = False, name = "Valentine")
```

```
'Hello, my name is Valentine.'
```

```
hello("Valentine", False)
```

```
'Hello, my name is Valentine.'
```

10.4 Output

If no `return` statement is given, then no output will be returned, but the function will still be run.

```
def hello(name):
  """Presenting myself."""
  print("We are inside the 'hello()' function.")
  presentation = f"Hello, my name is {name}."
```

```
print(hello("Valentine"))
```

```
We are inside the 'hello()' function.
None
```

The output can be of any type. If you have a lot of things to return, you might want to return a `list` or a `dict` for example.

```
def multiple_of_3(list_of_numbers):
  """Returns the number that are multiple of 3."""
  multiples = []
  for num in list_of_numbers:
    if num % 3 == 0:
      multiples.append(num)
```

```
  return multiples

multiple_of_3(range(1, 20, 2))
```

```
[3, 9, 15]
```

> **Note**
>
> This could be written as a one-liner.
>
> ```
> def multiple_of_3(list_of_numbers):
>   """Returns the number that are multiple of 3."""
>   multiples = [num for num in list_of_numbers if num % 3 == 0]
>   return multiples
>
> multiple_of_3(range(1, 20, 2))
> ```
>
> ```
> [3, 9, 15]
> ```

10.5 Exercise

> **Exercise 1**
>
> Write a function called `nucl_freq` to compute nucleotide frequency of a sequence. Given a sequence as input, it outputs a dictionnary with keys being the nucleotides `A`, `T`, `C` and `G`, and values being their frequency in the sequence. With the input given below, the output should be:
>
> ```
> def ...
>   # Your code here
>
> nucl_freq("ATTCCCGGGG")
> ```
>
> ```
> {'A': 0.1, 'G': 0.4, 'T': 0.2, 'C': 0.3}
> ```

11 File Handling

The key function to work with files in `open()`. It has two parameters `file` and `mode`.

```
# Write the correct path for you!
fasta_file = 'exercise/data/example.fasta'
f = open(fasta_file, mode = 'r')
```

The modes can be one of the following:

Mode	Description
`r`	Opens a file for reading, error if the file does not exist (default)
`a`	Opens a file for appending, creates the file if it does not exist
`w`	Opens a file for writing, creates the file if it does not exist
`x`	Creates the specified file, returns an error if the file exists

11.1 Reading

The `open()` function returns a file object, which has a `read()` method for reading the content of the file:

```
print(f.read())
```

```
>seq1
TTAGCTAAATAGCTAGCAAACTAGCTAGCTAAAAAAAAAAACTAGCTAGCT
>seq2
ATGCCAGCCAGCCAGCCAGCCAGCTCGCTCGCTCGCCAGCCAGCTAGCTA
```

```
>seq3
CCGGGCGGTCGATGGATGGAGGGAGCGAGCGATCGATCGGTCGATCGGTG
>seq4
GATCGATCGATCTTTTTATCGATCGATTGTTCTTTCGATCGTTCTATCGA
>seq5
ACGTACGTACGTACGTACGTACGTACGTACGTACGTACGTACGTACGTAT
```

The parameter `size =` can be added to specify the number of bytes (~ characters) to return.

```
# We need to re-open it because we have already parsed the whole file
f = open(fasta_file, mode = 'r')
print(f.read(2))
```

```
>s
```

You can return one line by using the `.readline()` method. By calling it two times, you can read the two first lines:

```
f = open(fasta_file, mode = 'r')
print(f.readline())
print(f.readline())
```

```
>seq1

TTAGCTAAATAGCTAGCAAACTAGCTAGCTAAAAAAAAAAACTAGCTAGCT
```

By looping through the lines of the file, you can read the whole file, line by line:

```
for i, line in enumerate(f):
  print(i, line)
```

```
0 >seq2

1 ATGCCAGCCAGCCAGCCAGCCAGCTCGCTCGCTCGCCAGCCAGCTAGCTA

2 >seq3
```

```
3 CCGGGCGGTCGATGGATGGAGGGAGCGAGCGATCGATCGGTCGATCGGTG

4 >seq4

5 GATCGATCGATCTTTTTATCGATCGATTGTTCTTTCGATCGTTCTATCGA

6 >seq5

7 ACGTACGTACGTACGTACGTACGTACGTACGTACGTACGTACGTACGTAT
```

It is a good practice to close the file when you are done with it.

```
f.close()
```

> **Warning**
>
> In some cases, changes made to a file may not show until you close the file.

> **Note**
>
> A common syntax to handle files that you might encounter is:
>
> ```
> with open(fasta_file, 'r') as f:
>   print(f.readline())
> ```
>
> ```
> >seq1
> ```
>
> This code is equivalent to
>
> ```
> f = open(fasta_file, 'r')
> try:
>   print(f.readline())
> finally:
>   f.close()
> ```
>
> ```
> >seq1
> ```

The `with` statement is an example of a context manager, i.e. it allows to allocate and release resources precisely, by cleaning up the resources once they are no longer needed.

11.2 Writting

To write into a file, you must have it open under a `w`, `a` mode.

Then, the method `write()` can be used.

```
txt_file = "exercise/data/some_file.txt"
f = open(txt_file, "w")
f.write("Woops! I have deleted the content!\n")
f.close()

# Read the current content of the file
f = open(txt_file, "r")
print(f.read())
```

Woops! I have deleted the content!

> **Warning**
>
> Be very careful when opening a file in `write` mode as you can delete its content without any way to retrieve the original file!

As you may have noticed, `write()` returns the number of characters written. You can prevent it from being printed by assigning the return value to a variable that will not be used.

```
f = open(txt_file, "a")
_ = f.write("Now the file has more content!\n")
f.close()

# Read the current content of the file
f = open(txt_file, "r")
print(f.read())
```

```
Woops! I have deleted the content!
Now the file has more content!
```

> **Note**
>
> You must specify a newline with the character:
>
> - `\n` in Linus/MacOS
> - `\r\n` in Windows
> - `\r` in MacOS before X

11.3 os module

Python has a built-in package called `os`, to interact with the operating system.

```
import os
```

Here are some useful functions from the `os` package.

Function	Description
`getcwd()`	Returns the current working directory
`chdir()`	Change the current working directory
`listdir()`	Returns a list of the names of the entries in a directory
`mkdir()`	Creates a directory
`makedirs()`	Creates a directory recursively

These functions can be useful if you don't manage to open a file, or don't find where you created it. Because it might just be that you are not in the directory you think:

```
# Verify your working directory
os.getcwd()
```

```
'/home/runner/work/python-intro/python-intro'
```

```
# Change you working directory if needed
os.chdir("/Users/gilbartv/Documents/git")
```

In other cases, to create a file, the folder it belongs to must already exist, so you need to create it automatically via python:

```
# Create a new directory recursively (if Documents/ does not exist it would be created)
# If the directory is already created, don't raise an error
os.makedirs("/Users/gilbartv/Documents/NewFolder", exist_ok=True)
```

11.4 Exercise

! Exercise 2

Create a function that:

- read the fasta file,
- calculate the nucleotide frequency for each sequence (using the previously defined function)
- create a new file as follow:

```
Seq A C T G
seq1 0.1 0.2 0.3 0.4
seq2 0.4 0.3 0.2 0.1
...
```

To make this easier, consider that the sequences in the fasta file are only in one line.
You might make good use of the method `str.strip()`.
You can take as input the file in `exercise/data/example.fasta` you should get the same result as `exercise/data/example.txt`.

```
def analyse_fasta(input_file, output_file):
  ...

input_file = "exercise/data/example.fasta"
output_file = "exercise/data/example.txt"

analyse_fasta(input_file, output_file)
```

12 Scientific packages

A python package contains a set of function to perform specific tasks.

A package needs to be **installed** to your computer one time.

> ⚠ Warning
>
> Installing a package is done outside of the python interpreter, in command line in a terminal.

You can install a package with `pip`. It should have been automatically installed with your python, to make sure that you have it you can run:

```
# In Linux/MacOS
python -m pip --version
# In Windows
py -m pip --version
```

If it does not work, check out pip documentation

To install a package called pandas, you must run:

```
# In Linux/MacOS
python -m pip install pandas
# In Windows
py -m pip install pandas
```

To get more information about `pip`, check out the full documentation.

When you wish to use a package in a python script, you'll need to import it, by writing inside of you script:

```
import pandas
```

12.1 Pandas

Pandas is a package used to work with data sets, in order to easily clean, manipulate, explore and analyze data.

12.1.1 Create pandas data

Pandas provides two types of classes for handling data:

- `Series`: a one-dimensional labeled array holding data of any type such as integers or strings. It is like a column in a table.

```
# If nothing else is specified, the values are labeled with their index number (starting from
myseries = pandas.Series([1, 7, 2], index = ["x", "y", "z"])
print(myseries)
```

```
x    1
y    7
z    2
dtype: int64
```

- `DataFrame`: a two-dimensional data structure that holds data like a two-dimension array or a table with rows and columns. It is like a table.

```
data = {
  "calories": [420, 380, 390],
  "duration": [50, 40, 45]
}

df = pandas.DataFrame(data)

print(df)
```

```
   calories  duration
0       420        50
1       380        40
2       390        45
```

You can also create a DataFrame from a file.

```
# Make sure this is the correct path for you! You are in the directory from where you execute t
df = pandas.read_csv('exercise/data/sample.csv')

print(df)
```

```
    Gene  Expression_Level Tissue
0  GeneA               8.7  Heart
1  GeneB               3.2  Heart
2  GeneA               7.0  Brain
3  GeneB              10.2  Brain
4  GeneA               6.6  Liver
5  GeneB               7.6  Liver
```

12.1.2 Index and columns

You get access to the index and column names with:

```
df.columns
```

```
Index(['Gene', 'Expression_Level', 'Tissue'], dtype='object')
```

```
df.index
```

```
RangeIndex(start=0, stop=6, step=1)
```

You can rename index and column names:

```
df = df.rename(index={0: 'a', 1: 'b', 2: 'c',
                      3: 'd', 4: 'e', 5 : 'f'})

df.index
```

```
Index(['a', 'b', 'c', 'd', 'e', 'f'], dtype='object')
```

You can select rows:

```
# Select one row by its label
df.loc[['a']]
```

```
/opt/hostedtoolcache/Python/3.10.17/x64/lib/python3.10/site-packages/IPython/core/formatters.py
  return method()
```

	Gene	Expression_Level	Tissue
a	GeneA	8.7	Heart

```
# Select one row by its index
df.iloc[[0]]
```

```
/opt/hostedtoolcache/Python/3.10.17/x64/lib/python3.10/site-packages/IPython/core/formatters.py
  return method()
```

	Gene	Expression_Level	Tissue
a	GeneA	8.7	Heart

```
# Select several rows by labels
df.loc[['a','c']]
```

```
/opt/hostedtoolcache/Python/3.10.17/x64/lib/python3.10/site-packages/IPython/core/formatters.py
  return method()
```

	Gene	Expression_Level	Tissue
a	GeneA	8.7	Heart
c	GeneA	7.0	Brain

```
# Select one row by index
df.iloc[[0,2]]
```

```
/opt/hostedtoolcache/Python/3.10.17/x64/lib/python3.10/site-packages/IPython/core/formatters.py
  return method()
```

	Gene	Expression_Level	Tissue
a	GeneA	8.7	Heart
c	GeneA	7.0	Brain

You can select columns:

```
# Select one column by label
df['Tissue'] # Series
```

	Tissue
a	Heart
b	Heart
c	Brain
d	Brain
e	Liver
f	Liver

```
df[['Tissue']] # DataFrame
```

```
/opt/hostedtoolcache/Python/3.10.17/x64/lib/python3.10/site-packages/IPython/core/formatters.py
  return method()
```

	Tissue
a	Heart
b	Heart
c	Brain
d	Brain
e	Liver
f	Liver

```
# Select several columns
df[['Gene','Expression_Level']]
```

```
/opt/hostedtoolcache/Python/3.10.17/x64/lib/python3.10/site-packages/IPython/core/formatters.py
  return method()
```

	Gene	Expression_Level
a	GeneA	8.7
b	GeneB	3.2
c	GeneA	7.0
d	GeneB	10.2
e	GeneA	6.6
f	GeneB	7.6

```
# Select several columns by index
df.iloc[:,[0,1]]
```

```
/opt/hostedtoolcache/Python/3.10.17/x64/lib/python3.10/site-packages/IPython/core/formatters.py
  return method()
```

	Gene	Expression_Level
a	GeneA	8.7
b	GeneB	3.2
c	GeneA	7.0
d	GeneB	10.2
e	GeneA	6.6
f	GeneB	7.6

You can select rows and columns as follows:

```
df.loc[['b'], ['Gene','Expression_Level']]
```

```
/opt/hostedtoolcache/Python/3.10.17/x64/lib/python3.10/site-packages/IPython/core/formatters.py
  return method()
```

	Gene	Expression_Level
b	GeneB	3.2

You can filter based on a condition as follows:

```
df[df['Expression_Level'] > 6]
```

```
/opt/hostedtoolcache/Python/3.10.17/x64/lib/python3.10/site-packages/IPython/core/formatters.py
  return method()
```

	Gene	Expression_Level	Tissue
a	GeneA	8.7	Heart
c	GeneA	7.0	Brain
d	GeneB	10.2	Brain
e	GeneA	6.6	Liver
f	GeneB	7.6	Liver

Note

To better understand how `df[df['Expression_Level'] > 6]` works, let's break it down.

