Introduction to Python

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I. A few words on formatting before we start

Throughout this document, I will use a few types of formatting. Normal text like this is just me rambling on insufferably, so **if you already know some Python**, you could ignore most of this black-and-white text. If you do not know much Python, I would advise against ignoring this type of text, as it contains most explanations.

Secondly, I will have to-the-point specific instructions that you should follow, in grey:

1. Follow the instructions in these grey blocks closely.

You can essentially just follow those blocks of grey text and you'd be mostly okay.

These specific instructions will be numbered continuously throughout this document.

Code blocks will be pretty obvious—in monospace font and coloured by syntax:

```
DEADLINE = 23
happy = True
day = 24

# Am I happy and is this day before the deadline?
if happy and day <= DEADLINE:
    print("Hello, World!")
else:
    # I either missed the deadline, or I'm unhappy :-(
    print("Good bye cruel world, I'm leaving you today." + 3*" Good bye...")
# ...extra points if you can tell where that line above came from.</pre>
```

I emphatically recommend that you **do not copy and paste my code into your editor**. Instead, **type the code yourself from scratch**. Neurologists and learning experts seem to believe that this should improve your learning process . In fact, if you want to get serious about programming, you could write your algorithms with pencil and paper before you actually code them!

Finally, I may occasionally give you a stark warning, such as:

You can ignore most black & white text, but **do not** ignore these red blocks or the grey ones! And with that, let's get started.

II. Installing Python and setting up

To write and run code in Python, we would generally need three things:

- The Python 3 engine itself, i.e. the software that interprets Python code.
- A text editor to write the code in.
- An interface to run this code using the engine.

The latter two tasks are typically combined into something called an **Integrated Development Environment (IDE)**, which is a type of editor in which you can both write your code and run it. Actually, if you're on a Mac or Linux machine, chances are you already have Python, so you could use the basic text editor app that came pre-installed on your system (you can't use MS Word because you need "plain text"), and you could run the code directly from the Terminal or Console. However, **this scenario isn't the most convenient**. Alternatively, you *could* (but shouldn't) go to Python's website itself (www.python.org) and download it from there. However, there is a far better way of doing all of this: Anaconda (or its lighter version, Miniconda).

Don't get Python from python.org—we'll use Anaconda instead.



II.1. Make sure you don't already have Anaconda or Miniconda!

Before we download Anaconda or Miniconda, let's make sure we don't already have either.

II.1.1. Mac/Linux

2. Open a terminal/console and type:

which conda

If your system can't find conda (it either doesn't print anything or it prints "conda not found"), you have neither Anaconda nor Miniconda. Read on to section II.2, where we will install it. If you did see a path to conda or a lot of text, then you already have conda, so skip to section II.3, where we will update it.

II.1.2. Windows

3. Hit the Windows key in your keyboard or the main icon at the bottom left of the task bar and start typing "Anacon..."

If you can't see anything that looks like "Anaconda 3 command prompt", you probably have neither version of conda, so read on to section II.2, where we will install it.

II.2. Downloading & Installing Anaconda or Miniconda

The best way to get Python is through **Anaconda**, a super useful package that contains Python and a large assortment of other tools pre-included, most notably a powerful package manager and two separate IDEs (Jupyter Notebook and Spyder).

Alternatively, if you have limited storage space or just like to keep things minimal, you may want to use **Miniconda**, which is a much lighter but just as powerful version of Anaconda. Both will work just fine for our purposes here. The main difference is Anaconda has a nice graphical user interface to manage packages (which we don't need to use here), and it comes with many pre-installed software and packages (which we don't need, we will install our own); because of this, Anaconda is far heavier, but they work equivalently.

4. Download and install

Anaconda from anaconda.com/products/individual

or...

Miniconda from docs.conda.io/en/latest/miniconda.html

These links are valid at the time of writing, but they do change every now and then. Once you have installed:

Open a **new** terminal window (Linux/Mac) or start the Anaconda Prompt (Windows), and type:

which conda

This time it should work.

II.3. Setting up conda

Let's update conda (yes, even if you just installed it).

6. With the terminal or Anaconda prompt open, type:

conda update --all -y

This will probably take a few minutes. The -y means "yes, I'm sure. Don't ask me to confirm". Remove it if you prefer more control.



II.3.1. Adding channels

7. Add channels to conda by running the following, one at a time:

```
conda config --add channels bioconda
conda config --add channels conda-forge
```

These channels are repositories where conda can find packages, such as the ones we will be installing in the next step.

II.3.2. Creating a conda environment

8. Create a conda environment in which you will do your Python work, with all the necessary packages. For example, for a basic bioinformatics setup, you could create an environment called bioinfo, containing the packages jupyter, jupyterlab, pandas, matplotlib, and numpy. For this, do:

conda create -n bioinfo -y jupyter jupyterlab pandas matplotlib numpy

This will take a while.

The greatest thing about conda is that it takes care of all dependencies, i.e. you don't have to check for compatibilities or libraries or anything, you just tell it what you need, and it finds anything that's required to run it and installs it for you.

9. Activate this environment:

conda activate bioinfo

II.3.3. Adding packages to a conda environment

Now that we have a working environment, we can add packages to it. For example, it would be good to have biopython and blast in our bioinformatics environment.

10. With the bioinfo environment activated (see the previous instruction), type:

conda install -y biopython blast spyder=4

We can just separate the different packages we want with a space. Note that for spyder, we **specify version** 4, otherwise at the time of writing it would install version 3 for some reason.

II.4. Checking that everything is working and starting Python on Spyder

When we created our Python environment via conda above, we also installed Spyder, the programming environment (IDE) that we will be using here.

- 11. With the bioinfo environment still active (see above), start spyder simply by typing "spyder" into the terminal (without the quotes) and pressing enter.
- 12. There should be a "Console" window on the lower-right quarter of Spyder. Click inside it and type:

print(1 + 2)

You should see a 3, of course. And that's it. We're ready to go!

II.5. Regularly updating your conda installation and environments

Actually, before we move on, a general note on updates. It is generally wise to keep your conda up to date.

13. In the terminal or anaconda prompt, run the following commands:

conda update --all

conda update -n bioinfo --all

And repeat that last line for every environment you have (we did it only for bioinfo here).



II.6. Other IDEs (optional)

There are probably hundreds of other IDEs (fancy code editors/runners/debuggers). Three worthy of mention are Visual Studio Code (code.visualstudio.com), PyCharm Community Edition (jetbrains.com/pycharm, make sure to follow the link to "Community", not "Professional"), and Jupyter Lab. All three are free and open source, and all are great. We won't really need them here because we already have two separate IDEs (Spyder and Jupyter Notebook), but you may want to consider them for the future work if you become a formal Python coder. Spyder is similar to VS Code and PyCharm, so if you end up liking Spyder I encourage you to try the other two also and see which one suits you better (warning: PyCharm has a bit of a learning curve). In any case, other than being light yet powerful, VS Code lets you easily copy and paste nicely formatted code into Word (which incidentally is how I did the beautifully coloured code snippets in this document). This isn't as easily done with the other two that we have installed. For any other intents and purposes in this workshop, Sypder is perfect.

VS code and PyCharm are great to code in in general but we won't be using them here.

With that said, Jupyter Notebooks are quickly becoming a (if not *the*) standard for sharing computational-science protocols, at least for Python code, so please do try to learn as much Jupyter as you can. I have a refresher of this course done on Jupyter, also at github.com/vsojo/Python Workshop (download the file JupyIntro_PythonRefresher.tar.gz).

II.6.1. What's the difference between Jupyter Notebook and Jupyter Lab?

Jupyter Notebooks are the format (file extension <code>.ipynb</code>), and they come with their own interface. This interface is formally discouraged now, you should move on to Jupyter Lab, which we installed above. In reality, they are extremely similar, other than perhaps Jupyter Lab feels a little more "modern".

Again, we won't be using Jupyter here. I would recommend learning Python with Spyder or VS Code, before moving on to Jupyter.

III. Mathematical operators

14. Take a look at the list of basic mathematical operators in Python:

Mathematical operators		Example	Result
Addition	+	2 + (-5)	-3
Subtraction	_	-7 + 9	2
Multiplication	*	3 * 2	6
"Floating-point" (real) division	/	6 / 2	3.0
Integer division quotient	//	13 // 5	2
Integer division remainder or "modulo"	%	13 % 5	3
Exponentiation (a ^b)	**	2 ** 3	8

Operation precedence works just like it did in middle school. If in doubt, just throw in a pair of parentheses, even if you think it's unnecessary but will make the code easier to read. Don't overdo it, though—try to keep your code readable, clean and pretty, in that order.



15. Go ahead and try all the examples in the table above in Spyder's Python console.

Note: here, Python won't care if you leave spaces or not. For other things that we will see later, Python is *extremely* nitpicky with spaces. I'll tell you when it becomes relevant.

You'll see that the **Python console** gives you the answer as screen output. It essentially behaves as a calculator.

There are some funny things happening, though. If you try 3*2 you get the integer 6, but if you try to reverse it with 6/2 you get 3.0, with a decimal point. That's because Python 3.x (but not Python 2.x), defaults to floating-point (float) division, i.e. it treats all numbers as Real and not integers. Conversely, multiplication defaults to integer (int) if all numbers being multiplied are integers, but float if at least one of them is a float (i.e. has decimals, even if the decimal is zero). You'll see in the table that you can actually get integer division by using a double //, but be careful:

```
// only gives you the exact value if the first integer is divisible by the second one (e.g. 4//2).

16. Try each of the following exercises, but predict their output before you run them.

6*3 \quad 6/3 \quad 6/4 \quad 6\%4 \quad (50-5*6)/4 \quad 3**2 \quad 9**(1/2) \quad 9**(1//2)
```

IV. The print() statement: the programmer's best friend

17. Let's do some of the same code above, but wrapped around a print() statement:

```
print(2 + 4)
print((50 - 5*6) / 4)
print(9**(1/2))
```

So far so good, we get essentially the same result as without the print statement. So why would we want to use print() at all? Well...

18. Try this:

```
print("I am", 3**2 - 7 + 38//3, "years old")
```

Pretty cool, innit? We will see more reasons to use print(), chiefly that when we write proper script files, Python won't print anything unless we actively tell it to.

