Basic Python

Content from Getting started

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OVERVIEW

Questions

- Programming - why bother?
- Why Python?
- How to learn it?

Objectives

- Understand the concept of programming
- Understand the basics of Python language

Programming — why bother?

Data handling and analysis in bio-research and medicine is best done using coding. In October 2017, the American technology magazine Wired published an article in which the author outlines reasons why several established bio-science researchers working in reputable institutions felt the need to learn coding — specifically in Python: “Want to Make It as a Biologist? Better Learn to Code”.

> THIS COURSE
>
> We focus on the Python programming language throughout this course, but we discuss universal principles shared amongst many programming languages. Through a diverse range of examples, we will be training these principles by solving problems that we face in biological and medical research.

Why Python?

Python is a general-purpose programming language. This means that it can be exploited to design any type of software, from desktop and web, to robotics and automation, to data analysis. The 2020 survey conducted by the Python Software Foundation and JetBrains® found that approximately 85% of respondents used Python as their first language to conduct data analysis.

In addition, the 2021 developer survey conducted by StackOverflow found that Python is the third most popular general-purpose programming language after JavaScript and HTML/CSS. This means that it enjoys a vibrant community that support and maintain its development, and the development of the libraries associated with it. This is confirmed by the fact that the language is ranked as the second most popular language on GitHub®, which is the primary code-sharing platform amongst programmers.

HOW TO LEARN?

Learning how to code as a beginner is akin to learning how to walk as a baby. You cannot learn programming by memorising directives; no matter how well you memorise them. To learn how to code, one must learn how think algorithmically; that is, how to break different tasks down into logical procedures. The only way to learn how to "think code" is to practice, make mistakes, and how to overcome those mistakes. It is common to make the same mistake more than once, especially in different contexts, and that can become frustrating at times. However, once you get it, you have it for life.

There are lots materials on the web, both free and paid, to assist with your learning. Use them to your advantage! Great programmers are not the ones who know every technical detail by heart; rather, they are the ones who know what they are looking for, and where they can find the answer.

KNOWN QUIRK

Unlike popular belief, the name **Python** has nothing to do with the snake. It is in fact derived from the popular British sketch comedy series Monty Python's Flying Circus, of which inventor Guido van Rossum was a self-confessed fan.

Python: The Programming Language

Python is a general-purpose, high-level programming language. It was invented by the Dutch computer programmer Guido van Rossum and was released for the first time in 1990.

A **high-level** programming language is a language that enjoys strong abstraction from computer details. This means that it is closer to the language that is spoken and understood by humans; put simply: it makes the language more enjoyable to work with.

CATEGORIES

In terms of compilation (the conversion of code into the binary symbols understood by a computer), programming languages may be divided into two different categories:

1 - **Compiled** These are languages whose code is translated (compiled) into machine language en-masse, and in advance, using a designated compiler programme — e.g. C, Rust, Haskell.

2- **Interpreted** These languages rely on and must *always* be accompanied by an interpreter, whose job is to translate the source code into machine language one line at a time — e.g. Python, R, MATLAB®.

KEY POINTS

- Programming is an important skill which is highly applicable to bio-research and medicine.
- Python is one of the most popular programming language for being general-purpose and high level language.
- Python uses an interpreter for line by line code translation.

Content from Variables, Types, and Operations

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OVERVIEW

Questions

- What are input and output (I/O) operations?
- What do variables do?
- Why are types and scopes of variables important?
- What types of operations are used?

Objectives

- Understanding I/O operations
- Build concepts of different types of variables
- Learning about type conversions and scope
- Understanding mathematical and logical operations

In programming, we process data and produce outputs. When data is being processed, it is stored in memory so that it is readily available, and can therefore be subject to the processes we want to apply.

In this lesson, we will discuss how to handle data in Python. We will start by displaying data on the screen, and understand how to receive input from a user. We can then use these techniques to perform different mathematical and logical operations. We will also cover the fundamental principles employed every time we code in Python. It is imperative that you understand everything before moving on.

I/O Operations

In computer science, input or output operations refer to the communication between an information processing system such as a computer, and the outside world, which may be a user or even another computer. Such communications are more commonly known as *I/O operations*. In general, this 'outside world' may be loosely defined as anything that falls outside of the coding environment.

REMEMBER

Only what we define within the environment and what we store in the memory is directly controlled by our application. We may access or take control over other environments, however, these interactions are classified as I/O operations. An example of this is interacting with a file on our computer. While we have complete control over a file while working on it (e.g. reading from it or writing to it), the access to the file and the transmission of data is in fact controlled and managed not by the programming environment but by the operating system of the computer.

In programming, I/O operations include, but are not limited to:

- Displaying the results of a calculation
- Requiring the user to enter a value
- Writing or reading data to and from a file or a database
- Downloading data from the Internet
- Operating a hardware (such as a robot, for example)

ADVANCED TOPIC

If you are interested in learning more about I/O systems and how they are handled at operating system level, you might benefit from chapter 13 of *Operating Systems Concepts, 10th ed.* by Abraham Silberschatz, Greg Gagne, and Peter Galvin.

I/O Operations in Python

Input and Output

In this section, we learn about two fundamental methods of I/O operations in Python. We will be using these methods throughout the course, so it is essential that you feel comfortable with them and the way they work before moving on.

PRODUCING AN OUTPUT

Print

The term `output` in reference to an application typically refers to data that has either been generated or manipulated by that application.

For example; calculating the sum of two numbers. The action of calculating the sum is itself a *mathematical operation*. The result of our calculation is called its `output`. Once we obtain the result, we might want to save it in a file or display it on the screen, in which case we will be performing an I/O operation. *I/O operation*.

The simplest and most frequently used method for generating output in almost every modern programming language is to display something on the screen. We recommend using Jupyter Notebooks to run our Python scripts, which defaults to displaying the output of a code cell beneath the code itself. We will start by calling a dedicated built-in function named `print()`.

> ## REMEMBER
>
> In programming, a `function` is essentially an isolated piece of code. It usually accepts input, *does* something to or with this, and produces `output`. A function can process input, often using several operations in a particular sequence or configuration, and process the input to give a final output. In Python programming syntax, a pair of (typically round) parentheses follows a function, and these provide the function with the *input arguments* it needs when we *call* it, so that it can do what we intend, to our data. We will explore functions in more details in Basic Python 4: Functions.

The `print()` function can take several inputs and performs different tasks. Its primary objective, however, is to take some values as input and display them on the screen. Here is how it works:

Suppose we want to display some text in the Terminal. To do so, we write the following into a cell of our Jupyter Notebook (or on the Terminal, a code editor or dedicated Integrated Development Environment (IDE)):

```
print('Welcome to L2D!!!')
```

This is now a fully functioning Python program that we can run using the Python interpreter.

If you are using an IDE (such as Mircosoft Visual Studio Code, for example) you must save the code in a file with the extension `.py`, in order to execute your code using the internal tools provided by that IDE. The specifics of how you do so depend on the IDE that you are using.

`.py` Python scripts can also be executed manually. To do so, we open the Terminal in MacOS or Linux or the command prompt (CMD) in Windows and navigate to the directory where we saved the script.

> ## NOTE
>
> If you don't know how to navigate in the Terminal, see the example in section How to use terminal environment? at the end of this chapter.

Once in the correct directory, we run a script called `script_a.py` by typing `python3 script_a.py` in our Terminal as follows:

BASH

```bash
python3 script_a.py
```

OUTPUT

```
Hello world!
```

This will call the Python 3 interpreter to execute the code we wrote in `script_a.py`. Once executed, we will see the output displayed in the Terminal window.

In a Jupyter Notebook we can press the keyboard shortcut 'shift+enter' to execute the code in a cell. The output will be displayed below the code cell.

You have now successfully written and executed your first program in Python.

REMEMBER

We know that `print()` is a *function* because it ends with a pair of parentheses, and it is written entirely in lowercase characters PEP-8: Function Names. Some IDEs change color when they encounter built-in functions, in order to signal to the user that the function is recognised, and available to use, and so that we don't accidentally overwrite them.

We can pass more than a single value to the `print()` function, provided that each value is separated from another, using a comma. For instance, if we write the code below and run the script, the results would be as shown in *output*.

PYTHON

```python
print('Hello', 'John')
```

OUTPUT

```
Hello John
```

Notice that there is a space between 'Hello' and 'John' even though we did not include a space in our text. This is the default behaviour of the `print()` function when it receives more than a single value (argument).

This default behaviour may be changed using a keyword argument called sep:

PYTHON

```python
print('Hello', 'John', sep='')
```

OUTPUT

```
HelloJohn
```

PYTHON

```python
print('Hello', 'John', sep='--')
```

OUTPUT

```
Hello--John
```

PYTHON

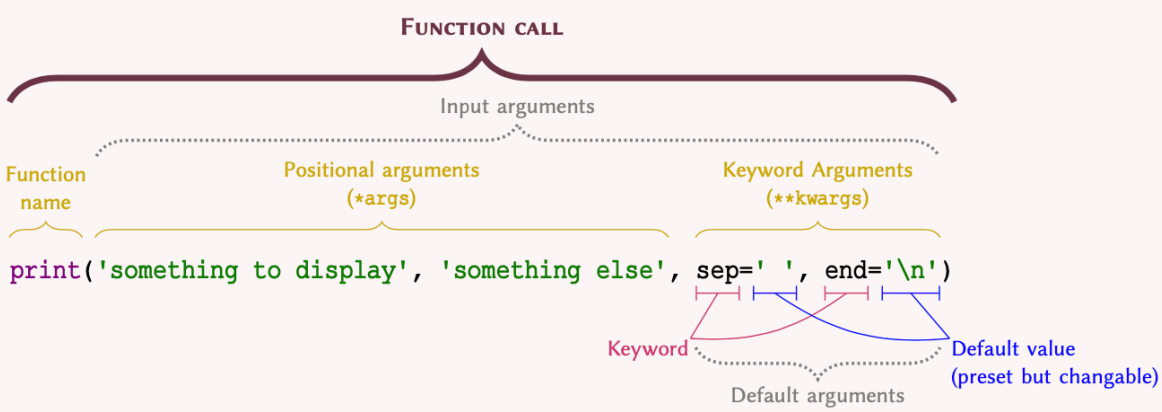
```python
print('Jane', 21, 'London', sep='.')
```

OUTPUT

```
Jane.21.London
```

Remember

In Python, values that do not require a name when passed to a function — *e.g.* `Jane`, `21`, or `London` in the last example, are known as *positional arguments*. On the other hand, values that require their name to be specified such as `sep=...` are referred to as *keyword arguments*. Values that do not require to be specified when calling a function and have a default value — *e.g.* `sep=' '`, are called *default arguments*.



The *input* and *output* arguments of a function are referred to as the **function signature**.

Explanation of a function call

PRACTICE EXERCISE 1

Write code that displays the following output:

Protein Kinase C (Alpha subunit)

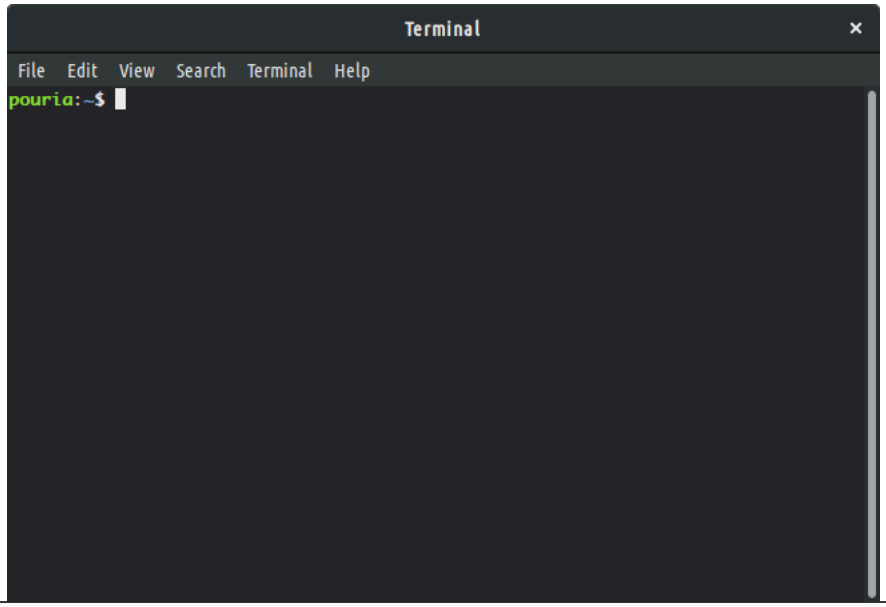
Solution

PYTHON

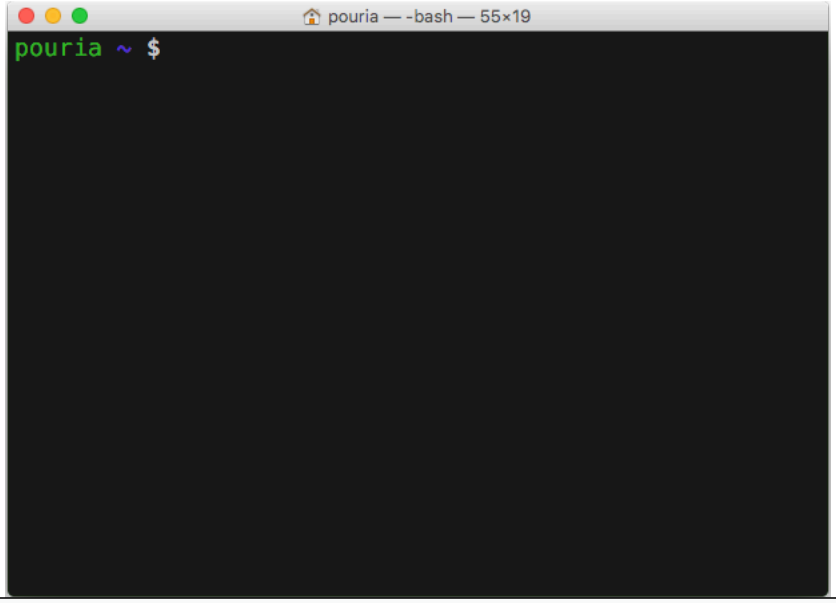
```python
print('Protein Kinase C (Alpha subunit)')
```

OUTPUT

```
Protein Kinase C (Alpha subunit)
```



Terminal window on a Linux computer



Terminal window on a Mac

RECEIVING AN INPUT

Input

Inputs are I/O operations that involve receiving some data from the outside world. This might include reading the contents of a file, downloading something from the internet, or asking the user to enter a value.

The simplest way to acquire an input is to ask the user to enter a value in the Terminal. To do so, we use a dedicated built-in function called `input()`.

> **NOTE**
>
> In a Unix system (Mac OS or Linux), a tilde (~) is an alias that is used to refer to a user's home directory.

This function takes a single *argument* called `prompt`. Prompt is the text displayed in the Terminal to ask the user for an input. Figure Terminal window on a Linux computer and Terminal window on a Mac, illustrates a screen shot of an example PC's prompt, where it displays a user name (i.e. `pouria`) followed by a tilde (~). A Terminal prompt may be different in each computer and operating system.

Here is how we implement the `input()` function:

```
input('Please enter your name: ')
```

which is exactly the same as:

```
input(prompt='Please enter your name: ')
```

If we save one of the above in a notebook and execute it, we will see:

```
python3 script_b.py

Please enter your name: _
```

The Terminal cursor, displayed as an underscore in our example, will be in front of the prompt (i.e. `'Please enter your name: '`) waiting for a response. Once it receives a response, it will proceed to run the rest of the code (if any), or terminate the execution.

We may store the user's response in a variable. Variables are the topic of the next episode in this learning material, where we shall also review more examples on `input()` and how we can use it to produce results based on the responses we receive from the user.

REMEMBER

Python is an interpreted language; this means that the code we write is executed by the Python interpreter one line at a time. The `input()` function performs a *blocking* process. This means that the execution of the code by the Python interpreter is halted upon encountering an `input()` function until the user enters a value. Once a value is entered, the interpreter then proceeds to execute the next line.

PRACTICE EXERCISE 2

Write a script that asks the user to enter the name of a protein in the Terminal.

Solution

```
input('Please enter the name of a protein: ')
```

Variables And Types

Variables are a type of data container, that we can use to store data to memory. Each variable has three main types of attribute: *scope*, *name*, and *type*. *Scope* and *name* must be mutually unique. Starting with *name*, we will discuss each of these attributes in more details throughout this chapter.

Variable names

PEP–8 Naming Conventions

The name that we give to a variable is, in fact, an alias for a location in the memory. You can think of it as a postbox, which is used as a substitute for an actual address. Similarly, we use variable names so we don't have to use the actual address to the location we want in the memory; because it would look something like this `0x106fb8348`.

There are some relatively simple rules to follow when defining variable names, which ultimately boil down to:

Validity	Example	Note
Invalid	`5mins = 5 * SEC_IN_MIN`	Variables cannot start with numbers — raises a `SyntaxError`.
Invalid	`if = 2`	Attempts to overwrite an internal syntax — raises a `SyntaxError`.
Worst	`j = 2`	Overwrites the internal identifier for complex numbers.
Worst	`int = 2`	Overwrites the internal definition for integer numbers.
Bad	`a = 4`	Meaningless name + hard to identify in code.
Okay	`var1 = 0`	Meaningless name + hard to distinguish.
Better	`var_1 = 0`	Meaningless name.
Good	`current_state = 0`	Good name + easy to distinguish.
Okay	`five_mins_in_sec = 5 * 60`	Good name, vague value.
Good	`SEC_IN_MIN = 60`	Good name + good value + distinguished as a constant (conventionally, names made exclusively of capital letters signify constants).
Good	`five_mins2sec = 5 * SEC_IN_MIN`	Good name + good value.
Good	`five_mins2sec = 5 * 60  # 5 min * 60 sec`	Good name + vague value clarified by a comment.
Good	`current_protein = 'DNA Polymerase III'`	Good name + good value.

REMEMBER

We should never overwrite an existing, built-in definition or identifier (e.g. `int` or `print`). We will be learning many such definitions and identifiers as we progress through this course. Nonetheless, the Jupyter Notebook as well as any good IDE highlights syntaxes and built-in identifiers in different colours. In Jupyter, the default for built-in definitions is green. The exact colouring scheme depends on the IDE being used, and the selected theme.

Once a variable is defined, its value may be altered or reset:

PYTHON

```python
total_items = 2
print(total_items)
```

OUTPUT

```
2
```

In Python, variables containing integer numbers are referred to as `int`, and those containing decimal numbers are referred to as `float`.

PYTHON

```python
total_items = 3
print(total_items)
```

OUTPUT

```
3
```

PYTHON

```python
total_values = 3.2
print(total_values)
```

OUTPUT

```
3.2
```

PYTHON

```python
temperature = 16.
print(temperature)
```

OUTPUT

```
16.0
```

Variables can contain data as characters as well; but to prevent Python from confusing them with meaningful commands, we use quotation marks. So long as we remain consistent, *it doesn't matter whether we use single or double quotations*. These data are known as `string` or `str`:

PYTHON

```python
forename = 'John'
surname = "Doe"


print('Hi,', forename, surname)
```

OUTPUT

```
Hi, John Doe
```

PRACTICE EXERCISE 3

Oxidised low-density lipoprotein (LDL) receptor 1 mediates the recognition, internalisation and degradation of oxidatively modified low-density lipoprotein by vascular endothelial cells. Using the Universal Protein Resource (UniProt) website, find this protein for humans, and identify:

- UniProt entry number.
- Length of the protein (right at the top).
- Gene name (right at the top).

Store the information you retrieved, including the protein name, in within four separate variables.

Display the values of these four variables in *one* line, and separate the items with three spaces, as follows:

```
Name EntryNo GeneName Length
```

Solution

PYTHON

```python
name = 'Oxidised low-density lipoprotein (LDL) receptor 1'

uniprot_entry = 'P78380'

gene_name = 'OLR1'

length = 273

print(name, uniprot_entry, gene_name, length, sep='   ')
```

OUTPUT

```
Oxidised low-density lipoprotein (LDL) receptor 1   P78380   OLR1   273
```

PRACTICE EXERCISE 4

1. Write a Python code that upon execution, asks the user to enter the name of an enzyme and then stores the response in an appropriately named variable.

2. Use the variable to display an output similar to the following:

`ENZYME_NAME is an enzyme.`

where `ENZYME_NAME` is the name of the enzyme entered in the prompt.

3. Now modify your script to prompt the user to enter the number of amino acids in that enzyme. Store the value in another appropriately named variable.

4. Alter the output of your script to display a report in the following format:

`ENZYME_NAME is an enzyme containing a total number of AMINO_ACIDS} amino acids.`

where `AMINO_ACIDS` is the number of amino acids.

Solution

```
enzyme = input('Please enter the name of an enzyme: ')

print(enzyme, 'is an enzyme.')

length = input('How many amino acids does the enzyme contain? ')

print(enzyme, 'is an enzyme containing a total number of', length, 'amino acids.')
```

Variable Types

Built-in Types

When it comes to types, programming languages may be divided into two distinct categories:

TYPES

- ☑**Statically typed** languages: these require the programmer to explicitly declare the type of each variable, and this type is checked at compile time.
- ☑**Dynamically typed** languages: the type of the variable is determined at run time, and variables can change types on the fly. The programmer is not required to explicitly define the type of a variable: the language infers the type of the variable, once it is assigned data.

Python is a dynamically typed language, and falls into this second category. This means that, unlike statically typed languages, we rarely need to worry about the *type* definitions because in the majority of cases, Python takes care of them for us, and automatically decodes the type of data being stored in a variable, once it is defined by the user.

REMEMBER

In a dynamically typed language, it is the value of a variable that determines the type. This is because the types are determined on the fly by the Python interpreter as and when it encounters different variables and values.

ADVANCED TOPIC

In computer programming, type systems are syntactic methods to enforce and/or identify levels of abstraction. This means that type systems take advantage of the syntax of a particular programming language, in order to enforce rules and identify types. This is important, as it can manage abstraction in data, by ensuring that differing data types interact meaningfully with one another. An entire field in computer science has been dedicated to the study of programming languages from a type–theoretic approach. This is primarily due to the implication of types and their underlying principles in such areas in software engineering as optimisation and security. To learn more about the study of type systems, refer to: Pierce B. Types and programming languages. Cambridge, Mass.: MIT Press; 2002.

NOTE

The values determine the type of a variable in dynamically typed languages. This is in contrast to statically typed languages, where a variable must be initialised using a specific type before a value.

Why learn about *types* in a dynamically typed programming language?

Python enjoys a powerful type system out of the box. The following table - Built-in types in Python - provides a comprehensive reference for the built-in types in Python. Built-in types already exist in the language, and do not require the use or implementation of any third-party libraries.

Type	Type Name	Specification	Numeric	Sequence	Iterable	Mutable	Container
`bool`	Boolean	`True` or `False`	✔				
`int`	Integer	An integer number: $x \in \mathbb{Z}$	✔				
`float`	Floating point	A rational number: $x \in \mathbb{Q}$	✔				
`complex`	Complex	A complex number: $x \in \mathbb{C}$	✔				
`bytes`*	Bytes	Single byte					
`bytearray`*	Byte Array	Array of bytes; *i.e.* binary		✔	✔	✔	
`str`	String	Array of characters; *i.e.* text.		✔	✔		
`list`	List	Array of any combination		✔	✔	✔	
`tuple`	Tuple	Array of any combination		✔	✔		
`set`	Set	Collection of unique members		✔		✔	✔
`frozenset`*	Frozen Set	Collection of unique members		✔			✔
`dict`	Dictionary	Mapping (associative array)		✔	✔ $	✔	✔

A comprehensive (but non-exhaustive) reference of built-in (native) types in Python 3.
* Not discussed in this course — included for reference only.
$ `dict` is not an iterable by default, however, it is possible to iterate through its keys.

Mutability is an important concept in programming. A mutable object is an object whose value(s) may be altered. This will become clearer once we study `list` and `tuple`. Find out more about mutability in Python from the documentation.

Complex numbers refer to a set of numbers that have both a real component, and an imaginary component; where the imaginary part is defined as \(\sqrt{-1}\). These numbers are very useful in the study of oscillatory behaviours and flow (e.g. heat, fluid, electricity). To learn more about complex numbers, watch this Khan Academy video tutorial.

Sometimes we might need want to explicitly know what the type of a variable is. To do this, we can use the build-in function `type()` as follows:

PYTHON

```python
total_items = 2

print(type(total_items))
```

OUTPUT

```
<class 'int'>
```

PYTHON

```python
total_values = 3.2

print(type(total_values))
```

OUTPUT

```
<class 'float'>
```

PYTHON

```python
temperature = 16.

print(type(temperature))
```

OUTPUT

```
<class 'float'>
```

PYTHON

```python
phase = 12.5+1.5j

print(type(phase))
```

OUTPUT

```
<class 'complex'>
```

PYTHON

```python
full_name = 'John Doe'

print(type(full_name))
```

OUTPUT

```
<class 'str'>
```

REMEMBER

In Python, a variable/value of a certain type may be referred to as an *instance* of that type. For instance, an integer value whose type in Python is defined as *int* is said to be an **instance of type** `int`.

PRACTICE EXERCISE 5

Determine and display the type for each of these values:

- 32
- 24.3454
- 2.5 + 1.5
- “RNA Polymerase III”
- 0
- .5 - 1
- 1.3e-5
- 3e5

The result for each value should be represented in the following format:

```
Value X is an instance of <class 'Y'>
```

Solution

PYTHON

```python
value = 32

value_type = type(value)

print('Value', value, 'is an instance of', value_type)
```

OUTPUT

```
Value 32 is an instance of <class 'int'>
```

PYTHON

```python
value = 24.3454

value_type = type(value)

print('Value', value, 'is an instance of', value_type)
```

OUTPUT

```
Value 24.3454 is an instance of <class 'float'>
```

PYTHON

```python
value = 2.5 + 1.5

value_type = type(value)

print('Value', value, 'is an instance of', value_type)
```

OUTPUT

```
Value 4.0 is an instance of <class 'float'>
```

PYTHON

```python
value = "RNA Polymerase III"

value_type = type(value)

print('Value', value, 'is an instance of', value_type)
```

OUTPUT

```
Value RNA Polymerase III is an instance of <class 'str'>
```

PYTHON

```python
value = 0

value_type = type(value)

print('Value', value, 'is an instance of', value_type)
```

OUTPUT

```
Value 0 is an instance of <class 'int'>
```

PYTHON

```python
value = .5 - 1

value_type = type(value)

print('Value', value, 'is an instance of', value_type)
```

OUTPUT

```
Value -0.5 is an instance of <class 'float'>
```

PYTHON

```python
value = 1.3e-5

value_type = type(value)

print('Value', value, 'is an instance of', value_type)
```

OUTPUT

```
Value 1.3e-05 is an instance of <class 'float'>
```

PYTHON

```python
value = 3e5

value_type = type(value)

print('Value', value, 'is an instance of', value_type)
```

OUTPUT

```
Value 300000.0 is an instance of <class 'float'>
```

Conversion of types

WHY CONVERT TYPES?

It is sometimes necessary to have the values returned by the `input()` function — *i.e.* the user's response, in other types. Imagine the following scenario:

"We ask our user to enter the total volume of their purified protein, so that we can work out the amount of assay they need to conduct a specific experiment. To calculate this assay volume using the volume of the purified protein, we need to perform mathematical calculations based on the response we receive from our user. It is not possible to perform mathematical operations on non-numeric values. Therefore, we ought to somehow convert the type from `str` to a numeric type."

The possibility of converting from one type to another depends entirely on the *value*, the *source type*, and the *target type*. For instance; we can convert an instance of type `str` (source type) to one of type `int` (target type) if and only if the source value consists entirely of numbers and there are *no* other characters.

REMEMBER

To convert a variable from one type to another, we use the *Type Name* of the target type (as described in Table Built-in types in Python and treat it as a function.

For instance, to convert a variable to integer, we:

- look up the *Type Name* for integer from Table Built-in types in Python
- then treat the *Type Name* as a function: `int()`
- use the function to convert our variable: new_var = `int`(old_var)

Here is an example of how we convert types in Python:

PYTHON

```python
value_a = '12'

print(value_a, type(value_a))
```

OUTPUT

```
12 <class 'str'>
```

PYTHON

```python
value_b = int(value_a)

print(value_b, type(value_b))
```

OUTPUT

```
12 <class 'int'>
```

If we attempt to convert a variable that contains non-numeric values, a `ValueError` is raised:

PYTHON

```python
value_a = '12y'

print(value_a, type(value_a))
```

OUTPUT

```
12y <class 'str'>
```

PYTHON

```python
value_b = int(value_a)
```

OUTPUT

```
ValueError: invalid literal for int() with base 10: '12y'
```

PRACTICE EXERCISE 6

In programming, we routinely face errors resulting from different mistakes. The process of finding and correcting such mistakes in the code is referred to as **debugging**.

We have been given the following piece of code written in Python:

```
value_a = 3
value_b = '2'

result = value_a + value_b
print(value_a, '+', value_b, '=', result)
```

But when the code is executed, we encounter an error message as follows:

```
Traceback (most recent call last):
File "<stdin>", line 1, in <module>
TypeError: unsupported operand type(s) for +: 'int' and 'str'
```

Debug the snippet so that the correct result is displayed:

```
3 + 2 = 5
```

Solution

PYTHON

```python
value_a = 3

value_b = '2'

result = value_a + int(value_b)

print(value_a, '+', value_b, '=', result)
```

OUTPUT

```
3 + 2 = 5
```

Handling Input Variables

DISCUSSION

When we use `input()` to obtain a value from the user, the results are by default an instance of type `str`. An `input()` function always stores the response as a `str` value, no matter what the user enters. However, it is possible to convert the type afterwards.

REMEMBER

The `input()` function *always* returns a value of type `str` regardless of the user's response. In other words, if a user's response to an `input()` request is numeric, Python will *not* automatically recognise it as a numeric type.

We may use *type conversion* in conjunction with the values returned by the `input()` function:

```
response = input('Please enter a numeric value: ')

response_numeric = float(response)

print('response:', response)
print('response type:', type(response))
print('response_numeric:', response_numeric)
print('response_numeric type:', type(response_numeric))
```

The output shows the results when we enter numeric values as directed.

PRACTICE EXERCISE 7

We know that each amino acid in a protein is encoded by a triplet of mRNA nucleotides.