```
df['Expression_Level']
```

	Expression_Level
a	8.7
b	3.2
c	7.0
d	10.2
e	6.6
f	7.6

```
rows_to_keep = df['Expression_Level'] > 6
rows_to_keep
```

```
/opt/hostedtoolcache/Python/3.10.17/x64/lib/python3.10/site-packages/IPython/core/formatters.
  return method()
```

	Expression_Level
a	True
b	False
c	True
d	True
e	True
f	True

Each value in `df['Expression_Level']` is being tested against the condition `> 6` and a boolean in being return.

```
df[rows_to_keep]
```

```
/opt/hostedtoolcache/Python/3.10.17/x64/lib/python3.10/site-packages/IPython/core/formatters.
  return method()
```

	Gene	Expression_Level	Tissue
a	GeneA	8.7	Heart
c	GeneA	7.0	Brain
d	GeneB	10.2	Brain
e	GeneA	6.6	Liver
f	GeneB	7.6	Liver

Rows of the DataFrame are being filtered by boolean values. If `True` the row is kept, if `False` it is dropped.

12.1.3 Useful methods

To explore the data set, use the following methods:

```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Index: 6 entries, a to f
Data columns (total 3 columns):
 #   Column            Non-Null Count  Dtype  
---  ------            --------------  -----  
 0   Gene              6 non-null      object 
 1   Expression_Level  6 non-null      float64
 2   Tissue            6 non-null      object 
dtypes: float64(1), object(2)
memory usage: 364.0+ bytes
```

```
df.describe()
```

```
/opt/hostedtoolcache/Python/3.10.17/x64/lib/python3.10/site-packages/IPython/core/formatters.py
  return method()
```

	Expression_Level
count	6.000000
mean	7.216667
std	2.358319
min	3.200000
25%	6.700000
50%	7.300000
75%	8.425000
max	10.200000

```
df.head()
```

```
/opt/hostedtoolcache/Python/3.10.17/x64/lib/python3.10/site-packages/IPython/core/formatters.py
  return method()
```

	Gene	Expression_Level	Tissue
a	GeneA	8.7	Heart
b	GeneB	3.2	Heart
c	GeneA	7.0	Brain
d	GeneB	10.2	Brain
e	GeneA	6.6	Liver

```
df.sort_values(by="Gene")
```

```
/opt/hostedtoolcache/Python/3.10.17/x64/lib/python3.10/site-packages/IPython/core/formatters.py
  return method()
```

	Gene	Expression_Level	Tissue
a	GeneA	8.7	Heart
c	GeneA	7.0	Brain
e	GeneA	6.6	Liver
b	GeneB	3.2	Heart
d	GeneB	10.2	Brain
f	GeneB	7.6	Liver

```
df['Expression_Level'].mean()

df.groupby("Gene")[['Expression_Level']].mean()
```

```
/opt/hostedtoolcache/Python/3.10.17/x64/lib/python3.10/site-packages/IPython/core/formatters.py
  return method()
```

Gene	Expression_Level
GeneA	7.433333
GeneB	7.000000

12.1.4 Learn More

To get more information on how to use pandas, check out:

- the documentation
- the cheat sheet
- any useful tutorial

12.1.5 Exercise

! Exercise 3

1. Create a pandas DataFrame from the file containing the frequency of each nucleotide per sequences (`exercise/data/example.txt`).
2. Make sure that `df.index` contains the name of the sequences, and `df.columns` contains the nucleotides.
3. Use `pandas.melt()` (see the example in the doc) to get the data in the following format:

```
     nucl  freq
Seq
seq1    A  0.46
seq2    A  0.20
```

```
seq3    A  0.16
seq4    A  0.18
seq5    A  0.26
seq1    T  0.22
seq2    T  0.12
...
```

4. Get the mean value of all nucleotide frequencies.
5. Get the mean value of frequencies per nucleotide.
6. Filter to remove values of seq1.
7. Recompute the mean value of frequencies per nucleotide.

12.2 Matplotlib

Matplotlib is a package to create visualizations in Python widely used in science.

To shorten the name of the package when we call its functions, we can import it with a nickname, as follows:

```
import pandas as pd

df = pd.read_csv('exercise/data/sample.csv')
```

For matplotlib, we usually import like so:

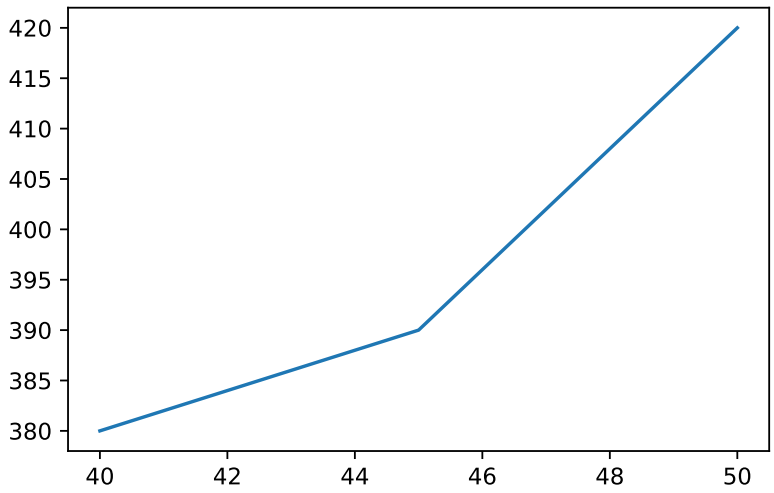
```
import matplotlib.pyplot as plt
```

pyplot is one of the modules of matplotlib. It contains functions to generate basic plots.

12.2.1 Create a plot

To create your first plot, you can use the function `plt.plot()` that draws points to plot, and by default draws a line from point to points:

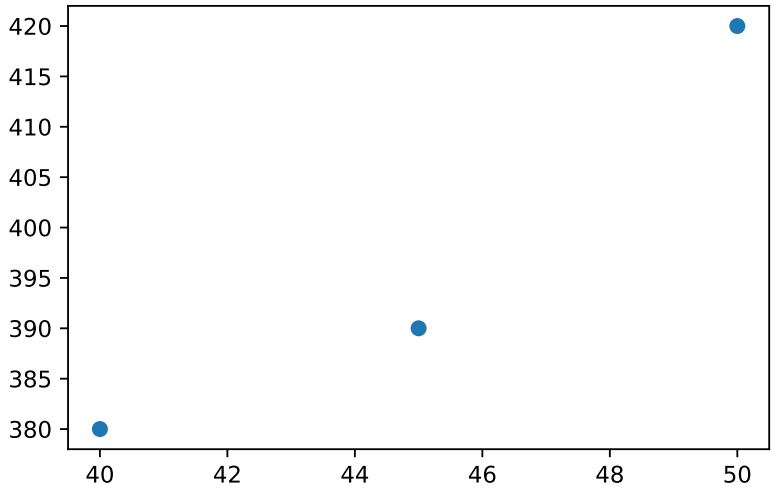
```
data = {
  "calories": [420, 380, 390],
  "duration": [50, 40, 45]
}
df = pd.DataFrame(data).sort_values(by="duration")

x = df['duration']
y = df['calories']

plt.plot(x, y)
plt.show()
```



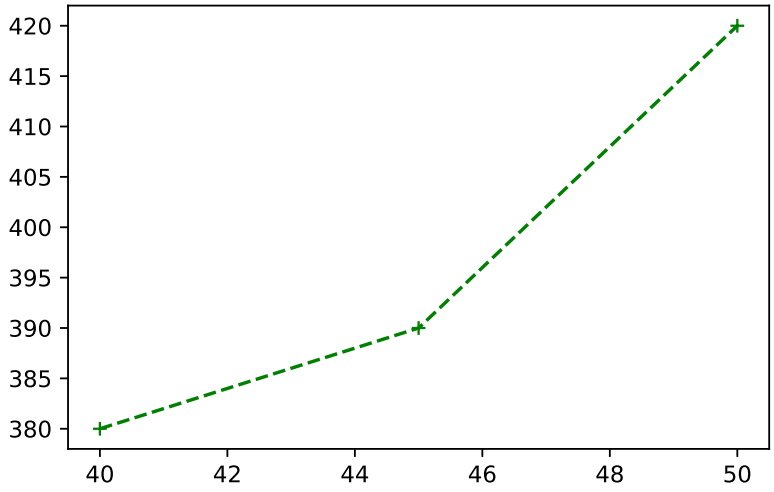
The first parameter is for the x-axis, and the second for the y-axis

To only plot the points, one can add the format (it can be color, marker, linestyle):

```
plt.plot(x, y, 'o') # point as markers
plt.show()
```



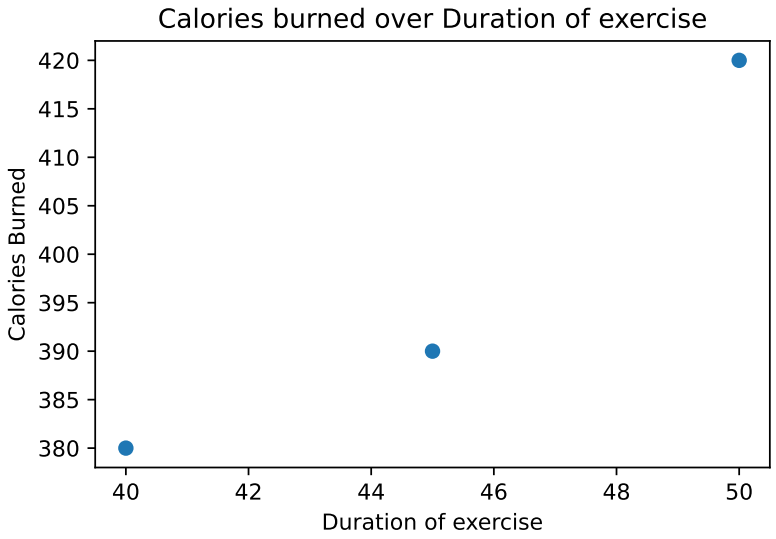

```
plt.plot(x, y, 'g+--') # Green as color, plus as marker, dash as line
plt.show()
```



X and y labels and plot title can be added:

```
plt.plot(x, y, 'o')

plt.xlabel("Duration of exercise")
plt.ylabel("Calories Burned")
plt.title("Calories burned over Duration of exercise")
```

```
plt.show()
```



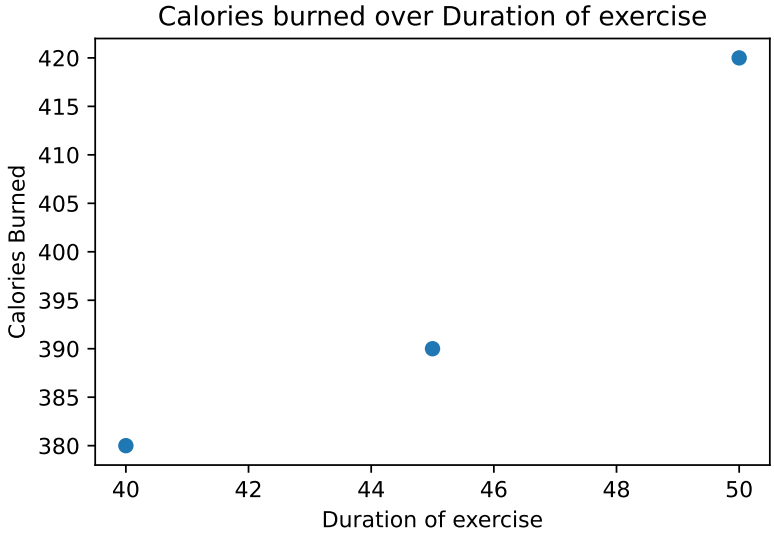
The first way of plotting is function-oriented. It relies on pyplot to implicitly create and manage the Figures and Axes, and use pyplot functions for plotting.

There is a second way of plotting called object-oriented. It needs to explicitly create Figures and Axes, and call methods on them (the "object-oriented (OO) style").

You might encounter both styles of coding.

In object-oriented, the plot above would be created like so:

```
fig, ax = plt.subplots(1) # Create the Figure and Axes

ax.plot(x, y, 'o') # Apply methods on the axes

ax.set_xlabel("Duration of exercise")
ax.set_ylabel("Calories Burned")
ax.set_title("Calories burned over Duration of exercise")

plt.show()
```



> **Note**
>
> Notice that the names of the functions/methods called are not the same: the function `xlabel()` is used for the function-oriented manner and the method `set_xlabel()` is used for the object-oriented.

12.2.2 Matplotlib anatomy

Matplotlib graphs your data on Figures, each of which can contain one or more Axes. An Axes is an area where points can be specified in terms of x-y coordinates.

Axes contains a region for plotting data and includes generally two Axis objects (2D plots), a title, an x-label, and a y-label. The Axes methods (e.g. `.set_xlabel()`) are the primary interface for configuring most parts of your plot (adding data, controlling axis scales and limits, adding labels etc.).

An Axis sets the scale and limits and generate ticks (the marks on the Axis) and ticklabels (strings labeling the ticks).

> **Note**
>
> Be aware of the difference between Axes and Axis.

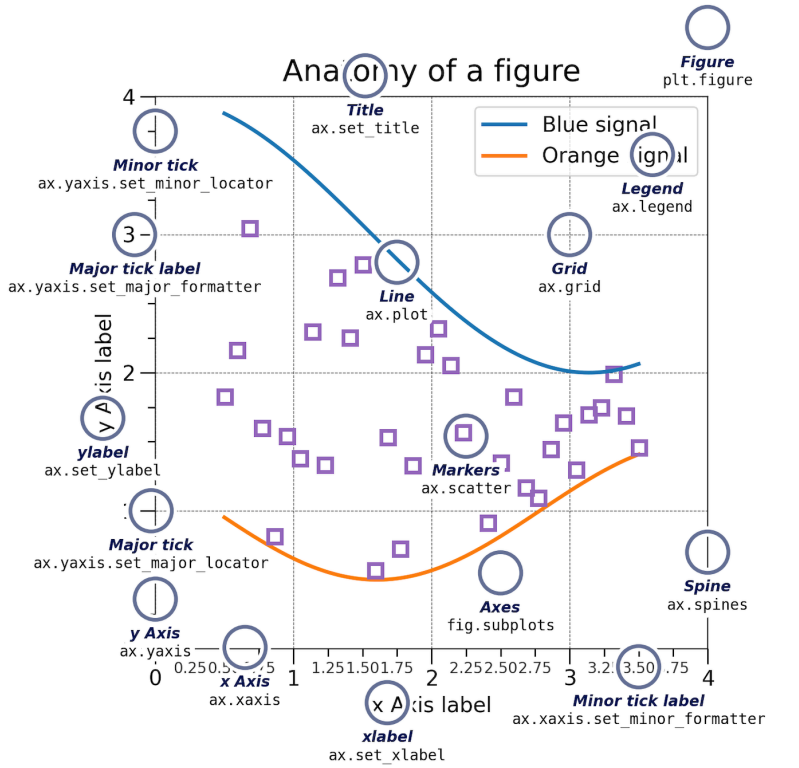
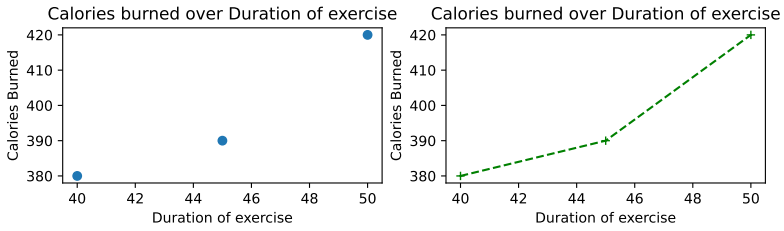


Figure 12.1: Anatomy of a matplotlib plot

To create a Figure with 2 Axes, run:

```
# a figure with a 1x2 (nrow x ncolumn) grid of Axes
# and of defined size figsize=(width,height)
fig, axs = plt.subplots(1, 2, figsize=(9,2))

axs[0].plot(x, y, 'o') # Apply methods on the axes
axs[0].set_xlabel("Duration of exercise")
axs[0].set_ylabel("Calories Burned")
axs[0].set_title("Calories burned over Duration of exercise")
```

```
axs[1].plot(x, y, 'g+--') # Apply methods on the axes
axs[1].set_xlabel("Duration of exercise")
axs[1].set_ylabel("Calories Burned")
axs[1].set_title("Calories burned over Duration of exercise")

plt.show()
```



There are many other plot available: `.scatter()`, `.bar()`, `.hist()`, `.pie()`, `.boxplot()`…

12.2.3 Save a figure

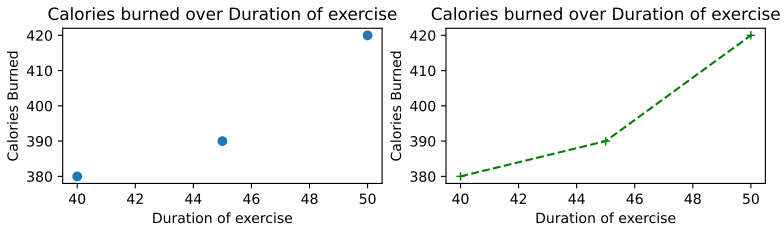
You can save a figure with the `savefig()` function:

```
plt.savefig('exercise/data/figure.png')
```

```
<Figure size 1650x1050 with 0 Axes>
```

> **Warning**
>
> Note that plt refer to a global figure variable and after a figure has been displayed to the screen (e.g. with plt.show) matplotlib will make this variable refer to a new empty figure. Therefore, make sure you call `plt.savefig` before the plot is displayed to the screen, otherwise you may find a file with an empty plot.

```
# a figure with a 1x2 (nrow x ncolumn) grid of Axes
# and of defined size figsize=(width,height)
fig, axs = plt.subplots(1, 2, figsize=(9,2))

axs[0].plot(x, y, 'o') # Apply methods on the axes
axs[0].set_xlabel("Duration of exercise")
axs[0].set_ylabel("Calories Burned")
axs[0].set_title("Calories burned over Duration of exercise")

axs[1].plot(x, y, 'g+--') # Apply methods on the axes
axs[1].set_xlabel("Duration of exercise")
axs[1].set_ylabel("Calories Burned")
axs[1].set_title("Calories burned over Duration of exercise")

plt.savefig('exercise/data/barplot.png')

plt.show()
```



The plot can also be save ad ps, pdf or svg. Moreover, the resolution can be modified. See the documentation of savefig.

12.2.4 Matplotlib documentation

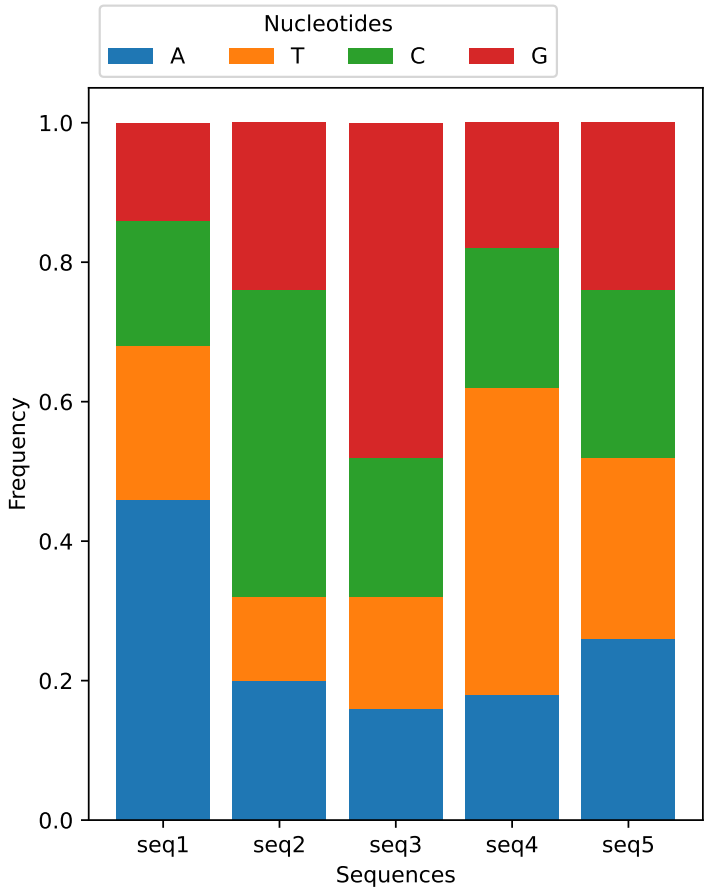
For more information, check out the following ressources:

- the documentation
- the cheat sheet
- any useful tutorial
- some inspiration

12.3 Exercise

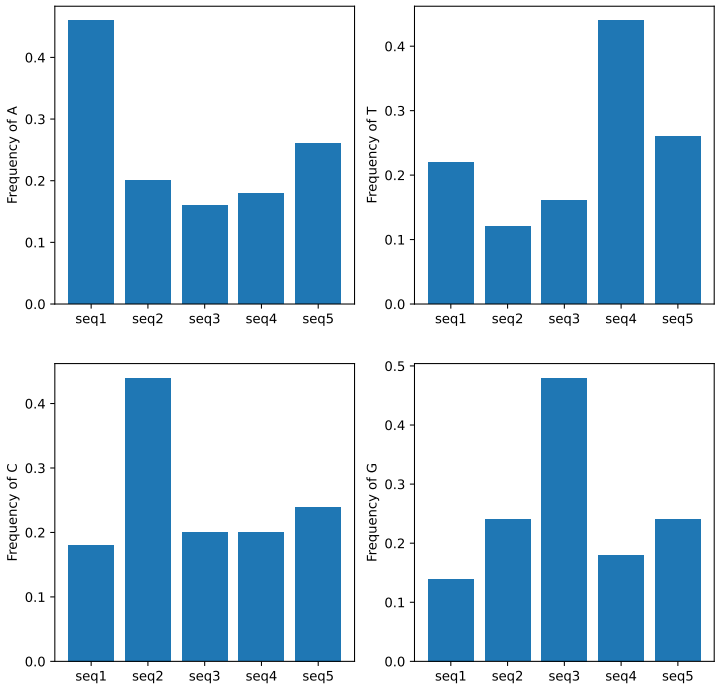
! Exercise 4

Create a script that gets nucleotide frequency data from a file in the format of `exercise/data/example.txt`, and visualizes it using Matplotlib and Pandas.
Your script should read the data, create a stacked bar chart showing the nucleotide frequencies for each sequence, and label the axes appropriately. Finally, save your plot as a png file. Here's the expected plot:



! Exercise 5

Create a figure of 4 bar plots, where each bar plot contains the frequency of one nucleotide for each sequences. Label the axes appropriately. Finally, save your plot as a png file. Here's the expected plot:



12.4 More packages

There are MANY packages available, here's a short list of some that might interest you:

Package	Usage	Example of usage
BioPython	Computational molecular biology	Sequence handling, access to NCBI databases

Package	Usage	Example of usage
NumPy	Numerical arrays	Data manipulation, mathematical operations, linear algebra
Seaborn	High-level interface for drawing plots	Data visualization, statistical graphics
HTSeq	High throughput sequencing	Quality and coverage, counting reads, read alignment
Scanpy	Single-Cell Analysis	Preprocessing, visualization, clustering
SciPy	Mathematical algorithms	Clustering, ODE, Fourier Transforms
Scikit-image	Image processing	Image enhancement, segmentation, feature extraction
Scikit-learn	Machine learning	Classification, regression, clustering, dimensionality reduction
TensorFlow and PyTorch	Deep learning	Neural networks, natural language processing, computer vision

13 Final tips and resources

Figure 13.1: Please, read the doc

Here are a couple of tips:

- Leave comments (think of your future self)
- Be consistent (quotes, indents…)
- Break down one complex task into lots of (easy) small tasks
- When using functions you are not comfortable with, verify the output and make sure it does what you expect in with small examples
- Don't re-invent the wheel, for common tasks, it's likely that a function already exists
- Read the documentation when using a new package or function
- Google It! Use the correct programming vocabulary to increase your chances of finding an answer. If you don't find anything, try wording it differently.
- Prompt it to AI! It works generally well to explain a code, and for small tasks using famous packages.
- The easiest way to learn is by example, so follow a tutorial with the example data, and then try to apply it to your own

You can follow some free tutorials on:

- Code Academy
- EdX
- Youtube!

References

Here are some references and ressources that inspired this class:

- Python doc
- w3schools
- pythonforbiologists
- justinbois's Bootcamp

Part I

Archive 2024

14 Lesson 1 - Introduction, Data types, Operators

15 Introduction

15.1 Aim of the class

At the end of this class, you will:

- Be familiar with the Python environment
- Understand the major data types in Python
- Manipulate variables with operators and built-in functions

Figure 15.1: Python logo

15.2 Requirements

You need to have a computer, and either:

- install Python 3.0.0 (or above) and install a text editor (Word is not a text editor!).

> **Note**
>
> An IDE (integrated development environment) is an improved text editor. It is a software that provides functionalities like syntax highlighting, auto completion, help, debugger… For example Visual Studio Code (install and learn how to use it with Python), but any other IDE will work.

- have a github account, create a new codespace, and select the Repository `vgilbart/python-intro` to copy from. This is a free solution up to 60 hours of computing and 15 GB per month.

15.3 What is Python?

Figure 15.2: Guido van Rossum

Python is a programming language first released in 1991 and implemented by Guido van Rossum.

It is widely used, with various applications, such as:

- software development
- web development
- data analysis
- ...

It supports different types of programming paradigms (i.e. way of thinking) including the procedural programming paradigm. In this approach, the program moves through a linear series of instructions.