The print statement is arguably the programmer's best friend. It is often used as a quick and cheap way of **debugging**, i.e. finding errors in code. There are fancier ways of debugging, but we won't be covering them here. I encourage you to read about it online if you get serious about coding. I'll limit myself to giving you the best advice I've ever read on the topic:

When debugging, don't try to figure out why your code *isn't* doing what you want it to do. Instead, try to understand why it *is* doing what it's doing.

V. Don't ever use the console, ever again – write scripts instead!

19. Let's make a deliberate error. Type and run the following in the Python console:



```
print("I am", 3**2 - 7 + 38//3, "years old)
```

Yes, it's the same code as before but leaving out the closing double-quote before the parenthesis.

Python will complain, and it will try to help us figure out what we did wrong. In this case the error message is not particularly helpful unless you already know a bit of coding:

SyntaxError: EOL while scanning string literal

What on Earth could that mean?

EOL means "End Of Line". It seems Python was scanning a "string literal" (whatever that may mean) and it reached the end of the line that we told it to execute before this "string literal" thing ended. Since we know what we broke, we can deduce what the message means: the string literal was the text, and Python reached the end of the line without understanding what was going on because we never told it where the text ended.

Annoyingly, we need to type or at best copy and paste the code again, correct the error, and run it again. There's a trick, though. In most consoles, you can use the up arrow in your keyboard to recover the preceding commands.

20. Use the up arrow in your keyboard to recover the previous command and correct it. But every time we run a line of code, it goes into the console and after a while we lose it. Sure, we can scroll up or hit the up arrow and recover it, but what if we want to build a more complex program? Writing and testing it line by line would be a real pain.

Instead, we write a **script**. A script is a text file with code that gets interpreted by the computer only when you tell it to, not every time you hit enter like in the console.

Don't ever use the console again, for anything other than testing some extremely basic Python command. If you want to use a calculator, just use the one that came with your operating system.

A script is just a text file. You can send it to your collaborators, share it with the community, update it, and so on. And you can keep all your code there and later delete anything that you don't want. Conversely, trying to get code out of the console can be very annoying and sometimes impossible.

So, if Spyder doesn't already have a text file open on the left, hit **File > New File** or **Cmd+N** on Mac, Ctrl+N on Windows/Linux.

- 21. Type or copy and paste some of your old code into the script in Spyder.
- 22. To run it, do not hit Enter, but **Ctrl+Enter**. Enter just adds a new line, like in MS Word. You can also hit the green "play" button at the top, near the left side.

You will see the output of your command on the console.

And that's it, we won't be using the console again here except to examine the output of our code.

VI.# Comment your code!

Comments are extremely important, and we will use them very generously here. They make your code readable—by you and by others—and they help you think about the code you're writing and why. Often while writing comments you will see that the code you wanted to write doesn't make sense or isn't necessary. I therefore recommend that you:

Write lots of comments and, as much as possible, write them **before** you even write the code that you are commenting!

Almost all programming languages have a way of adding comments. In Python there are two main ways: single-line comments, and multi-line comments.

VI.1. # Single-line comments

Created using the "hash", "numeral" or "number" sign # (for some strange reason called "pound" in some parts of North America). The convention is to leave a space after the #:

like this, with a space after the hash
#not like this (this is ugly and confusing, see next)



The space after the # is not obligatory, but it is strongly advisable because we normally **do not** leave a space when we're "commenting code out", i.e. when we have a line of code that we want to disable temporarily:

```
print("This code is fine.")
#print("But I don't want this code to run")
```

VI.2. """Multi-line comments"""

These are created between triple double-quotes:

```
This is a multi-line comment
I can write whatever I want here...

#%#%@^^!(!*!%!% Fja jas ;ljfl jdsfoae ou234@$@#$!$$! Absurd nonsensefd f dj jl!

print("...and none of this will run")

x = "because it's in a multi-line comment")

print(x, "so Python will ignore all of it!") BWAhahaha

"""
```

These comments can be very useful for temporarily commenting out large blocks of code, but other than that:

Refrain from using multi-line comments except to disable code temporarily. Triple-double-quote comments are typically reserved to describe functions and other things. We'll see how later.

In fact, you may have noticed that Spyder added a multi-line comment at the top of our script file. We're supposed to write into it what this file is supposed to do, who made it, when, for whom, and so on.

VII. Variables

Like in mathematics, <u>variables</u> in programming languages are symbols that represent values—but they can also represent other things. In Python, we use the equals sign = to <u>assign</u> a <u>value</u> to a <u>variable</u>.

Yes, equals = is used to **assign values to a variable**, not to compare things. For comparisons we use the double equals ==, as we will see later.

23. Predict the output of the following script, then write and run it:

```
width = 10
length = 2
height = 5
volume = width * length * height
```

...actually, if you're in Spyder, this script doesn't give you any output at all. Can you guess why? The reason is that we just told Python to multiply those three things, and it did it; fine. If we want to see the value, we have to tell Python to show it to us:

```
print(volume)
```

And now it does show it. In case you're wondering what would happen if you just throw volume on its own, i.e. removing the print statement:

```
volume
```

Go ahead try it. You'll get absolutely nothing. The reason is that computers respond only to commands, and you didn't give it any. If you tell it "volume", the computer just thinks "aha,

volume, it's worth 100, sure thing, I know what you mean". You didn't really tell it to do anything with that number, so it just looks at it, and then it just keeps going.

There's a caveat: if you try typing "volume" directly in the console instead, or in Jupyter, you'll see that it does actually print the result. This is because the console is meant as an interactive environment for immediate coding, so it was built to assume that you always want to see the value of a variable, even if you don't ask to print it. Once again: the console is not really meant to create lasting code, only for short tests. The same happens in Jupyter, but that's because the Notebooks were created for visualisation, so they show as much as possible.

One other thing is worth noting in the code above. If you try printing any of the three variables, you'll see that their values didn't change. So:

```
x = 1
print(x + 1)
print(x) # still the same original value
x = x + 1
print(x) # now it did change
# challenge: try x += 1
```

VII.1. Naming variables

Variable names must start with an English-language letter or underscore, and other than upper and lowercase letters, they can have numbers or underscores within. **No dashes or spaces**.

You don't have to, but please always start your variable names with lowercase letters. Starting uppercase letters are used for something else (Classes, if you must know). Python is casesensitive, i.e. the variables pYthon and pyThon are two different things. Needless to say, distinguishing your variables only by casing, although technically allowed, is a horrendous coding practice, so don't do it. In any case (forgive the pun), the convention in Python is to write every name in lowercase unless you have a compelling reason to do otherwise.

Constants, however, are normally written in all uppercase: AVOGADRO = 6.022e23

If you have a long variable name, somePeopleUseCamelCasing, whereas others prefer_to_use_snake_casing. The convention in Python is to use snake_casing for most things. CamelCasing is used only when defining classes in object-oriented programming.

VII.1.1. "Reserved" (i.e. forbidden) names

You can't use any name that Python is already using, such as print, if, else, for, while, and, or, and many others. The colour in your IDE often helps you a bit. Here's a sample from VS Code:

```
name = "NYC"
desc = "awesome"
type = "metropolis" # hm... maybe we need to use "kind" instead of "type"
```

VII.1.2. Using descriptive names

By all means, **give descriptive names to your variables**, but do try to keep them relatively short. I tend to prefer longer names like population_density far better than a confusing p, but some people prefer shorter code. Either way, **comment your code thoroughly** to indicate what each variable represents, even if you think it's obvious—it may not be obvious to everybody:

```
# Population density of New York City:
popdens_nyc = 10947 # persons/km2
```

Now whoever looks at our code knows that we're using persons/km², as opposed to persons/mi². Also, this:

```
popdens_bronx = 13231
popdens_brooklyn = 14649
popdens_manhattan = 27826
popdens_queens = 8354
popdens_staten_island = 3132
```

is much easier to read than this:

```
bronx_popdens = 13231
brooklyn_popdens = 14649
manhattan_popdens = 27826
queens_popdens = 8354
staten_island_popdens = 3132
```

All in all, please choose variable names that anybody can identify immediately if possible, even if they're completely unfamiliar with your code, or even with programming.

VII.2. Assigning multiple variables at the same time

Python is built for efficiency. You can assign multiple variables in one go. You just have to give a list of desired variables and their values.

24. Type and run the following (but predict the output before you run it!):

```
a, b, c = 1, 2, 3
print(c, a)
```

This is perhaps a little advanced and you may never need it, but the numbers don't really have to match, you can just make one of the variables a container for "everything else":

```
a, *b, c = 1, 2, 3, 4, 5, 6
print(a)
print(b)
print(c)
```

So, a takes the first value, c takes the last one, and since we gave b an asterisk, it takes everything else. Other than this exception, the numbers of variables and values typically must match.

The following will give an error:

```
a, b, c = 1, 2, 3, 4, 5, 6 # THIS WILL FAIL!
```

25. But... you can actually define multiple variables to the same value. Try the following:

```
x = y = z = -5
print(x, y, z)
```

VII.3. CHALLENGE: reassigning variables

26. Define two variables, x = 4 and y = 5. Now, **without** writing 4 or 5 again, make x have the original value of y (i.e. 5), and y the original value of x (i.e. 4).

Bonus points if you can do it in one line, but the traditional solution would have three.

VIII. Data types

27. Try the following:

```
print("Mary had " + "one" + " little lamb")
```



Cool. You can join bits of text using the + operator. This is very worth remembering. If you care to know, the process of joining text is almost always called **concatenation** in computer science. 28. Now try the following:

```
print("Mary had " + 1 + " little lamb") # will fail!
```

You'll get an interesting and very informative error. It tells you that you can only concatenate a str to another str, not an int. "str" is short for string, which is what computer people call text (think of text as being a *string* of characters, one after the other). "int" of course is short for integer. Essentially, you can't tell Python to just put these two things together, it doesn't understand what you mean. There are a few tricks you can use to solve this problem. The first:

```
print("Mary had", 1, "little lamb") # Good trick to remember: use comma instead of +
```

This will work, because the print function internally handles any **type conversion** necessary. It receives three separate bits, handles each of them independently making sure that they are all converted to string, and then concatenates them. But we can do the type conversion ourselves.