With that in mind, alter the script you wrote for Practice Exercise 3 and use the number of amino acids entered by the user to calculate the number of mRNA nucleotides.

Display the results in the following format:

```
ENZYME_NAME is an enzyme with AMINO_ACIDS amino acids and NUCLEOTIDES
nucleotides.
```

where `NUCLEOTIDES` is the total number of mRNA nucleotides that you calculated.

Note: Multiplication is represented using the asterisk (*) sign.

Solution

```
enzyme = input('Please enter the name of an enzyme: ')

length = input('How many amino acids does the enzyme contain? ')

nucleotides = 3 * int(length)

print(enzyme, 'is an enzyme with', length, 'amino acids and',  nucleotides, 'nucleotides.')
```

Variable scopes

Resolution of names

When defining a variable, we should always consider where in our program we intend to use it. The more localised our variables, the better. This is because local variables are easier to distinguish, and thus reduce the chance of making mistakes — e.g. unintentionally redefining or altering the value of an existing variable.

Therefore, the scope of a variable defines the ability to reference a variable from different *points* in our programs. The concept of local variables becomes clearer once we explore functions in programming in chapter Functions.

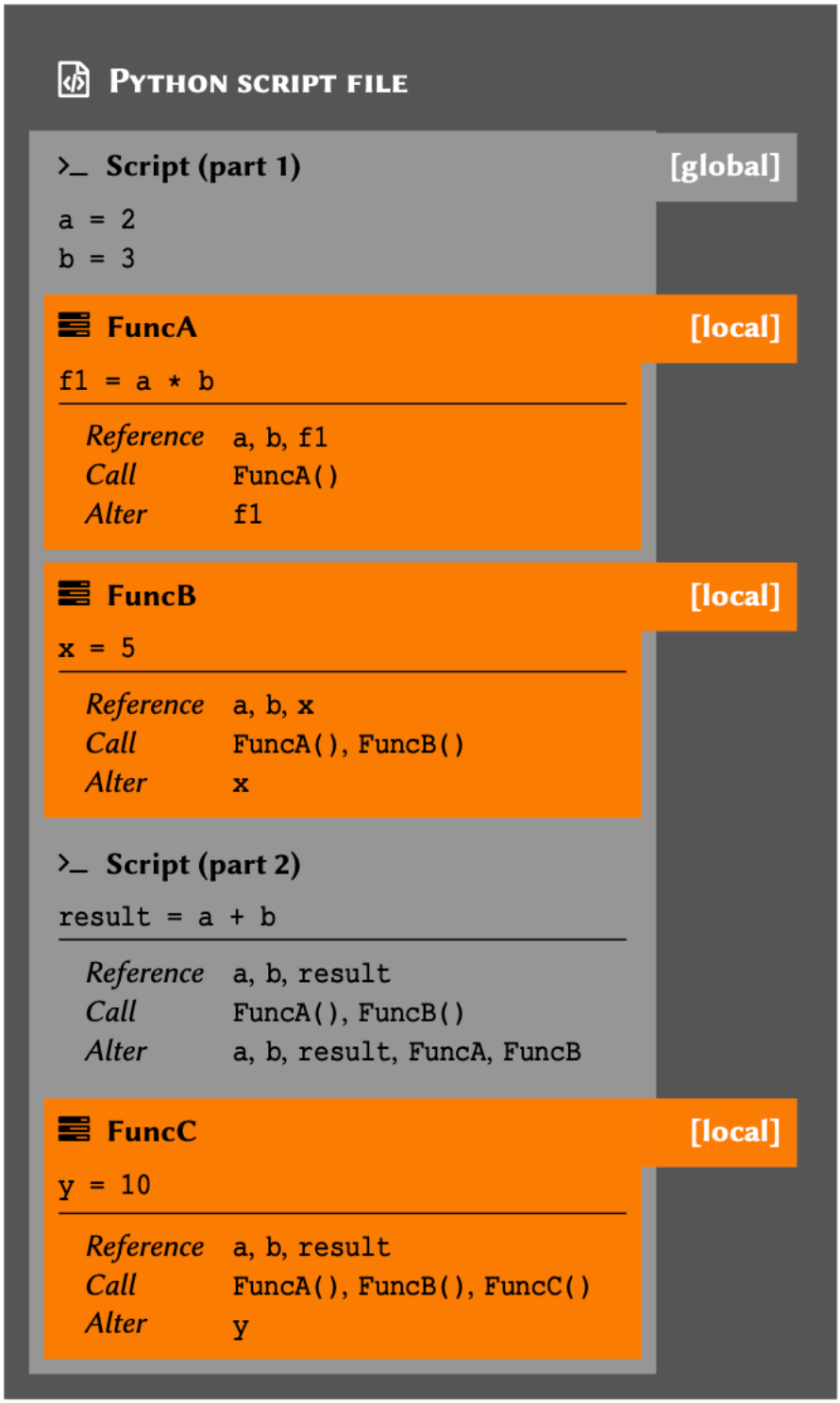
As displayed in Figure Variable scopes, the point *at* or *from* which a variable can be referenced depends on the location where the variable is defined.

In essence, there are three general rules to remember in relation to variable scopes in Python:

I. A variable that is defined in the outer scope, can be *accessed* or *called* in the inner scopes, but it cannot be *altered* implicitly. Not that such variables may still be altered using special techniques (not discussed).

II. A variable that is defined in the innermost scopes (local), can only be *accessed*, *called*, or *altered* within the boundaries of the scope it is defined in.

III. The inner scopes *from* which a variable is referenced must themselves be contained within the defining scope — e.g. in `FuncB` of Figure Variable scopes, we can reference `a`, `b`, and `x`; but not `f1`. This is because the scope of `f1` is `Script` → `FuncA`, so it can only be referenced from `Script` → `FuncA` → ..., but not `Script → ... or `Script` → `FuncB` → ...



Variable scopes in Python with respect to scripts and functions.

As we discussed earlier in this lesson, it is paramount to remember that Python is an interpreted language. This means that the Python interpreter goes through the codes that we write line by line, interpreting it to machine language. It is only then that the commands are processed and executed by the computer. On that account, a variable (or a function) can be referenced only *after* its initial definition. That is why, for instance, in `Script (part 2)` of Figure Variable scopes, we can reference every variable and function except for `FuncC`, which is declared further down in the code hierarchy.

Although scope and hierarchy appear at first glance as theoretical concepts in programming, their implications are entirely practical. The definition of these principles vary from one programming language to another. As such, it is essential to understand these principles and their implications in relation to any programming language we are trying to learn.

Optional: How to use Terminal environment?

How to navigate the terminal in Mac OS X and Linux?

The Unix terminal — *i.e.* the one used by Mac OS X® and Linux; uses a command language known as Bash, also referred to as the Unix Shell. This is not the topic of this book, so we won't discuss its properties and features in much detail.

Microsoft Windows®, on the other hand, relies on DOS (Microsoft Disk Operating System®) commands to navigate the terminal. The terminal environment in is sometimes referred to as the `CMD` or the command prompt.

The enviroment in which we can use Bash or DOS commands is known as the terminal. To use a terminal, we need a terminal emulator. Every operating system has a default terminal emulator, but you can always use an alternative software if you so wish.

Current working directory

To navigate the terminal environment, we should first find out where we are. Here is how we do that:

Unix	Microsoft Windows®
`pwd` ⏎	`pwd` ⏎

Remember that the path to an enviroment is displayed (and supplied differently in Unix and Microsoft Windows®). To that end, the response (output) to these commands may slightly vary:

Unix	Microsoft Windows®
`/home/UserName/Documents`	`C:\Documents`

Notice that in Microsoft Windows®, we separate directories using a backslash (\ ), whilst in Unix, we use a foreslash (/) for that purpose.

Changing the current directory

To navigate to another directory, we do as follows:

	Unix	Microsoft Windows®
Without spaces in the name	`cd /home/UserName/Documents/Python_Scripts` ⏎	`cd C:\Documents\Python_Scripts` ⏎
With spaces in the name	`cd "/home/UserName/Documents/Python Scripts"` ⏎	`cd "C:\Documents\Python Scripts"` ⏎

Note that paths containing one or more space characters must be encapsulated by double quotation marks (`"..."`).

If we are already in the `Documents` directory, and want to navigate onto `Python_Scripts`, we can use the following shorthand versions of the above method:

	Unix	Microsoft Windows®
Without spaces in the name	`cd Python_Scripts` ⏎	`cd Python_Scripts` ⏎
With spaces in the name	`cd "Python Scripts"` ⏎	`cd "Python Scripts"` ⏎

Parent directory

To navigate to the parent directory — *i.e.* from `Python_Scripts` to `Documents` in this example; we do:

Unix	Microsoft Windows®
`cd ..` ⏎	`cd ..` ⏎

Home directory

We can also navigate all the way back to the home directory in one go:

Unix	Microsoft Windows®
`cd` ⏎	`cd \` ⏎

Creating a new directory

We can create a new directory as follows:

Unix	Microsoft Windows®
`mkdir new_dir_name` ⏎	`md new_dir_name` ⏎

Contents of a directory

To see the contents of a directory, we use the following commands:

Unix	Microsoft Windows®
`ls` ⏎	`dir` ⏎

Operations

Through our experimentation with variable types, we already know that variables may be subjected to different operations.

When assessing type conversions, we also established that the operations we can apply to each variable depend on the *type* of that variable. To that end, we learned that although it is sometimes possible to mix variables from different types to perform an operation (for example multiplying a floating point number with an integer), there are some logical restrictions in place.

Throughout this section, we will take a closer look into different types of operations in Python. This will allow us to gain a deeper insight, and to familiarise ourselves with the underlying logic.

To recapitulate on what we have done so far, we start off by reviewing *additions* — the most basic of all operations.

Give the variable `total_items`:

PYTHON

```python
total_items = 2

print(total_items)
```

OUTPUT

```
2
```

We can increment the value of an *existing* variable by **1** as follows:

PYTHON

```python
total_items = total_items + 1

print(total_items)
```

OUTPUT

```
3
```

Given two different variables, each containing a different value; we can perform an operation on these values and store the result in *another* variable without altering the original variables in any way:

PYTHON

```python
old_items = 4
new_items = 3

total_items = old_items + new_items

print(total_items)
```

OUTPUT

```
7
```

We can change the value of an *existing* variable using a value stored in *another* variable:

PYTHON

```python
new_items = 5
total_items = total_items + new_items

print(total_items)
```

OUTPUT

```
12
```

There is also a shorthand method for applying this operation on an *existing* variable:

PYTHON

```python
total_items = 2

print(total_items)
```

OUTPUT

```
2
```

PYTHON

```python
total_items += 1

print(total_items)
```

OUTPUT

```
3
```

PYTHON

```python
new_items = 5
total_items += new_items

print(total_items)
```

OUTPUT

```
8
```

As highlighted in the introduction, different operations may be applied to any variable or value. We can now explore the most fundamental operations in programming, and learn about their implementation in Python.

REMEMBER

There are 2 very general categories of operations in programming: *mathematical*, and *logical*. Naturally, we use mathematical operations to perform calculations, and logical operations to perform tests.

Mathematical Operations

Suppose a and b are two variables representing integers, as follows:

```
a = 17
b = 5
```

Using a and b we can itemise built-in mathematical operations in Python as follows:

Operation	Notation	Result
Addition	`a + b`	22
Subtraction	`a - b`	12
Multiplication	`a * b`	85
Division	`a / b`	3.4
Floor quotient	`a // b`	3
Remainder	`a % b`	2
Quotient and remainder	`divmod(a, b)`	(3, 2)
Power	`a ** b`	1419857
Absolute value	`abs(b - a)`	12

Routine mathematical operations in Python

REMEMBER

As far as mathematical operations are concerned, variables a and b may be an instance of any *numeric* type. See Table Routine mathematical operations in Python to find out more about numeric types in Python.

Values of type `int` have been chosen in our examples to facilitate the understanding of the results.

PRACTICE EXERCISE 8

1. Calculate the following and store the results in appropriately named variables:

a. 5.8×3.3

b. $\frac{180}{6}$

c. $35 - 3.0$

d. $35 - 3$

e. 2^{1000}

Display the result of each calculation – including the type, in the following format:

```
Result: X is an instance of <class 'Y'>
```

2. Now using the results you obtained:
   I. Can you explain why the result of $35 - 3.0$ is an instance of type `float`, whilst that of $35 - 3$ is of type `int`?

II. Unlike the numeric types, string values have a length. To obtain the length of a string value, we use `len()`. Convert the result for 2^{1000} from `int` to `str`, then use the aforementioned function to work out the length of the number — i.e. how many digits is it made of?

If you feel adventurous, you can try this for 2^{10000} or higher; but beware that you might overwhelm your computer and need a restart it if you go too far (i.e. above $2^{1000000}$). Just make sure you save everything beforehand, so you don't accidentally lose your work.

Hint: We discuss `len()` in our subsection of arrays arrays lesson. However, at this point, you should be able to use the official function documentation to figure out how it works. To access a function's documentation or docstring within Jupyter Notebook, for example you can use `help(function_name)` to reveal it's documentation. Clicking within the function (for example, placing your cursor inside the function `len`) and using `shift+tab` can also be an easy shortcut for viewing a function's docstring.

Solution

PYTHON

```python
q1_a = 5.8 * 3.3
print('Result:', q1_a, 'is an instance of', type(q1_a))
```

OUTPUT

```
Result: 19.139999999999997 is an instance of <class 'float'>
```

PYTHON

```python
q1_b = 180 / 6
print('Result:', q1_b, 'is an instance of', type(q1_b))
```

OUTPUT

```
Result: 30.0 is an instance of <class 'float'>
```

PYTHON

```python
q1_c = 35 - 3.0
print('Result:', q1_c, 'is an instance of', type(q1_c))
```

OUTPUT

```
Result: 32.0 is an instance of <class 'float'>
```

PYTHON

```python
q1_d = 35 - 3
print('Result:', q1_d, 'is an instance of', type(q1_d))
```

OUTPUT

```
Result: 32 is an instance of <class 'int'>
```

PYTHON

```python
q1_e = 2 ** 1000
print('Result:', q1_e, 'is an instance of', type(q1_e))
```

OUTPUT

```
Result: 107150860718626732094842504906000181056140481170553360744375038837035105112493612249319837881569
```

Solution

In the case of \(35 - 3.0\) vs \(35 - 3\), the former includes a floating point number. Operations involving multiple numeric types always produce the results as an instance of the type that covers all of the operands – i.e. `float` covers `int`, but not vice-versa.

Solution

PYTHON

```python
big_num = 2 ** 1000
big_num_str = str(big_num)
big_num_len = len(big_num_str)

print('Length of 2**1000:', big_num_len)
```

OUTPUT

```
Length of 2**1000: 302
```

INTERESTING FACT

As of Python 3.6, you can use an underscores (`_`) *within* large numbers as a separator to make them easier to read in your code. For instance, instead of `x = 1000000`, you can write `x = 1_000_000`.

Shorthand:

When it comes to mathematical operations in Python, there is a frequently used shorthand method that every Python programmer should be familiar with.

Suppose we have a variable defined as `total_residues = 52` and want to perform a mathematical operation on it. However, we would like to store the result of that operation in `total_residues` instead of a new variable. We can do this as follows:

PYTHON

```python
total_residues = 52

# Addition:
total_residues += 8

print(total_residues)
```

OUTPUT

```
60
```

PYTHON

```python
# Subtraction:
total_residues -= 10

print(total_residues)
```

OUTPUT

```
50
```

PYTHON

```python
# Multiplication:
total_residues *= 2

print(total_residues)
```

OUTPUT

```
100
```

PYTHON

```python
# Division:
total_residues /= 4

print(total_residues)
```

OUTPUT

```
25.0
```

PYTHON

```python
# Floor quotient:
total_residues //= 2

print(total_residues)
```

OUTPUT

```
12.0
```

PYTHON

```python
# Remainder:
total_residues %= 5

print(total_residues)
```

OUTPUT

```
2.0
```

PYTHON

```python
# Power:
total_residues **= 3

print(total_residues)
```

OUTPUT

```
8.0
```

We can also perform such operations using multiple variables:

PYTHON

```python
total_residues = 52
new_residues = 8
number_of_proteins = 3

total_residues += new_residues

print(total_residues)
```

OUTPUT

```
60
```

PYTHON

```python
total_residues += (number_of_proteins * new_residues)

print(total_residues)
```

OUTPUT

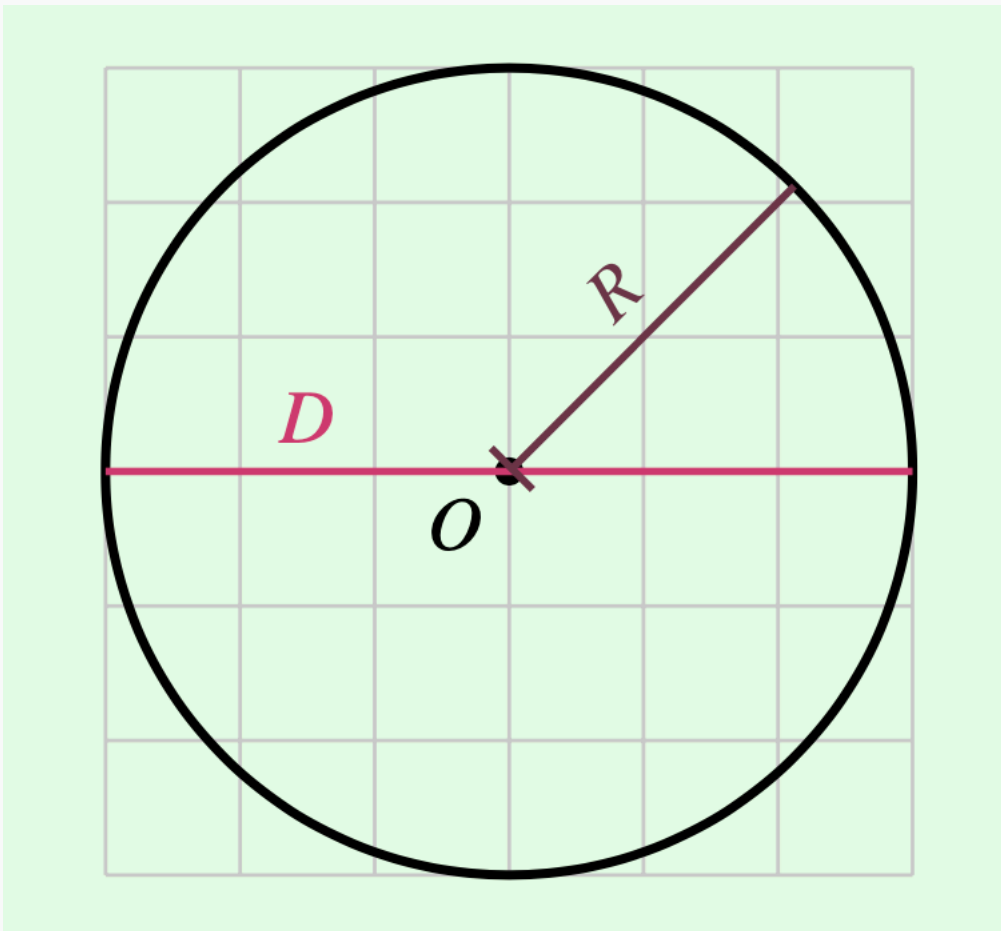
```
84
```

PRACTICE EXERCISE 9

1. Given:
   - Circumference: $C = 18.84956$
   - Radius: $R = 3$

and considering that the properties of a circle are defined as follows:

$$\pi = \frac{C}{D}$$ calculate π using the above equation and store it in a variable named `pi`:



Then round the results to 5 decimal places and display the result in the following format:

```
The value of pi calculated to 5 decimal places: X.XXXXX
```

Note: To round floating point numbers in Python, we use the function `round()`. This is a built-in function that takes two input arguments: the first is the variable/value to be rounded, and the second is the number of decimal places we wish to round to. Read more about the `round()` function in its official documentation.

2. Now without creating a new variable, perform the following operation:

$$pi = \frac{pi}{(3 \bmod 2) - 1}$$

where the expression "$(3 \bmod 2)$" represents the remainder for the division of 3 by 2.

Explain the output.

Solution

PYTHON

```python
c = 18.84956
r = 3
d = r * 2

pi = c / d

print('The value of pi calculated to 5 decimal places:', round(pi, 5))
```

OUTPUT

```
The value of pi calculated to 5 decimal places: 3.14159
```

Solution

```python
pi /= (3 % 2) - 1
```

The calculation raises a `ZeroDivisionError`. This is because division by zero is mathematically impossible.

Precedence:

In mathematics and computer programming, there are a series of conventional rules on the precedence of procedures to evaluate a mathematical expression. This collection of rules is referred to as the *order of operation* or *operator precedence*.

Suppose we have a mathematical expression as follows:

\[x = 2 + 3 \times 9\]
Such an expression can *only* be evaluated correctly if we do the multiplication first and then perform the addition. This means that the evaluation is done as follows:

\[given:3 \times 9 = 27\] \[\implies x = 2 + 27\] \[= 29\]

For instance, in an expression such as:

\[x = 2 \times (3 + (5 - 1)^2)\]

the evaluation workflow may be described as follows:

\[x = 2 \times (3 + 4^2)\] \[= 2 \times (3 + 16)\] \[= 38\]
The same principle applies in Python. This means that if we use Python to evaluate the above expression, the result would be identical:

PYTHON

```python
result = 2 * (3 + (5 - 1) ** 2)

print(result)
```

OUTPUT

```
38
```

REMEMBER

Operator precedence in mathematical operations may be described as follows:

1. Exponents and roots
2. Multiplication and division
3. Addition and subtraction

If there are any parentheses `( )` in the expression, the expression is evaluated from the innermost parenthesis, outwards.

PRACTICE EXERCISE 10

Display the result of each item in the following format:

```
EXPRESSION = RESULT
```

For example:

```
2 + 3 = 5
```

1. Calculate each expression *without* using parentheses:

a. $3 \times \frac{2}{4}$

b. $5 + 3 \times \frac{2}{4}$

c. $3 \times \frac{2}{4} + 5$

d. $\frac{2}{4} \times 3$

2. Calculate these expressions *using* parentheses:

a. $5 + \frac{2}{4} \times 3$

b. $5 + \frac{2 \times 3}{4}$

c. $5 + \frac{2}{4 \times 3}$

3. Given

```
a = 2
b = 5
```

use `a` and `b` to calculate the following expressions:

a. $(a + b)^2$

b. $a^2 + 2ab + b^2$

Solution

PYTHON

```python
q1_a = 3 * 2 / 4
print('3 * 2 / 4 =', q1_a)
```

OUTPUT

```
3 * 2 / 4 = 1.5
```

PYTHON

```python
q1_b = 5 + 3 * 2 / 4
print('5 + 3 * 2 / 4 =', q1_b)
```

OUTPUT

```
5 + 3 * 2 / 4 = 6.5
```

PYTHON

```python
q1_c = 3 * 2 / 4 + 5
print('3 * 2 / 4 + 5 =', q1_c)
```

OUTPUT

```
3 * 2 / 4 + 5 = 6.5
```

PYTHON

```python
q1_d = 2 / 4 * 3
print('2 / 4 * 3 =', q1_d)
```

OUTPUT

```
2 / 4 * 3 = 1.5
```

Solution

PYTHON

```python
q2_a = 5 + (2 / 4) * 3
print('5 + (2 / 4) * 3 =', q2_a)
```

OUTPUT

```
5 + (2 / 4) * 3 = 6.5
```

PYTHON

```python
q2_b = 5 + (2 * 3) / 4
print('5 + (2 * 3) / 4 =', q2_b)
```

OUTPUT

```
5 + (2 * 3) / 4 = 6.5
```

PYTHON

```python
q2_c = 5 + 2 / (4 * 3)
print('5 + 2 / (4 * 3) =', q2_c)
```

OUTPUT

```
5 + 2 / (4 * 3) = 5.166666666666667
```

Solution

PYTHON

```python
a = 2
b = 5

q3_a = (a + b) ** 2
print('(a + b)^2 =', q3_a)
```

OUTPUT

```
(a + b)^2 = 49
```

PYTHON

```python
q3_b = a ** 2 + 2 * a * b + b ** 2
print('a^2 + 2ab + b^2 =', q3_b)
```

OUTPUT

```
a^2 + 2ab + b^2 = 49
```

Non-numeric values

It sometimes makes sense to apply *some* mathematical operations to non-numeric variables, too.

We can multiply strings in order to repeat them. There is no specific advantage to using multiplication instead of manually repeating characters or words, but it does make our code look cleaner, which is ideal.

We can also add string values to each other. This is called *string concatenation*. It is a useful method for concatenating, and provides a useful method for combining multiple strings and/or string variables.

PYTHON

```python
SEPARATOR = '-' * 20
NEW_LINE = '\n'
SPACE = ' '

forename = 'Jane'
surname = 'Doe'
birthday = '01/01/1990'

full_name = forename + SPACE + surname

data = full_name + NEW_LINE + SEPARATOR + NEW_LINE + 'DoB: ' + birthday

print(data)
```

OUTPUT

```
Jane Doe
--------------------
DoB: 01/01/1990
```

REMEMBER

New line character or `'\n'` is a universal directive to induce a line-break in Unix-based operating systems (Mac OS) and Linux). In WINDOWS, we usually us `'\r'` or `'\r\n'` instead. These are known as escape sequences.

PRACTICE EXERCISE 11

Symptomatic Huntington's disease appears to increase in proportion to the number of `CAG` trinucleotide repeats (the codon for glutamine); once these exceed 35 repeats near the beginning of the Huntingtin (`IT15`) gene, the individual is phenotypic for the disease. These `CAG` repeats are also referred to as a polyglutamine or polyQ tract.

```
glutamine_codon = 'CAG'
```

1. Create a polynucleotide chain representing 36 glutamine codons. Store the result in a variable called `polyq_codons`.

Display the result as:

```
Polyglutamine codons with 36 repeats: XXXXXXXXX...
```

2. Use `len()` to work out the length of `polyq_codons`, and store the result in a variable called `polyq_codons_length`.

Display the result in the following format:

```
Number of nucleotides in a polyglutamine with 36 repeats: XXX
```

3. Use `len()` to work out the length of `glutamine_codon`, and store the result in variable `amino_acids_per_codon`.

4. Divide `polyq_codons_length` by `amino_acids_per_codon` to verify that the chain contains the total codons to encode exactly 36 amino acids. Store the result in a variable titled `polyq_peptide_length`.

Display the result in the following format:

```
Number of amino acids in a polyglutamine with 36 repeats: XXX
```

5. Determine the types for the following variable:

- amino_acids_per_codon
- polyq_codons_length
- polyq_peptide_length

  and display the result for each item in the following format:

```
Value: XXX - Type: <class 'XXXX'>
```

6. Are all the variables in task #5 of the same type? Why?

7. Repeat from task #4, but this time use an alternative method of division as outlined in See Table Routine mathematical operations in Python.

Solution

PYTHON

```python
glutamine_codon = 'CAG'

polyq_codons = glutamine_codon * 36

print('Polyglutamine codons with 36 repeats:', polyq_codons)
```

OUTPUT

```
Polyglutamine codons with 36 repeats: CAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAGCAG
```

Solution

PYTHON

```python
polyq_codons_length = len(polyq_codons)

print('Number of nucleotides in a polyglutamine with 36 repeats:', polyq_codons_length)
```

OUTPUT

```
Number of nucleotides in a polyglutamine with 36 repeats: 108
```

Solution

PYTHON

```python
amino_acids_per_codon = len(glutamine_codon)
```

Solution

PYTHON

```python
polyq_peptide_length = polyq_codons_length / amino_acids_per_codon

print('Number of amino acids in a polyglutamine with 36 repeats:', polyq_peptide_length)
```

OUTPUT

```
Number of amino acids in a polyglutamine with 36 repeats: 36.0
```

Solution

PYTHON

```python
print('Value:', amino_acids_per_codon, '- Type:', type(amino_acids_per_codon))

print('Value:', polyq_codons_length, '- Type:', type(polyq_codons_length))

print('Value:', polyq_peptide_length, '- Type:', type(polyq_peptide_length))
```

OUTPUT

```
Value: 3 - Type: <class 'int'>
Value: 108 - Type: <class 'int'>
Value: 36.0 - Type: <class 'float'>
```

Solution

No, `polyq_peptide_length` is an instance of type `float`. This is because we used the normal division (`/`) and not floor division (`//`}) to calculate its value. The result of normal division is always presented as a floating point number.

Solution

PYTHON

```python
polyq_peptide_length = polyq_codons_length // amino_acids_per_codon

print('Number of amino acids in a polyglutamine with 36 repeats:', polyq_peptide_length)

print('Value:', amino_acids_per_codon, '- Type:', type(amino_acids_per_codon))

print('Value:', polyq_codons_length, '- Type:', type(polyq_codons_length))

print('Value:', polyq_peptide_length, '- Type:', type(polyq_peptide_length))
```

OUTPUT

```
Number of amino acids in a polyglutamine with 36 repeats: 36
Value: 3 - Type: <class 'int'>
Value: 108 - Type: <class 'int'>
Value: 36 - Type: <class 'int'>
```

INTERESTING FACT

The Boolean data type is named after the English mathematician and logician George Boole (1815–1864).

Logical Operations

An operation may sometimes involve a comparison. The result of these operations may be either `True` or `False`. This is known as the *Boolean* or `bool` data type. In reality, however, computers record `True` and `False` as `1` and `0`, respectively.

Operations with Boolean results are referred to as *logical operations*. Testing the results of such operations is referred to as *truth value testing*.

Given the two variables `a` and `b` as follows:

```python
a = 17
b = 5
```

Boolean operations may be defined as outlined in this Table Routine logical operations in Python..

Logic	Statement	Result
Equivalence	`a == b`	`False`
Non-equivalence	`a != b`	`True`
Greater	`a > b`	`True`
Either greater or equal	`a >= b`	`True`
Smaller	`a < b`	`False`
Either smaller or equal	`a <= b`	`False`
Between	`5 < a < 20`	`True`

Table 2.2 Routine logical operations in Python.

Routine logical operations in Python.