```
# Create a string seq
seq = 'ATGAAGGGTCC'
# Call the function len() to retrieve the length of the string
size = len(seq)
# Call the function print() to print a text
print('The sequence has', size, 'bases.')
```

```
The sequence has 11 bases.
```

15.4 Why use Python?

- Easy-to-use and easy-to-read syntax
- Large standard library for many applications (`numpy` for tables/matrices, `matplotlib` for graphs, `scikit-learn` for machine learning...)
- Interactive mode making it easy to test short snippets of code
- Large community (stackoverflow)

Figure 15.3: Just google it!

15.5 How can I program in Python?

Python is an interpreted language, this means that all scripts written in Python need a software to be run. This software is called an interpreter, which "translate" each line of the code, into instructions that the computer can understand. By extension, the interpreter that is able to read Python scripts is also called Python. So, whenever you want your Python code to run, you give it to the Python interpreter.

15.5.1 Interactive mode

One way to launch the Python interpreter is to type the following, on the command line of a terminal:

```
python3
```

> **Note**
>
> You can also try `python`, `/usr/bin/env python3`, `/usr/bin/python3`... There are many ways to call python! You can see where your current python is located by running `which python3`.

From this, you can start using python interactively, e.g. run:

```
print("Hello world")
```

```
Hello world
```

To get out of the Python interpreter, type `quit()`or `exit()`, followed by `enter`. Alternatively, on Linux/Mac press `[ctrl + d]`, on Windows press `[ctrl + z]`.

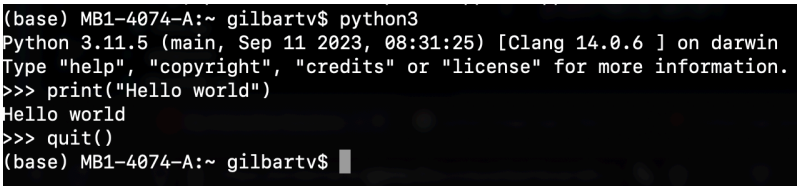


Figure 15.4: Interactive mode

15.5.2 Script mode

To run a script, create a folder named `script`, in which a file named `intro.py` contains:

```
#!/usr/bin/env python3
# -*- coding: UTF-8 -*-

print("Hello world")
```

and run

```
./script/intro.py
```

You should get the same output as before, that is:

```
Hello world
```

The shebang `#!` followed by the interpreter `/usr/bin/env python3` can be put at the beginning of the script in order to ommit calling `python3` in command-line. If you don't put it, you will have to run `python3 script/intro.py` instead of simply `./script/intro.py`.

The `-*- coding: UTF-8 -*-` specify the type of encoding to use. UTF-8 is used by default (which means that this line in the script is not necessary). This accepts characters from all languages. Other valid encoding are available, such as ascii (English characters only).

Warning

Some common errors can occur at this step:

- `bash: script/intro.py: No such file or directory` i.e. you are not in the right directory to run the file.

  Solution: run `ls */` and make sure you can find `script/: intro.py`, if not go to the correct directory by running `cd <insert directory name here>`

- `bash: script/intro.py: Permission denied` i.e. you don't have the right to execute your script.

  Solution: run `ls -l script/intro.py` and make sure you have at least `-rwx` (read, write, exectute rights) as the first 4 characters, if not run `chmod 744 script/intro.py` to change your rights.

16 Basic concepts

16.1 Values and variables

You will manipulate values such as integers, characters or dictionaries. These values can be stored in memory using variables. To assign a value to a variable, use the = operator as follow:

```
seq = 'ATGAAGGGTCC'
```

To output the variable value, either type the variable name or use a function like `print()`:

```
seq
```

```
'ATGAAGGGTCC'
```

```
print(seq)
```

```
ATGAAGGGTCC
```

We can change a variable value by assigning it a new one:

```
seq = seq + 'AAAA' # The + operator can be used to concatenate strings
seq
```

```
'ATGAAGGGTCCAAAA'
```

A variable can have a short name (like x and y) or a more descriptive name (seq, motif, genome_file). Rules for Python variable names:

- must start with a letter or the underscore character
- cannot start with a number
- can only contain alpha-numeric characters and underscores (A-z, 0-9, and _)
- are case-sensitive (seq, Seq and SEQ are three different variables)
- cannot be any of the Python keywords (run `help('keywords')` to find the list of keywords).

> ! Exercise
>
> Are the following variables names legal?
>
> - `2_sequences`
> - `_sequence`
> - `seq-2`
> - `seq 2`
>
> You can try to assign a value to these variable names to be sure of your answer!

16.2 Function calls

A function stores a piece of code that performs a certain task, and that gets run when called. It takes some data as input (parameters that are required or optional), and returns an output (that can be of any type). Some functions are predefined (but we will also learn how to create our own later on).

To run a function, write its name followed by parenthesis. Parameters are added inside the parenthesis as follow:

```
# round(number, ndigits=None)
x = round(number = 5.76543, ndigits = 2)
print(x)
```

```
5.77
```

Here the function `round()` needs as input a numerical value. As an option, one can add the number of decimal places to be used with digits. If an option is not provided, a default value is given. In the case of the option ndigits, `None` is the default. The function returns a numerical value, that corresponds to the rounded value. This value, just like any other, can be stored in a variable.

To get more information about a function, use the `help()` function.

> **Note**
>
> If you provide the parameters in the exact same order as they are defined, you don't have to name them. If you name the parameters you can switch their order. As good practice, put all required parameters first.

```
round(5.76543, 2)
```

```
5.77
```

```
round(ndigits = 2, number = 5.76543)
```

```
5.77
```

In Table 16.1 you will find some basic but useful python functions:

Table 16.1: List of useful Python functions.

Function	Description
`print()`	Print into the screen the values given in argument.
`help()`	Execute the built-in help system
`quit()` or `exit()`	Exit from Python
`len()`	Return the length of an object
`round()`	Round a numbers

> **Note**
>
> In python, you will also hear about methods. This vocabulary belongs to a programming paradigm called "Object-oriented programming" (OOP).
> A method is a function that belongs to a specific class of objects. It is defined within a class and operates only on objects from that class. Methods can access and modify the object's state.

16.3 Getting help

To get more information about a function or an operator, you can use the `help()` function. For example, in interactive mode, run `help(print)` to display the help of the `print()` function, giving you information about the input and output of this function. If you need information about an operator, you will have to put it into quotes, e.g. `help('+')`

> **Browse the help**
>
> If the help is long, press `[enter]` to get the next line or `[space]` to get the next 'page' of information.
> To quit the help, press `q`.

16.4 Comment your code

Except for the shebang and coding specifications seen before, all things after a hashtag `#` character will be ignored by the interpreter until the end of the line. This is used to add comments in your code.

Comments are used to:

- explain assumptions
- justify decisions in the code
- expose the problem being solved
- inactivate a line to help debug

- ...

17 How can I represent data?

Each programming language has its own set of data types, from the most basics (`bool`, `int`, `string`) to more complex structures (`list`, `tuple`, `set`…).

17.1 Simple data types

17.1.1 Boolean

Booleans represent one of two values: `True` or `False`.

When you compare two values, the expression is evaluated and Python returns the Boolean answer:

```
print(10 > 9)
```

```
True
```

17.1.2 Numeric

Python provides three kinds of numerical type:

- `int` ($\mathbb{Z}$), integers
- `float` ($\mathbb{R}$), real numbers
- `complex` ($\mathbb{C}$), complex numbers

Python will assign a numerical type automatically.

```
x = 1
y = 2.8
z = 1j + 2 # j is the convention in electrical engineering
```

```
type(x)
```

```
int
```

```
type(y)
```

```
float
```

```
type(z)
```

```
complex
```

17.1.3 Text

String type represents textual data composed of letters, numbers, and symbols. The character string must be expressed between quotes.

```
"""my string"""
'''my string'''
"my string"
'my string'
```

are all the same thing. The difference with triple quotes is that it allows a string to extend over multiple lines. You can also use single quotes and double quotes freely within the triple quotes.

```
# A multi-line string
my_str = '''This is a multi-line string. This is the first line.
This is the second line.
"What's your name?," I asked.
He said "Bond, James Bond."
'''

print(my_str)
```

```
This is a multi-line string. This is the first line.
This is the second line.
"What's your name?," I asked.
He said "Bond, James Bond."
```

You can get the number of characters inside a string with `len()`.

```
print(seq)
len(seq)
```

```
ATGAAGGGTCCAAAA
```

```
15
```

Strings have specific methods (i.e. functions specific to this class of object). Here are a few:

Method	Description
`.count()`	Returns the number of times a specified value occurs in a string
`.startswith()`	Returns true if the string starts with the specified value
`.endswith()`	Returns true if the string ends with the specified value
`.find()`	Searches the string for a specified value and returns the position of where it was found
`.replace()`	Returns a string where a specified value is replaced with a specified value

They are called like this:

```
seq.count('A')
```

```
7
```

> **Tip**
>
> To get the `help()` of the `.count()` method, you need to run `help(str.count)`.

> **Exercise**
>
> 1. Check if the sequence `seq` starts with the codon `ATG`
> 2. Replace all `T` into `U` in `seq`

17.2 Data structures

Data structures are a collection of data types and/or data structures, organized in some way.

17.2.1 List

List is a collection which is ordered and changeable. It allows duplicate members. They are created using square brackets `[]`.

```
seq = ['ATGAAGGGTCCAAAA', 'AGTCCCCGTATGAT', 'ACCT', 'ACCT']
```

List items are indexed, the first item has index `[0]`, the second item has index `[1]` etc.

```
seq[1]
```

```
'AGTCCCCGTATGAT'
```

> **Tip**
>
> You can count backwards, with the index `[-1]` that retrieves the last item.

As a list is changeable, we can change, add, and remove items in a list after it has been created.

```
seq[1] = 'ATG'
seq
```

```
['ATGAAGGGTCCAAAA', 'ATG', 'ACCT', 'ACCT']
```

You can specify a range of indexes by specifying the start (included) and the end (not included) of the range.

```
seq[0:2]
```

```
['ATGAAGGGTCCAAAA', 'ATG']
```

> **Tip**
>
> By leaving out the start value, the range will start at the first item:
>
> ```
> seq[:2]
> ```
>
> ```
> ['ATGAAGGGTCCAAAA', 'ATG']
> ```
>
> Similarly, by leaving out the end value, the range will end at the last item.

> **Note**
>
> Indexes also conveniently work on `str` types.

```
print(seq[0])
print(seq[0][0:5])
print(seq[0][2])
print(seq[0][-1])
```

```
ATGAAGGGTCCAAAA
ATGAA
G
A
```

You can get how many items are in a list with `len()`.

```
len(seq)
```

```
4
```

Lists have specific methods. Here are a few:

Method	Description
`.append()`	Inserts an item at the end
`.insert()`	Inserts an item at the specified index
`.extend()`	Append elements from another list to the current list
`.remove()`	Removes the first occurance of a specified item
`.pop()`	Removes the specified (by default last) index

! Exercise

1. Create a list `l = ['AAA', 'AAT', 'AAC']`, and add `AAG` at the end, using `.append()`.
2. Replace all `T` into `U` in the element `AAT`, using `.replace()`.

17.2.2 Tuple

Tuple is a collection which is ordered and unchangeable. It allows duplicate members. Tuples are written with round brackets `()`.

```
my_favorite_amino_acid = ('Y', 'Tyr', 'Tyrosine')
```

Just like for the list, you can get items with their index. The only difference is that you cannot change a tuple that has been created.

Tuples have specific methods. Here are a few:

Method	Description
`.count()`	Returns the number of times a specified value occurs
`.index()`	Searches for a specified value and returns the position of where it was found

> **!** Exercise
>
> Try to change the value of the first element of `my_favorite_amino_acid` and see what happens.

17.2.3 Set

Set is a collection which is unordered and unindexed. It does not allow duplicate members (they will be ignored). Sets are written with curly brackets `{}`.

```
seq = {'BRCA1', 'TP53', 'EGFR', 'MYC'}
```

Once a set is created, you cannot change its items directly (as they don't have index), but you modify the set by removing and adding items.

Sets have specific methods. Here are a few:

Method	Description
`.add()`	Adds an element to the set

Method	Description
`.difference()`	Returns a set containing the difference between two sets
`.intersection()`	Returns a set containing the intersection between two sets
`.union()`	Returns a set containing the union of two sets
`.remove()`	Remove the specified item
`.pop()`	Removes a random element

! Exercise

Get the common genes between the following sets:

```
organism1_genes = {'BRCA1', 'TP53', 'EGFR', 'MYC'}
organism2_genes = {'TP53', 'MYC', 'KRAS', 'BRAF'}
```

17.2.4 Dictionary

Dictionaries are used to store data values in `key: value` pairs. A dictionary is a collection which is ordered (as of Python >= 3.7), changeable and does not allow duplicates keys. Dictionaries are written with curly brackets `{}`, with keys and values.

```
organism1_genes = {
  #key: value;
  'BRCA1': 'DNA repair',
  'TP53': 'Tumor suppressor',
  'EGFR': 'Cell growth',
  'MYC': 'Regulation of gene expression'
}
```

Dictionary items can be referred to by using the key name.