VIII.1. Type conversion

29. Use the str() function to convert an integer to string:

```
print("Mary had " + str(1) + " little lamb") # will work :)
```

Nice! Now it works.

So, how many data types are there? Well, many. But here are the main ones:

30. Use the type() function to find out the main types of data in Python

```
type(1) # int
type(1.0) # float
type(True) # bool
type("número uno") # str
```

You can run type () on any variable in Python, so it's a good function to remember.

```
Try to remember those four main data types: int, float, bool, and str.
```

You'll be using them quite a bit whenever you write Python code.

Each of those types has its own type conversion or type casting function, called the same as the type itself, so...

VIII.2. CHALLENGE: type casting (a.k.a. type conversion, or type parsing)

31. Using either **Jupyter** or the **Spyder console**, predict the output of the following code snippets, **including quotes** 'and decimals, if you think there will be any.

```
float(1)
int(2.0)
int(2.9999)
str(2)
str(2) + str(3)
str(2) + float(3)
int(str(2) + str(float(3)))
int(True) + float(False)
```

VIII.3. Double quotes or single quotes?

Sometimes you'll see people write Python strings "like this", but sometimes 'like this'. Briefly, both are correct, but please use the double ones. There are two reasons for this. The first reason is that with double quotes you can easily write English-language strings such as "He ain't heavy, he's my brother". But there's another good reason to use double quotes for most of your strings, which I'll explain in the following sections (in short, we'll use them as the *index* or *key* of dictionaries).

IX. list, dict, tuple: Data structures

IX.1. Lists

Lists are collections of data, typically the same kind of data.

32. Create a list:

```
fruits = ["apple", "orange", "pineapple", "passion fruit", "coconut", "kiwi"]
```

Try printing the list with print(fruits). Nice. But what's coolest about lists is that you can do a lot of stuff with their individual members.

33. Let's access an element inside a list:

```
print(fruits[1])
```

Great! Or... hang on a sec... the 1st element was not the orange! The geekiest amongst you will know what's going on:

Many computer languages (including Python, but not R), start counting at zero!

This is crucial, and it's a major cause of headaches for beginning programmers, and for those of us who frequently have to switch between Python and R.

Anyhow, we can access elements inside a list by giving their index (remembering to subtract 1). 34. Cooler still, we can also access items backwards by giving a negative index:

```
print(fruits[-1]) # the last fruit (kiwi)
```

Ok, here the first index is actually -1 (not -0, which would make no sense)... just another thing to remember. The second one from the back is -2 and so on.

```
print(fruits[-2]) # the coconut
```

IX.1.1. Modifying values in a list

35. You can just change the value of any item in a list:

```
print(fruits)
fruits[2] = "tamarillo"
print(fruits)
```

IX.1.2. Slicing and stepping in a list

You can get "slices" of a list by using a colon:

```
36. Slice a list by using a colon, as in: my_list[start:stop]
```

```
print(fruits[2:4]) # This doesn't change the list itself, though
```

Nice! Oh... hang on again... index 4 is actually the 5th element, isn't it? So, that should have been the coconut! Why did we get only up to the previous one? Well... that's something you'll just have to learn to live with: when you're slicing or sub-setting a list (or tuple, or string), Python gets you up to the item *before* the one you gave it as stopping point.



37. You can slice backwards too:

```
print(fruits[-4:-2]) # Going backwards, Python also stops one earlier than you'd think
print(fruits[-4:-5]) # Nothing. That's an empty set. It's similar to doing this:
print(fruits[5:4]) # A nonsensical slice that will give you nothing, an empty set
```

38. You can indicate "everything else" by just leaving either of the two indices empty:

```
print(fruits[:4]) # start at the beginning, go until the 4th item
print(fruits[3:]) # start at the 4th item, go until the end
print(fruits[-3:]) # start at the antepenultimate item, go until the end
print(fruits[:]) # start at the beginning, go until the end, i.e., the whole list
```

Two weird things about Python indices to remember:

- Start counting at 0 if going forwards, but at -1 if going backwards.
- Sub-setting works until the number before the one you were aiming for.

This applies to strings, lists, tuples, and more.

39. Jump by specifying a step: my_list[start:stop:step]

```
print(fruits[:4:2]) # start at the beginning, go until the 5th item, but skip 2 by 2
print(fruits[::2]) # the whole list, but leaving every other item out
print(fruits[::-1]) # the whole list skipping backwards by 1... so, the reversed list!
```

Mind you, that last one is not the most efficient way to reverse a list, but coders sometimes use it because it makes them look cool, I suppose. We'll see the best way to reverse a string in the next section.

IX.1.3. Some very useful list functions

Note: many of the functions below also work for strings and tuples.

40. Create the following list

```
squares = [0, 1, 4, 9, 25, 36, 49, 64] # the squares from 0 to 8
print(squares)
```

41. Use the len() function to get the length of a list

```
print(len(squares))
```

Hm... the length is 8, but it should have been 9. Oh, I see what I did wrong, I forgot to add the square of 4 (i.e. 16). We can use the insert method for this.

42. Use insert(index, object_to_add) to add items to a list:

```
squares.insert(4, 16) # insert 16 at the 5th position (remember we start from zero)
print(squares)
```

43. Use pop() to remove items from a list and get the item removed at the same time:

```
squares.pop() # removes the last item
print(squares)
x = squares.pop(0) # removes the 0th (first) item. You can also use negative indices
print(squares)
print(x)
```

As you can see, pop does not just remove an item, it also "returns" the item removed, which you can assign to a variable. This is extremely useful and very much worth remembering.

44. Use append() to add elements to the end of a list:

```
squares.append(8**2) # adding the 64 back in, at the end of the list
print(squares)
```



45. Now that we're at it, let's append the squares of 9 and 10. But let's do it in one go:

```
squares.append([81, 100])
print(squares)
```

Hm... that didn't quite work out. *But*, we learned something useful: you can have lists inside other lists! In fact, **you can have all sorts of stuff inside lists**. We'll discuss this at the end of this section.

46. Mini-challenge: let's repair the squares list. Remove that last thing that we added.

```
squares.pop() # remove the last item
print(squares) # repaired now!
```

47. Use + or *extend() to join a list to another list:

```
squares.extend([81, 100]) # or:
squares += [121, 144] # same as squares = squares + [121, 144]. Print to see
```

48. Use the Boolean operator in to find out if something is in a list or not

```
print(4 in squares) # True
print(5 in squares) # False
```

49. Use index() to find where exactly stuff is in a list, if you're sure it's there:

```
squares.insert(3, 'papaya')
print(squares) # oops, it seems we put a fruit into the wrong list. Let's remove it.
# Let's assume we don't know where we put it. We can use .index() to find out:
idx = squares.index('papaya') # idx is just a variable to store the index that we need
squares.pop(idx)
print(squares) # great, fixed now!
```

Note: index() only works if the element you're looking for is definitely in the list. If you try squares.index('papaya') again, you'll get an error, because papaya is no longer there.

50. Use the reverse () method to reverse a list

```
revsquares = squares
revsquares.reverse()
print(revsquares) # nice! The new list is reversed
```

IX.1.4. Copying a list

Let's recover the code from the last exercise.

```
squares = [0, 1, 4, 9, 16, 25]
revsquares = squares # First we make a copy of the original list (...or do we?...)
revsquares.reverse() # then we reverse it
print(revsquares) # nice! revsquares is reversed now :)
print(squares) # what?!! We didn't do anything to squares! Why did it get reversed?!
```

Unlike for simple variables, using = on a list copies only the **pointer** to that list, not the list itself. The idea is that lists can be enormous, taking up a lot of memory. So, by default, Python copies only the bit that *points* to where a list is stored in memory, often known in computing as a *pointer*. 51. So, to copy a list, use the copy() method instead

```
# This is the preferred method on Python 3:
newlist = oldlist.copy() # best and clearest
# ...or you can use the list function:
newlist = list(oldlist) # a little more obscure, but still clear enough
# ...or you could use the old method of slicing from beginning to end:
newlist = oldlist[:] # uglier but typical in Python 2, so old Pythoners use it
```

These, however, give you what's called a "shallow copy" of the list. This is getting pretty technical, but briefly: if any of the elements of the list was itself a pointer to another list, then you only copied the pointer, not the internal list. And on that note...

52. You can throw all sorts of stuff into the same list:

```
x = [1234, "some text", ["another", "list"], {'a': "dict"}, ("and a", "tuple"), 3.14]
```

Many purists (particularly people coming into Python from C, C++ or Java) would recommend that you only put the same kind of data into a list. If you want to have mixed types of data within the same data structure, you should be using a tuple, they say. The reality is that most Python coders freely put all sorts of things into any of their data structures, and you can too unless you have a good reason to follow a tidier practice. If you can be tidy, by all means do so, but don't hesitate to use a dirty list if that's what's convenient.

IX.1.5. A few more list functions and properties

53. You can use the list() function itself to turn a string into a list:

```
mytext = "Hello, World!"
mylist = list(mytext)
print(mytext)
print(mylist)
```

54. If you only have numbers in a list, you can find their maximum and minimum easily:

```
geekyconstants = [2.71828, 3.14159, 6.022e23, -273.15]
print(max(geekyconstants))
print(min(geekyconstants))
```

55. There can be multiple repetitions of the same item in a list, and you can count them:

```
fruits = ["apple", "orange", "apple", "kiwi", "apples"] # someone really likes apples!
print(fruits.count("apple")) # only 2? Interesting...
```

Note that "apples" was not counted as matching "apple". Computers are very obedient... sometimes too much.

IX.2. Dictionaries (key: value pairs)

Dictionaries, or dict, are one of the coolest data structures in the galaxy. They work as key-value pairs, i.e. you can access the value using a key or index. This is more easily seen with an example.

56. Create two simple dictionaries

```
cat = {'lives': 9, 'goes': "meow", 'likes': "murdering beautiful things"}
dog = {'lives': 1, 'goes': "woof", 'likes': ["loving humans", "chasing cats"]}
```

Note: it's a very bad idea to have the 'likes' value be a simple string for the cat but a list for the dog. However, Python will not complain. It's up to us to write consistent code.