PRACTICE EXERCISE 12

We know that in algebra, the first identity (square of a binomial) is:

\[(a + b)^2 = a^2 + 2ab + b^2\] now given:

```
a = 15
b = 4
```

1. Calculate

\[y_1 = (a + b)^{2}\] \[y_2 = a^2 + 2ab + b^2\]

Display the results in the following format:

```
y1 = XX
y2 = XX
```

2. Determine whether or not `y_1` is indeed equal to `y_2`. Store the result of your test in another variable called `equivalence`. Display the results in the following format:

```
Where a = XX and b = XX:
y1 is equal to y2: [True/False]
```

Solution

PYTHON

```python
a = 15
b = 4

y_1 = (a + b) ** 2
y_2 = a ** 2 + 2 * a * b + b ** 2

print('y1 =', y_1)
print('y2 =', y_2)
```

OUTPUT

```
y1 = 361
y2 = 361
```

Solution

PYTHON

```python
equivalence = y_1 == y_2

print('Where a =', a, ' and b=', b)
print('y1 is equal to y2:', equivalence)
```

OUTPUT

```
Where a = 15  and b= 4
y1 is equal to y2: True
```

Negation

We can also use negation in logical operations. Negation in Python is implemented using `not`:

Logic	Statement	Result
Not equal	`not a == b`	`True`
Not greater	`not a > b`	`False`
Neither greater nor equal	`not a >= b`	`False`
Smaller	`not a < b`	`True`
Neither smaller nor equal	`not a <= b`	`True`

Negations in Python.

PRACTICE EXERCISE 13

Using the information from previous Practice Exercise 12:

1. Without using `not`, determine whether or not `y_1` is *not equal* to `y_2`. Display the result of your test and store it in another variable called `inequivalent`.
2. Negate `inequivalent` and display the result.

Solution

PYTHON

```python
inequivalent = y_1 != y_2

print(inequivalent)
```

OUTPUT

```
False
```

Solution

PYTHON

```python
inequivalent_negated = not inequivalent

print(inequivalent_negated)
```

OUTPUT

```
True
```

Disjunctions and Conjunctions:

Logical operations may be combined using conjunction with `and` and disjunction with `or` to create more complex logics:

Logic	Statement	Result
Either smaller or equal	`a < b or a == b`	`False`
Either greater or smaller	`a < b or a > b`	`True`
Either greater or equal	`a > b or a == b`	`True`
Greater but not greater than	`a > b and not a > 18`	`True`
Either equal or not between	`a == b or not b < a < 20`	`False`
Equal and between	`a == b and 5 <= a < 20`	`False`

PRACTICE EXERCISE 14

Given

```
a = True
b = False
c = True
```

Evaluate the following statements:

1. a == b
2. a == c
3. a `or` b
4. a `and` b
5. a `or` b `and` c
6. (a `or` b) `and` c
7. `not` a `or` (b `and` c)
8. `not` a `or` `not`(b `and` c)
9. `not` a `and` `not`(b `and` c)
10. `not` a `and` `not`(b `or` c)

Display the results in the following format:

```
1. [True/False]
2. [True/False]
   ...
```

Given that:

PYTHON

```
a = True
b = False
c = True
```

Solution

PYTHON

```python
print('1.', a == b)
```

OUTPUT

```
1. False
```

Solution

PYTHON

```python
print('2.', a == c)
```

OUTPUT

```
2. True
```

Solution

PYTHON

```python
print('3.', a or b)
```

OUTPUT

```
3. True
```

Solution

PYTHON

```python
print('4.', a and b)
```

OUTPUT

```
4. False
```

Solution

PYTHON

```python
print('5.', a or b and c)
```

OUTPUT

```
5. True
```

Solution

PYTHON

```python
print('6.', (a or b) and c)
```

OUTPUT

```
6. True
```

Solution

PYTHON

```python
print('7.', not a or (b and c))
```

OUTPUT

```
7. False
```

Solution

PYTHON

```python
print('8.', not a or not(b and c))
```

OUTPUT

```
8. True
```

Solution

PYTHON

```python
print('9.', not a and not(b and c))
```

OUTPUT

```
9. False
```

Solution

PYTHON

```python
print('10.', not a and not(b or c))
```

OUTPUT

```
10. False
```

Complex logical operations:

It may help to break down more complex operations, or use parentheses to make them easier to read and write:

Logic	Statement	Result
Complex logic	`a == b or (5 <= a or b < 20 and a < b)`	`True`
Complex logic	`a == b or (5 <= a or b < 20) and a < b`	`False`
Complex logic	`a == b or 5 <= a or (b < 20 and a < b)`	`True`

Complex Logical Operations in Python:

Notice that in the last example, all notations is essentially the same, and only varies in terms of the collective results as defined using parentheses. Always remember that in a logical statement:

LOGICAL STATEMENT

- ☑The statement in parentheses does **not** have precedence over the rest of the state (unlike mathematical statements). It merely defines an independent part of the operation whose response is evaluated separately.
- ☑The precedence is established on a first-come-first-serve basis (from left to right).
- ☑Always use parentheses in longer statements for clarification.
- ☑In disjunctive statements (such as a > 5 `or` b > 5) if the first part is `True`, the second part is *not* checked. In other words, if a is greater than 5, the computer does not proceed to check whether or not b is greater than 5.
- ☑In conjunctive statements (such as a > 5 `and` b > 5) the statement proceeds to the seconds part if the first part is `True`. In other words, the result of a conjunctive statement is only `True` if both a and b are greater than 5. If a is `False`, the entire statement will inevitably be `False`.
- ☑The longer the statement, the more difficult it would be to understand it properly, and by extension, the more likely it would be to cause problems.

PYTHON

```python
a, b, c = 17, 5, 2  # Alternative method to define variables.
```

PYTHON

```python
# Disjunction: false OR true.
a < b or b > c
```

OUTPUT

```
True
```

PYTHON

```python
# Disjunction: true OR true.
a > b or b > c
```

OUTPUT

```
True
```

PYTHON

```python
# Conjunction: true AND true.
a > b and b > c
```

OUTPUT

```
True
```

PYTHON

```python
# Conjunction: false and true.
a < b and b > c
```

OUTPUT

```
False
```

PYTHON

```python
# Disjunction and conjunction: true OR false AND true
a > b or b < c and b < a
```

OUTPUT

```
True
```

PYTHON

```python
# Disjunction and conjunction: false OR true AND false
a < b or b > c and b > a
```

OUTPUT

```
False
```

PYTHON

```python
# Disjunctions and conjunction: false OR true AND true
a < b or b > c and b < a
```

OUTPUT

```
True
```

PYTHON

```python
# Disjunction and negated conjunction and conjunction:
# true AND NOT false AND false
a < b or not b < c and b > a
```

OUTPUT

```
False
```

PYTHON

```python
# Disjunction and negated conjunction - similar to the
# previous example: true AND NOT (false AND false)
a < b or not (b < c and b > a)
```

OUTPUT

```
True
```

These are only a few examples. There are endless possibilities, try them yourself and see how they work.

REMEMBER

Some logical operations may be written in different ways. However, we should always use the notation that is most coherent in the context of our code. If in doubt, use the simplest or shortest notation.

To that end, you may want to use variables to break complex statements down into smaller fragments:

PYTHON

```python
age_a, age_b = 15, 35

are_positive = age_a > 0 and age_b > 0

a_is_older = are_positive and (age_a > age_b)
b_is_older = are_positive and (age_a < age_b)

a_is_teenager = are_positive and 12 < age_a < 20
b_is_teenager = are_positive and 12 < age_b < 20

a_is_teenager and b_is_older
```

OUTPUT

```
True
```

PYTHON

```python
a_is_teenager and a_is_older
```

OUTPUT

```
False
```

PYTHON

```python
a_is_teenager and (b_is_teenager or b_is_older)
```

OUTPUT

```
True
```

PRACTICE EXERCISE 15

Given

```
a = 3
b = 13
```

Test the following statements and display the results:

- \(a^2 < b\)
- \(3 - a^3 < b\)
- \(|25 - a^2| > b\)
- \(25 \bmod a^2 > b\)
- \(25 \bmod a^2 > b\) or \(25 \bmod b < a\)
- \(25 \bmod a^2 < b\) and \(25 \bmod b > a\)
- \(\frac{12}{a}\) and \(a\times4 < b\)

where "|...|" represents the absolute value, and "\(n \bmod m\)" represents the remainder for the division of \(n\) by \(m\).}

Display the results in the following format:

```
1. [True/False]
2. [True/False]
...
```

Solution

PYTHON

```python
#Given that:
a = 3
b = 13
print('1.', a**2 < b)
```

OUTPUT

```
1. True
```

Solution

PYTHON

```python
print('2.', (3 - a**3) < b)
```

OUTPUT

```
2. True
```

Solution

PYTHON

```python
print('3.', abs(25 - a**2) > b)
```

OUTPUT

```
3. True
```

Solution

PYTHON

```python
print('4.', (25 % a**2) > b)
```

OUTPUT

```
4. False
```

Solution

PYTHON

```python
print('5.', (25 % a**2) > b or (25 % b) < a)
```

OUTPUT

```
5. False
```

Solution

PYTHON

```python
print('6.', (25 % a**2) < b and (25 % b) > a)
```

OUTPUT

```
6. True
```

Solution

PYTHON

```python
print('7.', (12 / a) and (a * 4) < b)
```

OUTPUT

```
7. True
```

Exercises

END OF CHAPTER EXERCISES

1. Write and execute a Python code to display your own name as an output in the Terminal.
2. Write and execute a Python code that:

- Displays the text: `Please press enter to continue...`, and waits for the user to press enter.
- Once the user presses enter, the program should display `Welcome to my programme!` before terminating.

3. We have an enzyme whose reaction velocity is $v=50~mol \cdot L^{-1} \cdot s^{-1}$ at the substrate concentration of $[S] = K_{m} = 2.5~mol \cdot L^{-1}$. Work out the maximum reaction velocity or $V_{\max}$ for this enzyme using the Michaelis-Menten equation:

   $$v = \frac{V_{\max} [\textrm{S}]}{K_{m} + [\textrm{S}]}$$

Solution

KEY POINTS

- Two key functions for I/O operations are `print()` and `input()`
- Three most commonly used variables such as `int`, `float`, and `str`.
- Variable scope can be local or global depending where they are being used.
- Mathematical operations follow conventional rules of precedence
- Logical operations provide results in Boolean (True or False)

Content from Conditional Statements

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OVERVIEW

Questions

- What are conditional statements?
- How conditional statements are used to make decisions?
- Why indentation is so important in Python?
- Is there any hierarchical importance of conditional statements?

Objectives

- Understand the logic behind using conditional statements.
- Practice conditional statements.
- Learning structuring code using correct indentation.
- Understanding the hierarchy of conditional statements.

This chapter assumes that you are familiar with the following concepts in Python 3:

CHECKLIST

- ☑I/O Operations
- ☑Variables And Types
- ☑Mathematical Operation

When we construct logical expressions, we almost always do so because we need to test something. The definition of a process through which we test our logical expressions and provide directives on how to proceed is known in computer science as a *conditional statement*. Conditional statements are a feature of programming languages. This means that although their definitions and grammar may vary slightly from one programming language to another, their principles are almost universally identical.

Being a high-level programming language, defining conditional statements is very easy in Python. Before we start, however, let us briefly review the way conditional statements actually work. To help us with that, we use flowchart diagrams.

REMEMBER

The term *conditional statements* is often used in relation to imperative programming languages. In functional programming, however, it is more common to refer to them as *conditional expressions* or *conditional constructs*. Python supports both imperative and functional programming.

EXAMPLE: ALGORITHMS IN DAILY LIFE

We use algorithms in our life every day without realising it.

Suppose we enter a room poorly lit room to work. The first things that we notice is that the room is insufficiently lit. We check to see whether or not the light is on; *if* not, we find the switch to turn on the light. Likewise, *if* the light is on, we go ahead and turn on the desk lamp before we proceed with our business.

PROCESSES OF ALGORITHMS

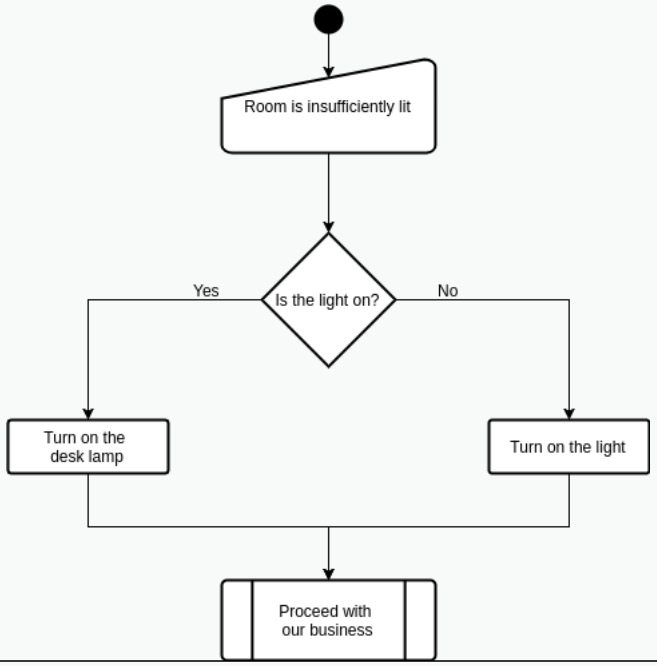
This scenario may be perceived as a set of processes. These processes include a set of procedures that may be outlined as follows:

1. `Action`: Enter the room.
2. `Input`: Determine that the room is insufficiently lit.
3. `Condition`: Is the light switched on?

- NO: `Action`: turn on the lights,
- YES: `Action`: turn on the desk lamp.

4. `Action`: Proceed with our business.

Now that we know what procedures are involved, we can draw a flowchart of the process:



Flowchart

Programming is not merely a hard skill. It is the door to a different way of thinking that enables one to break complex procedures down to simple, stepwise components and tasks. Flowcharts help us perceive processes as computers do — that is, one task or component at a time. As we progress in programming, our brains develop the ability to think in a procedural way. This is called *algorithmic thinking*, and is one of the most important soft-skills that a programmer can develop.

There are international competitions and comprehensive courses dedicated to this concept. At the end of the day, however, one can only acquire a skill through practice.

ADVANCED TOPIC

If you are keen to learn more about algorithms and algorithmic thinking, or just want to try out some of the problems, you may want to look into some of the past competition papers on Computational and Algorithmic Thinking (CAT) published by the Australian Mathematics Trust.

Exercise is provided to give you an idea of the type of problems that may be tackled in a procedural way.

PRACTICE EXERCISE 1

On a distant planet, the dominant carnivore, the zab, is nearing extinction. The number of zabs born in any year is one more than the (positive) difference between the number born in the previous year and the number born in the year before that.

Examples

- If 7 zabs were born last year and 5 the year before, 3 would be born this year.
- If 7 zabs were born last year and 10 the year before, 4 would be born this year.

If 2 zabs were born in the year 2000 and 9 zabs were born in 2001. What is the first year after 2000 when just 1 zab will be born?

a. 2009

b. 2011

c. 2013

d. 2015

e. 2017

Credit: This question is taken from the 2011 Computational and Algorithmic Thinking (CAT) Competition held by the Australian Mathematics Trust.}

Solution

To obtain the answer, we may write an algorithm in a pseudo-code format as follows:

```
  let a_total = 2

  let b_total = 9

  let current_total = absolute(a_total - b_total) + 1

  let a_total = b_total

  let b_total = current_total

  let current_year = 2002


  do {

    current_total = absolute(a_total - b_total) + 1

    a_total = b_total

    b_total = current_total

    current_year = current_year + 1

                } while current_total > 1


display current_year
```

Given:

```
  year = 2000; a_total = 2
  year = 2001; b_total= 9
```

the above process with repeat the section written in curly brackets for as long as current_total > 1:

```
  current_year: 2002; a_total = 2, b_total = 9, current_total = 8

Is current_total > 1 ? Yes:

  current_year: 2003; a_total = 9, b_total = 8; current_total = 2

Is current_total > 1 ? Yes:

  current_year: 2004; a_total = 8; b_total = 2; current_total = 7

Is current_total > 1 ? Yes:

  current_year: 2005; a_total = 2; b_total = 7; current_total = 6

Is current_total > 1 ? Yes:

  current_year: 2006; a_total = 7; b_total = 6; current_total = 2

Is current_total > 1 ? Yes:
```

```
  current_year: 2007; a_total = 6; b_total = 2; current_total = 5

Is current_total > 1 ? Yes:

  current_year: 2008; a_total = 2; b_total = 5; current_total = 4

Is current_total > 1 ? Yes:

  current_year: 2009; a_total = 5; b_total = 4; current_total = 2

Is current_total > 1 ? Yes:

  current_year: 2010; a_total = 4; b_total = 2; current_total = 3

Is current_total > 1 ? Yes:

  current_year: 2011; a_total = 2; b_total = 3; current_total = 2

Is current_total > 1 ? Yes:

  current_year: 2012; a_total = 3; b_total = 2; current_total = 2

Is current_total > 1 ? Yes:

  current_year: 2013; a_total = 2; b_total = 2; current_total = 1

Is current_total > 1 ? No:
```

The correct answer is **c)** 2013.

If this algorithm/pseudo-code is translated to Python language, it will look like this:

PYTHON

```python
a_total = 2

b_total = 9

current_year = 2002

current_total = abs(a_total - b_total) + 1
a_total = b_total
b_total = current_total

while (current_total > 1):
    current_total = abs(a_total - b_total) + 1
    a_total = b_total
    b_total = current_total
    current_year = current_year + 1

print(current_year)
```

OUTPUT

```
2013
```

REMEMBER

There is almost always more than one answer to any algorithmic problem; some answer might even be more efficient than other. The less repetition there is, the better more efficient an algorithm is considered to be.

Conditions in Python

`if` statments

To implement conditional statements in Python, we use 3 syntaxes:

- To initiate the statement, we use the syntax `if` followed by the condition and a colon;

PYTHON

```python
students_present = 15

# Conditional statement:
if students_present > 10:  # Initiation
    # Directive (must be indented).
    print('More than 10 students are present.')
```

OUTPUT

```
More than 10 students are present.
```

- To create an alternative condition after the first condition has been defined, we use the syntax `elif` followed by the new condition and a colon;

PYTHON

```python
students_present = 5

# Conditional statement:
if students_present > 10:  # Initiation

    # Directive (must be indented).
    print('More than 10 students are present.')

elif 0 < students_present < 10:
    print('Less than 10 students are present.')
```

OUTPUT

```
Less than 10 students are present.
```

- To introduce a default — i.e. where none of the above are `True`, we use the syntax `else`.

PYTHON

```python
students_present = 0

# Conditional statement:
if students_present > 10:  # Initiation
    # Directive (must be indented).
    print('More than 10 students are present.')

elif 0 < students_present < 10:  # Alternative condition
    # Alternative directive (must be indented).
    print('Less than 10 students are present.')

else:  # Default (none of the conditions are met).
    # Directive (must be indented).
    print('There is no one!')
```

OUTPUT

```
There is no one!
```

REMEMBER

We can use disjunctions or conjunctions, as discussed in topic Disjunctions and Conjunctions, to test for more than one condition at a time.

Indentation Rule

PEP-8: Indentation

Always use 4 spaces for indentation. Indentations are how the Python interpreter determines the code hierarchy. A consistent hierarchy is therefore essential for the interpreter to parse and execute our code.

The indented part of the code is known as a *block*. A block represents a part of the code that always "belongs" to (is the child process of) the first *un*indented (dedented) line that precedes it. In other words, the action(s) within a conditional statement (actions that are subject to a specific condition) must always be *indented*:

PYTHON

```python
value = 10

# Statement A:
if value > 0:

    # First dedented line before the block.
    # This is a block, and it belongs to the
    # preceding "if" (Statement A):
    print('The value is positive.')

    # We can have nested blocks too.
    # Statement B:
    if value > 9:
    # First dedented line before the block.
    # This is another block (nested).
    # This block belongs to the preceding "if" (Statement B).
        print('The value is not a single digit.')

    # Introducing a default behaviour for Statement B:
    else:
    # This block belongs to the preceding "else".
        print('The value is a single digit.')

# Introducing an alternative condition for Statement A:
elif value < 0:
# This block belongs to the preceding "elif".
    print('The value is negative.')

# Introducing a default behaviour for Statement A:
else:
# This block belongs to the preceding "else".
    print('The value is zero.')
```

OUTPUT

```
The value is positive.
The value is not a single digit.
```

It is not a good practice to have too many nested indentation. This would make the code more difficult to read. A rule of thumb is that you should not need more than 4 nested indentations in your code. If you do, you should reconsider the code structure to somehow simplify the process.

On that note, where possible, it is better to use conjunctions and disjunctions, or implement alternative conditions using `elif` instead of creating nested conditional statements. We can therefore restructure the previous example in a better, more coherent way as follows:

PYTHON

```python
value = 10

if value > 9:
  print('The value is positive.')
  print('The value is not a single digit.')
elif value > 0:
  print('The value is positive.')
  print('The value is a single digit.')
elif value < 0:
  print('The value is negative.')
else:
  print('The value is zero.')
```

OUTPUT

```
The value is positive.
The value is not a single digit.
```

It is customary and also best practice to use 4 spaces for indentation in Python. It is also paramount that all indentations throughout the code are consistent; that is, you may not use 4 spaces here and 3 spaces somewhere else in your code. Doing so will cause an `IndentationError` to be raised. It is recommended to *not* use `Tab` to indent your code; it is regarded as a bad practice in Python.

```
value = 10

if value > 0:
    print('The value is: ')  # Indented with 4 spaces.
   print('POSITIVE.')  # Indented with 3 spaces.
```

```
File <STDIN>, line 5
    print('POSITIVE.')  # Indented with 3 spaces.
                                                  ^
IndentationError: unindent does not match any outer indentation level
```

CALLOUT

`Tab` indentations represent different number of spaces on different computers and operating systems. It is therefore more than likely that they will lead to `IndentationError`. Additionally, Python 3 disallows the mixing of **tab** and **space** indentations. Some Python IDEs such as *PyCharm* automatically convert `Tab` indentations to 4 spaces. Some other IDEs (e.g. Jupyter) typically highlight `Tab` indentations to explicitly distinguish them and thereby notify the programmer of their existence. However, more often than not, IDEs and text editors tend to *ignore* this, which amounts to inconsistencies and subsequently `IndentationError`. This is a very common difficulty that new Python programmers face, and can be very confusing if not handled correctly.

PRACTICE EXERCISE 2

In previous chapter, Practice Exercise 11, we explored the implication of `CAG` repeats in Huntington's disease. We also created a polynucleotide chain containing 36 repetition of the `CAG` codons.

Write a conditional statement that tests the length of a polyQ tract to determine the *classification* and the *disease status* based on the following Table:

Number of repeats	Classification	Disease Status
< 26	Normal	Unaffected
27 — 35	Intermediate	Unaffected
36 — 40	Reduced Penetrance	+/- Affected
> 40	Full Penetrance	Affected

Using the technique you used in Practice Exercise 11, create 5 polyQ tracts containing 26, 15, 39, 32, 36, and 54 codons. Use these polynucleotide chains to test your conditional statement.

Display the result for each chain in the following format:

```
PolyQ chain with XXX number of CAG codons:
Status: XXX
Classification: XXX
```

Hint: The length of a polyQ tract represents the number of nucleotides, not the number of `CAG` codons. See task 4 of Practice Exercise 11 for additional information.

Solution

PYTHON

```python
#Constructing the codons:

glutamine_codon = 'CAG'

polyq_codons = glutamine_codon * 26


#Determining the length of our codon:

signle_codon = len('CAG')

len_polyq = len(polyq_codons)

polyq = len_polyq / signle_codon

#Constructing the conditional statement:

NORMAL = 26
INTERMEDIATE = 35
REDUCED_PENETRANCE = 40

classification = str()
status = str()

if polyq < NORMAL:

    classification, status = 'Normal', 'Unaffected'

elif polyq <= INTERMEDIATE:

    classification, status = 'Intermediate', 'Unaffected'

elif polyq <= REDUCED_PENETRANCE:
    classification, status = 'Reduced Penetrance', '+/- Affected'

else:
    classification, status = 'Full Penetrance', 'Affected'


#Displaying the results:

print('PolyQ chain with', polyq, 'number of CAG codons:')
print('Classification:', classification)
print('Status:', status)

#Repeat this with 15, 39, 32, 36, and 54 codons.
```

OUTPUT

```
PolyQ chain with 26.0 number of CAG codons:
Classification: Intermediate
Status: Unaffected
```

Hierarchy of conditional statements

The hierarchy of conditional statement is always the same. We start the statement with an `if` syntax (initiation). This is the only essential part to implement a conditional statement. Other parts include the `elif` and the `else` syntaxes. These are the non-essential part, and we implement these as and when needed. It is, however, important that we adhere to the correct order when we implement these:

- *Always* start with the initiation syntax `if`.
- *Where needed,* implement as many alternative conditions as necessary `elif`.
- *Where needed,* implement a default behaviour using `else`}.

In an `if...elif...else` hierarchy, once one condition in the hierarchy is `True`, all *subsequent* conditions in that group are skipped and would no longer be checked.

In the following example, the first condition is `True`, therefore its corresponding block is executed and the rest of this conditional statement is skipped:

PYTHON

```python
TATA_BOX = 'TATA'

promoter_region = 'GTAACTGTGGTATAATCGT'

if TATA_BOX in promoter_region:
    # This condition is "True", so this
    # and only this block is executed.
    print('There is a "TATA" box in this promoter region.')
else:
    # The last condition was "False", so this
    # block is skipped.
    print('There is no "TATA" box in this promoter region.')
```

OUTPUT

```
There is a "TATA" box in this promoter region.
```

REMEMBER

We already know from subsection Logical Operations that the value of a *boolean* (`bool`) variable is either `False` or `True`.

We have also learned that in conditional statements, we use *double* equals} or `... == ...` to test for equivalence. So naturally, one could test for the *truth value* of a `bool` variables as follows:

PYTHON

```python
variable = False

if variable == False:
    print('The variable is False.')
```

OUTPUT

```
The variable is False.
```

This works, and it looks simple enough. However, this is the **wrong approach** for testing the value of `bool` variables and should *not* be used. Whilst the answer is correct in the above example, using *double equals* for testing *boolean* variables can sometimes produce incorrect results.

The correct way to test the *truth value* of a *boolean* variable is by using `is` as follows:

PYTHON

```python
variable = False

if variable is False:
    print('The variable is False.')
```

OUTPUT

```
The variable is False.
```

and the negative test is:

PYTHON

```python
variable = True

if variable is not False:

    print('The variable is True.')
```

OUTPUT

```
The variable is True.
```

> In short; as far as *boolean* variables are concerned, we should always use `is` or `is not` to test for their *truth value* in a conditional statement.

Consequently, we can now write the example algorithm (room and light) as follows:

PYTHON

```python
light_status = False

if light_status is True:

    action = 'The light is on; you may want to turn off the desk light.'

else:
    action = 'The light is off... turn it on.'

print(action)
```

OUTPUT

```
The light is off... turn it on.
```

There are a few very popular shorthands in Python that you should be familiar with when writing or reading conditional statements:

In an `if` statement, Python expects the result of the condition to be `True`. As result of that, we can simplify the above example as follows:

PYTHON

```python
light_status = False

if light_status:

    action = 'The light is on; you may want to turn off the desk light.'

else:

    action = 'The light is off... turn it on.'

print(action)
```

OUTPUT

```
The light is off... turn it on.
```

Sometime, however, we might need to test for a `False` outcome. To do so, we can write a negated conditions as described in subsection Negation instead:

PYTHON

```python
# Note that we have changed the order of the condition
# and added a "not" before "light_status"
if not light_status:

    action = 'The light is off... turn it on.'

else:

    action = 'The light is on; you may want to turn off the desk light.'

print(action)
```

OUTPUT

```
The light is off... turn it on.
```

EXAMPLE: A FAMILIAR SCENARIO

Suppose we want to determine the classification of the final mark for a student.

The classification protocol is as follows:

- Above 70%: First class.
- Between 60% and 70%: Second class (upper division).
- Between 50% and 60%: Second class (lower division).
- Between 40% and 50%: Pass.
- Below 40%: Fail.

PYTHON

```python
mark = 63

# Thresholds
first = 70
second_upper = 60
second_lower = 50
passed = 40  # "pass" is a syntax in Python.

if mark >= first:
    classification = 'First Class'
elif mark >= second_upper:
    classification = 'Second Class (upper division)'
elif mark >= second_lower:
    classification = 'Second Class (lower division)'
elif mark >= passed:
    classification = 'Pass'
else:
    classification = 'Fail'

print('The student obtained a', classification, 'in their studies.')
```

OUTPUT

```
The student obtained a Second Class (upper division) in their studies.
```

Exercises

END OF CHAPTER EXERCISES

1. Protein Kinases have a phosphorylation site and a consensus sequence has been determined for these sites (Rust and Thompson, 2012). All the proteins incorporate either a Serine or a Threonine residue that gets phosphorylated. Naturally, the consensus sequence for each protein varies slightly from that of other proteins.

When studying a polypeptide in the lab, a colleague realised that it has a phosphorylated Serine. So they tried to sequence the polypeptide, and managed to obtain a sequence for the protein:

```
kinase_peptide = (
        "PVWNETFVFNLKPGDVERRLSVEVWDWDRTSRNDFMGAMSFGVSELLK"
        "APVDGWYKLLNQEEGEYYNVPVADADNCSLLQKFEACNYPLELYERVR"
        "MGPSSSPIPSPSPSPTDPKRCFFGASPGRLHISDFSFLMRRRKGSFGK"
        "VMLAERRGSDELYAIKILKKDVIVQDDDVDCTLVEKRVLALGGRGPGG"
        "RPHFLTQLHSTFQTPDRLYFVMEYVTGGDLMYHIQQLGKFKEPHAAFY"
        "AAEIAIGLFFLHNQGIIYRDLKLDNVMLDAEGHIKITDFGMCKENVF"
                )
```

Desperate to find a match, and knowing that we are good at doing `computer stuff`, they asked us if we can help them identify what protein kinase does the sequence correspond to?

So we extract the consensus sequence of 3 protein kinases from the paper:

- PKC-\(\eta\): either `RKGSFRR` or `RRRSFRR`
- PKC-\(\gamma\): either `RRRKGSF` or `RRRKKSF`
- DMPK-E: one of `KKRRRSL`, `RKRRRSL`, `KKRRRSV`, or `RKRRRSV`.