```
organism1_genes["BRCA1"]
```

```
'DNA repair'
```

Dictionaries have specific methods. Here are a few:

Method	Description
`.items()`	Returns a list containing a tuple for each key value pair
`.keys()`	Returns a list containing the dictionary's keys
`.values()`	Returns a list of all the values in the dictionary
`.pop()`	Removes the element with the specified key
`.get()`	Returns the value of the specified key

> ! Exercise
>
> From the dictionary `organism1_genes` created as example, get the value of the key `BRCA1`. If the key does not exist, return `Unknown` by default. Try your code before **and after** removing the `BRCA1` key:value pair.
> Check the help of `get` by running `help(dict.get)`.

17.3 Conversion between types

You can get the data type of any object by using the function `type()`. You can (more or less easily) convert between data types.

Function	Description
`bool()`	Convert to boolean type
`int()`, `float()`	Convert between integer or float types
`complex()`	Convert to complex type
`str()`	Convert to string type
`list()`, `tuple()`, `set()`	Convert between list, tuple, and set types

Function	Description
`dict()`	Convert a tuple of order (key, value) into a dictionary type

```
bool(1)
```

```
True
```

```
int(5.8)
```

```
5
```

```
str(1)
```

```
'1'
```

```
list({1, 2, 3})
```

```
[1, 2, 3]
```

```
set([1, 2, 3, 3])
```

```
{1, 2, 3}
```

```
dict((('a', 1),
      ('f', 2),
      ('g', 3)))
```

```
{'a': 1, 'f': 2, 'g': 3}
```

18 How can I manipulate data?

In the previous section we have learned how data can be represented in different types and gathered in various data structures. In this section we will see how we can manipulate data in order to do more complex tasks.

18.1 Operators

Operators are used to perform operations on variables and values. We will present a few common ones here.

18.1.1 Arithmetic operators

Arithmetic operators are used with numeric values to perform common mathematical operations:

Operator	Name
`+`	Addition
`-`	Substraction
`*`	Multiplication
`/`	Division
`**`	Power

> **Warning**
>
> Do not use the `^` operator to raise to a power. That is actually the operator for bitwise XOR, which we will not cover.

Python will convert data type according to what is necessary. Thus, when you divide two `int` you will obtain a `float` number, if you add a `float` to an `int`, you will get a `float`, …

```
# Example
2/10
```

```
0.2
```

> **Note**
>
> `+` also conveniently work on `str` types.
>
> ```
> 'AC' + 'AT'
> ```
>
> ```
> 'ACAT'
> ```

18.1.2 Assignment operators

Assignment operators are used to assign values to variables:

Operator	Example as	Same as
`=`	`x = 5`	`x = 5`
`+=`	`x += 5`	`x = x + 5`
`-=`	`x -= 5`	`x = x - 5`

> **Note**
>
> The same principle applies to multiplication, division and power, but are less commonly used.

18.1.3 Comparison operators

Comparison operators are used to compare two values:

Operator	Name
==	Equal
!=	Not equal
>	Greater than
>=	Greater than or equal to
<	Less than
<=	Less than or equal to

```
# Example
2 == 1 + 1
```

```
True
```

> **Warning**
>
> You should never use equalty operators (==or !=) with floats or complex values.
>
> ```
> # Example
> 2.1 + 3.2 == 5.3
> ```
>
> ```
> False
> ```
>
> This is a floating point arithmetic problem seen in other programming languages. It is due to the difficulty of having a fixed number of binary digits (bits) to accurately represent some decimal number. This leads to small rounding errors in calculations.
>
> ```
> 2.1 + 3.2
> ```
>
> ```
> 5.300000000000001
> ```
>
> If you need to use equalty operators, do it with a degree of freedom:
>
> ```
> tol = 1e-6 ; abs((2.1 + 3.2) - 5.3) < tol
> ```
>
> ```
> True
> ```

18.1.4 Logical operators

Logical operators are used to combine conditional statements:

Operator	Description
`and`	Returns True if both statements are true
`or`	Returns True if one of the statements is true
`not`	Reverse the result, returns False if the result is true

```
# Example
False and False, False and True, True and False, True and True
```

```
(False, False, False, True)
```

```
# Example
False or False, False or True, True or False, True or True
```

```
(False, True, True, True)
```

```
# Example
True or not True
```

```
True
```

18.1.5 Membership operators

Operator	Description
`in`	Returns True if a sequence with the specified value is present in the object
`not in`	Returns True if a sequence with the specified value is not present in the object

```
# Example
'ACCT' in seq
```

```
False
```

18.1.6 Operator precedence

Operator precedence describes the order in which operations are performed.

The precedence order is described in the table below, starting with the highest precedence at the top:

Operator	Description
`()`	Parenthesis
`**`	Power
`* /`	Multiplication, division
`+ -`	Addition, substraction
`==,!=,>,>=,<,<=,is,is not in, not`	Comparisons, identity, and membership operators
`not`	Logical NOT
`and`	AND
`or`	OR

If two operators have the same precedence, the expression is evaluated from left to right.

> **!** Exercise
>
> Try to guess what will output the following expressions:
>
> - `1+1 == 2 and "actg" == "ACTG"`
> - `True or False and True and False`
> - `"Homo sapiens" == "Homo" + "sapiens"`
> - `'Tumor suppressor' in organism1_genes`
>
> Verify with Python.

18.2 Conditionals

Conditionals allows you to make decisions in your code based on certain conditions.

```
if something is true:
    do task a
otherwise:
    do task b
```

The comparison (`==`, `!=`, `>`, `>=`, `<`, `<=`), logical (`and`, `or`, `not`) and membership (`in`, `not in`) operators can be used as conditions.

In Python, this is written with an `if ... elif ... else` statement like so:

```
# Define gene expression levels
gene1_expression = 100
gene2_expression = 50

# Analyze gene expression levels
if gene1_expression > gene2_expression:
  print("Gene 1 has higher expression level.")
elif gene1_expression < gene2_expression:
  print("Gene 2 has higher expression level.")
else:
  print("Gene 1 and Gene 2 have the same expression level.")
```

```
Gene 1 has higher expression level.
```

The `elif` keyword is Python's way of saying "if the previous conditions were not true, then try this condition". The following code is equivalent to the one before:

```
# Analyze gene expression levels
if gene1_expression > gene2_expression:
  print("Gene 1 has higher expression level.")
else:
```

```
  if gene1_expression < gene2_expression:
    print("Gene 2 has higher expression level.")
  else:
    print("Gene 1 and Gene 2 have the same expression level.")
```

```
Gene 1 has higher expression level.
```

! Exercise

Are these two codes equivalent?

```
# Code A
if "ATG" in dna_sequence:
  print("Start codon found.")
elif "TAG" in dna_sequence:
  print("Stop codon found.")
else:
  print("No interesting codon not found.")
```

```
# Code B
if "ATG" in dna_sequence:
  print("Start codon found.")
  if "TAG" in dna_sequence:
    print("Stop codon found.")
else:
  print("No interesting codon not found.")
```

An `if` statement cannot be empty, but if for some reason you have an if statement with no content, put in the `pass` statement to avoid getting an error.

```
a = 33
b = 200

if b > a:
  pass
```

18.3 Notes on indentation

> **Note**
>
> Python relies on **indentation** (the spaces at the beginning of the lines).

Indentation is not just for readability. In Python, you use spaces or tabs to indent code blocks. Python uses it to determine the scope of functions, loops, conditional statements, and classes.

Any code that is at the same level of indentation is considered part of the same block. Blocks of code are typically defined by starting a line with a colon (`:`) and then indenting the following lines.

When you have nested structures like a conditional statement inside another conditional statement, you must further to show the hierarchy. Each level of indentation represents a deeper level of nesting.

It's essential to be consistent with your indentation throughout your code. Mixing tabs and spaces can lead to errors, so it's recommended to choose one and stick with it.

> **Exercise**
>
> Here are three codes, they all are incorrect, can you tell why?
> Of course, you can run them and read the error that Python gives!

```
amino_acid_list = ["MET", "ARG", "THR", "GLY"]

if "MET" in amino_acid_list:
  print("Start codon found.")
  if "GLY" in amino_acid_list:
    print("Glycine found.")
else:
print("Start codon not found.")
```

```
dna_sequence = "ATGCTAGCTAGCTAG"

if "ATG" in dna_sequence:
  print("Start codon found.")
if "TAG" in dna_sequence
  print("Stop codon found.")
```

```
x = 7

if x > 5:
  print("x is greater than 5")
  if y > 10:
    print("x is greater than 10")
  elif y = 10:
    print("x equals 10")
  else:
    print("x is less than 10")
```

18.4 Iterations

Iteration involves repeating a set of instructions or a block of code multiple times.

There are two types of loops in python, `for` and `while`.

Iterating through data structures like lists allows you to access each element individually, making it easier to perform operations on them.

18.4.1 For loops

When using a for loop, you iterate over a sequence of elements, such as a list, tuple, or dictionary.

```
for item in data_structure:
    do task a
```

The loop will execute the indented block of code for each element in the sequence until all elements have been processed. This is particularly useful when you know the number of times you need to iterate.

```
all_codons = [
    'AAA', 'AAC', 'AAG', 'AAT',
    'ACA', 'ACC', 'ACG', 'ACT',
    'AGA', 'AGC', 'AGG', 'AGT',
    'ATA', 'ATC', 'ATG', 'ATT',
    'CAA', 'CAC', 'CAG', 'CAT',
    'CCA', 'CCC', 'CCG', 'CCT',
    'CGA', 'CGC', 'CGG', 'CGT',
    'CTA', 'CTC', 'CTG', 'CTT',
    'GAA', 'GAC', 'GAG', 'GAT',
    'GCA', 'GCC', 'GCG', 'GCT',
    'GGA', 'GGC', 'GGG', 'GGT',
    'GTA', 'GTC', 'GTG', 'GTT',
    'TAA', 'TAC', 'TAG', 'TAT',
    'TCA', 'TCC', 'TCG', 'TCT',
    'TGA', 'TGC', 'TGG', 'TGT',
    'TTA', 'TTC', 'TTG', 'TTT'
]

count = 0
for codon in all_codons:
  if codon[1] == 'T':
    count += 1

print(count, 'codons have a T as a second nucleotide.')
```

```
16 codons have a T as a second nucleotide.
```

What it does is the following: it processes each element in the list `all_codons`, called in the following code `codon`. If the `codon` has as a second character a `T`, it adds 1 to a counter (the variable called `count`).

> **Warning**
>
> You cannot modify an element of a list that way.

```
for codon in all_codons:
  if 'T' in codon :
    codon = codon.replace('T', 'U')

print(all_codons)
```

```
['AAA', 'AAC', 'AAG', 'AAT', 'ACA', 'ACC', 'ACG', 'ACT', 'AGA', 'AGC', 'AGG', 'AGT', 'ATA',
```

This is because `all_codons` was converted to an iterator in the `for` statement.

18.4.2 Iterators

An iterator is a special object that gives values in succession.

In the previous example, the iterator returns a copy of the item in a list, not a reference to it. Therefore, the `codon` inside the `for` block is not a view into the original list, and changing it does not do anything.

A way to modify the list would be to use an iterable to access the original data. The `range(start, stop)` function creates an iterable to count from one integer to another.

```
for i in range(2, 10):
    print(i, end='  ')
```

```
2  3  4  5  6  7  8  9
```

We could count from 0 to the size of the list, loop though every element of the list by calling them by their index, and modify them if necessary. That's what the following code does:

```
for i in range(0, len(all_codons)):
  if 'T' in all_codons[i] :
    all_codons[i] = all_codons[i].replace('T', 'U')

print(all_codons)
```

```
['AAA', 'AAC', 'AAG', 'AAU', 'ACA', 'ACC', 'ACG', 'ACU', 'AGA', 'AGC', 'AGG', 'AGU', 'AUA', 'AU
```

Another useful function that returns an iterator is `enumerate()`. It is an iterator that generates pairs of index and value. It is commonly used when you need to access both the index and value of items simultaneously.

```
seq = 'ATGCATGC'

# Print index and identity of bases
for i, base in enumerate(seq):
    print(i, base)
```

```
0 A
1 T
2 G
3 C
4 A
5 T
6 G
7 C
```

```
# Loop through sequence and print index of G's
for i, base in enumerate(seq):
    if base in 'G':
        print(i, end='  ')
```

```
2  6
```

18.4.3 While loops

A while loop continues executing a set of statement as long as a condition is true.

```
while condition is true:
    do task a
```

This type of loop is handy when you're not sure how many iterations you'll need to perform or when you need to repeat a block of code until a certain condition is met.

```
seq = 'TACTCTGTCGATCGTACGTATGCAAGCTGATGCATGATTGACTTCAGTATCGAGCGCAGCA'
start_codon = 'ATG'

# Initialize sequence index
i = 0
# Scan sequence until we hit the start codon
while seq[i:i+3] != start_codon:
  i += 1

# Show the result
print('The start codon begins at index', i)
```

```
The start codon begins at index 19
```

> **Warning**
>
> Remember to increment i, or you'll get stuck in a loop.

Actually, the previous code is quite dangerous. You can also get stuck in a loop... if the `start_codon` does not appear in `seq` at all.

Indeed, even when you go above the given length of `seq`, the condition `seq[i:i+3] != start_codon` will still be true because `seq[i:i+3]` will output an empty string.

Figure 18.1: Hopefully not you!