We probably should have put the 'likes' of the cat into a list, even if it has only one item. Anyhow, let's keep going. Oh, but before we go on, a short digression to discuss a main reason why I prefer using double quotes for normal text.

IX.2.1. So... "double quotes" or 'single quotes'?

This is very much a matter of personal choice. My own convention, which I highly recommend, is to use double quotes for any "free" text, "such as this one", and single quotes for strings that represent data, such as dictionary['keys'] or 'file_names.txt'. Using this convention helps me realise when a string is not supposed to contain spaces, for example, and

when it is supposed to have a very specific content that can't change freely (file names and dict indices don't typically change too often).

Easy rule of thumb for double vs. single quotes: if the text is for humans, double quotes; if it is for the computer, single.

OK, back to dictionaries.

IX.2.2. Accessing items inside a dictionary

57. Access the values of items inside a dictionary by giving the key:

```
print(cat) # the whole dict
print(cat['lives']) # get only one value, using its key
print(dog['goes'])
```

And you can use the print() function to get nice output:

```
animal = cat
print("Here's a riddle for you:\nThis animal has", animal['lives'], "lives, it goes",
... animal['goes'], "and it likes", animal['likes'], "\nCan you guess what it is?")
```

The three dots on the left mean that I ran out of space and the whole thing should be written in one line. Note that it is generally not great style to have a very long line. We could have done:

```
animal = cat
print("Here's a riddle for you:\nThis animal has"
   , animal['lives'], "lives, it goes", animal['goes']
   , "and it likes", animal['likes']
   , "\nCan you guess what it is?"
)
```

...which is much nicer to read. Python won't care much about any "whitespace" (that's the geeky name for it) added *inside* a **function call** (print() is the function here), so add it freely so that your code is easier to read. It will, however, care very much about whitespace when we start writing if statements and for loops. I'll discuss it then.

IX.3. Nested data structures

We can have dictionaries, lists, tuples, and pretty much any kind of object inside a dictionary, or inside a list, or inside a list that's inside another list inside a tuple inside a dictionary, and so on.

58. Try the following

```
FAVOURITE = 0
animals = {
    'cat': {'lives': 9, 'goes': "meow", 'likes': ["murdering beautiful things"]}
    ,'dog': {'lives': 1, 'goes': "woof", 'likes': ["loving humans", "chasing cats"]}
}
animal = 'cat'
print("The", animal, "'s favourite thing is", animals[animal]['likes'][FAVOURITE])
```

In the interest of full disclosure, I'd probably go with object-oriented programming for something like this. It would be way more versatile, more useful, and just prettier. But ignore that for now.

You'll notice an annoying space before the apostrophe. You can remove it using the sep=' ' parameter of the print() function, but then you'll have to add extra spaces. Don't worry too much about it right now, we'll see a better way to print later.

Also, you can now change the value of animal to 'dog', but it would be nice to have a way to see the data for each of the animals more efficiently. There is, and that's what loops are for (see what I did there? (a)). We'll get there shortly, but first, tuples.

IX.4. Tuples

Tuples look pretty much the same as lists, but they have one main technical difference: they are "immutable": once you put something in, you can't change it. The only caveat is you can still add stuff to the tuple, but once it's in, it stays as is for life:

```
# Lists
mylist = [1, 2, 99, 4, 5, 6] # SQUARE brackets [] to create and access
mylist[2] = 3 # let's fix that error
print(mylist) # nice, it's fixed now :)
# Tuples
mytuple = (1, 2, 99, 4, 5, 6) # ROUND brackets () to create, but square ones to access
mytuple[2] = 3 # ERROR! tuple can't be changed ...we can't fix it :(
```

IX.4.1. So, why on Earth would anybody ever want to use a tuple?!

Well, since tuples are immutable, you can use them as keys for a dictionary:

```
mymatrix = {
     (0,0): 2.2
     ,(0,1): 1.7
     ,(1,0): 1.8
     ,(1,1): 1.3
}
i, j = 1, 0
print(mymatrix[(i, j)])
```

Most coders don't really use tuples all that much, but Python itself does, a lot. Also, they can be very handy for, say, longitudes and latitudes of ecological locations, and what you found there. Below I discuss another good reason for tuples (spoiler: they use less memory).

IX.5. CHALLENGE: a dict indexed (keyed) with tuples to list values

59. Make a dictionary whose keys are tuples of potentially made-up latitudes and longitudes (in decimal degrees), and the value is an animal that you have seen there. For example, at the Museum, which is located at -73.974 degrees (west, but that's what the minus is for) and 40.781 degrees (north, so positive), I have seen a T. rex; and in my home city of Caracas I have seen a couple armadillos. Add as many animals and locations as you wish.

In all fairness, I'd rather just have the key of the dictionary be 'amnh', and have the value of that key be an inner dictionary that itself contains the latitude and longitude as elements, and a list of animals as a third element. This would be very much like what we did with the dog and cat in the Nested data structures section. But hey, I had to justify tuples somehow.

There are also sets, but those I won't even bother with here other than to say:

The main value of immutable collections such as tuples and sets is that, since they cannot change, they are a lot more efficient in how Python stores and accesses them in memory. Because lists and dictionaries can contain anything and change at any time, Python has to be a lot more flexible with the memory to store them, and therefore they are somewhat slower.

Imagine you had a mouse in this pocket, and now you go and change the mouse to an elephant: it has to be a pretty flexible pocket indeed. With a tuple or set, the mouse is a mouse forever, so Python knows it will never need more space (memory) to store it. For most purposes, though, lists and dicts do the job just fine, and that's what most coders use most of the time.

Note: when computer scientists talk about memory, they almost always mean active memory, such as the RAM (random access memory), not the more passive hard-drive space.

X. for and while loops: iterative statements to do repetitive tasks

Loops are absolutely awesome. Together with control statements (if and else), they form the core of computer programming. The main type of loop, at least as Python is concerned, is the for loop, so we start with that. There is also the while loop, which we will mention briefly.

X.1. A simple for loop

60. Try the following, very basic for loop.

```
for i in range(5):
    print("Hello", i, "times!")
```

Pretty simple, but extremely powerful, so do not underestimate it. You'll probably be writing thousands upon thousands of these in your life. Two things to note: First, remember that Python starts counting at \emptyset . Second, you don't have to use i at all, but it's very common to do so for basic loops in which you just need a simple counter and have no reason to call it anything else.

CRUCIAL: that space before print() is extremely important. If you don't put it there, or if you use that space inconsistently, you'll get an IndentationError, a bane of Python coding.

61. You can specify from where to where, and by how much, the range goes:

```
for i in range(20, 5, -2):
    print("Hello", i, "times!")
```

So, the first number is the start, the second is the stop, and the third is the step. As you can see, we can even go backwards if we wish.

62. See what happens if you swap around the 20 and the 5 in the last example. Why?

X.2. Nested for loops

Perhaps not surprisingly, you can have a for loop inside another for loop.

63. Write the following fragment to print a 5×3 matrix

```
ROWS = 5 # remember that use ALLUPPERCASE for constants

COLS = 3
for i in range(ROWS):
    for j in range(COLS):
        print i+j
```

...that's all right, I suppose, but it looks nothing like a matrix. We can do better. We need to store each row of the column, and print the row once it is complete, i.e. when the second loop finishes.

64. Improve the matrix printing nested loops by storing and printing each row.

```
for i in range(ROWS):
    this_row = ""
    for j in range(COLS):
        this_row += str(i+j)
    print(this_row)
```

Much better. Maybe we should add some spacing there, to make it look pretty. A tab would be good ($^{\prime}\$ \t^{\dagger}).

X.3. Challenge: nested for loops

65. Improve the code above so that it prints all the numbers sequentially from 1 to 15; i.e. on the first row we should have 1\t2\t3, then 4\t5\t6, and so on.

Nested for loops are often the only possible solution (e.g. if you really have to check all the cells in a grid one by one). You must keep in mind that, although they are deceivingly easy to write, they can be **extremely expensive computationally**. So, make sure you really need to use them.

X.4. Using a for loop to go over a list

Since we can use the len() function to find out how long a list is, we can do the following:

66. Go over a list the poor way:

```
fruits = ["apple", "orange", "pineapple", "passion fruit", "kiwi"]
for i in range(len(fruits)):
    print("I want to eat a delicious", fruits[i])
```

Fine... but Python is far too cool for that!

67. Go over a list the amazing Pythonic way:

```
for fruit in fruits:
    print("I want to eat a delicious", fruit)
```

Ain't that neat?

But what if, for some reason, you want to have a counter as well as the item itself?

68. Use enumerate() to go over the list items **and** also get a counter at each step!:

```
for i, fruit in enumerate(fruits):
    print("On day", i+1, "I want to eat a delicious", fruit)
```

You've got to be enjoying this stuff (the coding, I mean; the fruits also if you wish)! I do, anyway.

X.5. Using a for loop to go over a dict

```
mybasket = {'loo rolls': 96, 'bottles of sanitiser': 25, 'packs of flour': 17}
print("On my next coronapanic shopping spree, I will get:")
for product in mybasket:
    print("+", product)
```

Hm... that's all right, but we didn't quite get the numbers of each. We can just use the properties of dictionaries:

```
print("On my next coronapanic shopping spree, I will get:")
for product in basket:
    print("+", basket[product], product)
```

Nice! But Python can do better.

69. Use the *items() method of dictionaries to get both the keys and their values at the same time. Beautiful stuff!:

```
print("On my next coronapanic shopping spree, I will get:")
for product, howmany in basket.items():
    print("+", howmany, product)
```

X.6. CHALLENGE: using a for loop to go over dicts inside a dict

70. Let's bring back our murderous cats. Iterate over them with a for loop the same way we did above, and print a nice string that tells us something about each animal.

```
animals = {
    'cat': {'lives': 9, 'goes': "meow", 'likes': ["murdering beautiful things"]}
    ,'dog': {'lives': 1, 'goes': "woof", 'likes': ["humans", "bones", "chasing cats"]}
    ,'pig': {'lives': 0, 'goes': "oink", 'likes': ["not being turned to bacon", "mud"]}
} # your loop below. Tell us something about what each animal says, likes and so on.
```

We may want to do something nicer with that list of things that the animal likes, but without knowing a little more Python, it would be rather tricky.