Now all we need is to write a conditional statement in Python to identify which of the above protein kinases, if any, does our sequence correspond to. That is, which one of the consensus peptides exists in our mystery sequence?

If there is a match, our programme should display the name of the corresponding protein kinase; otherwise, it should say `No matches found` for good measures.

Solution

KEY POINTS

- Python used `if, elif and else` as conditional statements.
- In Python, there is an indentation rule of 4 spaces.
- The hierarchy of conditional statement is always the same.

Content from Introduction to Arrays

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Mandatory Lesson Feedback Survey

OVERVIEW

Questions

- What are the different types of arrays?
- How is data stored and retrieved from an array?
- What are nested arrays?
- What are tuples?

Objectives

- Understanding difference between lists and tuples.
- Understanding operations on arrays.
- Storing multidimensional data.
- Understanding the concepts of mutability and immutability.

Arrays: Nested Arrays in Python

Arrays: Numpy Arrays in Python

PREREQUISITE

- Variables and Types
- Logical Operations
- Conditional Statements

So far, we have been using variables to store individual values. In some circumstances, we may need to access multiple values in order to perform operations. On such occasions, defining a variable for every single value can become very tedious. To address this, we use **arrays**.

Arrays are variables that hold any number of values. Python provides three types of built-in arrays. These are: `list`, `tuple`, and `set`. There are a several common features among all arrays in Python; however, each type of array enjoys its own range of unique features that facilitates specific operations.

REMEMBER

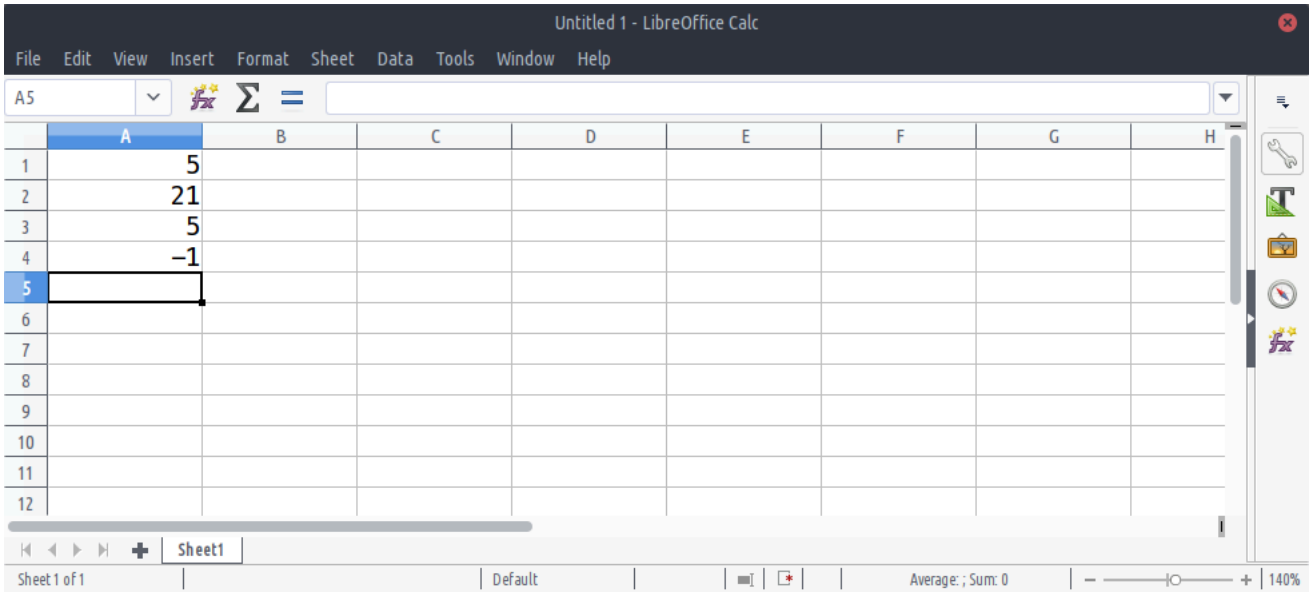
Each item inside an array may be referred to as an *item* or a *member* of that array.

Lists

Resource for Lists

Lists are the most frequently-used type of arrays in Python. It is therefore important to understand how they work, and how can we use them, and the features they offer, to our advantage.

The easiest way to imagine how a `list` works, is to think of it as a table that can have any number of rows. This is akin to a spreadsheet with one column. For instance, suppose we have a table with four rows in a spreadsheet application, as follows:



The number of rows in an array determines its *length*. The above table has four rows; therefore it is said to have a *length* of 4.

Implementation

REMEMBER

In order to implement a `list` in Python, we place values into this list and separate them from one another using commas inside **square brackets**: list = [1,2,3].

PYTHON

```python
table = [5, 21, 5, -1]

print(table)
```

OUTPUT

```
[5, 21, 5, -1]
```

PYTHON

```python
print(type(table))
```

OUTPUT

```
<class 'list'>
```

PRACTICE EXERCISE 1

Implement a `list` array called fibonacci, whose members represent the first 8 numbers of the Fibonacci sequence as follows:

FIBONACCI NUMBERS (FIRST 8)							
1	1	2	3	5	8	13	21

Solution

PYTHON

```python
fibonacci = [1, 1, 2, 3, 5, 8, 13, 21]
```

Indexing

In an array, an index is an integer (whole number) that corresponds to a specific item in that array.

You can think of an index as a *unique reference* or *key* that corresponds to a specific row in a table. We don't always write the row number when we create a table. However, we always know that the third row of a table refers to us starting from the first row (row #1), counting three rows down and there we find the third row.

Python, however, uses what we term **zero-based** indexing. We don't count the first row as row #1; instead, we consider it to be row #0. As a consequence of starting from #0, we count rows in our table down to row #2 instead of #3 to find the third row. So our table may,essentially, be visualised as follows:

Index	Value
0	5
1	21
2	5
3	-1

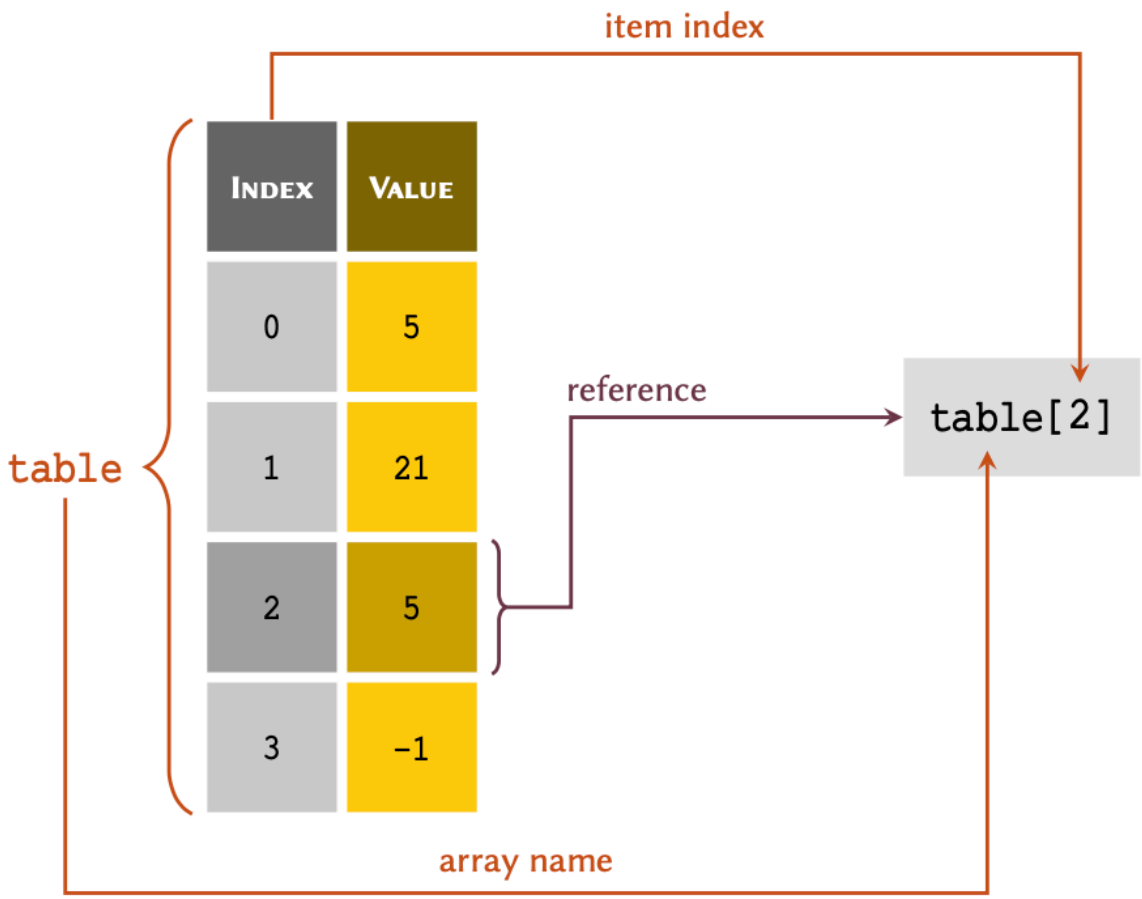
> REMEMBER
>
> Python uses **zero-based** indexing system. This means that the first row of an array, regardless of its type, is always referred to with index #0.

With that in mind, we can use the index for each item in the list, in order to retrieve it from a `list`.

Given the following `list` of four members stored in a variable called table:

```
table = [5, 21, 5, -1]
```

we can visualise the referencing protocol in Python as follows:



As illustrated in this figure; in order to retrieve a member of an array through its index, we write the name of the variable immediately followed by the index value inside a pair of square brackets — *e.g.* table[2]. Note, you may have noticed our interchangeable use of the terms 'list' and 'array'. That is because a list, in Python, can be considered as a type of dynamic array (they can increase or decrease in size, as required).

PYTHON

```python
print(table[2])
```

OUTPUT

```
5
```

PYTHON

```python
print(table[0])
```

OUTPUT

```
5
```

PYTHON

```python
item = table[3]

print(item)
```

OUTPUT

```
-1
```

PRACTICE EXERCISE 2

Retrieve and display the 5th Fibonacci number from the `list` you created in the previous Practice Exercise 1.

Solution

PYTHON

```python
print(fibonacci[4])
```

OUTPUT

```
5
```

It is sometimes more convenient to index an array, backwards — that is, to reference the members from the bottom of the array, first. This is termed **negative indexing**, and is particularly useful when we are dealing with lengthy arrays. The indexing system in Python support both positive and negative indexing systems.

The table above therefore may also be represented, as follows:

Index		Value
−4	0	5
−3	1	21
−2	2	5
−1	3	−1

REMEMBER

Unlike the normal indexing system, which starts from #0, negative indexes start from #-1. This serves to definitely highlight which indexing system is being used.

If the index is a negative number, the indices are counted from the end of the `list`. We can implement negative indices in the same way as positive indices:

PYTHON

```python
print(table[-1])
```

OUTPUT

```
-1
```

PYTHON

```python
print(table[-2])
```

OUTPUT

```
5
```

PYTHON

```python
print(table[-3])
```

OUTPUT

```
21
```

We know that in table, index #-3 refers the same value as index #1. So let us go ahead and test this:

PYTHON

```python
equivalence = table[-3] == table[1]

print(equivalence)
```

OUTPUT

```
True
```

If the index requested is larger than the length of the `list` minus one, an `IndexError` will be raised:

PYTHON

```python
print(table[4])
```

OUTPUT

```
IndexError: list index out of range
```

REMEMBER

The values stored in a `list` may be referred to as the **members** of that `list`.

PRACTICE EXERCISE 3

Retrieve and display the *last* Fibonacci number from the `list` you created in Practice Exercise 1.

Solution

PYTHON

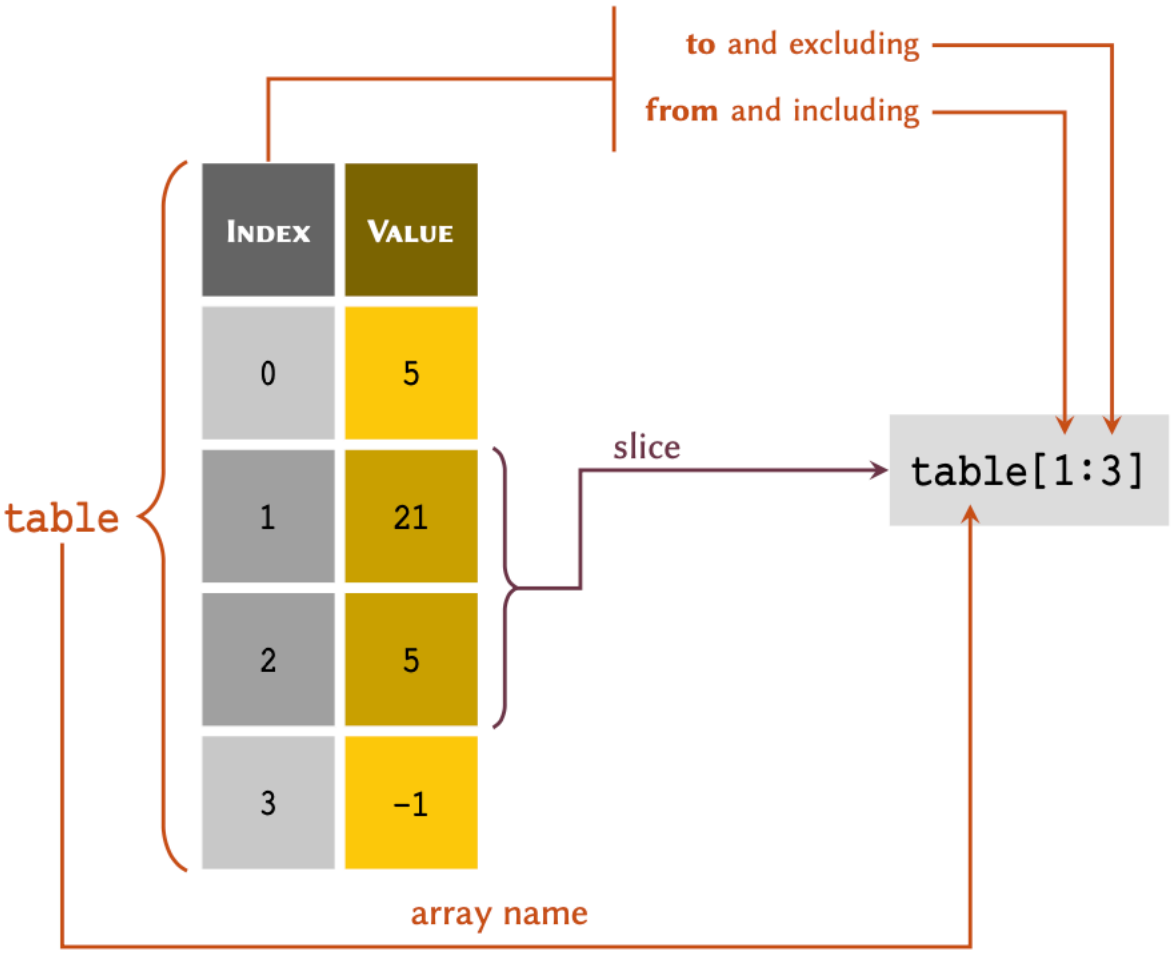
```python
print(fibonacci[-1])
```

OUTPUT

```
21
```

Slicing

It is also possible that you may wish to retrieve more than one value from a `list` at a time, as long as the values are in *consecutive* rows. This process is is termed , and may be visualised, as follows:



REMEMBER

Python is a **non-inclusive** language. This means that in table[a:b], a *slice* includes all the values from, and including index a right down to, but *excluding*, index b.

Given a `list` representing the above table:

```
table = [5, 21, 5, -1]
```

we may retrieve a slice of table, as follows:

PYTHON

```python
my_slice = table[1:3]

print(my_slice)
```

OUTPUT

```
[21, 5]
```

```python
print(table[0:2])
```

If the first index of a slice is #0, the slice may also be written as:

PYTHON

```python
print(table[:2])
```

OUTPUT

```
[5, 21]
```

Negative slicing is also possible:

PYTHON

```python
# Retrieves every item from the first member down
# to, but excluding the last one:
print(table[:-1])
```

OUTPUT

```
[5, 21, 5]
```

PYTHON

```python
print(table[1:-2])
```

OUTPUT

```
[21]
```

If the second index of a slice represents the last index of a `list`, it would be written as:

PYTHON

```python
print(table[2:])
```

OUTPUT

```
[5, -1]
```

PYTHON

```python
print(table[-3:])
```

OUTPUT

```
[21, 5, -1]
```

We may also store indices and slices in variables:

PYTHON

```python
start, end = 1, 3
new_table = table[start:end]

print(new_table)
```

OUTPUT

```
[21, 5]
```

The `slice()` function may also be used to create a slice variable:

PYTHON

```python
my_slice = slice(1, 3)

print(table[my_slice])
```

OUTPUT

```
[21, 5]
```

PRACTICE EXERCISE 4

Retrieve and display a slice of Fibonacci numbers from the `list` you created in Practice Exercise 1 that includes all the members from the second number onwards — *i.e.* the slice must not include the first value in the `list`.

Solution

PYTHON

```python
print(fibonacci[1:])
```

OUTPUT

```
[1, 2, 3, 5, 8, 13, 21]
```

NOTE

Methods are features of Object-Oriented Programming (OOP) - a programming paradigm that we do not discuss in the context of this course. You can think of a *method* as a *function* that is associated with a specific *type*. The job of a *method* is to provide a certain functionality unique to the *type* it is associated with. In this case, `.index()` is a *method* of type `list` that, given a value, finds and produces its index from the `list`.

From value to index

Given a `list` entitled table as:

PYTHON

```python
table = [5, 21, 5, -1]
```

we can also determine the index of a specific value. To do so, we use the `.index()` *method*:

PYTHON

```python
print(table.index(21))
```

OUTPUT

```
1
```

PYTHON

```python
last_item = table.index(-1)

print(last_item)
```

OUTPUT

```
3
```

If a value is repeated more than once in the `list`, the index corresponding to the *first* instance of that value is returned:

PYTHON

```python
print(table.index(5))
```

OUTPUT

```
0
```

If a value does *not* exist in the `list`, using `.index()` will raise a `ValueError`:

PYTHON

```python
print(table.index(9))
```

OUTPUT

```
ValueError: 9 is not in list
```

PRACTICE EXERCISE 5

Find and display the index of these values from the `list` of Fibonacci numbers that you created in Practice Exercise 1:

- 1
- 5
- 21

Solution

PYTHON

```python
print(fibonacci.index(1))

print(fibonacci.index(5))

print(fibonacci.index(21))
```

OUTPUT

```
0
4
7
```

Mutability

Mutability is a term that we use to refer to a structure's capability of being change, once it is created. Arrays of type `list` are *modifiable*. That is, we can add new values, change the existing ones or remove them from the array, altogether. Variable types that allow their contents to be modified are referred to as *mutable types* in programming.

Addition of new members

Given a `list` called table, we can add new values to it using `.append()`:

PYTHON

```python
table.append(29)

print(table)
```

OUTPUT

```
[5, 21, 5, -1, 29]
```

PYTHON

```python
table.append('a text')

print(table)
```

OUTPUT

```
[5, 21, 5, -1, 29, 'a text']
```

Sometimes, it may be necessary to insert a value at a specific position or index in a `list`. To do so, we may use `.insert()`, which takes two input arguments; the first representing the index, and the second the value to be inserted:

PYTHON

```python
table.insert(3, 56)

print(table)
```

OUTPUT

```
[5, 21, 5, 56, -1, 29, 'a text']
```

PRACTICE EXERCISE 6

Given fibonacci - the `list` representing the first 8 numbers in the Fibonacci sequence that you created in Practice Exercise 1:

1. The 10th number in the Fibonacci sequence is 55. Add this value to fibonacci.
2. Now that you have added 55 to the `list`, it no longer provides a correct representation of the Fibonacci sequence. Alter fibonacci and insert the missing number such that the list correctly represents the first 10 numbers in the Fibonacci sequence, as follows:

FIBONACCI NUMBERS (FIRST 8)									
1	1	2	3	5	8	13	21	34	55

Solution

PYTHON

```python
fibonacci.append(55)
```

Solution

PYTHON

```python
fibonacci.insert(8, 34)
```

Modification of members

Given a `list` as:

PYTHON

```python
table = [5, 21, 5, 56, -1, 29, 'a text']
```

we can also modify the exiting value or values inside a `list`. This process is sometimes referred to as *item assignment*:

PYTHON

```python
# Changing the value of the 2nd member.

table[1] = 174

print(table)
```

OUTPUT

```
[5, 174, 5, 56, -1, 29, 'a text']
```

PYTHON

```python
table[-4] = 19

print(table)
```

OUTPUT

```
[5, 174, 5, 19, -1, 29, 'a text']
```

It is also possible to perform *item assignment* over a *slice* containing any number of values. Note that when modifying a slice, the replacement values must be *the same length* as the slice we are trying to replace:

PYTHON

```python
print('Before:', table)

replacement = [-38, 0]

print('Replacement length:', len(replacement))
print('Replacement length:', len(table[2:4]))

# The replacement process:
table[2:4] = replacement

print('After:', table)
```

OUTPUT

```
Before: [5, 174, 5, 19, -1, 29, 'a text']
Replacement length: 2
Replacement length: 2
After: [5, 174, -38, 0, -1, 29, 'a text']
```

PYTHON

```python
# Using the existing value to determine the new value:
table[2] = table[2] + 50

print(table)
```

OUTPUT

```
[5, 174, 12, 0, -1, 29, 'a text']
```

PRACTICE EXERCISE 7

Create a `list` containing the first 10 prime numbers as:

```python
primes = [2, 3, 5, 11, 7, 13, 17, 19, 23, 29]
```

Values 11 and 7, however, have been misplaced in the sequence. Correct the order by replacing the slice of primes that represents [11, 7] with [7, 11].

Solution

```python
primes = [2, 3, 5, 11, 7, 13, 17, 19, 23, 29]

primes[3:5] = [7, 11]
```

Removal of members

When removing a value from a `list`, we have two options depending on our needs: we either remove the member and retain the value in another variable, or we remove it and dispose of the value, completely.

To remove a value from a `list` without retaining it, we use `.remove()`. The method takes one input argument, which is the value we would like to remove from our `list`:

```python
table.remove(174)

print(table)
```

```
[5, 12, 0, -1, 29, 'a text']
```

Alternatively, we can use `del`; a Python syntax that we can use, in this context, to delete a specific member using its index:

```python
del table[-1]

print(table)
```

```
[5, 12, 0, -1, 29]
```

As established above, we can also delete a member and retain its value. Of course we can do so by holding the value inside another variable before deleting it.

Whilst this is a valid approach, Python's `list` provide us with `.pop()` to simplify the process even further. The method takes one input argument for the index of the member to be removed. It removes the member from the `list` and returns its value, so that we can retain it in a variable:

```python
removed_value = table.pop(2)

print('Removed value:', removed_value)
print(table)
```

OUTPUT

```
Removed value: 0
[5, 12, -1, 29]
```

PRACTICE EXERCISE 8

We know that the nucleotides of DNA include Adenosine, Cytosine, Threonine and Glutamine: A, C, T, and G.

Given a `list` representing a nucleotide sequence:

```
strand = ['A', 'C', 'G', 'G', 'C', 'M', 'T', 'A']
```

1. Find the index of the invalid nucleotide in strand.

2. Use the index you found to remove the invalid nucleotide from strand and retain the value in another variable. Display the result as:

```
Removed from the strand: X
New strand: [X, X, X, ...]
```

3. What do you think happens once we run the following code, and why? What would be the final result displayed on the screen?

```
strand.remove('G')

print(strand)
```

Solution

PYTHON

```python
strand = ['A', 'C', 'G', 'G', 'C', 'M', 'T', 'A']

outlier_index = strand.index('M')
```

Solution

PYTHON

```python
outlier_value = strand.pop(outlier_index)

print('Removed from the strand:', outlier_value)
print('New strand:', strand)
```

OUTPUT

```
Removed from the strand: M
New strand: ['A', 'C', 'G', 'G', 'C', 'T', 'A']
```

Solution

One of the two G nucleotides, the one at index 2 of the original array, is removed. This means that the `.remove()` method removes only *first* instance of a member in an array. The output would therefore be:

```
['A', 'C', 'G', 'C', 'M', 'T', 'A']
```

Method–mediated operations

We already know that *methods* are akin to functions that are associated with a specific type. In this subsection, we will be looking at how operations are performed using *methods*. We will not be introducing anything new, but will recapitulate what we already know from, but from different perspectives.

So far in this chapter, we have learned how to perform different operations on `list` arrays in Python. You may have noticed that some operations return a result that we can store in a variable, while others change the original value.

With that in mind, we can divide operations performed using *methods* into two general categories:

1. Operations that return a result *without* changing the original array:

PYTHON

```python
table = [1, 2, 3, 4]

index = table.index(3)

print(index)
print(table)
```

OUTPUT

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

2. Operations that use specific **methods** to *change* the original array, but do *not* necessarily return anything (in-place operations):

PYTHON

```python
table = [1, 2, 3, 4]

table.append(5)

print(table)
```

OUTPUT

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

If we attempt to store the output of an operation that does not a return result, and store this into a variable, the variable will be created, but its value will be set to `None`, by default:

PYTHON

```python
result = table.append(6)

print(result)
print(table)
```

OUTPUT

```
None
[1, 2, 3, 4, 5, 6]
```

It is important to know the difference between these types of operations. So as a rule of thumb, when we use *methods* to perform an operation, we can only change the original value if it is an instance of a *mutable* type. See Table to find out which of Python's built-in types are mutable.

The *methods* that are associated with *immutable* objects always return the results and do not provide the ability to alter the original value:

- In-place operation on a *mutable* object of type `list`:

PYTHON

```python
table = [5, 6, 7]

table.remove(6)

print(table)
```

OUTPUT

```
[5, 7]
```

- In-place operation on an *immutable* object of type `str`:

PYTHON

```python
string = '567'

string.remove(20)
```

OUTPUT

```
AttributeError: 'str' object has no attribute 'remove'
```

PYTHON

```python
print(string)
```

OUTPUT

```
567
```

- Normal operation on a *mutable* object of type `list`:

PYTHON

```python
table = [5, 6, 7]

ind = table.index(6)

print(ind)
```

OUTPUT

```
1
```

- Normal operation on a *mutable* object of type `list`:

PYTHON

```python
string = '567'

ind = string.index('6')

print(ind)
```

OUTPUT

```
1
```

List members

A `list` is a collection of members that are independent of each other. Each member has its own type, and is therefore subject to the properties and limitations of that type:

PYTHON

```python
table = [1, 2.1, 'abc']

print(type(table[0]))
print(type(table[1]))
print(type(table[2]))
```

OUTPUT

```
<class 'int'>
<class 'float'>
<class 'str'>
```

For instance, mathematical operations may be considered a feature of all numeric types demonstrated in Table. However, unless in specific circumstance described in subsection Non-numeric values, such operations do not apply to instance of type `str`.

PYTHON

```python
table = [1, 2.1, 'abc']

table[0] += 1
table[-1] += 'def'

print(table)
```

OUTPUT

```
[2, 2.1, 'abcdef']
```

A `list` in Python plays the role of a container that may incorporate *any number* of values. Thus far, we have learned how to handle individual members of a `list`. In this subsection, we will be looking at several techniques that help us address different circumstances where we look at a `list` from a 'wholist' perspective; that is, a container whose members are unknown to us.

Membership test

Membership test operations [advanced]

We can check to see whether or not a specific value is a member of a `list` using the operator syntax `in`:

PYTHON

```python
items = [1, 2.4, 'John', 5, 4]

print(2.4 in items)
```

OUTPUT

```
True
```

PYTHON

```python
print(3 in items)
```

OUTPUT

```
False
```

The results may be stored in a variable:

PYTHON

```python
has_five = 5 in items

print(has_five)
```

OUTPUT

```
True
```

Similar to any other logical expression, we can negate membership tests by using :

PYTHON

```python
expr = 10 not in items

print(expr)
```

OUTPUT

```
True
```

PYTHON

```python
expr = 5 not in items

print(expr)
```

OUTPUT

```
False
```

REMEMBER

When testing against `str values` — *i.e.* text; don't forget that in programming, operations involving texts are *always* case-sensitive.