```
seq[9999:9999+3]
```

```
''
```

So, once the end of the sequence is reached, the condition `seq[i:i+3] != start_codon` will always be true, and you'll get stuck in an infinite loop.

> **Note**
>
> To get interrupt a process, press `[ctrl + c]`.

18.4.4 Break statement

Iteration stops in a `for` loop when the iterator is exhausted. It stops in a `while` loop when the conditional evaluates to `False`. There is another way to stop iteration: the `break` keyword. Whenever `break` is encountered in a `for` or `while` loop, the iteration stops and execution continues outside the loop.

```
seq = 'ACCATTTTTTGGGGGGGCGGGGGGAGGGGGGG'
start_codon = 'ATG'

# Initialize sequence index
i = 0
# Scan sequence until we hit the start codon
while seq[i:i+3] != start_codon:
  i += 1
  if i+3 > len(seq): # Get out of the loop if we parsed the full seq
    print('Codon not found in sequence.')
    break
else:
  print('The start codon starts at index', i)
```

```
Codon not found in sequence.
```

> **Note**
>
> Also, note that the `else` statement can be used in `for` and `while` loops. In `for` loops it is executed when the **loop is finished**. In `while` loops, it is executed when the condition is **no longer true**. In both case, the loops need to **not** encounter a `break` to enter in the `else` block.

18.4.5 Continue statement

In addition to the break statement, there is also the continue statement in Python that can be used to alter the flow of iteration in loops. When continue is encountered within a loop, it skips the remaining code inside the loop for the current iteration and moves on to the next iteration.

Here's an example showcasing the continue statement in a loop:

```
# List of DNA sequences
dna_sequences = ['ATGCTAGCTAG', 'ATCGATCGATC', 'ATGGCTAGCTA', 'ATGTAGCTAGC']

# Find sequences starting with a start codon
for sequence in dna_sequences:
    if sequence[:3] != 'ATG':  # Check if the sequence does not start with a start codon
        print(f"Sequence '{sequence}' does not start with a start codon. Skipping analysis.")
        continue  # Skip further analysis for this sequence
    print(f"Analyzing sequence '{sequence}' for protein coding regions...")
    # Additional analysis code here
else:
  print('All sequences were processed.')
```

```
Analyzing sequence 'ATGCTAGCTAG' for protein coding regions...
Sequence 'ATCGATCGATC' does not start with a start codon. Skipping analysis.
Analyzing sequence 'ATGGCTAGCTA' for protein coding regions...
Analyzing sequence 'ATGTAGCTAGC' for protein coding regions...
All sequences were processed.
```

The continue statement in this example skips the analysis code for sequence that does not start with a start codon.

18.4.6 Exercises

! Exercise 1

Given a list of DNA sequences, find the first sequence that contains a specific motif `'TATA'`, print the sequence, and stop the process. If no sequence contains the motif, print a message accordingly. You must use only one `for` loop. With the input given below, the output should look like this:

```
# List of DNA sequences with a TATA
dna_sequences = [
'ATGCTACAGCTAG',
'ATCGATATAATC', # TATA
'ATGGCTAGCTA',
'ATGTAGCTAGC',
'ATGTAGCTATA'   # TATA
]

for ...
  # Your code here
```

```
Sequence 'ATCGATATAATC' contains the 'TATA' motif.
```

```
# List of DNA sequences without a TATA
dna_sequences = [
'ATGCTACAGCTAG',
'ATCGATACAATC',
'ATGGCTAGCTA',
'ATGTAGCTAGC'
]

for ...
  # Your code here
```

```
No sequence contains the 'TATA' motif.
```

! Exercise 2

Analyze a DNA sequence to count the number of consecutive `'A'` nucleotides. You must use only one `while` loop. With the input given below, the output should look like this:

```
# DNA sequence to analyze
dna_sequence = 'ATGATAAGAGAAAGTAAAAGCGATCGAAAAAA'

while ...
  # Your code here
```

```
Number of consecutive 'A's: 6
```

19 Conclusion

Congrats! You now know the (very) basics of Python programming.

If you want to keep on practising with simple exercises, you can check out w3schools.

For more biology-related exercises check out pythonforbiologist.org, they have exercises availables in each chapters.

For french speakers, the AFPy (Association Francophone Python) has a learning tool called HackInScience.

Or keep on googling for more python exercises!

To continue your learning journey, follow lesson 2.

References

A python conference organized by the AFPy (Association Francophone Python) is held in Strasbourg in the end of October 2024!

Here are some references and ressources that (greatly) inspired this class:

- Python doc
- w3schools
- pythonforbiologists
- justinbois's Bootcamp

20 Lesson 2 - Functions, Errors, File Handling, Scientific Packages

21 Introduction

21.1 Aim of the class

At the end of this class, you will be able to:

- Create simple functions
- Handle some errors
- Ask for input from the user
- Upload, modify and download files into Python
- Import packages (and use in a simple manner some scientific packages)

21.2 Requirements

Remembering some of lesson 1.

22 Function

A function stores a piece of code that performs a certain task, and that gets run when called. It takes some data as input (parameters that are required or optional), and returns an output (that can be of any type).

> Tip
>
> We already learned how to run a predefined function in the last lesson. You need to write its name followed by parenthesis. Parameters are added inside the parenthesis as follow:
>
> ```
> # round(number, ndigits=None)
> x = round(number = 5.76543, ndigits = 2)
> print(x)
> ```
>
> ```
> 5.77
> ```
>
> To get more information about a function, use the `help()` function.

We will now learn how to create our own function.

22.1 Syntax

In python, a function is declared with the keyword `def` followed by its name, and the arguments inside parenthesis. The next block of code, corresponding to the content of the function, must be indented. The output is defined by the `return` keyword.

```
def hello(name):
  """Presenting myself."""
  presentation = "Hello, my name is {0}.".format(name)
  return presentation
```

```
text = hello(name = "Valentine")
print(text)
```

```
Hello, my name is Valentine.
```

22.2 Documentation

As you may have noticed, you can also add a description of the function directly after the function definition. It is the message that will be shown when running `help()`. As it can be along text over multiple lines, it is common to put it inside triple quotes `"""`.

```
help(hello)
```

```
Help on function hello in module __main__:

hello(name)
    Presenting myself.
```

22.3 Arguments

You can have several arguments. They can be mandatory or optional. To make them optional, they need to have a default value assigned inside the function definition, like so:

```
def hello(name, french = True):
  """Presenting myself."""
  if french:
    presentation = "Bonjour, je m'appelle {0}."
  else:
```

```
    presentation = "Hello, my name is {0}."
  return presentation.format(name)
```

The parameter `name`is mandatory, but `french` is optional.

```
hello("Valentine")
```

```
"Bonjour, je m'appelle Valentine."
```

```
hello(french = False)
```

```
TypeError: hello() missing 1 required positional argument: 'name'
---------------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)
Cell In[7], line 1
----> 1 hello(french = False)
TypeError: hello() missing 1 required positional argument: 'name'
```

> **Note**
>
> Reminder: if you provide the parameters in the exact same order as they are defined, you don't have to name them. If you name the parameters you can switch their order. As good practice, put all required parameters first.
>
> ```
> hello(french = False, name = "Valentine")
> ```
>
> ```
> 'Hello, my name is Valentine.'
> ```
>
> ```
> hello("Valentine", False)
> ```
>
> ```
> 'Hello, my name is Valentine.'
> ```

22.4 Output

If no `return` statement is given, then no output will be returned, but the function will still be run.

```
def hello(name):
  """Presenting myself."""
  print("We are inside the 'hello()' function.")
  presentation = "Hello, my name is {0}.".format(name)
```

```
print(hello("Valentine"))
```

```
We are inside the 'hello()' function.
None
```

The output can be of any type. If you have a lot of things to return, you might want to return a `list` or a `dict` for example.

```
def multiple_of_3(list_of_numbers):
  """Returns the number that are multiple of 3."""
  multiples = []
  for num in list_of_numbers:
    if num % 3 == 0:
      multiples.append(num)
  return multiples

multiple_of_3(range(1, 20, 2))
```

```
[3, 9, 15]
```

> **Note**
>
> This could be written as a one-liner.
>
> ```
> def multiple_of_3(list_of_numbers):
>   """Returns the number that are multiple of 3."""
>   multiples = [num for num in list_of_numbers if num % 3 == 0]
>   return multiples
>
> multiple_of_3(range(1, 20, 2))
> ```
>
> ```
> [3, 9, 15]
> ```

22.5 Exercise

! Exercise

Write a function called `nucl_freq` to compute nucleotide frequency of a sequence. Given a sequence as input, it outputs a dictionnary with keys being the nucleotides `A`, `T`, `C` and `G`, and values being their frequency in the sequence. With the input given below, the output should be:

```
def ...
  # Your code here

nucl_freq("ATTCCCGGGG")
```

```
{'T': 0.2, 'G': 0.4, 'C': 0.3, 'A': 0.1}
```

23 Exceptions Handling

23.1 Syntax

It is possible to handle errors (in python, they are also called exceptions), using the following statements:

- `try` to test a block of code for errors
- `except` to handle the error
- `else` to excute code if there is no error
- `finally` to excute code, regardless of the result of the try and except blocks

```
# The try block will generate an exception, because some_undefined_variable is not defined:
try:
  print(some_undefined_variable)
except:
  print("Oops... Something went wrong")
```

```
Oops... Something went wrong
```

```
# Without the try block, the program will crash and raise an error:
print(some_undefined_variable)
```

```
NameError: name 'some_undefined_variable' is not defined
---------------------------------------------------------------------------
NameError                                 Traceback (most recent call last)
Cell In[17], line 2
      1 # Without the try block, the program will crash and raise an error:
----> 2 print(some_undefined_variable)
NameError: name 'some_undefined_variable' is not defined
```

```
try:
  print(some_undefined_variable)
except:
  print("Oops... Something went wrong")
else:
  print("Nothing went wrong")
finally:
  print("The 'try except' is finished")
```

```
Oops... Something went wrong
The 'try except' is finished
```

23.2 Raising exceptions

Here is a table of some of the built-in exceptions in python.

Exception	Description
`IndexError`	Raised when the index of a sequence is out of range.
`KeyError`	Raised when a key is not found in a dictionary.
`KeyboardInterrupt`	Raised when the user hits the interrupt key (Ctrl+c or Delete).
`NameError`	Raised when a variable is not found in the local or global scope.
`TypeError`	Raised when a function or operation is applied to an object of an incorrect type.
`ValueError`	Raised when a function receives an argument of the correct type but of an incorrect value.
`RuntimeError`	Raised when an error occurs that do not belong to any specific exceptions.
`Exception`	Base class of exceptions.

You can use them to be more specific about the type of exception occurring.

```
try:
  print(some_undefined_variable)
except NameError:
  print("A variable is not defined")
except:
  print("Oops... Something went wrong")
else:
  print("Nothing went wrong")
finally:
  print("The 'try except' is finished")
```

```
A variable is not defined
The 'try except' is finished
```

You can also use them to throw an exception if a condition occurs, by using the `raise` keyword.

```
x = "hello"
try:
  if not isinstance(x, int):
    raise TypeError("Only integers are allowed")
  if x < 0:
    raise ValueError("Sorry, no numbers below zero")
  print(x, "is a positive integer.")
except NameError:
  print("A variable is not defined")
else:
  print("Nothing went wrong")
finally:
  print("The 'try except' is finished")
```

```
The 'try except' is finished

TypeError: Only integers are allowed
---------------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)
```

```
Cell In[20], line 4
      2 try:
      3   if not isinstance(x, int):
----> 4     raise TypeError("Only integers are allowed")
      5   if x < 0:
      6     raise ValueError("Sorry, no numbers below zero")
TypeError: Only integers are allowed
```

23.3 Exercise

! Exercise

Let's make our previous function even better by adding some exception handling. Raise a `TypeError` if the input is not a string. Raise a `ValueError` if the input string contains something else than the nucleotides `A`, `C`, `T`, `G`.
With the input given below, the output and errors should be:

```
def ...
  # Your code here

nucl_freq(5474)
nucl_freq("ATTCXCCGGGG")
nucl_freq("ATTCCCGGGG")
```

```
TypeError: Input must be a string.
---------------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)
Cell In[21], line 15
     12     freq[nucl] = seq.count(nucl)/n
     13   return freq
---> 15 nucl_freq(5474)
     16 nucl_freq("ATTCXCCGGGG")
     17 nucl_freq("ATTCCCGGGG")
Cell In[21], line 3, in nucl_freq(seq)
      1 def nucl_freq(seq):
      2   if not isinstance(seq, str):
```

```
----> 3     raise TypeError("Input must be a string.")
      4   valid_nucl = {"A", "T", "C", "G"}
      5   seq_nucl = set(seq)
TypeError: Input must be a string.
```

24 User-defined input

There are some interesting ways to get input from the user:

- `input()` receives input from the keyboard. This means that the input is defined *while* the python script is being executed.
- `sys.argv` takes arguments provided in command line after the name of the program. This means that the input is defined *before* the python script is being executed.
- `argparse` is similar to `sys.argv`, with the advantage of being able to give specific names to arguments.

24.1 input

Python stops executing when it comes to the `input()` function, and continues when the user has given some input.

In a file called `username-1.py`, write the following:

```
username = input("Enter username: ")
print("Username is: " + username)
```

Then in the terminal, run:

```
#| eval: False
python username-1.py
```

You should be asked, in command line, to enter a username. When you write it, and press Enter, it gets printed.