X.7. Using zip to go over two lists at the same time within the same for loop

71. Try the following code

```
numbers = [1, 2, 3, 4, 5]
squares = [1, 4, 9, 16, 25]
cubes = []
for num, squ in zip(numbers, squares):
    cubes.append(num * squ) # compute the cube as the number times its own square
print(numbers, squares, cubes, sep='\n')
```

The sep parameter tells print() how to separate the different bits. Here we used a newline.

X.8. Using continue to skip an iteration

72. You can use continue to leap to the next iteration, ignoring the rest of the code in a loop:

```
for i in range(10):
    if i == 3: # we will see how "if" works later, but it should be obvious here
        continue # stop this iteration here and go on with the next one
    print("I am doing iteration #", i)
```

This will ignore the fourth iteration, in which 1 = 3, but it will do all the others normally.

73. **Challenge:** use continue to print only the odd numbers between 1 and 10.

X.9. Using break to stop a loop entirely

```
for i in range(10):
    if i == 3:
        break # stop the loop entirely
    print("I am doing iteration #", i)
print("Moving on, now.")
```

This completely breaks out of the loop at the fourth iteration, in which i is 3, and it will not do any of the remaining iterations at all.

Note: Some (chiefly old-school) programmers consider the use of continue and break to be poor programming. You are supposed to solve every problem with if and else statements (which we will see soon), they say. I find that this tends to make my code longer and more convoluted than it needs to be, so I do use continue and break—if sparingly, and typically only at the start of a loop to check if this iteration makes sense or the loop itself makes sense.

One scenario to use break could be in processing a long genome file and we only want consecutive lines that match a certain gene name, but we don't know the gene name beforehand,

we find it during the program's run. In this case, we detect the gene name, then keep processing lines that contain it, and as soon as the gene name changes, we break out of the loop. It may not be elegant, but it can be the most efficient way, so do keep continue and break in mind.

X.10. A simple while loop

While loops operate as long as a condition is True... hence the name while.

74. Try the following while loop:

```
fruits = ["apple", "orange", "apple", "kiwi", "níspero"]
while len(fruits):
    fruit = fruits.pop()
    print("Ñam, ñam, I ate a delicious", fruit)
print("\nNow I have", len(fruits), "fruits left :(\n")
```

Important side note: the uppercase \tilde{N} (an awesome letter, by the way), does not seem to print in my version of VS Code, but it does in Spyder and Jupyter Notebook. If you'll be using non-English characters, you need to check that they work in the medium you intend them to.

We'll leave while loops at that, other than to say that they can get dangerous if you're sloppy:

```
x = 5
while x > 0:
    function_that_fills_up_the_memory_with(huge_things)
x -= 1
```

Can you spot the error? This code will run forever and potentially crash the computer (or worse, the department's calculation cluster, depending on how it's managed) because x will always be greater than 0. We should have had the x -= 1 at the end of the while loop, but still *inside* the loop (remember that x -= 1 is the same thing as x = x - 1, just a tiny bit shorter).

Because for loops take care of this kind of controls for us, it is strongly advisable to use for whenever possible. But don't disregard while loops entirely, they can be very useful sometimes. In any case, all this discussion of while loops running only while a condition is True, brings us to our next big topic: Boolean (i.e. True/False) logic.

XI. Logical (Boolean) operators

Boolean logic is a stunningly beautiful and crucial sub-universe of human thinking, and we only have time to scratch its surface here. Suffice it to say that computers are based on it, so you will encounter quite a bit of it in coding. In brief, this means questions of whether something is strictly true or not, 1 or 0, on or off. In Python terms, this is typically expressed as True or False (mind the first uppercase letters).

The table below presents the main list of logical operators in Python

Try to think of each of these Boolean operators as a question, not an affirmation.

Logical operators	¿?	Example	Result
Equality (is 1 st equal to 2 nd ?)	==	2 == 1+1	True
Inequality (≠)	!=	2 != 1+1	False
Greater than (>)	>	2 > 1	True
Greater than or equal to (≥)	>=	1 >= 1	True
And (are 1 st and 2 nd both true?)	and	0 > 3 and $2 > 1$	False



Or (is either of the two true?)	or	0 > 3 or 2 > 1	True
In (is 1 st contained in 2 nd ?)	in	2 in [0, 1, 2, 3]	True

Important: Remember that we use *one* equals to assign a value to a variable, *two* to compare:

```
x = 5 # means that x is DEFINITELY equal to 5, because we just made it so x == 5 # is wondering whether x is equal to 5 or not
```

75. Try all of the examples in the table above, one by one.

There is also a **Boolean inverter**, not, which takes any Boolean value and flips it.

76. Try running the following in the Spyder console, one by one, predicting the output before you run them (if you don't do it in the console, you'll need to print each line)

```
not True
not False
not 5 > 4
not 1 + 1 == 2
not 5 in [1, 2, 3, 4]
5 not in [1, 2, 3, 4, 5]
True and False
True or False
True or False and True
True and False or True # compare me to the one above! Are we the same? Use () to check
```

Cool! Let's look at a few other interesting examples:

```
True == True

False == False # is a false thing false?

"Hello, World!" == "Hello, " + "World!" # mind your punctuation and spaces!

"2" + "3" == "5"

"23" == 23

5 == 5.000e0

[1, 2, 3] + [4, 5] == [1, 2, 3, 4, 5]
```

And here are a few others:

```
not 1 # also try bool(1) to see what you get
not 0
not -5
not 5
not None
not "" # an empty str
not [] # an empty list
not () # an empty tuple
not {} # an empty dict
```

Remember that True, False and None must start with uppercase, but or, and, in and not must start with lowercase. Python is very finicky about this.

These last examples are very interesting. Let's see what they mean. First, 1 and 0: for a computer, this is fundamental, zero means nothing, so it's False. Any other number is True (including negative numbers).

That's why the first while loop above in section X.7 works! Python computes the length of the list, and as long as there are one or more things in there, the number is not zero, so the condition

is True and the loop keeps going. Eventually, we manage to empty the list, its length becomes zero, and so the condition fails (it is False), so we exit the loop.

this applies to many programming languages, but not all.

Ok, back to the list here. Next after the numbers is a custom Python value, None, and it does what it says on the tin. Then we have an empty string "", i.e. empty text, which is considered False in Python. Finally, the square [], round () and curly brackets {} are an empty list, tuple and dictionary, respectively. Since they're empty, Python considers them False.

You may be wondering why we've been covering all of this technical computer-sciencey logical mathsy stuff. Well, it is essential for a major bedrock of computer programming: conditional statements, i.e. whether to do something or not depending on specific conditions. We will study them next.

XII. if, elif, else: determining what happens with control statements

We have come to the other main pillar of computer programming (together with loops). **Control statements** allow us to decide what happens given certain conditions, so obviously programmers use them extremely frequently.

XII.1. A simple if

77. Write the following simple if:

```
x = 1 # try changing this to 1+1, 2, -2, and run again
if x == 2: # note the double equals for comparisons!
    print("x equals two") # if you're copy-pasting, make sure to do the indentations!
    print("We're still inside the if")
print("And now we're outside the if")
```

That should be pretty obvious. One thing to notice again is the space at the beginning of each line inside the if. **Be extremely careful with these** *indentations*. Make sure they are the same for blocks of code that belong together. It doesn't matter how many spaces, as long as it's the same for all (it's typically between 2 and 4, but it could be anything, or also a TAB. Don't use 1, though).

XII.2. Nested ifs

We can have ifs inside other ifs:

78. Predict the output of the following code:

```
things_it_does = ["growls", "bites", "howls at the Moon"]
if "growls" in things_it_does:
    if "howls at the Moon" in things_it_does:
        print("It's a wolf!")
    if "loves humans" in things_it_does:
        print("It's a dog!")
```

...yes, I know that wolves don't actually howl to the Moon but to each other.

XII.3. A simple else

Maybe we'd like to do something in case a condition is True, but something else if it isn't. That's what else is for.

79. You can use else to specify what happens if a condition is not True (i.e. False):

```
x = 1 # try changing this to other numbers and run again
if x < 0:
    print(x, "is a negative number.")
else:
    print("Maybe", x,"is a positive number, maybe it's zero, I dunno!")
# end if: is x positive or negative? # This line is not necessary, but I like it</pre>
```

As I mentioned at the end, that last line is just a comment, so it's certainly not necessary. However, I really like closing my if, for, while, def, and with blocks (we'll see the latter two soon) with such a comment. I think it makes my code much easier to read, but this is by no means a standard practice (most coders in fact don't do it... and their code is uglier than mine).

XII.4. Using elif (short for "else-if") to provide intermediate conditions

```
x = 1 # try testing this with 1-1, -5, -2**0, 0**0 and run again
if x < 0:
    print(x, "is a negative number.")
elif x > 0:
    print(x, "is a positive number.")
else:
    print("I think x has to be zero!")
    print("...or... hang on a sec, let me check...")
    if x == 0: # an unnecessary nested if block inside the other if block
        print("Yep, x is zero, look: x =", x) # note deeper indentation of this line!
    # end if: useless confirmation that x really is zero. Of course it is!
# end if: is x positive, negative, or zero?
```

Hm... some weird behaviour there with -2**0 and 0**0, but other than that, it works like a charm! Obviously, **the inner** if **is not necessary**, because any self-respecting number is either positive, negative, or zero. There are, of course, *imaginary* numbers, but those are no self-respecting numbers, as everyone knows. Try to keep your code **robust**, but don't write unnecessary clutter. Go on and get rid of that inner if. I just wrote it to show again that **you can have "nested" if blocks inside other if blocks**. Note how the indentation got one level deeper.

XII.5. CHALLENGE: loops with conditionals!

80. Generate a dictionary called oddsquares that contains the squares of all the odd numbers between 0 and N, where N can be altered at will. Use the odd number as the dictionary key and its square as the value, i.e. it should be something like {1: 1, 3: 9, 5: 25, ...}. Test it with N = 20.

Hint: you may need to create an empty dict (or "declare" it, in computer jargon) *before* the for loop, then proceed to fill it *inside* the loop.