PYTHON

```python
items = [1, 2.4, 'John', 5, 4]

john_capital = 'John'
john_small = 'john'

print(john_capital in items)
print(john_small in items)
```

OUTPUT

```
True
False
```

For *numeric* values, `int` and `float` may be used interchangeably:

PYTHON

```python
print(4 in items)
```

OUTPUT

```
True
```

PYTHON

```python
print(4.0 in items)
```

OUTPUT

```
True
```

Similar to other logical expression, membership tests may be incorporated into conditional statements:

PYTHON

```python
if 'John' in items:
    print('Hello John')
else:
    print('Hello')
```

OUTPUT

```
Hello John
```

PRACTICE EXERCISE 9

Given a `list` of randomly generated peptide sequences as:

PYTHON

```python
peptides = [
  'FAEKE', 'DMSGG', 'CMGFT', 'HVEFW', 'DCYFH', 'RDFDM', 'RTYRA',
  'PVTEQ', 'WITFR', 'SWANQ', 'PFELC', 'KSANR', 'EQKVL', 'SYALD',
  'FPNCF', 'SCDYK', 'MFRST', 'KFMII', 'NFYQC', 'LVKVR', 'PQKTF',
  'LTWFQ', 'EFAYE', 'GPCCQ', 'VFDYF', 'RYSAY', 'CCTCG', 'ECFMY',
  'CPNLY', 'CSMFW', 'NNVSR', 'SLNKF', 'CGRHC', 'LCQCS', 'AVERE',
  'MDKHQ', 'YHKTQ', 'HVRWD', 'YNFQW', 'MGCLY', 'CQCCL', 'ACQCL'
  ]
```

Determine whether or not each of the following sequences exist in peptides; and if so, what is their corresponding index:

- IVADH
- CMGFT
- DKAKL
- THGYP
- NNVSR

Display the results in the following format:

```
Sequence XXXXX was found at index XX
```

Solution

PYTHON

```python
sequence = "IVADH"
if sequence in peptides:
    index = peptides.index(sequence)
    print('Sequence', sequence, 'was found at index',  index)
```

Solution

PYTHON

```python
sequence = "CMGFT"
if sequence in peptides:
    index = peptides.index(sequence)
    print('Sequence', sequence, 'was found at index',  index)
```

OUTPUT

```
Sequence CMGFT was found at index 2
```

Solution

PYTHON

```python
sequence = "DKAKL"
if sequence in peptides:
    index = peptides.index(sequence)
    print('Sequence', sequence, 'was found at index',  index)
```

Solution

PYTHON

```python
sequence = "THGYP"
if sequence in peptides:
    index = peptides.index(sequence)
    print('Sequence', sequence, 'was found at index',  index)
```

Solution

PYTHON

```python
sequence = "NNVSR"
if sequence in peptides:
    index = peptides.index(sequence)
    print('Sequence', sequence, 'was found at index',  index)
```

OUTPUT

```
Sequence NNVSR was found at index 30
```

Length

Built-in functions: len

The number of members contained within a `list` defines its length. Similar to the length of `str` values as discussed in mathematical operations Practice Exercise 8 and Practice Exercise 11, we use the built-in function `len()` also to determine the length of a `list`:

PYTHON

```python
items = [1, 2.4, 'John', 5, 4]

print(len(items))
```

OUTPUT

```
5
```

PYTHON

```python
print(len([1, 5, 9]))
```

OUTPUT

```
3
```

The `len()` function *always* returns an integer value (`int`) equal to, or greater than, zero. We can store the length in a variable and use it in different mathematical or logical operations:

PYTHON

```python
table = [1, 2, 3, 4]
items_length = len(items)
table_length = len(table)

print(items_length + table_length)
```

OUTPUT

```
9
```

PYTHON

```python
print(len(table) > 2)
```

OUTPUT

```
True
```

We can also use the length of an array in conditional statements:

PYTHON

```python
students = ['Julia', 'John', 'Jane', 'Jack']
present = ['Julia', 'John', 'Jane', 'Jack', 'Janet']

if len(present) == len(students):
    print('All the students are here.')
else:
    print('One or more students are not here yet.')
```

OUTPUT

```
One or more students are not here yet.
```

REMEMBER

Both `in` and `len()` may be used in reference to any *type* of array or sequence in Python.

See Table to find out which of Python's built-in types are regarded as a sequence.

PRACTICE EXERCISE 10

Given the `list` of random peptides defined in Practice Exercise 9:

1. Define a `list` called overlaps, containing the sequences whose presence in peptides you previously confirmed in Practice Exercise 9.
2. Determine the length of peptides.
3. Determine the length of overlaps.

Display yours results as follows:

```
overlaps = ['XXXXX', 'XXXXX', ...]
Length of peptides: XX
Length of overlaps: XX
```

Solution

PYTHON

```python
overlaps = list()

sequence = "IVADH"
if sequence in peptides:
    overlaps.append(sequence)

sequence = "CMGFT"
if sequence in peptides:
    overlaps.append(sequence)

sequence = "DKAKL"
if sequence in peptides:
    overlaps.append(sequence)

sequence = "THGYP"
if sequence in peptides:
    overlaps.append(sequence)

sequence = "NNVSR"
if sequence in peptides:
    overlaps.append(sequence)

print('overlaps:', overlaps)
```

OUTPUT

```
overlaps: ['CMGFT', 'NNVSR']
```

Solution

PYTHON

```python
print('Length of peptides:', len(peptides))
```

OUTPUT

```
Length of peptides: 42
```

Solution

PYTHON

```python
print('Length of overlaps:', len(overlaps))
```

OUTPUT

```
Length of overlaps: 2
```

Weak References and Copies

In our discussion on mutability, we also explored some of the in-place operations such as `.remove()` and `.append()`, that we can use to modify an existing `list`. The use of these operations gives rise the following question: What if we need to perform an in-place operation, but also want to preserve the original array?

In such cases, we create a *deep copy* of the original array before we call the method and perform the operation.

Suppose we have:

PYTHON

```python
table_a = [1, 2, 3, 4]
```

A weak reference for table_a, also referred to as an alias or a symbolic link, may be defined as follows:

PYTHON

```python
table_b = table_a

print(table_a, table_b)
```

OUTPUT

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

Now if we perform an in-place operation on only *one* of the two variables (the original or the alias) as follows:

PYTHON

```python
table_a.append(5)
```

we will effectively change *both* of them:

PYTHON

```python
print(table_a, table_b)
```

OUTPUT

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

This is useful if we need to change the name of a variable under certain conditions to make our code more explicit and legible; however, it does *nothing* to preserve an actual copy of the original data.

To retain a copy of the original array, however, we must perform a *deep copy* as follows:

PYTHON

```python
table_c = table_b.copy()

print(table_b, table_c)
```

OUTPUT

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

where table_c represents a *deep copy* of table_b.

In this instance, performing an in-place operation on one variable would *not* have any impacts on the other:

PYTHON

```python
table_b.append(6)

print(table_a, table_b, table_c)
```

OUTPUT

```
[1, 2, 3, 4, 5, 6] [1, 2, 3, 4, 5, 6] [1, 2, 3, 4, 5]
```

where both the original array and its weak reference (table_a and table_b) changed without influencing the *deep copy* (table_c).

There is also a shorthand for the `.copy()` method to create a *deep copy*. As far as arrays of type `list` are concerned, writing:

```python
new_table = original_table[:]
```

is exactly the same as writing:

```python
new_table = original_table.copy()
```

Here is an example:

PYTHON

```python
table_a = ['a', 3, 'b']
table_b = table_a
table_c = table_a.copy()
table_d = table_a[:]

table_a[1] = 5

print(table_a, table_b, table_c, table_d)
```

OUTPUT

```
['a', 5, 'b'] ['a', 5, 'b'] ['a', 3, 'b'] ['a', 3, 'b']
```

Whilst both the original array and its weak reference (table_a and table_b) changed in this example; the *deep copies* (table_c and table_d) have remained unchanged.

PRACTICE EXERCISE 11

When defining a consensus sequence, it is common to include annotations to represent ambiguous amino acids. Four such annotations are as follows:

Residues		Annotation	
Names	**1-letter**	**3-letter**	**1-letter**
Any / Unknown	All	Xaa	X
Asparagine / Aspartic Acid	D / B	Asx	B
Glutamine / Glutamic Acid	E / Q	Glx	Z
Leucine / Isoleucine	I / L	Xle	J

Given a `list` of amino acids as:

PYTHON

```python
amino_acids = [
    'A', 'R', 'N', 'D', 'C', 'E', 'Q', 'G', 'H', 'I',
    'L', 'K', 'M', 'F', 'P', 'S', 'T', 'W', 'Y', 'V'
  ]
```

1. Use amino_acids to create an independent `list` called amino_acids_annotations that contains all the standard amino acids.
2. Add to amino_acids_annotations the **1-letter** annotations for the ambiguous amino acids, as outlined in the table.
3. Evaluate the lengths for amino_acids and amino_acids_annotations and retain the result in a new `list` called lengths.
4. Using logical operations, test the two values stored in lengths for equivalence and display the result as a boolean (`True` or `False`) output.

Solution

PYTHON

```python
amino_acid_annotations = amino_acids.copy()
```

Solution

PYTHON

```python
ambiguous_annotations = ['X', 'B', 'Z', 'J']

amino_acid_annotations.extend(ambiguous_annotations)
```

Solution

PYTHON

```python
lengths = [len(amino_acids), len(amino_acid_annotations)]
```

Solution

PYTHON

```python
equivalence = lengths[0] == lengths[1]

print(equivalence)
```

OUTPUT

```
False
```

Conversion to list

As highlighted earlier in this section, arrays in Python can contain any value - regardless of type. We can exploit this feature to extract some interesting information about the data we store in an array.

To that end, we can convert any sequence to a `list`. See Table to find out which of the built-in types in Python are considered to be a sequence.

Suppose we have the sequence for Protein Kinase A Gamma (catalytic) subunit for humans as follows:

PYTHON

```python
# Multiple lines of text may be split into
# several lines inside parentheses:

human_pka_gamma = (
  'MAAPAAATAMGNAPAKKDTEQEESVNEFLAKARGDFLYRWGNPAQNTASSDQFERLRTLGMGSFGRVMLV'
  'RHQETGGHYAMKILNKQKVVKMKQVEHILNEKRILQAIDFPFLVKLQFSFKDNSYLYLVMEYVPGGEMFS'
  'RLQRVGRFSEPHACFYAAQVVLAVQYLHSLDLIHRDLKPENLLIDQQGYLQVTDFGFAKRVKGRTWTLCG'
  'TPEYLAPEIILSKGYNKAVDWWALGVLIYEMAVGFPPFYADQPIQIYEKIVSGRVRFPSKLSSDLKDLLR'
  'SLLQVDLTKRFGNLRNGVGDIKNHKWFATTSWIAIYEKKVEAPFIPKYTGPGDASNFDDYEEEELRISIN'
  'EKCAKEFSEF'
        )

print(type(human_pka_gamma))
```

OUTPUT

```
<class 'str'>
```

We can now *convert* our sequence from its original type of `str` to `list` by using `list()` as a *function*. Doing so will automatically decompose the text down into individual characters:

PYTHON

```python
# The function "list" may be used to convert string
# variables into a list of characters:
pka_list = list(human_pka_gamma)

print(pka_list)
```

OUTPUT

```
['M', 'A', 'A', 'P', 'A', 'A', 'A', 'T', 'A', 'M', 'G', 'N', 'A', 'P', 'A', 'K', 'K', 'D', 'T', 'E', 'Q', 'E
```

PRACTICE EXERCISE 12

Ask the user to enter a sequence of single-letter amino acids in *lower case*. Convert the sequence to `list` and:

1. Count the number of serine and threonine residues and display the result in the following format:

```
Total number of serine residues: XX
Total number of threonine residues: XX
```

2. Check whether or not the sequence contains both serine and threonine residues:

- If it does, display:

```
The sequence contains both serine and threonine residues.
```

- if it does not, display:

```
The sequence does not contain both serine and threonine residues.
```

Solution

```python
sequence_str = input('Please enter a sequence of signle-letter amino acids in lower-case: ')

sequence = list(sequence_str)

ser_count = sequence.count('s')
thr_count = sequence.count('t')

print('Total number of serine residues:', ser_count)

print('Total number of threonine residues:', thr_count)
```

Solution

```
if ser_count > 0 and thr_count > 0:
    response_state = ''
else:
    response_state = 'not'

print(
    'The sequence does',
    'response_state',
    'contain both serine and threonine residues.'
                )
```

ADVANCED TOPIC

Generators represent a specific type in Python whose results are *not* immediately evaluated. A generator is a specific type of iterable (an object capable of returning elements, one at a time), that can return its items, lazily. This means that it generates values on the fly, and only as and when required in your program. Generators can be particularly useful when working with large datasets, where loading all the data into memory can be computationally expensive. Using genarators with such data, can help to process it in more manageable units.

Generators' lazy evaluation in functional programming is often used in the context of a `for-loop`: which we will explore in a later L2D lesson on iterations. We do not further explore generators on this course, but if you are interested to learn more, you can find plenty of information in the following official documentation.

Useful methods

Data Structures: More on Lists

In this subsection, we will be reviewing some of the useful and important *methods* that are associated with object of type `list`. We will make use of snippets of code that exemplify such *methods*, in practice. The linked cheatsheet of the *methods* associated with the built-in arrays in Python can be helpful.

Method	list	tuple	set
.append()	+		
.extend()	+		
.insert()	+		
.index()	+	+	
.sort()	+		
.reverse()	+		
.copy()	+		+
.clear()	+		+
.pop()	+		+
.count()	+	+	
.remove()	+		+
.add()			+
.intersection()			+
.difference()			+
.isdisjoint()			+
.issubset()			+
.issuperset()			+
.union()			+
.symmetric_difference()			+
.discard()			+
.update()			+

Common operations for list, tuple and set arrays in Python.

The *methods* outlined here are not individually described; however, at this point, you should be able to work out what they do by looking at their names and respective examples.

Count a specific value within a `list`:

PYTHON

```python
table_a = [1, 2, 2, 2]
table_b = [15, 16]

print(table_a.count(2))
```

OUTPUT

```
3
```

Extend a `list`:

PYTHON

```python
table_a = [1, 2, 2, 2]
table_b = [15, 16]

table_c = table_a.copy()  # deep copy.
table_c.extend(table_b)

print(table_a, table_b, table_c)
```

OUTPUT

```
[1, 2, 2, 2] [15, 16] [1, 2, 2, 2, 15, 16]
```

Extend a `list` by adding two lists to each other. Note: adding two lists to each other is *not* considered an in-place operation:

PYTHON

```python
table_a = [1, 2, 2, 2]
table_b = [15, 16]

table_c = table_a + table_b

print(table_a, table_b, table_c)
```

OUTPUT

```
[1, 2, 2, 2] [15, 16] [1, 2, 2, 2, 15, 16]
```

PYTHON

```python
table_a = [1, 2, 2, 2]
table_b = [15, 16]

table_c = table_a.copy()  # deep copy.
table_d = table_a + table_b

print(table_c == table_d)
```

OUTPUT

```
False
```

We can also reverse the values in a `list`. There are two methods for doing so. Being a generator means that the output of the function is not evaluated immediately; and instead, we get a generic output. The first of these two methods is:

1. Through an in-place operation using `.reverse()`

PYTHON

```python
table = [1, 2, 2, 2, 15, 16]
table.reverse()

print("Reversed:", table)
```

OUTPUT

```
Reversed: [16, 15, 2, 2, 2, 1]
```

2. And secondly, using `reversed()` - which is a built-in generator function.

PYTHON

```python
table = [1, 2, 2, 2, 15, 16]
table_rev = reversed(table)

print("Result:", table_rev)
print("Type:", type(table_rev))
```

OUTPUT

```
Result: <list_reverseiterator object at 0x7f951f886590>
Type: <class 'list_reverseiterator'>
```

We can, however, force the evaluation process by converting the generator results into a `list`:

PYTHON

```python
table_rev_evaluated = list(table_rev)

print('Evaluated:', table_rev_evaluated)
```

OUTPUT

```
Evaluated: [16, 15, 2, 2, 2, 1]
```

Members of a `list` may also be sorted in-place, as follows:

PYTHON

```python
table = [16, 2, 15, 1, 2, 2]
table.sort()

print("Sorted (ascending):", table)
```

OUTPUT

```
Sorted (ascending): [1, 2, 2, 2, 15, 16]
```

ADVANCED TOPIC

There is also a further function built into Python: `sorted()`. This works in a similar manner to `reversed()`. Also a generator function, it offers more advanced features that are beyond the scope of this course. You can find out more about it from the official documentation and examples.

The `.sort()` method takes an optional keyword argument entitled *reverse* (default: `False`). If set to `True`, the method will perform a descending sort:

PYTHON

```python
table = [16, 2, 15, 1, 2, 2]
table.sort(reverse=True)

print("Sorted (descending):", table)
```

OUTPUT

```
Sorted (descending): [16, 15, 2, 2, 2, 1]
```

We can also create an empty `list`, so that we can add members to it later in our code using `.append()`, or `.extend()` or other tools:

PYTHON

```python
table = list()

print(table)
```

OUTPUT

```
[]
```

PYTHON

```python
table.append(5)

print(table)
```

OUTPUT

```
[5]
```

PYTHON

```python
another_table = ['Jane', 'Janette']
table.extend(another_table)

print(another_table)
```

OUTPUT

```
['Jane', 'Janette']
```

PRACTICE EXERCISE 13

Create a `list`, and experiment with each of the methods provided in the above example. Try including members of different *types* in your `list`, and see how each of these methods behave.

Solution

This practice exercise was intended to encourage you to experiment with the methods outlined.

Nested Arrays

At this point, you should be comfortable with creating, handling and manipulating arrays of type `list`, in Python. It is important to have a foundational understanding of the principles outlined in this section so far, before starting to learn about *nested arrays*.

We have already established that arrays can contain any value - regardless of type. This means that they can also contain other arrays. An array that includes at least one member that is, itself, an array is referred to as a **nested array**. This can be thought of as a table with more than one column:

Index rows	Value		
0	1	2	3
1	4		
2	7	8	
Index columns	0	1	2

REMEMBER

Arrays can contain values of any *type*. This rule applies to nested arrays too. We have exclusively included `int` numbers in our table in order to simplify the above example.

Implementation

The table can be written in Python as a nested array:

PYTHON

```python
# The list has 3 members, 2 of which
# are arrays of type list:
table = [[1, 2, 3], 4, [7, 8]]

print(table)
```

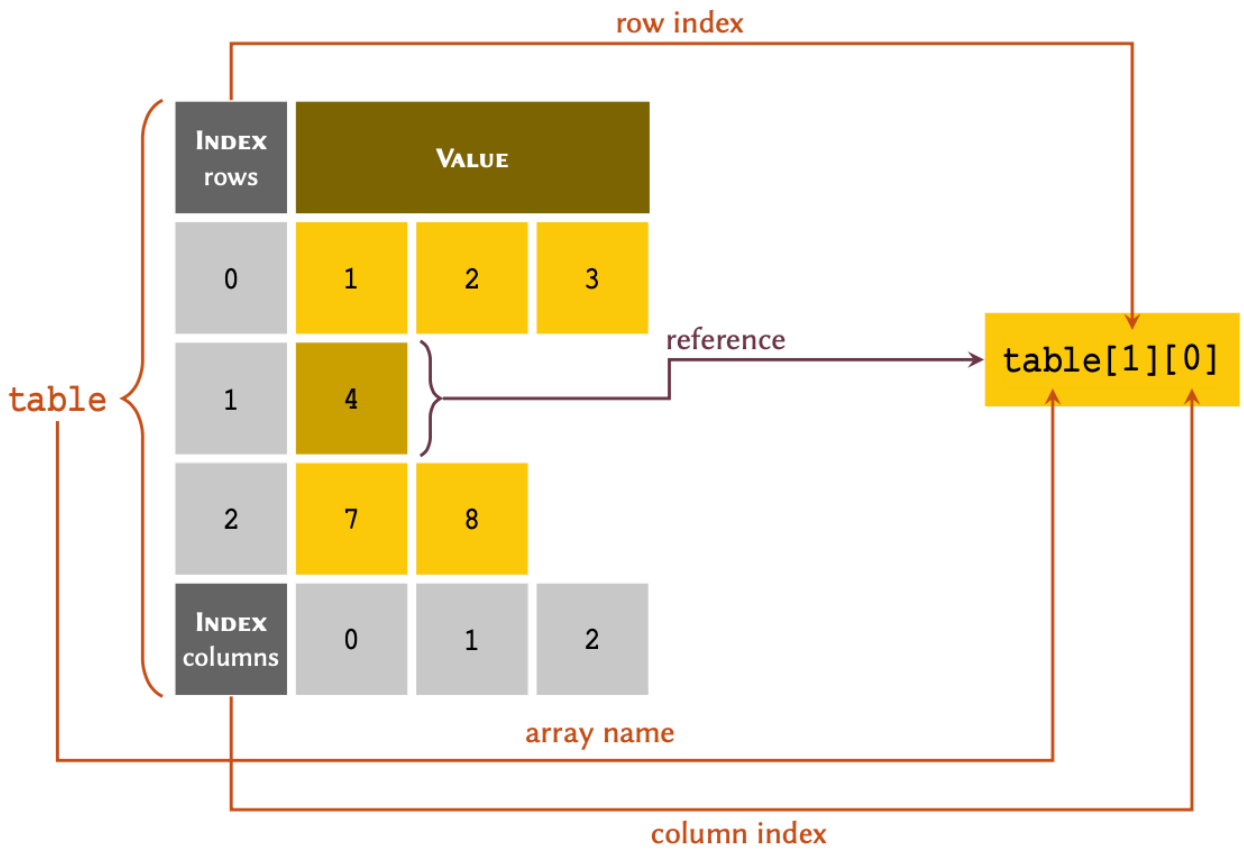
OUTPUT

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

Indexing

The indexing principles for nested arrays are slightly different to those we have familiarised with, up to this point. To retrieve an individual member in a nested `list`, we always reference the *row index*, followed by the *column index*.

We may visualise the process as follows:



To retrieve an entire row, we only need to include the reference for that row. All the values within the row are referenced, implicitly:

PYTHON

```
print(table[0])
```

OUTPUT

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

and to retrieve a specific member, we include the reference for both the row and column:

PYTHON

```
print(table[0][1])
```

OUTPUT

```
2
```

We may also extract slices from a nested array. The protocol is identical to normal arrays, described in the previous section of this lesson on slicing. In nested arrays, however, we may take slices from the columns as well as the rows:

PYTHON

```python
print(table[:2])
```

OUTPUT

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

PYTHON

```python
print(table[0][:2])
```

OUTPUT

```
[1, 2]
```

Note that only 2 of the 3 members in table are arrays of type `list`:

PYTHON

```python
print(table[0], type(table[0]))
```

OUTPUT

```
[1, 2, 3] <class 'list'>
```

PYTHON

```python
print(table[2], type(table[2]))
```

OUTPUT

```
[7, 8] <class 'list'>
```

However, there is another member that is not an array:

PYTHON

```python
print(table[1], type(table[1]))
```

OUTPUT

```
4 <class 'int'>
```

In most circumstances, we would want all the members in an array to be *homogeneous* in type — *i.e.* we want them all to have the same type. In such cases, we can implement the table as:

PYTHON

```python
table = [[1, 2, 3], [4], [7, 8]]

print(table[1], type(table[1]))
```

OUTPUT

```
[4] <class 'list'>
```

An array with only one member — *e.g.* [4], is sometimes referred to as a *singleton* array.

PRACTICE EXERCISE 14

Given the following Table of pathogens and their corresponding diseases:

Pathogen Type	Gram	Pathogen Name	Disease
Bacterium	Negative	*Shigella flexneri*	Bacillary dysentery
Prion	N/A	PrP(sc)	Transmissible spongiform encephalopathies
Bacterium	Negative	*Vibrio cholerae*	Cholera
Bacterium	Negative	*Listeria monocytogenes*	Listeriosis
Virus	N/A	Hepatitis C	Hepatitis
Bacterium	Negative	*Helicobacter pylori*	Peptic ulcers
Bacterium	Negative	*Mycobacterium tuberculosis*	Tuberculosis
Bacterium	Negative	*Chlamydia trachomatis*	Chlamydial diseases
Virus	N/A	Human Immunodeficiency Virus	Human Immunodeficiency

1. Substitute N/A for `None`, and create an array to represent the table in its presented order. Retain the array in a variable, and display the result.

2. Modify the array you created so that its members are sorted *descendingly*, and display the result.

Solution

PYTHON

```python
disease_pathogen = [
  ["Bacterium", "Negative", "Shigella flexneri" , "Bacillary dysentery"],
  ["Prion", None, "PrP(sc)", "Transmissible spongiform encephalopathies"],
  ["Bacterium", "Negative", "Vibrio cholerae", "Cholera"],
  ["Bacterium", "Negative", "Listeria monocytogenes", "Listeriosis"],
  ["Virus", None, "Hepatitis C", "Hepatitis"],
  ["Bacterium", "Negative", "Helicobacter pylori", "Peptic ulcers"],
  ["Bacterium", "Negative", "Mycobacterium tuberculosis", "Tuberculosis"],
  ["Bacterium", "Negative", "Chlamydia trachomatis", "Chlamydial diseases"],
  ["Virus", None, "Human Immunodeficiency Virus", "Human Immunodeficiency"]
  ]

print(disease_pathogen)
```

OUTPUT

```
[['Bacterium', 'Negative', 'Shigella flexneri', 'Bacillary dysentery'], ['Prion', None, 'PrP(sc)', 'Trans
```

Solution

PYTHON

```python
disease_pathogen.sort(reverse=True)

print(disease_pathogen)
```

OUTPUT

```
[['Virus', None, 'Human Immunodeficiency Virus', 'Human Immunodeficiency'], ['Virus', None, 'Hepatitis C
```

Dimensions

A nested array is considered *two-dimensional* or *2D* when:

- *All* of its members in a nested array are arrays, themselves;
- *All* sub-arrays are of **equal length** — *i.e.* all the columns in the table are filled and have the same number of rows; and,
- *All* members of the sub-arrays are *homogeneous* in type — *i.e.* they all have the same type (*e.g.* `int`).

A two dimensional arrays may be visualised as follows:

Index rows	Value		
0	1	2	3
1	4	5	6
2	7	8	9
Index columns	0	1	2

ADVANCED TOPIC

Nested arrays may, themselves, be nested. This means that, if needed, we can have 3, 4 or *n* dimensional arrays, too. Analysis and organisation of such arrays is an important part of a field known as optimisation in computer science and mathematics. Optimisation is the cornerstone of machine learning, and addresses the problem known as curse of dimensionality.

Such arrays are referred to in mathematics as a matrix. We can therefore represent a two-dimensional array as a mathematical matrix. To that end, the above array would translate to the annotation displayed in equation below.

$$table=\begin{bmatrix} 1&2&3\\ 4&5&6\\ 7&8&9\\ \end{bmatrix}$$

The implementation of these arrays is identical to the implementation of other nested arrays. We can therefore code our table in Python as:

PYTHON

```python
table = [
  [1, 2, 3],
  [4, 5, 6],
  [7, 8, 9]
  ]

print(table)
```

OUTPUT

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

PYTHON

```python
print(table[2])
```

OUTPUT

```
[7, 8, 9]
```

PYTHON

```python
print(table[1][0])
```

OUTPUT

```
4
```

PYTHON

```python
print(table[:2])
```

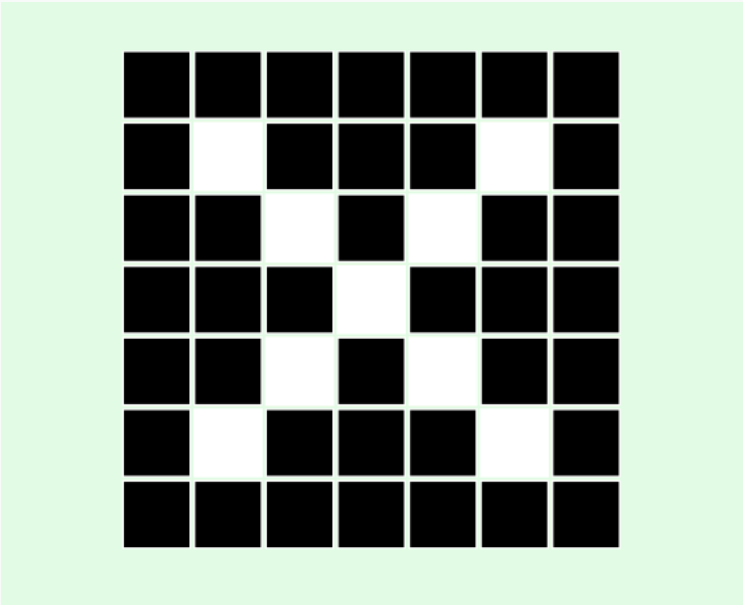
OUTPUT

```
[[1, 2, 3], [4, 5, 6]]
```

PRACTICE EXERCISE 15

Computers see images as multidimensional arrays (matrices). In its simplest form, an image is a two-dimensional array containing only two colours.

Given the following black and white image:



1. Considering that black and white squares represent zeros and ones respectively, create a two-dimensional array to represent the image. Display the results.

2. Create a new array, but this time use `False` and `True` to represent black and white respectively.

Display the results.

Solution

PYTHON

```python
cross = [
                    [0, 0, 0, 0, 0, 0, 0],
                    [0, 1, 0, 0, 0, 1, 0],
                    [0, 0, 1, 0, 1, 0, 0],
                    [0, 0, 0, 1, 0, 0, 0],
                    [0, 0, 1, 0, 1, 0, 0],
                    [0, 1, 0, 0, 0, 1, 0],
                    [0, 0, 0, 0, 0, 0, 0]
                ]

print(cross)
```

OUTPUT

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

Solution

PYTHON

```python
cross_bool = [
  [False, False, False, False, False, False, False],
  [False, True, False, False, False, True, False],
  [False, False, True, False, True, False, False],
  [False, False, False, True, False, False, False],
  [False, False, True, False, True, False, False],
  [False, True, False, False, False, True, False],
  [False, False, False, False, False, False, False]
  ]

print(cross_bool)
```

OUTPUT

```
[[False, False, False, False, False, False, False], [False, True, False, False, False, True, False], [Fal
```

Summary

At this point, you should be familiar with arrays and how they work, in general. Throughout this section, we extensively covered the Python `list`, which is one of the language's most popular types of *built-in* arrays. We also learned:

- How to `list` from the scratch;
- How to *manipulate* a `list` using different *methods*;
- How to use *indexing* and *slicing* techniques to our advantage;
- *Mutability* — a concept we revisit in the forthcoming lessons;
- *In-place operations*, and the difference between *weak references* and *deep copies*;
- *Nested* and *multi-dimensional* arrays; and,
- How to *convert* other sequences (*e.g.* `str`) to `list`.

Tuple

Data Structures: Tuples and Sequences

Another of Python's built-in array types is called a `tuple`. A tuple is an immutable alternative to `list`. That is, once a tuple has been created, its contents cannot be modified in any way. Tuples are often used in applications where it is imperative that the contents of an array cannot be changed.

For instance, we know that in the Wnt signaling pathway, there are two co-receptors. This is final, and would not change at any point in our program.

REMEMBER

The most common way to implement a `tuple` in Python, is to place our comma-separated values inside round parentheses: (1, 2, 3, ...). While there is no specific theoretical term for a tuple instantiated with round parentheses, we can refer to this type of tuple as an **explicit tuple**.

You can also instantiate a tuple without parentheses, as well: (1, 2, 3, ...). In this case, Python acknowledges that a tuple is implied, and is therefore assumed. Thus, we often refer to this type of tuple as an **implicit tuple**, and these are created using an operation called *packing*.

For the time being, we will be making use of explicit tuples, as they are the clearest and most explicit in annotation, and therefore easiest to program with and recognise.