```
Enter username: vgilbart
Username is: vgilbart
```

24.2 sys.argv

To use `sys.argv` you need to import a module called `sys`. It is part of the standard python library, so you should not have to install anything in particular.

In a file called `username-2.py`, write the following:

```
import sys

print("Username is: " + sys.argv[1])
```

Then in the terminal, run:

```
#| eval: False
python username-2.py vgilbart
```

Arguments are given in command line, seperated by `[space]`.

```
Username is: vgilbart
```

> **Note**
>
> What is the type of `sys.argv`? Remember that in python index begins at `0`. What do you think is `sys.argv[0]`? Verify!
> Also, what happens if you run `python username-2.py valentine gilbart` ?

24.3 argparse

Just like for `sys`, you need to import `argparse`.

In a file called `username-3.py`, write the following:

```
import argparse
parser = argparse.ArgumentParser()
parser.add_argument('--username', action="store")

args = parser.parse_args()
print("Username is: " + args.username)
```

Then in the terminal, run:

```
#| eval: False
python username-3.py --username vgilbart
```

Arguments are given in command line, but they have specific names.

> **Note**
>
> `argparse` is a very useful module when creating programs! You can easily specify the expected type of argument, whether it is optional or not, and create a help for your script. Check their tutorial for more information.

25 File Handling

The key function to work with files in `open()`. It has two parameters `file` and `mode`.

```
# Write the correct path for you!
fasta_file = 'exercise/data/example.fasta'
f = open(fasta_file, mode = 'r')
```

The modes can be one of the following:

Mode	Description
`r`	Opens a file for reading, error if the file does not exist (default)
`a`	Opens a file for appending, creates the file if it does not exist
`w`	Opens a file for writing, creates the file if it does not exist
`x`	Creates the specified file, returns an error if the file exists

25.1 Reading

The `open()` function returns a file object, which has a `read()` method for reading the content of the file:

```
print(f.read())
```

```
>seq1
TTAGCTAAATAGCTAGCAAACTAGCTAGCTAAAAAAAAAAACTAGCTAGCT
>seq2
ATGCCAGCCAGCCAGCCAGCCAGCTCGCTCGCTCGCCAGCCAGCTAGCTA
```

```
>seq3
CCGGGCGGTCGATGGATGGAGGGAGCGAGCGATCGATCGGTCGATCGGTG
>seq4
GATCGATCGATCTTTTTATCGATCGATTGTTCTTTCGATCGTTCTATCGA
>seq5
ACGTACGTACGTACGTACGTACGTACGTACGTACGTACGTACGTACGTAT
```

The parameter `size =` can be added to specify the number of bytes (~ characters) to return.

```
# We need to re-open it because we have already parsed the whole file
f = open(fasta_file, mode = 'r')
print(f.read(2))
```

```
>s
```

You can return one line by using the `.readline()` method. By calling it two times, you can read the two first lines:

```
f = open(fasta_file, mode = 'r')
print(f.readline())
print(f.readline())
```

```
>seq1

TTAGCTAAATAGCTAGCAAACTAGCTAGCTAAAAAAAAAAACTAGCTAGCT
```

By looping through the lines of the file, you can read the whole file, line by line:

```
for i, line in enumerate(f):
  print(i, line)
```

```
0 >seq2

1 ATGCCAGCCAGCCAGCCAGCCAGCTCGCTCGCTCGCCAGCCAGCTAGCTA

2 >seq3
```

```
3 CCGGGCGGTCGATGGATGGAGGGAGCGAGCGATCGATCGGTCGATCGGTG

4 >seq4

5 GATCGATCGATCTTTTTATCGATCGATTGTTCTTTCGATCGTTCTATCGA

6 >seq5

7 ACGTACGTACGTACGTACGTACGTACGTACGTACGTACGTACGTACGTAT
```

It is a good practice to close the file when you are done with it.

```
f.close()
```

> **Warning**
>
> In some cases, changes made to a file may not show until you close the file.

> **Note**
>
> A common syntax to handle files that you might encounter is:
>
> ```
> with open(fasta_file, 'r') as f:
>   print(f.readline())
> ```
>
> ```
> >seq1
> ```
>
> This code is equivalent to
>
> ```
> f = open(fasta_file, 'r')
> try:
>   print(f.readline())
> finally:
>   f.close()
> ```
>
> ```
> >seq1
> ```

The `with` statement is an example of a context manager, i.e. it allows to allocate and release resources precisely, by cleaning up the resources once they are no longer needed.

25.2 Writting

To write into a file, you must have it open under a `w`, `a` mode.

Then, the method `write()` can be used.

```
txt_file = "exercise/data/some_file.txt"
f = open(txt_file, "w")
f.write("Woops! I have deleted the content!\n")
f.close()

# Read the current content of the file
f = open(txt_file, "r")
print(f.read())
```

Woops! I have deleted the content!

> **Warning**
>
> Be very careful when opening a file in `write` mode as you can delete its content without any way to retrieve the original file!

As you may have noticed, `write()` returns the number of characters written. You can prevent it from being printed by assigning the return value to a variable that will not be used.

```
f = open(txt_file, "a")
_ = f.write("Now the file has more content!\n")
f.close()

# Read the current content of the file
f = open(txt_file, "r")
print(f.read())
```

```
Woops! I have deleted the content!
Now the file has more content!
```

> **Note**
>
> You must specify a newline with the character:
>
> - `\n` in Linus/MacOS
> - `\r\n` in Windows
> - `\r` in MacOS before X

25.3 os module

Python has a built-in package called `os`, to interact with the operating system.

```
import os

print("Current working directory:", os.getcwd())
os.chdir('../')
print("Current working directory:", os.getcwd())
```

```
Current working directory: /home/runner/work/python-intro/python-intro
Current working directory: /home/runner/work/python-intro
```

Here are some useful functions from the `os` package.

Function	Description
`getcwd()`	Returns the current working directory
`chdir()`	Change the current working directory
`listdir()`	Returns a list of the names of the entries in a directory
`mkdir()`	Creates a directory
`mkdirs()`	Creates a directory recursively

25.4 Regular expression

A regular expression is a sequence of characters that forms a search pattern.

Python has a built-in package called `re`, to work with regular expressions.

```
import re

x = re.findall("hello", "hello world, hello you!")
print(x)
```

```
['hello', 'hello']
```

Here are some useful functions from the `re` package.

Function	Description
`findall()`	Returns a list containing all matches
`search()`	Returns a Match object if there is a match anywhere in the string
`split()`	Returns a list where the string has been split at each match
`sub()`	Replaces one or many matches with a string

To be more specific about a sequence search, regular expression uses metacharacters (i.e characters with sepecial meaning)

Metacharacters	Description	Example
[]	A set of characters	`[a-m]`
\	Signals a special sequence (can also be used to escape special characters)	`\n`
.	Any character (except newline character)	`he..o`
^	Starts with	`^hello`
$	Ends with	`hello$`
*	Zero or more occurrences	`he.*o`

Metacharacters	Description	Example
+	One or more occurrences	`he.+o`
?	Zero or one occurrences	`he.?o`
{}	Exactly the specified number of occurrences	`he.{2}o`
|	Either or	`hello|bonjour`
()	Captures and group	`hello (.+) \1` in which `\1` correspond to what is being captured in `(.+)`

> **Note**
>
> To build and test a regex, you can use regex101.com, or any website equivalent, in which you can write your regex, and some string to test, to see how it matches.

A Match Object is an object containing information about the search and the result.

```
x = re.search("hello .*",
"""
hello world
hello you
bonjour
""")
print(x)
```

```
<re.Match object; span=(1, 12), match='hello world'>
```

The Match object has methods used to retrieve information about the search, and the result:

- `.span()` returns a tuple containing the start and end positions of the match.
- `.group()` returns the part of the string where there was a match

```
print(x.group())
```

```
hello world
```

> **!** Exercise
>
> From the list `dna_sequences = ["ATGCGAATTCAC", "ATGAC", "ATGCCCGGGTAA", "ATGACGTACGTC", "ATGAGGGGTTCA"]`,
>
> 1. Extract all sequences that start with `ATG` and end with `AC` or `AA`.
> 2. Extract all sequences that contain either `G` or `C` repeated three times consecutively.
>
> You should get the following results:
>
> ```
> Sequences starting with 'ATG' and ending with 'AC' or 'AA':
> ['ATGCGAATTCAC', 'ATGAC', 'ATGCCCGGGTAA']
> Sequences containing 'G' or 'C' repeated three times consecutively:
> ['ATGCCCGGGTAA', 'ATGAGGGGTTCA']
> ```

25.5 Exercise

> **!** Exercise
>
> Create a program, that you can run on command line as follow `./analyse_fasta.py path/to/fasta/file path/to/output/file`. It should:
>
> - read the fasta file,
> - calculate the nucleotide frequency for each sequence (using the previously defined function)
> - create a new file as follow:
>
> ```
> Seq A C T G
> seq1 0.1 0.2 0.3 0.4
> seq2 0.4 0.3 0.2 0.1
> ```

...

To make this easier, consider that the sequences in the fasta file are only in one line.
You might make good use of the method `str.strip()`.
You can take as input the file in `exercise/data/example.fasta` you should get the same result as `exercise/data/example.txt`.

26 Scientific packages

A python package contains a set of function to perform specific tasks.

A package needs to be **installed** to your computer one time.

You can install a package with `pip`. It should have been automatically installed with your python, to make sure that you have it you can run:

```
#| eval: false
# In Linux/MacOS
python -m pip --version
# In Windows
py -m pip --version
```

If it does not work, check out pip documentation.

To install a package called pandas, you must run:

```
#| eval: false
# In Linux/MacOS
python -m pip install pandas
# In Windows
py -m pip install pandas
```

To get more information about `pip`, check out the full documentation.

> ⚠ Warning
>
> Installing a package is done outside of the python interpreter, in command line in a terminal.

When you wish to use a package in a python script, you'll need to import it, by writing inside of you script:

```
import pandas
```

26.1 Pandas

Pandas is a package used to work with data sets, in order to easily clean, manipulate, explore and analyze data.

26.1.1 Create pandas data

Pandas provides two types of classes for handling data:

- `Series`: a one-dimensional labeled array holding data of any type such as integers or strings. It is like a column in a table.

```
# If nothing else is specified, the values are labeled with their index number (starting from
myseries = pandas.Series([1, 7, 2], index = ["x", "y", "z"])
print(myseries)
```

```
x    1
y    7
z    2
dtype: int64
```

- `DataFrame`: a two-dimensional data structure that holds data like a two-dimension array or a table with rows and columns. It is like a table.

```
data = {
  "calories": [420, 380, 390],
  "duration": [50, 40, 45]
}

df = pandas.DataFrame(data)

print(df)
```

```
   calories  duration
0       420        50
1       380        40
2       390        45
```

You can also create a DataFrame from a file.