XII.6. List/dict comprehensions

Ok, I'm sure your solution to the last challenge was very cool, but take a look at mine 😎:

```
N = 20
oddsquares = {num:num**2 for num in range(N+1) if num%2 != 0}
print(oddsquares)
```

My solution is what's called a **comprehension**, in this case a **dictionary comprehension**. Here's a simpler one without the if bit, in this case a **list comprehension**:

```
doubles = [2*i for i in range(10)]
print(doubles)
```

We don't really have time to delve any deeper into comprehensions, but they are one of the major elements of the concept of "**pythonicness**", i.e. writing the most Python-like code possible. Sometimes that gets dangerously close to snobbism in my opinion: it can render code that's impossible to read for anyone who is not very familiar with Python. But sometimes it really gives you much more efficient and prettier code, so it's worth keeping comprehensions in mind.

XIII. Functions and their arguments, parameters and returns: reusing code

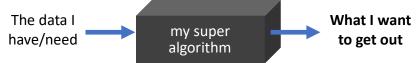
A function is a **reusable** piece of code that does a particular job. It is defined with a unique **name** by which it can be **called** as many times as desired. For example, we've been using the print() function frequently here, but we can write our own too, and we can have them return output.

DRY (Don't Repeat Yourself): write functions whenever a piece of code is used more than once. It is a very good habit to write a """long multi—line comment"" at the beginning of a function definition, describing what it does, what it takes in as arguments, and what it returns. Most people write this comment only after they're done with writing their function, if at all. I strongly advise and encourage you to do it the other way around: always write what the function is supposed to do before you write any code into it. The reason is that this helps guide the code that you will write, and often prevents you from making silly mistakes or writing a function that you don't really need. Actually, I'll make a brief stop here and talk a little about software engineering. Just a minute, please bear with me.

81. Use the black-box approach to design functions and code in general.

By this I mean, imagine the code as a magical black box that does anything it needs to do, perfectly. What you really need to know before you write any of that code is two things:

- 1. What data do you have or need? (actually, think about this secondly).
- 2. What do you want to do to it? What should the code give you? (start here!)



I know it sounds obvious, but it is extremely common to skip this and start coding before you even know exactly what kind of data you have or even what exactly you want to do to it. **Don't**.

Try to always start your code scribbling with pencil and paper... i.e. without any code at all!

82. **Define** (i.e. write) the following simple function, then **call** it (i.e. use it):

```
# The function DEFINITION:
def say_hello():
    print("Hello!")
# And now the function CALL:
say_hello()
```

...well that's truly one rather mediocre function! Surely, we can do better than that.

83. Pass an **argument/parameter** to a function, inside the parenthesis:

```
def say_something(thing):
    """This function says anything you want it to say, using the argument <thing>"""
    print(thing)
# end def: say_something()
say_something("Fare thee well!")
```

Other than the new argument called thing, whose behaviour should hopefully be quite obvious, I have added two optional bits:

- 1. The multi-line comment that describes the function (ok, it only has one line here, but it could have many). This is called a "docstring" for "documentation string".
- 2. A closing comment that marks where the function definition ends. This is very much a personal choice of mine. Most Python coders don't use it, but I think it makes code easier (for me) to read.

Suit yourself regarding the second, but please, and to reiterate:

Once more: do add a multi-line comment at the beginning of every function you write. I'll insist:

XIII.1. Docstrings (function documentation strings)

The reason for adding that multi-line comment at the very beginning of a function def is not only that it makes your code much easier to read and maintain but, significantly, that many IDEs actually use that text to give users information about the function. Here are Spyder and VS Code:

Spyder:

```
def say_someth say_something(thing)
print(thin # end def say_

This function says anything you want it to say, using the argument <thing>
say_something()
```

VS Code:

VS Code seems to make better use of the information than Spyder, but both are helpful. Jupyter on the other hand doesn't initially seem to use the docstring information at all, but actually, it will show us quite a bit of information if we hit Shift+Tab inside a function call:

Jupyter:

So... always write the """docstring""" at the beginning of each and every function.

Also: remember that the docstring must always start on the very first line. Ok, back to functions.

XIII.2. Default and multiple values

84. Give the parameter (or argument) a default value:

```
def say_something(thing="Hello Roger!"):
    """
    Says anything you want it to say, using the argument <thing>,
    which defaults to "Hello Roger!" if you don't specify anything.
    """
    print(thing)
# end def: say_something()
say_something(thing = "Good bye, Roger darling.")
say_something("Good bye, Roger darling.")
say_something()
```

You'll see that you can either specify the argument name or not. For this function, it's fine not to bother specifying the name of the argument because there's only one, and from the name of the function it's pretty obvious what will happen. But when we start defining more complex functions, or using those created by other people, at times it may be best to specify the arguments by name, so that your code is easier to read (by you and others).

85. When defining a function with multiple arguments, those without a default value must come before those with a default:

```
def say_something_many_times(thing, times=1):
    """
    Says any <thing> you want it to say and repeats it a specified number of <times>.
    # PARAMETERS:
    <thing> has no default, you must specify it!
    <times> defaults to 1 if you don't specify anything else.
    """
    for i in range(times):
        print(thing, i+1, "times.")
        # end for: printing the message <times> times
# end def: say_something_many_times()
```

86. Good. Let's test it now:

```
say_something_many_times(thing="Farewell", times=4)
say_something_many_times("Farewell", 4) # same as above, still works
say_something_many_times(times=4, thing="Good bye") # this also works!
say_something_many_times(4, "Adieu") # but this will fail, wrong order
say_something_many_times("Adieu") # this is fine, <times> will use its default of 1
say_something_many_times() # another error, <thing> always needs a value
say_something_many_times(4) # MINI-CHALLENGE: will this work or fail?
```

You'll see that you can actually invert the order of the arguments as long as you specify their names.

Note: Whether you call the stuff that the function takes in an **argument** or a **parameter** is a mathematical/comp-sci discussion that I will not be dragged into here. Call them what you will. Ok, fine: formally, a **parameter** is a *variable* that you put into the function *definition*, whereas an **argument** is the *data* that you send (or *assign*) into that variable when you *call* the function. I think mathematicians may actually have a different opinion about this, but I'll leave it at that.

XIII.3. returning values from a function

Besides performing a job, you can have your function give a return value. This is really useful:

87. Create a function that returns the maximum between two numbers

```
def max_between_two_nums(num1, num2):
    """Returns the maximum between two numbers.
    Fails if the numbers are the same"""
    maximum = None
    if num1 > num2:
        maximum = num1
    elif num2 > num1:
        maximum = num2
    else:
        raise ValueError("ARGH, I don't know what to do, the numbers are the same!")
    # end if: testing which number is larger
    return maximum
# end def max_between_two_nums()
```

88. Ok, now try it:

```
print(max_between_two_nums(5, 23))
print(max_between_two_nums(5, -23))
print(max_between_two_nums(5, 5))
```

Hopefully that should be clear. You'll notice that we never used the word max, which is short and neat and would have been a great function or variable name. The thing is, Python is already using that name (for precisely the same purpose), so we can't use it to name our own stuff.

You'll see that we raised an error if the numbers are the same. The best solution if the numbers are the same would of course be to just pick one of the two and return that one, but I wanted to show you the principle of raising errors. Python comes with a bunch of pre-defined errors (such as ValueError), and you can define your own freely to match the kind of data you expect your users to give you. We unfortunately don't have time to cover errors more formally here, but:

Defining (or borrowing) and raising informative errors to your users is a very good practice.



89. You can return multiple values:

```
def triplet_inverter(x, y, z):
    """Gets three values as input, and returns them swapped around"""
    return z, y, x
# end def: triplet_inverter()

print(triplet_inverter(1,2,3))
```

Not my most impressive function, I'll admit, but it does the job.

XIII.4. CHALLENGE: a function to get the minimum and maximum in a list

90. Create a function minmax (the_list) that returns the minimum and maximum from a list of numbers, such as nums = [1, 45, 3.9, -7, 8].

We'll have to go over the whole list and check if what we thought was the maximum is still the maximum, and same for the minimum.

XIII.5. Getting variable numbers of arguments with *args and **kwargs

This is a little advanced, but, wouldn't it be cool if we could take our triplet_inverter() function above and turn it into a multiplet_inverter() that can take any number of arguments?

91. Use *args to tell Python that you're probably expecting some arguments, but you don't know how many:

```
def multiplet_inverter(*args):
    """Gets a tuple of any length as input, and returns its contents swapped around"""
    #print(type(args)) # it's a tuple!
    outlist = []
    for num in args:
        outlist.insert(0, num) # add each subsequent number to the start of the list
    # end for: adding each
    # because we received a tuple as input, it's fair to give a tuple back
    return tuple(outlist)
# end def: multiplet_inverter()
print(multiplet_inverter(1, 2, 3, 4, 5))
```

Of course, there are better ways to invert a tuple, but this was just a proof of principle.

Cooler still, you can have an unspecified number of named arguments also!

92. Use **kwargs to specify arguments with a unique name, even without defining them into the function as parameters.

```
def privacy_violator(name, **kwargs):
    """Can deal with any number of named arguments"""
    print("name =", name)
    for stuff in kwargs:
        print(stuff, "=", kwargs[stuff])
    # end for: printing all the stuff in kwargs
# end def: privacy_violator()
privacy_violator("Jonnie", hometown="NYC", mother="Gina", password="12345")
```

Actually, the names *args and **kwargs are purely convention, you can change them if you wish (don't!). What really matters are the *single and **double asterisks preceding them.

XIV. Working with strings and text

XIV.1. Common properties between lists and strings

Strings are seen by many programmers as lists of characters, so the creators of Python made many of the methods, functions and behaviours the same between the two classes.

93. Try the following examples, in which strings behave just like lists:

```
mystr = "New York City"
print("ork" in mystr) # oh no, there's an ork in New York City! :0
print(mystr.index("ork")) # Python starts counting at zero!
print(mystr[2:6]) # remember the weird Python index counting
print(mystr[::-3]) # print every 3rd character, going backwards
```

XIV.2. Some useful string functions

94. Use replace() to ... erm... replace:

```
# Let's get rid of that evil ork from NYC and replace it with a lovely elf:
print(mystr.replace("ork", "elf"))
print(mystr) # oh well, it seems the original remains unchanged
# What if we try to replace something that appears many times?:
print(mystr.replace(" ", "$")) # all the spaces get replaced with $... damn Wall St!
print(mystr.replace(" ", "$", 1)) # you can limit how many times you replace
```

Most of these functions don't really change the original string. You'd need to store the changes into a new variable (or replace the original on the fly).