Similarly, we can briefly demonstrate that removing round parentheses, or instantiating a implicit tuple, is categorised in the same way, in Python:

PYTHON

```python
pathway = 'Wnt Signaling'
coreceptors = ('Frizzled', 'LRP')

print(type(coreceptors))
```

OUTPUT

```
<class 'tuple'>
```

PYTHON

```python
print(coreceptors)
```

OUTPUT

```
('Frizzled', 'LRP')
```

PYTHON

```python
wnt = (pathway, coreceptors)

print(type(wnt))
```

OUTPUT

```
<class 'tuple'>
```

PYTHON

```python
print(wnt)
```

OUTPUT

```
('Wnt Signaling', ('Frizzled', 'LRP'))
```

PYTHON

```python
print(wnt[0])
```

OUTPUT

```
Wnt Signaling
```

Indexing and slicing principles for a `tuple` are identical to those of a `list`, aforementioned in this lesson's subsections on indexing and slicing.

Conversion to tuple

Similar to `list`, we can convert other sequences to `tuple`:

PYTHON

```python
numbers_list = [1, 2, 3, 4, 5]

print(type(numbers_list))
```

OUTPUT

```
<class 'list'>
```

PYTHON

```python
numbers = tuple(numbers_list)

print(numbers)
```

OUTPUT

```
(1, 2, 3, 4, 5)
```

PYTHON

```python
print(type(numbers))
```

OUTPUT

```
<class 'tuple'>
```

PYTHON

```python
text = 'This is a string.'

print(type(text))
```

OUTPUT

```
<class 'str'>
```

PYTHON

```python
characters = tuple(text)

print(characters)
```

OUTPUT

```
('T', 'h', 'i', 's', ' ', 'i', 's', ' ', 'a', ' ', 's', 't', 'r', 'i', 'n', 'g', '.')
```

PYTHON

```python
print(type(characters))
```

OUTPUT

```
<class 'tuple'>
```

Immutability

In contrast with `list`, however, if we attempt to change the contents of a `tuple`, a `TypeError` is raised:

PYTHON

```python
coreceptors[1] = 'LRP5/6'
```

OUTPUT

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

Even though `tuple` is an immutable type, it can contain both mutable and immutable objects:

PYTHON

```python
# (immutable, immutable, immutable, mutable)
mixed_tuple = (1, 2.5, 'abc', (3, 4), [5, 6])

print(mixed_tuple)
```

OUTPUT

```
(1, 2.5, 'abc', (3, 4), [5, 6])
```

and mutable objects inside a `tuple` may still be changed:

PYTHON

```python
print(mixed_tuple, type(mixed_tuple))
```

OUTPUT

```
(1, 2.5, 'abc', (3, 4), [5, 6]) <class 'tuple'>
```

PYTHON

```python
print(mixed_tuple[4], type(mixed_tuple[4]))
```

OUTPUT

```
[5, 6] <class 'list'>
```

ADVANCED TOPIC

Why and how can we change mutable objects inside a tuple, when a `tuple` is considered to be an immutable data structure:

Members of a `tuple` are not directly stored in memory. An immutable value (*e.g.* an integer: `int`) has an existing, predefined reference, in memory. When used in a `tuple`, it is this reference that is *associated* with the `tuple`, and not the value itself. On the other hand, a mutable object does not have a predefined reference in memory, and is instead created on request somewhere in your computer's memory (wherever there is enough free space).

While we can never change or redefine a predefined reference, we can always manipulate something we have defined ourselves. When we make such an alteration, the location of our mutable object in memory may well change, but its reference — which is what is stored in a `tuple`, remains identical. In Python, it is possible to discover the reference an object is using, with the function `id()`. Upon experimenting with this function, you will notice that the reference to an immutable object (*e.g.* an `int` value) will never change, no matter how many times you define it in a different context or variable. In contrast, the reference number to a mutable object (*e.g.* a `list`) is changed every time it is defined, even if it contains exactly the same values.

PYTHON

```python
# Lists are mutable, so we can alter their values:
mixed_tuple[4][1] = 15

print(mixed_tuple)
```

OUTPUT

```
(1, 2.5, 'abc', (3, 4), [5, 15])
```

PYTHON

```python
mixed_tuple[4].append(25)

print(mixed_tuple)
```

OUTPUT

```
(1, 2.5, 'abc', (3, 4), [5, 15, 25])
```

PYTHON

```python
# We cannot remove the list from the tuple,
# but we can empty it by clearing its members:
mixed_tuple[4].clear()

print(mixed_tuple)
```

OUTPUT

```
(1, 2.5, 'abc', (3, 4), [])
```

Tuples may be empty or have a single value (singleton):

PYTHON

```python
member_a = tuple()

print(member_a, type(member_a), len(member_a))
```

OUTPUT

```
() <class 'tuple'> 0
```

PYTHON

```python
# Empty parentheses also generate an empty tuple.
# Remember: we cannot add values to an empty tuple, later.
member_b = ()

print(member_b, type(member_b), len(member_b))
```

OUTPUT

```
() <class 'tuple'> 0
```

PYTHON

```python
# Singleton - Note that it is essential to include
# a comma after the value in a single-member tuple:
member_c = ('John Doe',)

print(member_c, type(member_c), len(member_c))
```

OUTPUT

```
('John Doe',) <class 'tuple'> 1
```

PYTHON

```python
# If the comma is not included, a singleton tuple
# is not constructed:
member_d = ('John Doe')

print(member_d, type(member_d), len(member_d))
```

OUTPUT

```
John Doe <class 'str'> 8
```

Packing and unpacking

As previously discussed, a `tuple` may also be constructed without parentheses. This is an implicit operation and is known as *packing*.

REMEMBER

Implicit processes must be used sparingly. As always, the more coherent the code, the better it is.

PYTHON

```python
numbers = 1, 2, 3, 5, 7, 11

print(numbers, type(numbers), len(numbers))
```

OUTPUT

```
(1, 2, 3, 5, 7, 11) <class 'tuple'> 6
```

PYTHON

```python
# Note that for a singleton, we still need to
# include the comma.
member = 'John Doe',

print(member, type(member), len(member))
```

OUTPUT

```
('John Doe',) <class 'tuple'> 1
```

The reverse of this process is known as unpacking. Unpacking is no longer considered an implicit process because it replaces unnamed values inside an array, with named variables:

PYTHON

```python
dimensions = 14, 17, 12

x, y, z = dimensions

print(x)
```

OUTPUT

```
14
```

PYTHON

```python
print(x, y)
```

OUTPUT

```
14 17
```

PYTHON

```python
member = ('Jane Doe', 28, 'London', 'Student', 'Female')
name, age, city, status, gender = member

print('Name:', name, '- Age:', age)
```

OUTPUT

```
Name: Jane Doe - Age: 28
```

PRACTICE EXERCISE 16

Given:

PYTHON

```python
protein_info = ('GFP', 238)
```

Unpack protein_info into two distinct variables: protein_name and protein_length.

Solution

PYTHON

```python
protein_name, protein_length = protein_info
```

NOTE

There is another type of `tuple` in Python referred to as a `namedtuple`. This allows for the members of a `tuple` to be named independently (*e.g.* `member.name` or `member.age`), and thereby eliminates the need for unpacking. It was originally implemented by Raymond Hettinger, one of Python's core developers, for Python 2.4 (in 2004) but was neglected at the time. It has since gained popularity as a very useful tool. `namedtuple` is not a built-in tool, so it is not discussed here. However, it is included in the default library and is installed as a part of Python. If you are feeling ambitious and would like to learn more, please take a look at the official documentations and examples. Raymond is also a regular speaker at PyCon (International Python Conferences), recordings of which are available online. He also often uses his Twitter/X account to talk about small, but important features in Python; which could be worth throwing him a follow.

Summary

In this section of our Basic Python 2 lesson, we learned about `tuple` - another type of built-in array within Python, and one which is *immutable*. This means that once it is created, the array can no longer be altered. We saw that trying to change the value of a `tuple` raises a `TypeError`. We also established that `list` and `tuple` follow an identical indexing protocol, and that they have 2 methods in common: `.index()()` and `.count()`. Finally, we talked about *packing* and *unpacking* techniques, and how they improve the quality and legibility of our code.

If you are interested in learning about `list` and `tuple` in more depth, have a look at the official documentation of Sequence Types – list, tuple, range.

INTERESTING FACT

Graph theory was initially developed by the renowned Swiss mathematician and logician Leonhard Euler (1707 – 1783). Howeve graphs, in the sense discussed here, were introduced by the English mathematician James Joseph Sylvester (1814 – 1897).

Exercises

END OF CHAPTER EXERCISES

1. We have

```
table = [[1, 2, 3], ['a', 'b'], [1.5, 'b', 4], [2]]
```

What is the length of table and why?

Store your answer in a variable and display it using `print()`.

2. Given the sequence for the Gamma (catalytic) subunit of the Protein Kinase A as:

```
human_pka_gamma = (
  'MAAPAAATAMGNAPAKKDTEQEESVNEFLAKARGDFLYRWGNPAQNTASSDQFERLRTLGMGSFGRVML'
  'VRHQETGGHYAMKILNKQKVVKMKQVEHILNEKRILQAIDFPFLVKLQFSFKDNSYLYLVMEYVPGGEM'
  'FSRLQRVGRFSEPHACFYAAQVVLAVQYLHSLDLIHRDLKPENLLIDQQGYLQVTDFGFAKRVKGRTWT'
  'LCGTPEYLAPEIILSKGYNKAVDWWALGVLIYEMAVGFPPFYADQPIQIYEKIVSGRVRFPSKLSSDLK'
  'DLLRSLLQVDLTKRFGNLRNGVGDIKNHKWFATTSWIAIYEKKVEAPFIPKYTGPGDASNFDDYEEEEL'
  'RISINEKCAKEFSEF'
  )
```

Using the sequence;

- Work out and display the number of Serine (S) residues.
- Work out and display the number of Threonine (T) residues.
- Calculate and display the total number of Serine and Threonine residues in the following format:

```
Serine: X
Threonine: X
```

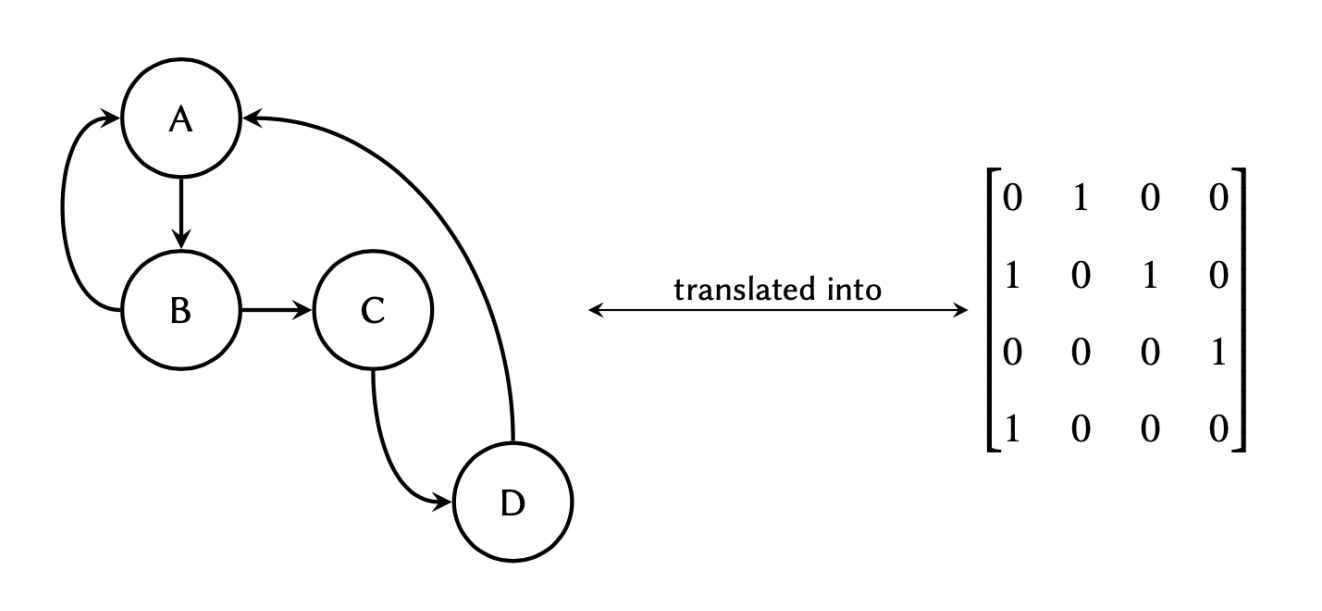
- Create a nested array to represent the following table, and call it :

Row		Value
0	S	*Number of* Ser *residues*
1	T	*Number of* Thr *residues*
Column	0	1

3. Explain why in the previous question, we used the term *nested* instead of *two-dimensional* in reference to the array? Store your answer in a variable and display it using `print()`.

4. Graph theory is a prime object of discrete mathematics utilised for the non-linear analyses of data. The theory is extensively used in systems biology, and is gaining momentum in bioinformatics too. In essence, a graph is a structure that represents a set of object (nodes) and the connections between them (edges).

The aforementioned connections are described using a special binary (zero and one) matrix known as the adjacency matrix. The elements of this matrix indicate whether or not a pair of nodes in the graph are adjacent to one another.

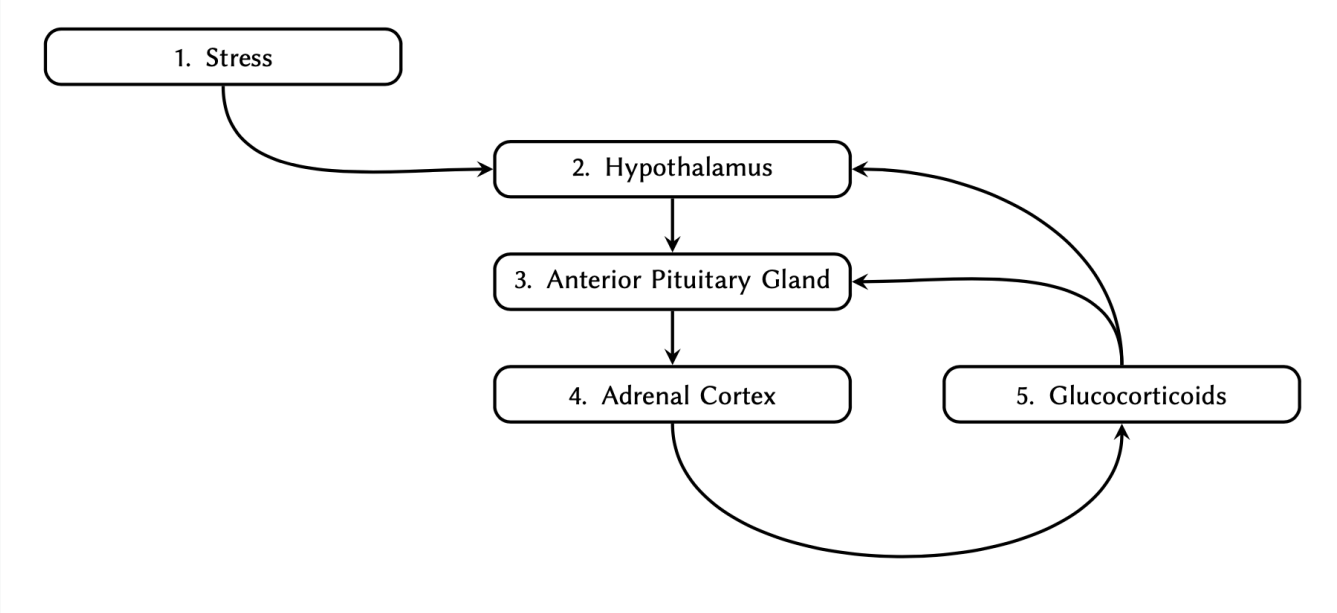


where each row in the matrix represents a node of origin in the graph, and each column a node of destination:

	A	B	C	D
A	0	1	0	0
B	1	0	1	0
C	0	0	0	1
D	1	0	0	0

If the graph maintains a connection (edge) between two nodes (*e.g.* between nodes A and B in the graph above), the corresponding value between those nodes would be #1 in the matrix, and if there are no connections, the corresponding value would #0.

Given the following graph:



Determine the adjacency matrix and implement it as a two-dimensional array in Python. Display the final array.

Solution

KEY POINTS

- `lists` and `tuples` are 2 types of arrays.
- An index is a unique reference to a specific value and Python uses a zero-based indexing system.
- `lists` are mutable because their contents can be modified.
- `slice()`, `.pop()`, `.index()`, `.remove()` and `.insert()` are some of the key functions used in mutable arrays.
- `tuples` are immutable, which means that their contents cannot be modified.

Content from Iterations

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Mandatory Lesson Feedback Survey

OVERVIEW

Questions

- What do we mean by *iterations* and *loops*?
- How are `for`-loops implemented?
- Can conditional statements be used in iterations?
- What are `while`-loops, and how these used?

Objectives

- Understanding the concepts behind iterations and loops.
- Learning the processes involved in `for`-loops implementation.
- Building conditional statements into loops.
- Understanding the concept of `while`-loops, and when to use them.

For Loop with Python List

For Loop through Numpy array

This chapter assumes that you are familiar with the following concepts in Python:

PREREQUISITE

- I/O Operations
- Variables and Types
- Mathematical Operation
- Logical Operations
- Indentation Rule
- Conditional Statements
- Arrays

Additionally, make sure that you are comfortable with the principles of indexing in arrays before commencing this lesson. It is very important that you have a good understanding of arrays and sequences, because the concept of iteration in programming deals *almost* exclusively with these subjects.

NOTE

You can practice everything in this lesson as you have been doing so far. However, if you find it hard to grasp some of the concepts, do not worry. It takes practice. To help you with that, Philip Guo from UC San Diego (Calif., USA) has developed PythonTutor.com - an excellent online tool for learning Python. On that website, write, or paste your code into the editor, and click *Visualize Execution*. In the new page, use the *forward* and *back* buttons to see a step-by-step graphical visualisation of the processes that occur during the execution of your code. Try it on the examples in this section.

The concept

We make use of iterations and loops in programming to perform repetitive operations. A repetitive operation is where one or several defined operations that are repeated multiple times.

For instance, suppose we have a `list` of 5 numbers as follows:

```
numbers = [-3, -2, 5, 0, 12]
```

Now we would like to multiply each number by 2. Based on what we have learned thus far, this is how we would approach this problem:

PYTHON

```python
numbers = [-3, -2, 5, 0, 12]

numbers[0] *= 2
numbers[1] *= 2
numbers[2] *= 2
numbers[3] *= 2
numbers[4] *= 2

print(numbers)
```

OUTPUT

```
[-6, -4, 10, 0, 24]
```

Whilst this does the job, it is clearly very tedious. Furthermore, if we have an array of several thousand members, this approach quickly becomes infeasible.

The process of multiplying individual members of our array by 2 is a very simple example of a repetitive operations.

REMEMBER

In programming, there is a universally appreciated golden principle known as the **DRY** rule; and this is what it stands for:

Don't **R**epeat **Y**ourself

So if you find yourself doing something again and again, it is fair to assume that there might a better way of getting the results you're looking for.

Some programmers (with questionable motives) have created **WET** rule too. Find out more about DRY and WET from Wikipedia.

There are some universal tools for iterations that exist in all programming languages — *e.g.* `for` and `while`-loops. There are also other tools such as vectorisation or generators, that are often unique to one or several specific programming languages.

In this section of the lesson, we will discuss iterations via `for` and `while`-loops, and review some real-world examples that may only be addressed using iterative processes.

for-loops

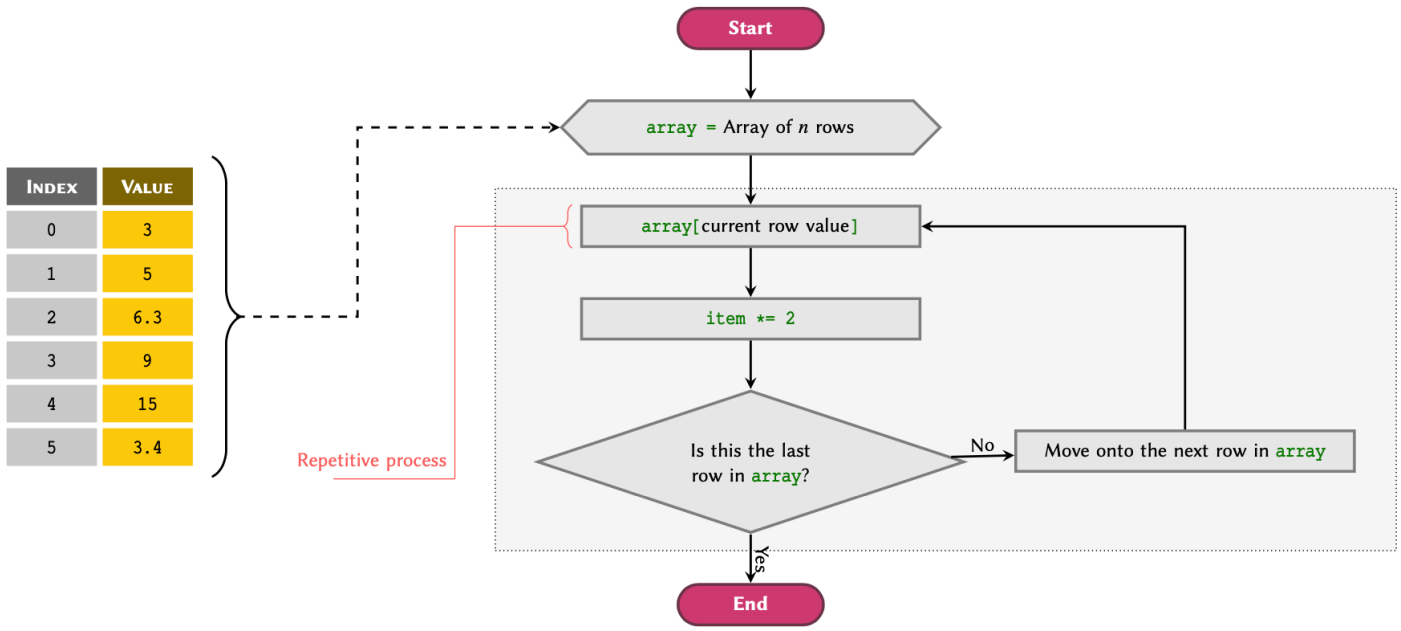
There is evidence that up to 80% of all conventional iterations are implemented as `for`-loops. Whether or not it is the best choice in of all these cases is subject to opinion. What is important, however, is to learn the difference between the two methods, and feel comfortable with how they work.

Implementation of `for`-loops in Python is simple compared to other programming languages. It essentially iterates through an existing *iterable* variable — (such as an array) and retrieves the values from it one by one, from the beginning through to the end.

REMEMBER

In Python, *iterable* is a term used to refer to a variable that can be iterated through. Any variable type that can be used in a `for`-loop *without* any modifications, is therefore considered an *iterable*.

Most arrays and sequences are iterable. See Table to find out which native types in Python are iterable. A rule of thumb is that if an array or a sequence is numerically indexed (e.g. `list`, `tuple`, or `str`), then it is considered an iterable.



Flowchart of a `for`–loop workflow applied to a `list` array.

Figure illustrates a flowchart to visualise the workflow of an iterative process using `for`-loops in Python. The process depicted in the flowchart may be described as follows:

PROCESS

1. A `for`-loop is initialised using an array or a sequence, and begins its process by sequentially going through the values, starting at the array's first row.
2. **Iterative Process:** The value of the *current row* is retrieved and given the alias item, which now represents a single variable within the context of the loop.
3. **Repetitive Operation(s):** Designated operations are performed using the value of item:
   - item *= 2
4. **Loop Condition:** The `for`-loop *automatically* checks whether or not it has reached the last row of the sequence. Depending on the outcome of this check:
   - **NO (last value not reached):** Move onto the next row and *repeat* the process from step 2.
   - **YES (last value reached):** Exit the loop.

We write this process in Python as follows:

PYTHON

```python
numbers = [3, 5, 6.3, 9, 15, 3.4]

for item in numbers:
    item *= 2
    # Display the item to see the results:
    print(item)
```

OUTPUT

```
6
10
12.6
18
30
6.8
```

We can see that the result for each iteration is displayed on a new line. Example outlines other such applications and expands on repetitive operations that may be simplified using `for`-loops.

ADVANCED TOPIC

An iterable is a Python variable that contains the built–in method `.__iter__()`. Methods starting and ending with two underscores (dunderscores) are also known as *magic methods* in Python. See the official Python documentations for additional information.

REMEMBER

A `for`-loop is always initialised as:

```
for variable_name in an_array:
  # An indented block of processes
  # we would like to perform on the
  # members of our array one by one.
```

where `an_array` is an *iterable* variable, and `variable_name` is the name of the variable we temporarily assign to a member of `an_array` that corresponds to the current loop cycle (iteration). The number of loop cycles performed by a `for`-loop is equal to the length (number of members) of the array that we are iterating through, which in this case is called `an_array`.

You can think of each iteration cycle as pulling out a row from the table that is our array (as exemplified in the lesson on arrays) and temporarily assigning its corresponding value to a variable until the next iteration cycle.

See subsection List Members to find the length of an array.

PRACTICE EXERCISE 1

Given:

PYTHON

```python
peptides = [
    'GYSAR',
    'HILNEKRILQAID',
    'DNSYLY'
                ]
```

write a `for`-loop to display each item in peptides alongside its index and length. Display the results in the following format:

`Peptide XXXX at index X contains X amino acids.`

Solution

PYTHON

```python
for sequence in peptides:
    length = len(sequence)
    index = peptides.index(sequence)

    print('Peptide', sequence, 'at index', index, 'contains', length, 'amino acids.')
```

OUTPUT

```
Peptide GYSAR at index 0 contains 5 amino acids.
Peptide HILNEKRILQAID at index 1 contains 13 amino acids.
Peptide DNSYLY at index 2 contains 6 amino acids.
```

EXTENDED EXAMPLE OF ITERATIONS USING `for`-LOOPS

When using a `for`-loop, we can also reference other variables that have already been defined outside of the loop block:

PYTHON

```python
numbers = [3, 5, 6.3, 9, 15, 3.4]
counter = 0

for item in numbers:
    item *= 2

    # Display the item to see the results:
    print('Iteration number', counter, ':', item)

    counter += 1
```

OUTPUT

```
Iteration number 0 : 6
Iteration number 1 : 10
Iteration number 2 : 12.6
Iteration number 3 : 18
Iteration number 4 : 30
Iteration number 5 : 6.8
```

It is also possible to define new variables inside the loop, but remember that the value of any variables defined inside a loop is reset with each iteration cycle:

PYTHON

```python
numbers = [3, 5, 6.3, 9, 15, 3.4]
counter = 0

for item in numbers:
    new_value = item * 2

    # Display the item to see the results:
    print('Iteration number', counter, ':', item, '* 2 =', new_value)

    counter += 1
```

OUTPUT

```
Iteration number 0 : 3 * 2 = 6
Iteration number 1 : 5 * 2 = 10
Iteration number 2 : 6.3 * 2 = 12.6
Iteration number 3 : 9 * 2 = 18
Iteration number 4 : 15 * 2 = 30
Iteration number 5 : 3.4 * 2 = 6.8
```

PRACTICE EXERCISE 2

Write a `for`-loop to display the values of a `tuple` defined as:

PYTHON

```python
protein_kinases = ('PKA', 'PKC', 'MPAK', 'GSK3', 'CK1')
```

such that each protein is displayed on a new line and follows the phrase `Protein Kinase X:` as in

```
Protein Kinase 1: PKA
Protein Kinase 2: PKC
```

and so on.

Solution

PYTHON

```python
counter = 1

for protein in protein_kinases:
    print('Protein Kinase ', counter, ': ', protein, sep='')
    counter += 1
```

OUTPUT

```
Protein Kinase 1: PKA
Protein Kinase 2: PKC
Protein Kinase 3: MPAK
Protein Kinase 4: GSK3
Protein Kinase 5: CK1
```

Retaining the new values

It is nice to be able to manipulate and display the values of an array but in the majority of cases, we need to retain the new values and use them later.

In such cases, we have two options:

- Create a new array to store our values.
- Replace the existing values with the new ones by overwriting them in the same array.

Creating a new array to store our values is very easy. We must firstly create a new `list` and add values to it with each iteration. In other words, we start off by creating an empty `list`; to which we then iteratively add members using the `.append()` method inside our `for`-loop. The process of creating a new `list` and using the `.append()` method to values to an existing `list` are discussed in Useful Methods and mutability, respectively.

PYTHON

```python
numbers = [-4, 0, 0.3, 5]
new_numbers = list()

for value in numbers:
    squared = value ** 2
    new_numbers.append(squared)

print('numbers:', numbers)
```

OUTPUT

```
numbers: [-4, 0, 0.3, 5]
```

PYTHON

```python
print('new_numbers:', new_numbers)
```

OUTPUT

```
new_numbers: [16, 0, 0.09, 25]
```

PRACTICE EXERCISE 3

Given:

PYTHON

```python
peptides = [
    'GYSAR',
    'HILNEKRILQAID',
    'DNSYLY'
                ]
```

write a `for`-loop in which you determine the length of each sequence in peptides, and then store the results as a `list` of `tuple` items as follows:

```
[('SEQUENCE_1', X), ('SEQUENCE_2', X), ...]
```

Solution

PYTHON

```python
peptides_with_length = list()

for sequence in peptides:
    length = len(sequence)
    item = (sequence, length)

    peptides_with_length.append(item)
```

The replacement method uses a slightly different approach. Essentially, what we are trying to achieve is:

- Read the value of an item in an array;
- Manipulate the value via operations;
- Return the value back into the original array through *item assignment*, thereby replacing the existing value.

We learned about modifying an existing value in a `list` in our discussion of mutability, where we discussed the concept of *item assignment*. The process of replacing the original values of an array in a `for`-loop is identical. An important point to be aware of, however, is that we make use of the correct *index* for the specific item in the array that we are trying to modify. Additionally, don't forget that *item assignment* is only possible in mutable arrays such as `list`. See Table to see which types of array are mutable in Python.