```
# Make sure this is the correct path for you! You are in the directory from where you execute t
df = pandas.read_csv('exercise/data/sample.csv')

print(df)
```

You get access to the index and column names with:

```
df.columns
df.index
```

You can rename index and column names:

```
df = df.rename(index={0: 'a', 1: 'b', 2: 'c', 3: 'd', 4: 'e', 5 : 'f'})

df.index
```

You can select rows:

```
# Select one row by its label
print(df.loc[['a']])
# Select one row by its index
print(df.iloc[[0]])

# Select several rows by labels
print(df.loc[['a','c']])
# Select one row by index
print(df.iloc[[0,2]])
```

You can select columns:

```
# Select one column by label
df['Tissue'] # Series
df[['Tissue']] # DataFrame

# Select several columns
df[['Gene','Expression_Level']]

# Select several columns by index
df.iloc[:,[0,1]]
```

You can select rows and columns as follows:

```
df.loc[['b'], ['Gene','Expression_Level']]
```

You can filter based on a condition as follows:

```
df[df['Expression_Level'] > 6]
```

26.1.2 Useful methods

To explore the data set, use the following methods:

```
df.info()
```

```
df.describe()
```

```
df.head()
```

```
#| eval: false

df.sort_values(by="Gene")
```

```
df['Expression_Level'].mean()

df.groupby("Gene")[['Expression_Level']].mean()
```

26.1.3 Learn More

To get more information on how to use pandas, check out:

- the documentation
- the cheat sheet
- any useful tutorial

26.1.4 Exercise

! Exercise

1. Create a pandas DataFrame from the file containing the frequency of each nucleotide per sequences (`exercise/data/example.txt`).
2. Make sure that `df.index` contains the name of the sequences, and `df.columns` contains the nucleotides.
3. Use `pandas.melt()` (see the doc) to get the data in the following format:

```
    nucl  freq
Seq
seq1    A  0.46
seq2    A  0.20
seq3    A  0.16
seq4    A  0.18
seq5    A  0.26
seq1    T  0.22
seq2    T  0.12
...
```

4. Get the mean value of all nucleotide frequencies.
5. Get the mean value of frequencies per nucleotide.
6. Filter to remove values of seq1.
7. Recompute the mean value of frequencies per nucleotide.

26.2 Matplotlib

Matplotlib is a package to create visualizations in Python widely used in science.

To shorten the name of the package when we call its functions, we can import it as follows:

```
import matplotlib.pyplot as plt

df = pandas.read_csv('exercise/data/sample.csv')

# The data for GeneA and GeneB is extracted from the DataFrame 'df'
serieA = df[df['Gene'] == 'GeneA']['Expression_Level']
serieB = df[df['Gene'] == 'GeneB']['Expression_Level']

# Create a new figure
fig = plt.figure()

# Create a boxplot showing the expression levels of GeneA and GeneB
plt.boxplot([serieA, serieB], # List of series
            labels=['GeneA', 'GeneB'])

# Set the label for the x-axis
plt.xlabel('Gene')
# Set the label for the y-axis
plt.ylabel('Expression Level')
# Set the title of the plot
plt.title('Expression of Genes in Different Tissues')
# Display the boxplot
plt.show()
# Save the plot as a PNG file with a resolution of 300 dots per inch (dpi)
# The file will be saved in the specified location
fig.savefig('exercise/data/my-figure.png', dpi=300)
```

The following code is equivalent.

```
# Create a new figure
fig, ax = plt.subplots(1, figsize=(5, 4))
```

```
ax.boxplot([serieA, serieB], # List of series
           labels=['GeneA', 'GeneB'])
ax.set_xlabel('Gene')
ax.set_ylabel('Expression Level')
ax.set_title('Expression of Genes in Different Tissues')
ax.legend()
plt.show()

# Save the plot as a PNG file with a resolution of 300 dots per inch (dpi)
# The file will be saved in the specified location
fig.savefig('exercise/data/my-figure-2.png', dpi=300)
```

> **Note**
>
> The first way of plotting is function-oriented, and the second is object-oriented. You might encounter both styles of coding.

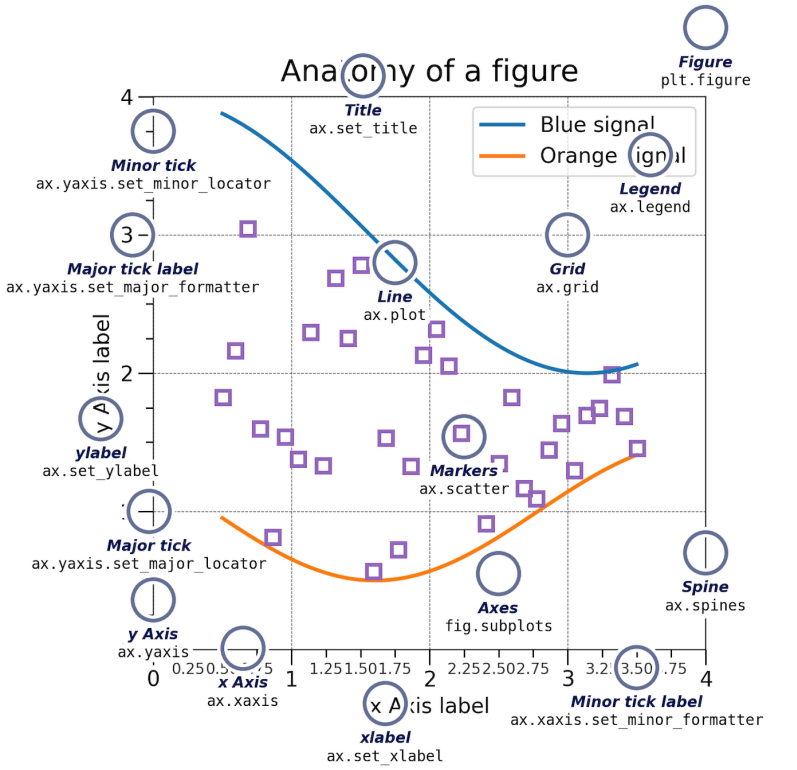


Figure 26.1: Anatomy of a matplotlib plot

Many visualizations are available (static, animated, interactive). For more information, check out:

- the documentation
- the cheat sheet
- any useful tutorial
- some inspiration

26.3 Exercise

> **!** Exercise
>
> Create a script that gets nucleotide frequency data from a file in the format of `exercise/data/example.txt`, and visualizes it using Matplotlib and Pandas.
> Your script should read the data, create a stacked bar chart showing the nucleotide frequencies for each sequence, and label the axes appropriately. Here's the expected plot:

26.4 More packages

There are MANY packages available, here's a short list of some that might interest you:

Package	Usage	Example of usage
BioPython	Computational molecular biology	Sequence handling, access to NCBI databases
NumPy	Numerical arrays	Data manipulation, mathematical operations, linear algebra
Seaborn	High-level interface for drawing plots	Data visualization, statistical graphics
HTSeq	High throughput sequencing	Quality and coverage, counting reads, read alignment
Scanpy	Single-Cell Analysis	Preprocessing, visualization, clustering
SciPy	Mathematical algorithms	Clustering, ODE, Fourier Transforms
Scikit-image	Image processing	Image enhancement, segmentation, feature extraction

Package	Usage	Example of usage
Scikit-learn	Machine learning	Classification, regression, clustering, dimensionality reduction
TensorFlow and PyTorch	Deep learning	Neural networks, natural language processing, computer vision

27 Final tips and resources

Figure 27.1: Please, read the doc

Here are a couple of tips:

- Leave comments (think of your future self!)
- Be consistent (quotes, indents…)
- Don't re-invent the wheel, for common tasks, it's likely that a function already exists
- Read the documentation when using a new package or function!
- Google It! Use the correct programming vocabulary to increase your chances of finding an answer. If you don't find anything, try wording it differently.
- The easiest way to learn is by example, so follow a tutorial with the example data, and then try to apply it to your own!

You can follow some free tutorials on:

- Code Academy
- EdX
- Youtube!

Finally, you should able to use Github Copilot (AI coding assistant), as it is free for students: https://education.github.com/benefits.

References

A python conference organized by the AFPy (Association Francophone Python) is held in Strasbourg in the end of October 2024!

Here are some references and ressources that inspired this class:

- Python doc
- w3schools
- pythonforbiologists
- justinbois's Bootcamp

28 Lesson 3 - Conway's Game of Life

29 Introduction

29.1 Aim of the class

This last class is to pratice the notions learned on a couple of (larger) exercises.

The exercises have one provided solution, but it is not the only one. We all have a different coding style, and it evolves with time. So do not worry if you have a different solution, as long as your result is correct, that's already great!

"the best way to learn a language
is to speak to natives"
the guy learning Python:

Figure 29.1: *psssssss*

29.2 Requirements

Remembering some of lesson 1 and 2.

30 Conway's Game of Life (basic)

30.1 Instructions

Create an implementation of Conway's Game of Life in a script called `conway_life_basic.py`.

The game consists in initializing a 2D matrix of binary value (0 or 1), and, by following certain rules, observing its evolution at each generation.

Each value represent a cell, that can either be live (0) or dead (1).

30.2 Rules

Cells interact with their neighbors such that:

- Any live cell with fewer (<) than two live neighbors dies (as if by underpopulation)
- Any live cell with more than three (>) live neighbors dies (as if by overpopulation)
- Any live cell with two or three live neighbors lives on to the next generation
- Any dead cell with exactly three live neighbors becomes a live cell (as if by reproduction)

The new matrix created corresponds to a new generation.

The original game is played on a infinite board, but we'll implement it to a finite board. When a cell is in a corner, it has 3 neighbors. When a cell is on a side it has 5 neighbors.

30.3 Functions to create

You should create:

- a `count_neighbors` function that counts the number of live neighbors around a cell
- a `survival` function that determines if a cell survives or dies based on the rules of the game
- a `generation` function that generate the next generation of the game
- an `animate_life` function that animate the game of life

You should use basic python, and print each generation to the terminal as follows:

- live cells are represented by a `*`
- dead cells are represented by a `.`

e.g. the following 3-by-3 2D matrix has one live cell in the center:

```
. . .
. * .
. . .
```

You will need to initialize a matrix to begin the game, then it should run on its own for a defined amount of generations.

30.4 Optional function

As an option, you can create a function called `initialize_universe` to initialize the grid with one of the following seeds that have specific proprieties:

```
# Dictionary containing different seed patterns for the game
seeds = {
    "diehard": [
        [0, 0, 0, 0, 0, 0, 1, 0],
        [1, 1, 0, 0, 0, 0, 0, 0],
```

```
        [0, 1, 0, 0, 0, 1, 1, 1],
    ],
    "boat": [[1, 1, 0], [1, 0, 1], [0, 1, 0]],
    "r_pentomino": [[0, 1, 1], [1, 1, 0], [0, 1, 0]],
    "pentadecathlon": [
        [1, 1, 1, 1, 1, 1, 1, 1],
        [1, 0, 1, 1, 1, 1, 0, 1],
        [1, 1, 1, 1, 1, 1, 1, 1],
    ],
    "beacon": [[1, 1, 0, 0], [1, 1, 0, 0], [0, 0, 1, 1], [0, 0, 1, 1]],
    "acorn": [[0, 1, 0, 0, 0, 0, 0], [0, 0, 0, 1, 0, 0, 0], [1, 1, 0, 0, 1, 1, 1]],
    "spaceship": [[0, 0, 1, 1, 0], [1, 1, 0, 1, 1], [1, 1, 1, 1, 0], [0, 1, 1, 0, 0]],
    "block_switch_engine": [
        [0, 0, 0, 0, 0, 0, 1, 0],
        [0, 0, 0, 0, 1, 0, 1, 1],
        [0, 0, 0, 0, 1, 0, 1, 0],
        [0, 0, 0, 0, 1, 0, 0, 0],
        [0, 0, 1, 0, 0, 0, 0, 0],
        [1, 0, 1, 0, 0, 0, 0, 0],
    ],
    "infinite": [
        [1, 1, 1, 0, 1],
        [1, 0, 0, 0, 0],
        [0, 0, 0, 1, 1],
        [0, 1, 1, 0, 1],
        [1, 0, 1, 0, 1],
    ],
}
```

30.5 Exemple of input and output

Here's an example of input, and the desired output:

```
# Initialize by hand
universe = [
  [0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
  [0, 0, 1, 1, 1, 0, 1, 0, 0, 0],
  [0, 0, 1, 0, 0, 0, 0, 0, 0, 0],
```

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

animate_life(universe, generations = 3, delay=0.5)
```

```
. . . . . .
. . . * . . .
. . * * . . .
. . * . * . .
. . . * * * .
. . . * * . *
. . . . * . .
. . . . . . .
. . . . . . .
. . . . . . .
```

```
. . . . . . .
. . * * . . .
. . * . * . .
. . * . . * .
. . * . . . .
. . . . . * *
. . . * * * .
. . . . . . .
. . . . . . .
. . . . . . .
```

```
. . . . . . .
. . * * . . .
. * * . . . .
. * * . . . .
. . . . . * *
. . . * * * .
```

```
. . . . * * * . . .
. . . . * . . . . .
. . . . . . . . . .
. . . . . . . . . .
```

The same matrix can be initialized by the following (if you are doing the optional `initialize_universe` function):

```
# Initialize with a seed
universe = initialize_universe(universe_size = (10, 10), seed = "infinite", seed_position = (2
for row in universe:
  print(row)
```

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

With this matrix, if the number of generations increases (> 30), it should stabilize over:

```
. . . . . . . . . .
. . . . . . . . . .
. . . . . . . . . .
. . . . . . . . . .
. . . . . . . * * .
. . * * . . * . . *
. . * * . . . * . *
. . . . . . . . * .
. . . . . . . . . .
. . . . . . . . . .
```

30.6 Tips

- Take an exemple and do it by hand to better understand the game.
- Before jumping into coding, try to have a plan of how you will implement it all. Imagine what will be the input and output of each function.
- To visualize the evolution of the grid, you can print it, and then can clean the terminal by using `os.system('cls' if os.name == 'nt' else 'clear')` (you will need to `import os` at the beginning of your script).
- To wait between two generations you can use `time.sleep(delay)` (you will need to `import time` at the beginning of your script).

31 Conway's Game of Life (advanced)

31.1 Instructions

Create another implementation of Conway's Game of Life, with the following characteristics:

- the file parses arguments from command line (if you use argparse, you can check the help of your function by running in the terminal `python conway_life_advanced.py --help`)
- use pandas (or numpy as there it is only numerical data) to deal with the matrix
- use matplotlib to plot each generation, and create a final gif

Example of a final gif generated from the same universe matrix as the one from basic implementation

32 Solutions

Both solutions are available in the folder `exercise/script/`.

33 References