95. Use split() to turn a string into a list, splitting at whichever character (or string) you choose:

```
mystr = "Methinks it is like a weasel"
print(mystr.split())
print(mystr) # good to know that the original remains unchanged by .split()
```

So, if you don't specify anything to split, it just breaks at any space. Actually, it breaks at any whitespace, which includes new lines (\n), tabs (\t), carriage returns (\n), and simple spaces. But nothing stops you from using some other character if you wish:

```
print(mystr.split('i'))
```

Actually, you don't have to use a single character. You can use a longer string:

```
print(mystr.split('s '))
print(mystr.split('thinks it '))
```

96. The good brother of the evil split(), is join(), which needs a joining string as its base, and a list (or technically, any iterable object) as its input:

```
mylist = ["1", "2.07", "tomato", "more things", "-8", "9"]
print(' AND '.join(mylist))
```

All members of the list must be strings themselves, that's why the quotes around the numbers. But we could use a fancy **list comprehension** if we have numbers that need to be **parsed** to str:

```
mylist = [1, 2.07, "tomato", "more things", -8, 9]
print(' AND '.join([str(item) for item in mylist]))
```

Both of split and join will be extremely useful when we read and write comma-separated values (CSV) files (or tab-separated, which I like to call TSV, but not everyone does).

There are many more string functions, such as strip() to remove whitespace to the sides (we will use it later), and a bunch more. Do search for "python string functions" if you wish.

XIV.3. Printing pretty output with f"strings"

97. Precede a string with f to use {variables} inside it:

```
x = 5
day = "Friday"
print(f"I called you {x} times last {day} and you didn't pick up!")
```

98. You can use functions and do operations inside an f-string:

```
ages = [17, 72, 34, 55]
print(f"The oldest person is at least {max(ages) * 12} months old.")
```

But f-strings are much cooler than that, you can format strings in very advanced ways:

```
nums = {'money':752, 'base rate':1.4, 'c':0.4, 'age':19, 'pi':3.14159}
for num, val in nums.items():
    print(f"#{num:^12.3}:{val:>010.2f}") # try changing the > to ^ or <</pre>
```

We won't go into further details, just search for "python f strings" or something like that.

XV. Getting input from the user

99. Getting input from the user is very easily done in Python:

```
name = input("Please enter your name: ")
age = input("Now please enter your age: ")
print("Thank you, " + name + ". I hope you had a wonderful " + age + "th birthday!")
```

Actually, now that we know how to use f-strings, we can make that code prettier:

100. Change the last line to an f-string:

```
print(f"Thank you, {name}. I hope you enjoyed your {age}th birthday!")
```

Maybe we could improve that a bit, to respond correctly to years ending in 1, 2, or 3, so that they get "st", "nd", and "rd" as opposed to "th"... but actually only if the number is not 11, 12, or 13, in which case it actually should still end with "th"... anyhow, it can get tricky, but you're an if-elif-else master by now, so you could do it without much problem ©

We have to trust that the user gives us a proper name and an integer as their age. This should be handled with Exceptions, assertions, trys, and Errors, which we won't cover here.

101. Mini-challenge: give the user good wishes for their next birthday instead.

XV.1. CHALLENGE: read and process user input

102. Write a script that asks the user how many days ago they followed the installation instructions at the beginning of this guide. The script should distinguish between and give different messages to four groups of people: those who installed only up to 1 day ago, those who installed between 2 and 4 days ago, those who installed between 5 and 9 days ago, and those who installed 10 days ago or earlier.

In truth, most Python coders don't really take user input very often, they mostly read data from files, so that's what we'll learn next.

XVI. Reading and writing files

103. Go to my GitHub (github.com/vsojo/Python Workshop) and get the two CSV files:

- A list of (fake) attendees to the workshop.
- Global population data from the UN.

You'll probably need to click on "Raw" near the top-right to get the actual files.

If the size of the files is not too large, it's always a good idea to try to open them to take a look. For a CSV, by all means go ahead and open it in MS Excel or similar spreadsheet software (size allowing). Also take a look in a simple text editor—you can use Spyder itself, vim/emacs if you're a geek, or you could consider the awesome Notepad++ for Windows or BB-Edit for Mac.

Note: these files are both small, but if the file is very large (hundreds of MB or more), you may want to use the head command on the Linux or Mac terminal to take a peek at the top lines. If you're on Windows... why?

XVI.1. Reading a whole file to a string using . read()

There are many ways to read files in Python. Technically, you have to open the file, read it, and then close it. My understanding is that the best way to do that is to use a with statement, which takes care of closing the file safely even if something fails within your code. So, we'll do that.

104. To read an entire file safely, in one go, use with, open(), and read():

```
with open('PythonWorkshop_Attendees.csv') as f:
    filecontents = f.read()
    print(filecontents)
```

This code assumes that you put the file in the same folder as your Python script.

105. In case you didn't put the file in the same place, and just to be super safe, let's go and specify a directory, so that we can always find the file:

```
WD = '/Where/ever/you/put/the/downloaded/files/' # no spaces, and mind the final '/'
with open(WD + 'PythonWorkshop_Attendees.csv') as f:
    filecontents = f.read()
    print(filecontents)
```

That text above is for Mac and Linux. On **Windows**, you'll need to use the typical Windows file structure: WD = 'C:/I/Dont/Know/Where/Your/Stuff/Is/But/You/Should/'. **It must be forward slashes** (Python uses the backward ones for something else that we'll mention later).

Note: WD is just a text variable. I like to call it WD for "working directory", but you can call it anything you want, and you don't even have to use it at all, you can just specify the entire path inside the open('/full/path/to/your_file'). I like to use a variable to store the directory because if I'm opening and closing many files, they probably all live in the same place or very close to each other, so a WD variable that only needs to change once at the top of the script is a good idea.

I am using ALL_CAPS to remind myself that it's a constant; the working directory is not supposed to be changing. By the way, Python doesn't really care about what we consider to be a constant or not. If something is constant, just don't change it. That's why the convention of using ALL_CAPS is even more important in Python than in other languages that do have explicit constants.

Ok, back to the code. We opened and read the whole file into a string, and because we did it inside a with block, Python took care of closing it for us. We could also read the lines separately, so let's try that next.

XVI.2. Reading a whole file to a list of lines using . readlines()

Instead of loading the entire file to a single string, we can load its lines into a list of strings:

106. To read all lines of a file in one go and store them into a list, use readlines():

```
with open(WD + 'PythonWorkshop_Attendees.csv') as f:
    filecontents = f.readlines()
print(filecontents)
```

Note that now we're printing outside the with block. In this case, it's exactly the same as printing inside it as we did above. I just wanted to show you a weird thing about Python:

If you're coming from another programming language such as C++, you'll find it very weird that Python recognizes the variable filecontents outside the with block. That's just the way Python works. This applies also to for loops and if statements, but not function definitions. If this paragraph sounds like gibberish to you, just ignore it.

Ok, having each line in a list is good, we could now use a for loop to go over each line (for line in filecontents:) and do something to it. That would work, but it's not necessarily a great idea. Whether you use read() or readlines() is the same:

Reading files all in one go is generally a bad idea, especially for data scientists (such as biologists). That's because our files can get huge, so you should instead read the file line by line, and I strongly recommend that this is the main if not only way you read your files from now on. See next.

XVI.3. Reading a file one line at a time using a for loop (do it this way!)

Instead of loading the entire file to a string or list, we can read it one line at a time its lines one by , each into a list:

107. To read a file **efficiently** one line at a time use a for loop:

```
with open(WD + 'PythonWorkshop_Attendees.csv') as f:
    for line in f:
        print(line)
    # end for: reading the file line by line
# end with: processing the file
```

This method is waaaay more efficient than the other two that we used before. My recommendation therefore that you always read files line by line, such as in this code above, unless you know exactly why you're loading the whole file, and you're sure it's not too big.

Imagine you're processing human genomes, or transcriptomic data from a population study with thousands of individuals... you most certainly do not want to load all of that stuff into memory at the same time unless you really need them all at the same time. In this case—and in most cases—we don't, so we can just process each line one at a time, get what we need out of it, then forget about it—quite literally, since we remove it from memory by loading the next line into the same variable (which we called line here, but we can call it anything we wish).

Both f and line, as well as WD are arbitrary names. We could have used studentsfile, studentline and mydir, but using line and f is typical.

Again, if you put the files in the same place as your script (and you're not using VS Code) you should be able to just leave the working-directory variable blank ($WD = \ \ \ \ \ \)$ or just out entirely. Either way, I'll assume you know where to find your files.

Note also the last two comment lines in the code above. We've mentioned these before. They are just my personal preference. **Most coders don't use that kind of closing comment**, but I think it makes my code much easier to read, particularly when the with and for blocks get very long, which they nearly always do. That said, I learned to code in C++, so this may just be an old habit (because in C++ you always have to close your blocks of code explicitly, but in Python you just open them and whenever you move the indentation back to the left the interpreter knows that the block is over).

Ok, let's look at the output. The script goes and reads and then prints every line of the file, one by one. But the lines look pretty spaced out, don't they? That's because all lines in a text file end with a newline character "\n", and Python kept this character when reading, for some reason. We could just cut that last character out by doing something like line = line[:-1], but it's more elegant to use Python's in-built method strip():

108. Add the following line before the print call in the code above (inside the for loop):

would return "text more text.". All padding "whitespace" was removed.