To perform *item assignment*, we can use a variable to represent the current iteration cycle in our `for`-loop. We do so by initialising the variable with a value of 0, and adding 1 to its value at the end of each cycle. We can then use that variable as an *index* in each iteration cycle:

PYTHON

```python
numbers = [-4, 0, 0.5, 5]

# Variable representing the
# index (iteration cycle):
index = 0

for value in numbers:
    new_value = value ** 5

    # Putting it back into
    # the original array:
    numbers[index] = new_value

    # Adding one to the index for
    # the next iteration cycle:
    index += 1

print(numbers)
```

OUTPUT

```
[-1024, 0, 0.03125, 3125]
```

ADVANCED TOPIC

The `enumerate()` function actually returns a *generator* of `tuple` items each time it is called in the context of a `for`-loop. A generator is, in principle, similar to a normal array; however, unlike an array, the values of a generator are not evaluated by the computer until the exact time at which they are going to be used. This is an important technique in functional programming known as *lazy evaluation*. It is primarily utilised to reduce the workload on the computer (both the processor and the memory) by preventing the execution of processes that could otherwise be delayed to a later time. In the case of the `enumerate()` function, the values are evaluated at the beginning of each iteration cycle in a `for`-loop. Learn more about lazy evaluation in Wikipedia or read more on generators in Python in the official documentations.

This is a perfectly valid approach and it is used in many programming languages. However, Python makes this process even easier by introducing the function `enumerate()`. We often use this function at the initiation of a `for`-loop. The function takes an array as an input and as the name suggests, enumerates them; thereby simplifying the indexing process. The previous example may, therefore, be written more concisely in Python, as follows:

PYTHON

```python
numbers = [-4, 0, 0.5, 5]

for index, value in enumerate(numbers):
    # Manipulating the value:
    new_value = value ** 5
    numbers[index] = new_value

print(numbers)
```

OUTPUT

```
[-1024, 0, 0.03125, 3125]
```

PRACTICE EXERCISE 4

Given:

PYTHON

```python
characters = ['1', '2', '3', '4']
```

Display each item in characters as many times in one line as the index of that item in characters. The results should appear as follows:

```
2
33
444
```

Solution

PYTHON

```python
for index, item in enumerate(characters):
    print(item * index)
```

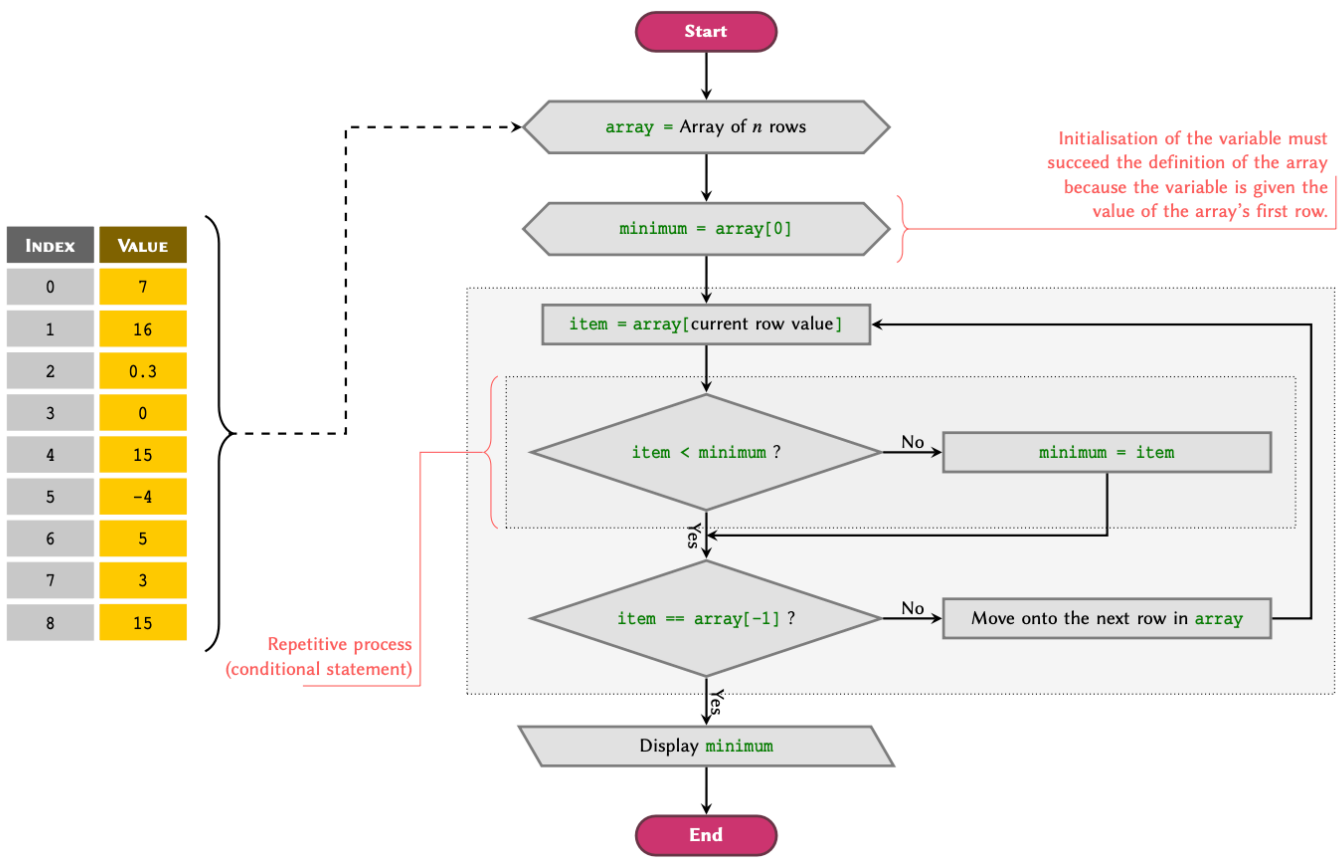
OUTPUT

```
2
33
444
```

for-loop and conditional statements

We can use conditional statements within `for`-loops to account for and handle different situations.

Suppose we want to find the smallest value (the minimum) within a `list` of numbers using a `for`-loop. The workflow of this process is displayed as a flowchart diagram in figure below.



Index	Value
0	7
1	16
2	0.3
3	0
4	15
5	-4
6	5
7	3
8	15

Given an array, we can break down the problem as follows:

1. Define the variable `minimum` outside our `for`-loop, and set its value to be equal to the value of the first row in our array.
2. A `for`-loop is initialised using an array or a sequence and begins its process by going through the array values from the first row.
3. **Iterative Process:** The value of the *current row* is retrieved and given the alias `item`, which now represents a variable in the context of the loop.
4. **Repetitive Operation(s):** Designated operations are performed using the value of `item`:
   - Compare the value of `minimum` with the value of every row in the array at each iteration cycle as test if `item < minimum`:
     - `True`: update the value of `minimum` to be `minimum = item`.
     - `False`: do nothing and proceed to the next step.
5. **Loop Condition:** The `for`-loop *automatically* checks whether or not it has reached the last row of the sequence:
   - **NO:** Move onto the next row and *repeat* the process from #3.
   - **YES:** Exit the loop.

Finally, we can implement the process displayed in figure as follows:

PYTHON

```python
numbers = [7, 16, 0.3, 0, 15, -4, 5, 3, 15]

minimum = numbers[0]

for value in numbers:
    if value < minimum:
        minimum = value

print('The minimum value is:', minimum)
```

OUTPUT

```
The minimum value is: -4
```

PRACTICE EXERCISE 5

Given:

PYTHON

```python
peptides = [
  'FAEKE',
  'CDYSK',
  'ATAMGNAPAKKDT',
  'YSFQW',
  'KRFGNLR',
  'EKKVEAPF',
  'GMGSFGRVML',
  'YSFQMGSFGRW',
  'YSFQMGSFGRW'
                ]
```

Using a `for`-loop and a conditional statement, find and display the sequences in peptides that contain the amino acid serine (S) in the following format:

```
Found S in XXXXX.
```

Solution

PYTHON

```python
target = 'S'

for sequence in peptides:
    if target in sequence:
        print('Found', target, 'in', sequence)
```

OUTPUT

```
Found S in CDYSK
Found S in YSFQW
Found S in GMGSFGRVML
Found S in YSFQMGSFGRW
Found S in YSFQMGSFGRW
```

Sequence of numbers in for-loops

In order to produce a sequence of `int` numbers for use in a `for`-loop, we can use the built-in `range()` function. The function takes in three positional arguments representing *start*, *stop*, and *step*. Note that `range()` is *only* capable of producing a sequence of integer numbers.

REMEMBER

The `range()` function does not create the sequence of numbers immediately. Rather, it behaves in a similar way to the `enumerate()` function does (as a generator).

Displaying the output of the `range()` function is not an array of numbers, as you might expect:

PYTHON

```python
range_generator = range(0, 10, 2)

print(range_generator)
```

OUTPUT

```
range(0, 10, 2)
```

It is, however, possible to evaluate the values outside of a `for`-loop. To do so, we need to convert the output of the function to `list` or a `tuple`:

PYTHON

```python
range_sequence = list(range_generator)

print(range_sequence)
```

OUTPUT

```
[0, 2, 4, 6, 8]
```

REMEMBER

The `range()` function is *non-inclusive*. That is, it creates a sequence that starts from and includes the value given as the *start* argument, up to but *excluding* the value of the *end* argument. For instance, `range`(1, 5, 1) creates a sequence starting from 1, which is then incremented 1 step at a time right up to 5, resulting in a sequence that includes the following numbers: 1, 2, 3, 4

EXAMPLE: SEQUENCE COMPARISON, DOT PLOTS AND `for` LOOPS

There are different methods to evaluate the similarity of two or more polypeptide or polynucleotide sequences. The *dot matrix* (also known as the *dot plot*) is one such method. A *dot matrix* is in essence a two-dimensional array of binary values — *i.e.* it only contains zeros and ones, or `True` and `False`.

For instance, given the following polypetide sequences, extracted from the **CFTR** (Cystic fibrosis transmembrane conductance regulator) protein in humans and mice:

In [1]:
```
cftr_human = 'GRMMMKYRDQRAGKISERLVITSEMIENIQSVKAYCWEEAMEKMIENLRQTELKLTRKAA'
cftr_mouse = 'GKMMVKYRDQRAAKINERLVITSEIIDNIYSVKAYCWESAMEKMIENLREVELKMTRKAA'
```

we can go ahead and construct a dot matrix by comparing each residue in `cftr_human` with every residue in `cftr_mouse`.

On this occasion, D is an $n \times m$ matrix, where:

- n is equal to the number of residues in `cftr_human`; and,
- m is equal to that of `cftr_mouse`.

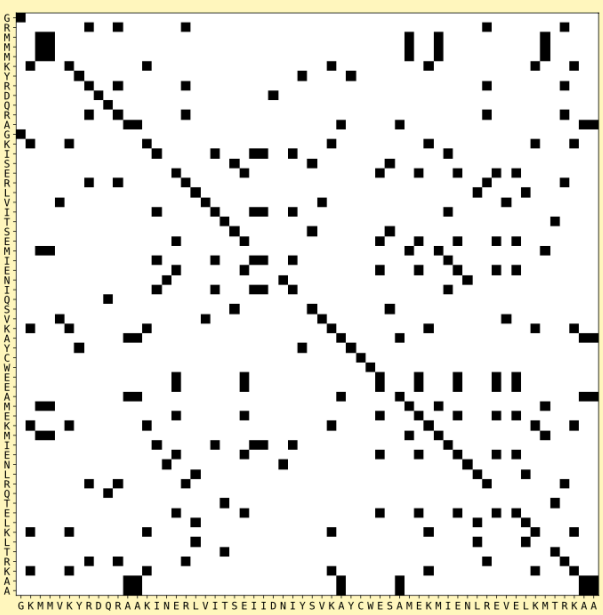
Therefore, each element in D may be referred to as $D_{i,j}$, where i and j represent the index of a residue in `cftr_human` and `cftr_mouse` respectively. The value of each element is either `0` or `1` depending on their similarity — *i.e.* if `cftr_human[i]` is identical to `cftr_mouse[j]`, then $D_{i,j}$ is `1`, otherwise it is `0`.

It is beyond the scope of this book to discuss the interpretation of dot plots. However, in general, the existence of a diagonal line in the final matrix or the dot plot would imply a high degree of similarity between the two sequence. This means that if we compare `cftr_human` with a randomly shuffled version of `cftr_mouse`, we should lose the diagonal line. To test this, we will additionally create a surrogate sequence of the `cftr_mouse` sequence:

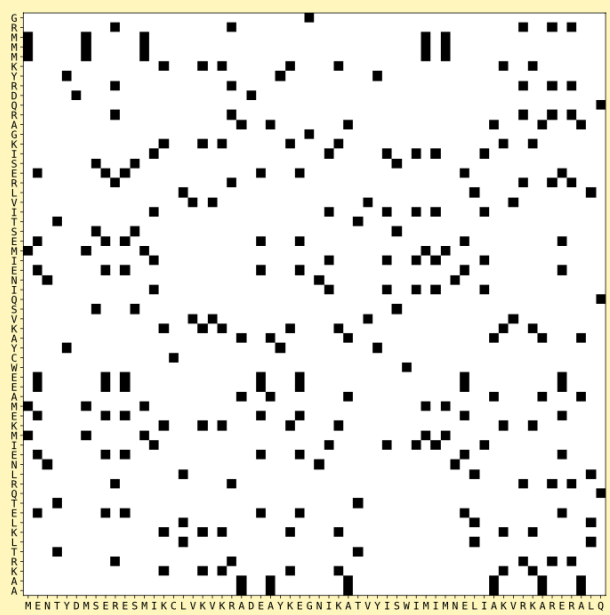
```
cftr_mouse_surrogate = 'MENTYDMSERESMIKCLVKVKRADEAYKEGNIKATVYISWIMIMNELIAKVRKARERALQ'
```

The visualisation of the dot matrices determined for the sequences we have defined are as follows, where black dots represent a value of `1` (identical residues):

`cftr_human` vs `cftg_mouse`



`cftr_human` vs `cftr_mouse_surrogate`



Implementation

We can create the above matrix by implementing a nested for-loop, which we then use to construct a nested array, one element at a time. This might appear somewhat difficult to grasp; however, it becomes clear once you investigate the code and the go through the workflow.

In [2]:

```
dot_matrix = list()

for residue_a in cftr_human:
    row = list()

    for residue_b in cftr_mouse:
        if residue_a == residue_b:
            row.append(1)
        else:
            row.append(0)

    dot_matrix.append(row)

print(dot_matrix)
```

To achieve a binary matrix, we compare every character in `cftr_human` to every character in `cftr_mouse`. In other words, we iterate through `cftr_human`, and during each iteration, we also iterate through `cftr_mouse`. This allows us to compare each character in `cftr_human`, to every character in `cftr_mouse`. Given that each sequence in our example has a length of 60 characters, we will essentially complete 60 iterations for `cftr_humans` (outter loop), and $60 \times 60 = 3600$ iterations for `cftr_mouse` (inner loop). This number is equal to the number of squares displayed in the above dot matrix.

In the context of the inner loop, depending on whether or not the two characters (or amino acid residues) are identical, we append a value of #0 or #1 to the row. Each row represents a `list` and corresponds to the `cftr_human` residue in the current iteration. This means that each column (each item added to the row) represents one residue in `cftr_mouse`.

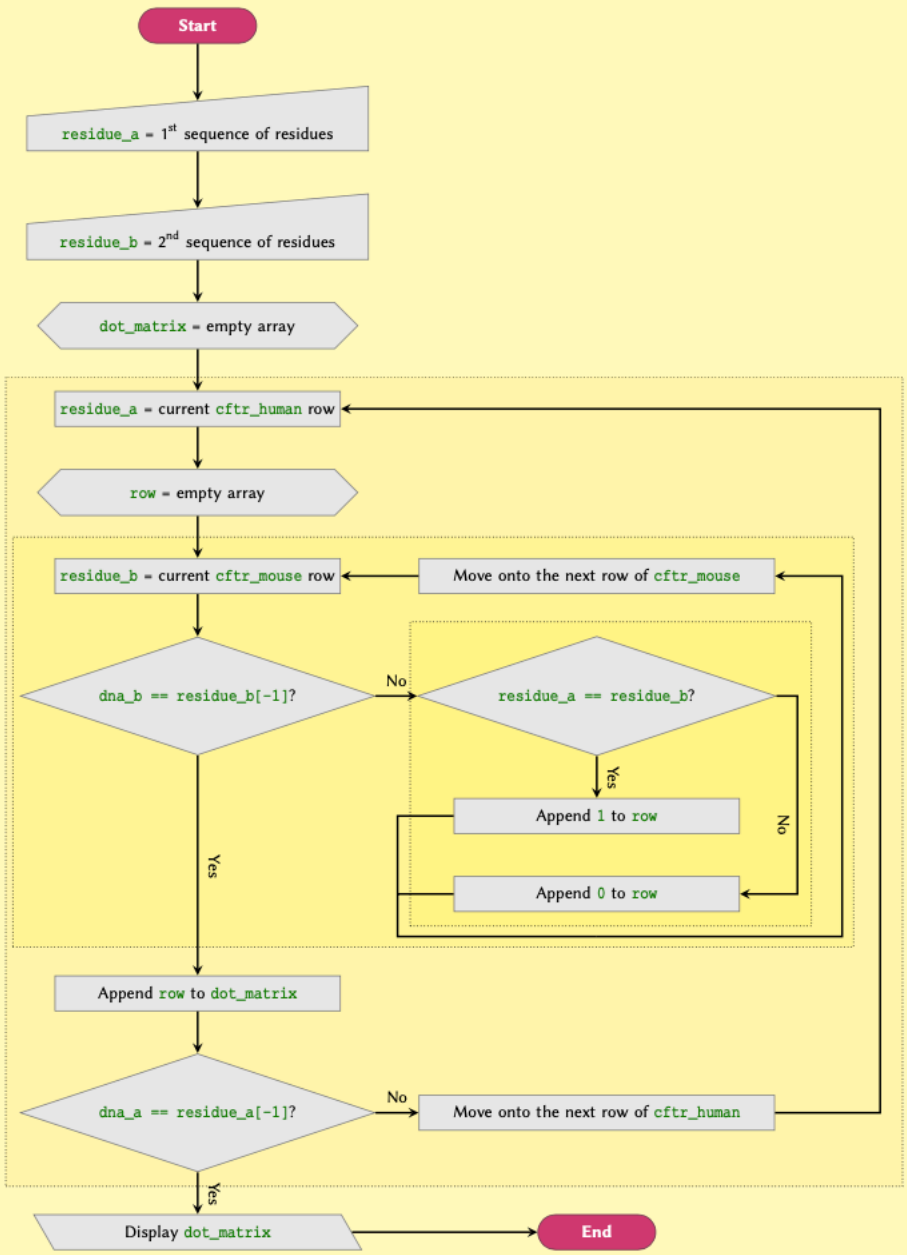
The output of the code will thus be a matrix of zeros and ones, as follows:

Out [2]:

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

Workflow

The algorithm that we implemented to create the dot matrix may appear relatively complex. However, it demonstrates the important and complementary relationship between for-loops and sequences in programming. The logic of the code is best described as a flowchart.



Visualisation

Dot plots are typically visualised as a heatmap. We do not investigate visualisation techniques here. Nonetheless, we shall take this opportunity to visualise the dot matrix we have created.

Visualisation and plotting in Python is done using external libraries, of which there are many varieties to choose from. For the purpose of this example, we will be using `matplotlib`, an extensive and powerful library for producing publication quality figures in Python. The library is installed automatically as a part of the Anaconda distribution. See the official documentations, examples, and tutorials for `matplotlib` to find out more.

Use the following code to produce a heatmap of the dot matrix:

In [3]:

```python
from matplotlib.pyplot import subplots, show


# Initialising a figure and its axis:
fig, ax = subplots(figsize=(10, 10))

# Plotting a heatmap of the matrix with
# equal axes,  and a reversed grayscale
# colour map:
ax.imshow(dot_matrix, aspect='equal', cmap='gray_r')

# Determining the length of each sequence:
human_len, mouse_len = len(human_cftr), len(mouse_cftr)

# Creating a sequence of numbers to use
# for tick positions in our plot:
human_ticks, mouse_ticks = range(human_len), range(mouse_len)

# Setting tick positions:
ax.set_yticks(human_ticks)
ax.set_xticks(mouse_ticks)

# Setting tick labels:
ax.set_yticklabels(human_cftr, fontsize=8)
ax.set_xticklabels(mouse_cftr, fontsize=8)

# Display the figure:
show()
```

Try this code with other polypeptide or polynucleotide sequences and experiment with the LIB `matplotlib` options as described in its documentations.

LEARN MORE

To learn more about sequence comparison methods, including how to interpret dot plots, read:

- Orengo, C.A., Jones, D.T., Thornton, J.M. (2005). *Bioinformatics*. 1st ed. New York: Taylor & Francis, pp. 33-34.
- Lesk, A. (2014). *Introduction to bioinformatics*. Oxford: Oxford University Press. pp. 176-181.

while-loops

In our discussion of `for` loop mediated iterations above, we learned that they are *exclusively* applied to iterable objects — such as arrays and sequences. This is because, as demonstrated in workflow figure, at the end of each iteration, the *implicit* termination condition that is inherent in the process tests whether or not the end of the sequence being iterating through, has been reached.

It may, however, be deemed necessary to apply iterative processes based on conditions other than those embedded within the `for`-loop. In such cases, we use a different class of iterations known as a `while`-loop.

REMEMBER

The termination condition of a `while`-loop is manually defined by the programmer. It is therefore paramount to ensure that the termination condition is somehow satisfied at some point in process. If the termination condition is implemented incorrectly such that the condition is never met, the iteration process would *never* end. In that case, the programme falls into what is known as the *infinite loop* state.

This is bound to happen to every programmer at some point. It is, however, important to know how to break out of an *infinite loop*:

IDE In most IDEs — *e.g.* PyCharm® or Jupyter, the programme may be terminated using the tools provided in the environment. Such tools often appear in the shape of a *stop* button in the shape of ■ or ⊙, and are positioned near the *start* / *execute* button.

Terminal To abort the current task and stop the execution of a programme, we send a `SIGINT` signal in the terminal as follows:

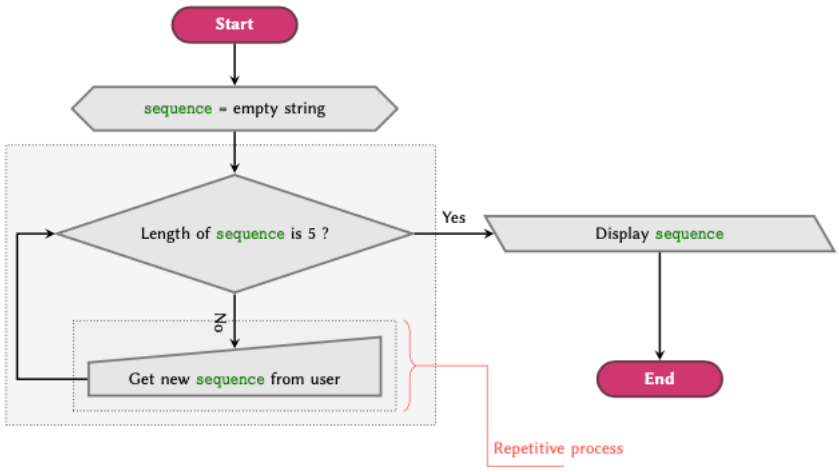
- in Linux or Microsoft Windows®, press ctrl + c
- in Mac OS X®, press ⌘ + c

Other Try to close the window manually. This will force the termination of your programme. However, if your computer freezes, the only remaining option would be to restart the computer.

Consider the following:

> We want to ask a user to enter a sequence of exactly five amino acids in single-letter code. If the provided sequence is more or less than five letters long, we would like to display a message and ask them to try again; otherwise, we will display the process and terminate the program.

It is impossible to write such a process using a `for`-loop. This is because when we initialise the iteration process in a `for`-loop, the number of loops we need is unknown. In other words, we simply do not know how many times the user would need enter said sequence before they get it right.



To simplify the understanding of the concept, we can visualise the process in a flowchart, as displayed in figure. In this flowchart, you can see that the only way to exit the loop is to enter a sequence of exactly five characters. Doing anything else — such as entering a different number of letters – is equivalent to going back to the beginning of the loop. The process may be described verbally as follows:

1. Initialise the variable sequence and assign an empty string to it.
2. *While* the length of sequence is not equal to 5:
   - Ask the user to enter a new sequence.
   - Go back to step #2.
3. Display the value of sequence.

Implementation

We instantiate `while`-loop using the `while` syntax, immediately followed by the loop condition.

We can now implement the process displayed in figure as follows:

```
sequence = str()

while len(sequence) != 5:
    sequence = input('Enter a sequence of exactly 5 amino acids: ')

print(sequence)
```

When executed, the above code will prompt the user to enter a value:

```
Enter a sequence of exactly 5 amino acids: GCGLLY
Enter a sequence of exactly 5 amino acids: GCGL
Enter a sequence of exactly 5 amino acids: GC
Enter a sequence of exactly 5 amino acids: GCGLL

GCGLL
```

As expected, the user is repetitively asked to enter a five-character sequence until they supply the correct number of letters.

PRACTICE EXERCISE 6

1. Write a script which prompts the user to enter a number, then:
    - If the second power of the number is smaller than 10, repeat the process and ask again;
    - If the second power of the number is equal or greater than 10, display the original value and terminate the program.

Hint: Don't forget to convert the value entered by the user to an appropriate numeric type *before* you perform any mathematical operations.

2. We learned in subsection Sequence of Numbers that the built-in function `range()` may be utilised to produce a sequence of *integer* numbers. The function takes 3 input arguments in the following order: stop, start, step.

We now need a sequence of floating-point numbers with the following criteria:

```
stop = 10
start = 0
step = 0.5
```

The use of a floating-point number as step means that we cannot use `range()` to create the desired sequence. Write a script in which you use a `while`-loop to produce a sequence of floating-point numbers with the above criteria and display the result.

The resulting sequence must be:

- Presented as an instance of type `list`;
- Similar to `range()`, the sequence must be non-inclusive — *i.e.* it must include the value of start, but not that of stop.

Solution

```
value = 0

while value ** 2 < 10:
    response = input('Enter a number: ')
    value = float(response)

print(value)
```

Solution

PYTHON

```python
stop = 10
start = 0
step = 0.5

number = start
sequence = list()

while number < stop:
    sequence.append(number)
    number += step

print(sequence)
```

OUTPUT

```
[0, 0.5, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 4.5, 5.0, 5.5, 6.0, 6.5, 7.0, 7.5, 8.0, 8.5, 9.0, 9.5]
```

Solution

PYTHON

```python
# A smarter solution, however, would be:
stop = 10
start = 0
step = 0.5

sequence = [start]

while sequence[-1] < stop - step:
    sequence.append(sequence[-1] + step)

print(sequence)
```

OUTPUT

```
[0, 0.5, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 4.5, 5.0, 5.5, 6.0, 6.5, 7.0, 7.5, 8.0, 8.5, 9.0, 9.5]
```

Breaking a while-loop

Unlike `for`-loops, it is common to *break* out of a `while`-loop, mid-process. This is also known as *premature termination*.

To consider a situation that may necessitate such an approach, we shall modify our scenario as follows:

> We want to ask the user to enter a sequence of exactly five amino acids. If the sequence the user provides is more or less than five letters long, we would like to display a message and ask them to try again; otherwise, we will display the sequence and terminate the program. Additionally, the loop should be terminated: - upon three failed attempts; or, - if the user enters the word exit instead of a five-character sequence.

In the former case, however, we would also like to display a message and inform the user that we are terminating the programme because of three failed attempts.

To implement the first addition to our code, we will have to make the following alterations in our code:

- Define a variable to hold the iteration cycle, then test its value at the beginning of each cycle to ensure that it is below the designated threshold. Otherwise, we manually terminate the loop using the `break` syntax.
- Create a conjunctive conditional statement for the `while`-loop to make, so that it is also sensitive to our exit keyword.

```
sequence = str()
counter = 1
max_counter = 3
exit_keyword = 'exit'

while len(sequence) != 5 and sequence != exit_keyword:
    if counter == max_counter:
        sequence = "Three failed attempt - I'm done."
        break

    sequence = input('Enter a sequence of exactly 5 amino acids or [exit]: ')

    counter += 1

print(sequence)
```

Exercises

END OF CHAPTER EXERCISES

1. Can you explain the reason why, in the example given in subsection for-loop and conditional statements we set minimum to be equal to the first value of our array instead of, for instance, zero or some other number?

Store your answer in a variable and display it using `print()`.

2. Write a script that using a `for`-loop, calculates the sum of all numbers in an array defined as follows:

```
numbers = [0, -2.1, 1.5, 3]
```

and display the result as:

```
Sum of the numbers in the array is 2.4
```

3. Given an array of integer values as:

```
numbers = [2, 1, 3]
```

write a script using `for`-loops, and display each number in the list as many times as the number itself. The program must therefore display '2' twice, '1' once, and '3' three times.

4. Given a `list` of numbers defined as:

```
numbers = [7, 16, 0.3, 0, 15, -4, 5, 3, 15]
```

write a script that using (at most) two `for`-loops, finds the *variance* of the numbers, and display the **mean**, and the **variance**. Note that you will need to calculate the *mean* as a part of your calculations to find the *variance*.

The equation for calculating variance is:

$$\sigma^2 = \frac{\sum^{n}_{i=1}(x_i - \mu)^2}{n}$$

Hint: *Breaking down the problem into smaller pieces will simplify the process of translating it into code and thereby solving it:*

a. Work out the Mean or μ (the simple average of the numbers): $$\mu = \frac{\sum^{n}_{i=1} x_i}{n}$$

b. Calculate the sum of: each number (x_i) subtracted by the Mean (μ) and square the result.

c. Divide the resulting number by the length of number.

Display the results in the following format:

```
Mean: XXXX
Variance: XXXX
```

Solution

KEY POINTS

- Iterations and loops are used to perform repetitive operations.
- Implementation of `for`-loops involves four steps.
- Conditional statements are used within loops to handle different situations.
- `while`-loops are most suitable when an exact number of conditions/iterations is unknown.

Content from Dictionaries

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Mandatory Lesson Feedback Survey

OVERVIEW

Questions

- What is a dictionary, in Python?
- What are the ways to interact with a dictionary?
- Can a dictionary be nested?

Objectives

- Understanding the structure of a dictionary.
- Accessing data from a dictionary.
- Applying nested dictionaries to deal with complex data.