The file is a CSV, i.e. a comma-separated-values file. That means that it is composed of values that are—surprise!—separated by commas. Anyhow, let's extract the data using split():

109. Use split(',') to split a line of a csv file into a list. Actually, let's go ahead and assign values on the fly by "unpacking" the list as we create it on the 4th line:

```
with open(WD + 'PythonWorkshop_Attendees.csv') as f:
    for line in f:
        line = line.strip() # remove the newline character at the end
        name, age, institution = line.split(',') # split at the ',' and unpack values
        print(name, age, institution)
```

Hm, it seems the first four students worked without problem, but the fifth one failed. If we take another look at the raw text file, we will see:

```
given name,age,institution
Arianna,27,AMNH
Felix,25,CUNY
John,35,AMNH
Mehdi,33,NYU
Mike,27
Monica,31,CUNY
```

We don't have an institution for Mike, his line only has 2 values. That's why the code failed: the list unpacking on the penultimate line was expecting 3 values (name, age, institution), but it only found 2. I suppose we could open the file in Excel or a plain text editor (Notepad++ for Windows and BBEdit for Mac are great options) and add "Unknown" as Mike's institution. But what if we have thousands of entries, some with missing data, some not? Maybe it's best to store the split values in a list and process case by case, checking whether anything is missing, especially age and institution.



110. Store the split items into a list, to process the cases that have information missing:

```
with open(WD + 'PythonWorkshop Attendees.csv') as f:
    for line in f:
        fields = line.strip().split(',') # Nifty! The whole thing in a single line!
        if len(fields) == 3:
            name, age, institution = fields
        elif len(fields) == 2:
            name, age = fields
            institution = "(unknown)"
        elif len(fields) == 1:
            name = fields[0]
            age = -999
            institution = "(unkown)"
        else: # fields should not have any other length
            raise IndexError(f"This file has too many values per line: {len(fields)}."
                +"\nAre you sure this is the right file?")
        # end if: testing if the line has the right number of fields
        print(f"{name} is {age} years old and works at {institution}.")
    # end for: reading the file line by line
# end with: processing the file
```

Cool! This is beginning to look a lot more like real-life code now. An age of -999 is so ludicrous that it will make you realise that something is wrong or missing. I like to use numbers like that when something is missing or cannot be. I also wrapped "(unknown)" in parentheses, for the same reason.

XVI.4. CHALLENGEs: operations on data read from files

- 111. Calculate the mean age of the workshop attendees.
- 112. Bigger challenge: how many times does each letter in the alphabet appear across the names of all attendees? i.e. in the first two names there are 3a, 1r, 2i, 2n, 1f, 1e, and 1x. Count them all and put the result into a dictionary with letters as keys and counts as values.
- 113. Find out how to sort a dictionary by keys and by values, then print the letters in descending order of frequency, and in alphabetical order, showing how many times each letter appears.

XVI.5. Writing new files using the 'w' mode

Writing files is very easily done in Python, and it looks very similar to reading:

114. Create and write to a file by specifying the 'w' mode when you open the file:

```
with open('myfile.txt', 'w') as f:
    f.write("Rubbish sent to a file")
```

Great!... but dangerous. Let's do something stupid.

115. Add your own name to the names file:

```
with open(wd + 'PythonWorkshop_Attendees.csv', 'w') as f:
    # Add a new attendee,age,institution
    f.write("Juanito,52,AMNH")
```

Ok, now go and take a look at the file...

Evil thing! ...it did add the new attendee but otherwise it emptied the whole file! >=(

The write mode is meant to create **new** files, so if you give it the name of an **existing** file, it will obediently destroy the original without warning you!

116. Now you'll need to go and download the attendee-names file again, since you just destroyed it. Consider yourself lucky that the file is still there and it didn't take you 3 days to generate.

I know, it's annoying. Now you need to scroll up and find the address to my GitHub again. I could just paste it again here, but I deliberately won't, so that the pain reminds you that you need to be careful with your data files and not write to them.

Writing is to create new files! If you just want to add stuff to a file, you need to use the append mode instead.

XVI.6. Appending to a file using the 'a' mode

117. Add your own name to the names file:

```
with open(wd + 'PythonWorkshop_Attendees.csv', 'a') as f:
    # Add a new student,age,institution
    f.write("Juanito,52,AMNH")
```

Same code as above, but with append instead of write mode. Much nicer. Now it does add to the end instead of just replacing the whole file.

In case you care to know, there's also an 'r' mode, for "read". That's the default, so you don't really need to specify it. However:

We didn't do it above, but I recommend that you do specify 'r' when you read files, to make your code even clearer.

XVI.7. Adding large amounts of data to a file

If you need to write plenty of stuff to a file, e.g. in a big for loop, one way to do it would be to just store all of the information into a text variable, add a \new line character at the end of each line, and then print the whole thing:

(Note that in the code below we've used \t, i.e. tabs, instead of commas to separate the items, and so we named our file *tsv instead of *csv. This is very common too, and easier to read for humans, so some people prefer it. This is just personal choice, but I recommend that you stick to the extensions *csv and *tsv depending on which of the two separators you're using).

118. Writing large amounts of data to a file **THE WRONG WAY**:



You can probably tell why this is a terrible idea. 10 is of course not a gigantic number, and this line with squares and cubes is pretty short, so all in all outtxt will be small here. But if the gigantic number truly were gigantic, and the very-super-duper-ultra long line were truly very-super-duper-ultra long (e.g. if you were working with genomic data), we'd be filling up the memory with stuff that we don't need. In this code, once a line is calculated, it's not needed anymore, so the best way to go about this would be to just send each line to the file one by one. So:

119. **Challenge:** Write large amounts of data to a file the right way, i.e., one line at a time. **Solution** (please don't read this before you try it):

You'll need to create the file (in write mode) before you go into the loop, sending only the header. Then you go into the loop and write to the file using the appropriate mode (append) at every iteration. So, all in all, you won't need the outtxt variable at all.

I recommend that you define a file_name variable at the beginning, and then use it in the two occasions that you'll need it. It's better this way in case you choose to change the file name. Of course, if your code uses more than one file, then file_name is a terrible name for a variable. Remember to use descriptive names.

XVII. Turning your Python code into an independent script

You can have a more professional-looking script that can be used via the Terminal by non-coders, just like we've been using conda activate and other such commands.

120. Create a new file in Spyder and save it as attendee_reprinter.py, some place where you can find it (e.g. Desktop/PyWorkshop/).

121. Add a simple line at the end, something like print ("Hello, World!").

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

Created on Mon May 20 10:07:20 2020

@author: vsojo
"""

print("Hello, World!")
```

The first line is called a "shebang" (I have no idea why and I don't know if I want to know, so I won't Google it, but be my guest). It tells the console where to find the software that can run this script, in this case my version of python3. Chances are your Spyder found the proper python for your code, so you might just want to leave it as is, but note that:

If you redistribute your code, your users may need to change that first line to point to where their python is located.

But you actually don't need to worry too much about this, since you can always specify to the console that you want it to use python to process this file.

122. Depending on Mac/Linux/Windows, open a Terminal/Console/Anaconda-Prompt-(anaconda3), navigate to where the script file is, and run it:

```
myuser % conda activate pyworkshop
myuser % cd /Users/myuser/Desktop/PyWorkshop
myuser % python attendee_reprinter.py
```

(You can ignore that myuser % bit, it's just meant to indicate the input prompt of the console)



Note: if you're in Windows, the file system is different, so you may have to do something like:

```
myuser % conda activate pyworkshop
myuser % cd C:\Users\User\Desktop\PyWorkshop
myuser % python attendee_reprinter.py
```

Or something of the sort. Remember to use TAB to help you fill out that stuff without typing. The second line in the script specifies the "coding" of the document, in this case UTF-8. This tells the computer what kind of characters it should expect. If you will be using special characters such as French, Czech, Arabic, Spanish and so on, the computer needs to know, otherwise it will get very confused. It's generally advisable to avoid non-standard characters, but what qualifies as standard differs from region to region, of course.

Ok, let's move on. You should have seen the code print "Hello, World!". Not too fancy, but hey, we have a working command-line script! Let's get it to do something useful now. What we would really like to do is specify an input file to the script via the command line, so that it can read and process it. To do that, we need to import a package called argparse, which comes with Python already. That means we don't have to *install* it, but we do have to *import* it because Python doesn't load it by default the way it always loads things like for, print, True or def. Python comes with a lot of stuff that it doesn't load by default, and there's tons more that can be installed using the Anaconda Navigator or via the terminal (e.g. conda install matplotlib would install a really cool plotting library, but that's another matter for another time).

123. Use argparse to get arguments from the console/terminal/prompt

```
#!/usr/bin/env python3
# -*- coding: utf-8 -*-
<attendee reprinter.py>
Takes a CSV file with a list of workshop attendees, and reprints it as TSV.
Version: 0.01
Author: Victor Sojo, vsojo@amnh.org
import argparse
# Create the argument parser, and give it a description for the script's help:
parser = argparse.ArgumentParser(
    description = "Reads a list of attendees as CSV and prints it to screen as TSV."
# Add arguments to the parser:
parser.add argument(
    'filename'
    ,help = "CSV file with <attendee_name,age,institution> in each line."
# Execute the parser to read any arguments given to the script on the command line:
args = parser.parse_args()
# And let's open the file now
with open(args.filename, 'r') as f:
    for line in f:
        print(line.strip().replace(',', '\t'))
```



Very nice. Hopefully that's working for you. Let's test it.

124. Check if the command-line argument was read properly by doing an actual test run on the console. Try all of the following:

```
myuser % python attendee_reprinter.py
myuser % python attendee_reprinter.py -h
myuser % python attendee_reprinter.py PythonWorkshop_Attendees.csv
myuser % python attendee_reprinter.py somefilethatdoesntexist.fake
```

The first one will complain that the script wants a filename. This is really cool!

The second one prints the script's help. Also really cool! It uses that description and help that we wrote for the parser and argument to provide the user with some general idea about what the script does and what arguments should be given.

Assuming you have your attendees file in the same directory as the script, the third line should work without problem. If it didn't, you may need to give a full path to where the file is.

Finally, the fourth line points to a file that doesn't exist. The software fails telling you that the file was not found. Very nice again.

Formal script production can and should get a lot more complex than this, but all in all, this is pretty cool behaviour already, and we have a working script!

XVIII. Where to from here

You may want to look into the following topics and tools: NumPy, Pandas, MatPlotLib, BioPhython, RegEx, GeoPy, Jupyter Notebooks, debugging, and a whole lot more!