This chapter assumes that you are familiar with the following concepts in Python:

PREREQUISITE

- Indentation Rule
- Conditional Statements
- Arrays
- Loops and Iterations

Dictionary

Mapping Types – `dict`

Google search

StackOverflow python-3.x dictionaries

YouTube Tutorial Dictionaries

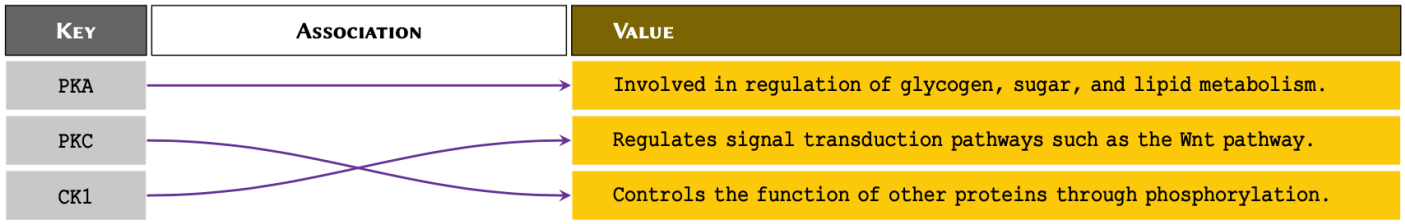
Dictionaries are one of the most valuable in-build tools in Python, and are characterised by being able to associate a set of *values* with a number of *keys*.

Think of a paperback dictionary, where we have a range of words together with their definitions. The words are the *keys*, and the definitions are the *values* that are associated with those keys. A Python dictionary works in the same way.

Consider the following scenario:

> Suppose we have a number of protein kinases, and we would like to associate them with their descriptions for future reference.

This is an example of association in arrays. We may visualise this problem as displayed in Figure.



One way to associate the proteins with their definitions would be to make use of nested arrays, as covered in Basic Python 2. However, this would make it difficult to retrieve the values at a later point in time. This is because in order to retrieve these values, we would need to know the numerical index at which a given protein is stored, and the level it's stored at.

As an alternative to using normal arrays in such cases, we can make use of *associative arrays*. The most common method for constructing an associative array in Python is to create dictionaries or `dict`.

REMEMBER

To implement a `dict` in Python, we place our entries within **curly brackets**, separated using a comma. We separate *keys* and *values* using a colon — e.g. {'key': 'value'}. The combination of dictionary *key* and its associated *value* is referred to as a dictionary *item*.

NOTE

When constructing a long `dict` with several *items* that span over several lines, it is not necessary to write one *item* per line, nor to use indentations for each *item* or line. All we need to do is to write key-value pairs as {'key': 'value'} in curly brackets, and separate each pair using a comma. However, it is good practice to write one *item* per line and use indentations as it makes it considerably easier to read the code and understand the hierarchy.

We can therefore implement the diagram displayed in Figure in Python as follows:

PYTHON

```python
protein_kinases = {
  'PKA': 'Involved in regulation of glycogen, sugar, and lipid metabolism.',
  'PKC': 'Regulates signal transduction pathways such as the Wnt pathway.',
  'CK1': 'Controls the function of other proteins through phosphorylation.'
  }

print(protein_kinases)
```

OUTPUT

```
{'PKA': 'Involved in regulation of glycogen, sugar, and lipid metabolism.', 'PKC': 'Regulates signal transdu
```

PYTHON

```python
print(type(protein_kinases))
```

OUTPUT

```
<class 'dict'>
```

PRACTICE EXERCISE 1

Use the Universal Protein Resource (UniProt) database to find the following human proteins:

- Axin-1
  - Rhodopsin

Construct a dictionary for these proteins and the number amino acids within each of them. The *keys* should represent the name of the protein. Display the result.

Solution

PYTHON

```python
proteins = {
  'Axin-1': 862,
  'Rhodopsin': 348
  }

print(proteins)
```

OUTPUT

```
{'Axin-1': 862, 'Rhodopsin': 348}
```

Now that we have created a dictionary; we can test whether or not a specific *key* exists our dictionary:

PYTHON

```python
'CK1' in protein_kinases
```

OUTPUT

```
True
```

PYTHON

```python
'GSK3' in protein_kinases
```

OUTPUT

```
False
```

PRACTICE EXERCISE 2

Using the dictionary you created in Practice Exercise 1, test to determine whether or not a protein called **ERK** exists as a *key* in your dictionary. Display the result as a Boolean value.

Solution

PYTHON

```python
print('ERK' in proteins)
```

OUTPUT

```
False
```

Interacting with a dictionary

In programming, we have already learned that the more explicit our code is, the better it is. Interacting with dictionaries in Python is very easy, coherent and explicit. This makes them a powerful tool that we can exploit for different purposes.

In arrays, specifically in `list` and `tuple`, we routinely use indexing techniques to retrieve *values*. In dictionaries, however, we use *keys* to do that. Because we can define the *keys* of a dictionary ourselves, we no longer have to rely exclusively on numeric indices.

As a result, we can retrieve the *values* of a dictionary using their respective *keys* as follows:

PYTHON

```python
print(protein_kinases['CK1'])
```

OUTPUT

```
Controls the function of other proteins through phosphorylation.
```

However, if we attempt to retrieve the *value* for a *key* that does not exist in our `dict`, a `KeyError` will be raised:

PYTHON

```python
'GSK3' in protein_kinases
```

OUTPUT

```
False
```

PYTHON

```python
print(protein_kinases['GSK3'])
```

OUTPUT

```
KeyError: 'GSK3'
```

PRACTICE EXERCISE 3

Implement a `dict` to represent the following set of information:

Cystic Fibrosis:

Full Name	Gene	Type
Cystic fibrosis transmembrane conductance regulator	CFTR	Membrane Protein

Using the dictionary you implemented, retrieve and display the *gene* associated with cystic fibrosis.

Solution

PYTHON

```python
cystic_fibrosis = {
  'full name': 'Cystic fibrosis transmembrane conductance regulator',
  'gene': 'CFTR',
  'type': 'Membrane Protein'
  }

print(cystic_fibrosis['gene'])
```

OUTPUT

```
CFTR
```

REMEMBER

Whilst the *values* in a `dict` can be of virtually any type supported in Python, the *keys* may only be defined using immutable types.

To find out which types are immutable, see Table. Additionally, the *keys* in a dictionary must be unique.

If we attempt to construct a `dict` using a mutable value as *key*, a `TypeError` will be raised.

For instance, `list` is a mutable type and therefore cannot be used as a *key*:

PYTHON

```python
test_dict = {
  ['a', 'b']: 'some value'
  }
```

OUTPUT

```
TypeError: unhashable type: 'list'
```

But we can use any immutable type as a *key*:

PYTHON

```python
test_dict = {
  'ab': 'some value'
  }

print(test_dict)
```

OUTPUT

```
{'ab': 'some value'}
```

PYTHON

```python
test_dict = {
  ('a', 'b'): 'some value'
  }

print(test_dict)
```

OUTPUT

```
{('a', 'b'): 'some value'}
```

If we define a *key* more than once, the Python interpreter constructs the entry in `dict` using the last defined instance of that key.

In the following example, we repeat the *key* 'pathway' twice; and as expected, the interpreter only uses the last instance, which in this case represents the value 'Canonical':

PYTHON

```python
signal = {
  'name': 'Wnt',
  'pathway': 'Non-Canonical',  # first instance
  'pathway': 'Canonical'  # second instance
  }

print(signal)
```

OUTPUT

```
{'name': 'Wnt', 'pathway': 'Canonical'}
```

Mutability

Like lists, dictionaries are mutable. This means that we can alter the contents of a dictionary, after it has been instantiated. We can make any alterations to a dictionary as long as we use *immutable* values for the *keys*.

Suppose we have a dictionary stored in a variable called `protein`, holding some information about a specific protein:

PYTHON

```python
protein = {
  'full name': 'Cystic fibrosis transmembrane conductance regulator',
  'alias': 'CFTR',
  'gene': 'CFTR',
  'type': 'Membrane Protein',
  'common mutations': ['Delta-F508', 'G542X', 'G551D', 'N1303K']
  }
```

We can add new *items* to our dictionary or alter the existing ones:

PYTHON

```python
# Adding a new item:
protein['chromosome'] = 7

print(protein)

print(protein['chromosome'])
```

OUTPUT

```
{'full name': 'Cystic fibrosis transmembrane conductance regulator', 'alias': 'CFTR', 'gene': 'CFTR', 'type'
7
```

We can also alter an existing *value* in a dictionary using its *key*. To do so, we simply access the *value* using its *key*, and treat it as a normal variable; the same way we would treat members of a `list`:

PYTHON

```python
print(protein['common mutations'])
```

OUTPUT

```
['Delta-F508', 'G542X', 'G551D', 'N1303K']
```

PYTHON

```python
protein['common mutations'].append('W1282X')
print(protein)
```

OUTPUT

```
{'full name': 'Cystic fibrosis transmembrane conductance regulator', 'alias': 'CFTR', 'gene': 'CFTR', 'type'
```

PRACTICE EXERCISE 4

Implement the following dictionary:

```
signal = {'name': 'Wnt', 'pathway': 'Non-Canonical'}}
```

with respect to signal:

- Correct the *value* of pathway to “Canonical”;
- Add a new *item* to the dictionary to represent the *receptors* for the canonical pathway as “Frizzled” and “LRP”.

Display the altered dictionary as the final result.

Solution

PYTHON

```python
signal = {'name': 'Wnt', 'pathway': 'Non-Canonical'}

signal['pathway'] = 'Canonical'
signal['receptors'] = ('Frizzled', 'LRP')

print(signal)
```

OUTPUT

```
{'name': 'Wnt', 'pathway': 'Canonical', 'receptors': ('Frizzled', 'LRP')}
```

ADVANCED TOPIC

Displaying an entire dictionary using the `print()` function can look a little messy because it is not properly structured. There is, however, an external library called `pprint` (Pretty-Print) that behaves in very similar way to the default `print()` function, but structures dictionaries and other arrays in a more presentable way before displaying them. We do not elaborate on Pretty-Print in this course, but it is a part of Python’s default library, and is therefore installed with Python automatically. To learn more about it, have a read through the official documentation for the library and review the examples.

Because a dictionary’s *keys* are immutable, they cannot be altered. However, we can get around this limitation in the following manner. It is possible to introduce a new *key* and assigning the *values* of the old *key* to this new key. Once we have done this, we can go ahead and *remove*

the old *item*. The easiest way to remove an *item* from a dictionary is to use the syntax `del`:

PYTHON

```python
# Creating a new key and assigning to it the
# values of the old key:
protein['human chromosome'] = protein['chromosome']

print(protein)
```

OUTPUT

```
{'full name': 'Cystic fibrosis transmembrane conductance regulator', 'alias': 'CFTR', 'gene': 'CFTR', 'type'
```

PYTHON

```python
# Now we remove the old item from the dictionary:
del protein['chromosome']

print(protein)
```

OUTPUT

```
{'full name': 'Cystic fibrosis transmembrane conductance regulator', 'alias': 'CFTR', 'gene': 'CFTR', 'type'
```

We can simplify the above operation using the `.pop()` method, which removes the specified *key* from a dictionary and returns any *values* associated with it:

PYTHON

```python
protein['common mutations in caucasians'] = protein.pop('common mutations')

print(protein)
```

OUTPUT

```
{'full name': 'Cystic fibrosis transmembrane conductance regulator', 'alias': 'CFTR', 'gene': 'CFTR', 'type'
```

PRACTICE EXERCISE 5

Implement a dictionary as:

PYTHON

```python
signal = {'name': 'Beta-Galactosidase', 'pdb': '4V40'}
```

with respect to signal:

- Change the *key* name from 'pdb' to 'pdb id' using the `.pop()` method.
- Write a code to find out whether the dictionary:
  - contains the new *key* (i.e. 'pdb id').
  - confirm that it no longer contains the old *key* (i.e. 'pdb')

If both conditions are met, display:

```
Contains the new key, but not the old one.
```

Otherwise:

```
Failed to alter the dictionary.
```

Solution

PYTHON

```python
signal = {
                    'name': 'Beta-Galactosidase',
                    'pdb': '4V40'
        }

signal['pdb id'] = signal.pop('pdb')

if 'pdb id' in signal and 'pdb' not in signal:
    print('Contains the new key, but not the old one.')
else:
    print('Failed to alter the dictionary.')
```

OUTPUT

```
Contains the new key, but not the old one.
```

Nested dictionaries

As explained earlier the section, dictionaries are among the most powerful built-in tools in Python. As we have previously done with arrays, it is also possible to construct nested dictionaries in order to organise data in a hierarchical fashion. This useful technique is outlined extensively in example.

It is very easy to implement nested dictionaries:

PYTHON

```python
# Parent dictionary
pkc_family = {
    # Child dictionary A:
    'conventional': {
      'note': 'Require DAG, Ca2+, and phospholipid for activation.',
      'types': ['alpha', 'beta-1', 'beta-2', 'gamma']
    },
    # Child dictionary B:
    'atypical': {
        'note': (
            'Require neither Ca2+ nor DAG for'
            'activation (require phosphatidyl serine).'
        ),
        'types': ['iota', 'zeta']
    }
}
```

and we follow similar principles to access, alter or remove the *values* stored in nested dictionaries:

PYTHON

```python
print(pkc_family)
```

OUTPUT

```
{'conventional': {'note': 'Require DAG, Ca2+, and phospholipid for activation.', 'types': ['alpha', 'beta-1'
```

PYTHON

```python
print(pkc_family['atypical'])
```

OUTPUT

```
{'note': 'Require neither Ca2+ nor DAG foractivation (require phosphatidyl serine).', 'types': ['iota', 'zeta
```

PYTHON

```python
print(pkc_family['conventional']['note'])
```

OUTPUT

```
Require DAG, Ca2+, and phospholipid for activation.
```

PYTHON

```python
print(pkc_family['conventional']['types'])
```

OUTPUT

```
['alpha', 'beta-1', 'beta-2', 'gamma']
```

PYTHON

```python
print(pkc_family['conventional']['types'][2])
```

OUTPUT

```
beta-2
```

PYTHON

```python
apkc_types = pkc_family['conventional']['types']
print(apkc_types[1])
```

OUTPUT

```
beta-1
```

PRACTICE EXERCISE 6

Implement the following table of genetic disorders as a nested dictionary:

	Full Name	Gene	Type
Cystic fibrosis	Cystic fibrosis transmembrane conductance regulator	CFTR	Membrane Protein
Xeroderma pigmentosum A	DNA repair protein complementing XP-A cells	XPA	Nucleotide excision repair
Haemophilia A	Haemophilia A	F8	Factor VIII Blood-clotting protein

Using the dictionary, display the *gene* for *Haemophilia A*.

Solution

PYTHON

```python
genetic_diseases = {
    'Cystic fibrosis': {
        'name': 'Cystic fibrosis transmembrane conductance regulator',
        'gene': 'CFTR',
        'type': 'Membrane Protein'
    },
    'Xeroderma pigmentosum A': {
        'name': 'DNA repair protein complementing XP-A cells',
        'gene': 'XPA',
        'type': 'Nucleotide excision repair'
    },
    'Haemophilia A': {
        'name': 'Haemophilia A',
        'gene': 'F8',
        'type': 'Factor VIII Blood-clotting protein'
    }
}

print(genetic_diseases['Haemophilia A']['gene'])
```

OUTPUT

```
F8
```

EXAMPLE: NESTED DICTIONARIES IN PRACTICE

We would like to store and analyse the structure of several proteins involved in the *Lac operon* - a commonly-studied operon fundamental to the metabolism and transport of lactose in many species of enteric bacteria. To do so, let's create a Python `dict` to help us organise our data.

Let's begin by creating an empty dictionary to store our structures:

PYTHON

```python
structures = dict()
```

We then move on to depositing our individual entries to structures by adding new *items* to it.

Each *item* has a *key* that represents the name of the protein we are depositing, and a *value* that is itself a dictionary consisting of information regarding the structure of that protein:

PYTHON

```python
structures['Beta-Galactosidase'] = {
    'pdb id': '4V40',
    'deposit date': '1994-07-18',
    'organism': 'Escherichia coli',
    'method': 'x-ray',
    'resolution': 2.5,
    'authors': (
        'Jacobson, R.H.', 'Zhang, X.',
        'Dubose, R.F.', 'Matthews, B.W.'
    )
}
```

PYTHON

```python
structures['Lactose Permease'] = {
    'pdb id': '1PV6',
    'deposit data': '2003-06-23',
    'organism': 'Escherichia coli',
    'method': 'x-ray',
    'resolution': 3.5,
    'authors': (
        'Abramson, J.', 'Smirnova, I.', 'Kasho, V.',
        'Verner, G.', 'Kaback, H.R.', 'Iwata, S.'
    )
}
```

Dictionaries don't have to be homogeneous. In other words, each entry can contain different *items* within it.

For instance, the 'LacY' protein contains an additional *key* entitled 'note':

PYTHON

```python
structures['LacY'] = {
    'pdb id': '2Y5Y',
    'deposit data': '2011-01-19',
    'organism': 'Escherichia coli',
    'method': 'x-ray',
    'resolution': 3.38,
    'note': 'in complex with an affinity inactivator',
    'authors': (
        'Chaptal, V.', 'Kwon, S.', 'Sawaya, M.R.',
        'Guan, L.', 'Kaback, H.R.', 'Abramson, J.'
    )
}
```

The variable structure which is an instance of type `dict`, is now a nested dictionary:

PYTHON

```python
print(structures)
```

OUTPUT

```
{'Beta-Galactosidase': {'pdb id': '4V40', 'deposit date': '1994-07-18', 'organism': 'Escherichia coli', '
```

We know that we can extract information from our nested `dict` just like we would with any other `dict`:

PYTHON

```python
print(structures['Beta-Galactosidase'])
```

OUTPUT

```
{'pdb id': '4V40', 'deposit date': '1994-07-18', 'organism': 'Escherichia coli', 'method': 'x-ray', 'resc
```

PYTHON

```python
print(structures['Beta-Galactosidase']['method'])
```

OUTPUT

```
x-ray
```

PYTHON

```python
print(structures['Beta-Galactosidase']['authors'])
```

OUTPUT

```
('Jacobson, R.H.', 'Zhang, X.', 'Dubose, R.F.', 'Matthews, B.W.')
```

PYTHON

```python
print(structures['Beta-Galactosidase']['authors'][0])
```

OUTPUT

```
Jacobson, R.H.
```

Sometimes, particularly when creating longer dictionaries, it might be easier to store individual entries in a variable beforehand and add them to the parent dictionary later on.

Note that our parent dictionary in this case is represented by the variable structure.

PYTHON

```python
entry = {
    'Lac Repressor': {
        'pdb id': '1LBI',
        'deposit data': '1996-02-17',
        'organism': 'Escherichia coli',
        'method': 'x-ray',
        'resolution': 2.7,
        'authors': (
            'Lewis, M.', 'Chang, G.', 'Horton, N.C.',
            'Kercher, M.A.', 'Pace, H.C.', 'Lu, P.'
        )
    }
}
```

We can then use the `.update()` method to update our structures dictionary:

PYTHON

```python
structures.update(entry)

print(structures['Lac Repressor'])
```

OUTPUT

```
{'pdb id': '1LBI', 'deposit data': '1996-02-17', 'organism': 'Escherichia coli', 'method': 'x-ray', 'resc
```

Sometimes, we need to see what *keys* our dictionary contains. In order to obtain an array of *keys*, we use the method `.keys()` as follows:

PYTHON

```python
print(structures.keys())
```

OUTPUT

```
dict_keys(['Beta-Galactosidase', 'Lactose Permease', 'LacY', 'Lac Repressor'])
```

Likewise, we can also obtain an array of *values* in a dictionary using the `.values()` method:

PYTHON

```python
print(structures['LacY'].values())
```

OUTPUT

```
dict_values(['2Y5Y', '2011-01-19', 'Escherichia coli', 'x-ray', 3.38, 'in complex with an affinity inacti
```

We can then extract specific information to conduct an analysis. Note that the `len()` function in this context returns the number of *keys* in the parent dictionary only.

PYTHON

```python
sum_resolutions = 0
res = 'resolution'

sum_resolutions += structures['Beta-Galactosidase'][res]
sum_resolutions += structures['Lactose Permease'][res]
sum_resolutions += structures['Lac Repressor'][res]
sum_resolutions += structures['LacY'][res]

total_entries = len(structures)

average_resolution = sum_resolutions / total_entries

print(average_resolution)
```

OUTPUT

```
3.0199999999999996
```

Useful methods for dictionary

Next, we can demonstrate some of the useful *methods* that are associated with `dict` in Python.

Given a dictionary as:

PYTHON

```python
lac_repressor = {
            'pdb id': '1LBI',
            'deposit data': '1996-02-17',
            'organism': 'Escherichia coli',
            'method': 'x-ray',
            'resolution': 2.7,
}
```

We can create an array of all *items* in the dictionary using the `.items()` method:

PYTHON

```python
print(lac_repressor.items())
```

OUTPUT

```
dict_items([('pdb id', '1LBI'), ('deposit data', '1996-02-17'), ('organism', 'Escherichia coli'), ('method',
```

Similar to the `enumerate()` function, the `.items()` method also returns an array of `tuple` members. Each `tuple` itself consists of two members, and is structured as ('key': 'value'). On that account, we can use its output in the context of a `for`–loop as follows:

PYTHON

```python
for key, value in lac_repressor.items():
    print(key, value, sep=': ')
```

OUTPUT

```
pdb id: 1LBI
deposit data: 1996-02-17
organism: Escherichia coli
method: x-ray
resolution: 2.7
```

PRACTICE EXERCISE 7

Try `.items()` on a nested `dict`, and see how it works.

Solution

PYTHON

```python
nested_dict = {
    'L1-a': {
        'L2-Ka': 'L2_Va',
        'L2-Kb': 'L2_Vb',
    },
    'L1-b': {
        'L2-Kc': 'L2_Vc',
        'L2-Kd': 'L3_Vd'
    },
    'L3-c': 'L3_V'
}

print(nested_dict.items())
```

OUTPUT

```
dict_items([('L1-a', {'L2-Ka': 'L2_Va', 'L2-Kb': 'L2_Vb'}), ('L1-b', {'L2-Kc': 'L2_Vc', 'L2-Kd': 'L3_Vd'
```

We learned earlier that if we try to retrieve a *key* that is not in the `dict`, a `KeyError` will be raised. If we anticipate this, we can handle it using the `.get()` method. The method takes in the *key* and searches the dictionary to find it. If found, the associated *value* is returned. Otherwise, the method returns `None` by default. We can also pass a second value to `.get()` to replace `None` in cases that the requested *key* does not exist:

PYTHON

```python
print(lac_repressor['gene'])
```

OUTPUT

```
KeyError: 'gene'
```

PYTHON

```python
print(lac_repressor.get('gene'))
```

OUTPUT

```
None
```

PYTHON

```python
print(lac_repressor.get('gene', 'Not found...'))
```

OUTPUT

```
Not found...
```

PRACTICE EXERCISE 8

Implement the lac_repressor dictionary and try to extract the *values* associated with the following *keys*:

- organism
- authors
- subunits
- method

If a *key* does not exist in the dictionary, display No entry instead.

Display the results in the following format:

```
organism: XXX
authors: XXX
```

Solution

PYTHON

```python
lac_repressor = {
    'pdb id': '1LBI',
    'deposit data': '1996-02-17',
    'organism': 'Escherichia coli',
    'method': 'x-ray',
    'resolution': 2.7,
}

requested_keys = ['organism', 'authors', 'subunits', 'method']

for key in requested_keys:
    lac_repressor.get(key, 'No entry')
```

OUTPUT

```
'Escherichia coli'
'No entry'
'No entry'
'x-ray'
```

`for`-loop and dictionary

Dictionaries and `for`-loops used together can synergise into a powerful combination. We can leverage the accessibility of dictionary *values* through specific *keys* that we define ourselves in a loop in order to extract data iteratively, and repeatedly.

One of the most useful tools that we can create using nothing more than a `for`-loop and a dictionary, in only a few lines of code, is a sequence converter.

Here, we are essentially iterating through a sequence of DNA nucleotides (sequence), extracting one character per loop cycle from our string (nucleotide). We then use that character as a *key* to retrieve its corresponding *value* from our dictionary (dna2rna). Once we get the *value*, we add it to the variable that we initialised using an empty string outside the scope of our `for`-loop (rna_sequence) as discussed here. At the end of the process, the variable rna_sequence will contain a converted version of our sequence.

PYTHON

```python
sequence = 'CCCATCTTAAGACTTCACAAGACTTGTGAAATCAGACCACTGCTCAATGCGGAACGCCCG'

dna2rna = {"A": "U", "T": "A", "C": "G", "G": "C"}

rna_sequence = str()  # Creating an empty string.

for nucleotide in sequence:
    rna_sequence += dna2rna[nucleotide]

print('DNA:', sequence)
print('RNA:', rna_sequence)
```

OUTPUT

```
DNA: CCCATCTTAAGACTTCACAAGACTTGTGAAATCAGACCACTGCTCAATGCGGAACGCCCG
RNA: GGGUAGAAUUCUGAAGUGUUCUGAACACUUUAGUCUGGUGACGAGUUACGCCUUGCGGGC
```

PRACTICE EXERCISE 9

We know that in reverse transcription, RNA nucleotides are converted to their complementary DNA nucleotides as shown:

Type	Direction	Nucleotides
RNA	5'...'	U A G C
cDNA	5'...'	A T C G

with this in mind:

1. Use the table to construct a dictionary for reverse transcription, and another dictionary for the conversion of cDNA to DNA.

2. Using the appropriate dictionary, convert the following mRNA (exon) sequence for human G protein-coupled receptor to its cDNA.

PYTHON

```python
human_gpcr = (
    'AUGGAUGUGACUUCCCAAGCCCGGGGCGUGGGCCUGGAGAUGUACCCAGGCACCGCGCAGCCUGCGGCCCCCAACACCACCUC'
    'CCCCGAGCUCAACCUGUCCCACCCGCUCCUGGGCACCGCCCUGGCCAAUGGGACAGGUGAGCUCUCGGAGCACCAGCAGUACG'
    'UGAUCGGCCUGUUCCUCUCGUGCCUCUACACCAUCUUCCUCUUCCCCAUCGGCUUUGUGGGCAACAUCCUGAUCCUGGUGGUG'
    'AACAUCAGCUUCCGCGAGAAGAUGACCAUCCCCGACCUGUACUUCAUCAACCUGGCGGUGGCGGACCUCAUCCUGGUGGCCGA'
    'CUCCCUCAUUGAGGUGUUCAACCUGCACGAGCGGUACUACGACAUCGCCGUCCUGUGCACCUUCAUGUCGCUCUUCCUGCAGG'
    'UCAACAUGUACAGCAGCGUCUUCUUCCUCACCUGGAUGAGCUUCGACCGCUACAUCGCCCUGGCCAGGGCCAUGCGCUGCAGC'
    'CUGUUCCGCACCAAGCACCACGCCCGGCUGAGCUGUGGCCUCAUCUGGAUGGCAUCCGUGUCAGCCACGCUGGUGCCCUUCAC'
    'CGCCGUGCACCUGCAGCACACCGACGAGGCCUGCUUCUGUUUCGCGGAUGUCCGGGAGGUGCAGUGGCUCGAGGUCACGCUGG'
    'GCUUCAUCGUGCCCUUCGCCAUCAUCGGCCUGUGCUACUCCCUCAUUGUCCGGGUGCUGGUCAGGGCGCACCGGCACCGUGGG'
    'CUGCGGCCCCGGCGGCAGAAGGCGCUCCGCAUGAUCCUCGCGGUGGUGCUGGUCUUCUUCGUCUGCUGGCUGCCGGAGAACGU'
    'CUUCAUCAGCGUGCACCUCCUGCAGCGGACGCAGCCUGGGGCCGCUCCCUGCAAGCAGUCUUUCCGCCAUGCCCACCCCCUCA'
    'CGGGCCACAUUGUCAACCUCACCGCCUUCUCCAACAGCUGCCUAAACCCCCUCAUCUACAGCUUUCUCGGGGAGACCUUCAGG'
    'GACAAGCUGAGGCUGUACAUUGAGCAGAAAACAAAUUUGCCGGCCCUGAACCGCUUCUGUCACGCUGCCCUGAAGGCCGUCAU'
    'UCCAGACAGCACCGAGCAGUCGGAUGUGAGGUUCAGCAGUGCCGUG'
)
```

Solution

PYTHON

```python
mrna2cdna = {
    'U': 'A',
    'A': 'T',
    'G': 'C',
    'C': 'G'
}

cdna2dna = {
    'A': 'T',
    'T': 'A',
    'C': 'G',
    'G': 'C'
}
```

Q2

PYTHON

```python
cdna = str()
for nucleotide in human_gpcr:
    cdna += mrna2cdna[nucleotide]

print(cdna)
```

OUTPUT

```
TACCTACACTGAAGGGTTCGGGCCCCGCACCCGGACCTCTACATGGGTCCGTGGCGCGTCGGACGCCGGGGGTTGTGGTGGAGGGGGCTCGAGTTGGACAGGGTC
```

Summary

In this section we explored dictionaries: one of the most powerful in-built types in Python. We covered:

- How to create dictionaries in Python.
- Methods to alter or manipulate both normal and nested dictionaries.
- Two different techniques for changing an existing *key*.
- Examples of how dictionaries can organise data and retrieve specific items and entries as and when required.

Finally, we also explored instantiating *iterables* (discussed here) from dictionary *keys* or *values* using the `.key()`, the `.values()`, and/or `.items()` methods.

Exercises

END OF CHAPTER EXERCISES

We know that the process of protein translation begins by transcribing a gene from DNA to RNA *nucleotides*, followed by translating the RNA *codons* into protein.

Conventionally, we write DNA sequences from their 5'-end to their 3'-end. The transcription process, however, begins from the 3'-end of a gene, through to the 5'-end (anti-sense strand), resulting in a sense mRNA sequence complementing the sense DNA strand. This is because RNA polymerase can only add nucleotides to the 3'-end of the growing mRNA chain, which eliminates the need for the Okazaki fragments as seen in DNA replication.

Example: The DNA sequence ATGTCTAAA is transcribed into AUGUCUAAA.

Given a conversion table:

DNA	A	T	C	G
cDNA	T	A	G	C
RNA	A	U	C	G

and this 5'- to 3'-end DNA sequence of 717 nucleotides for the Green Fluorescent Protein (GFP) mutant 3 extracted from Aequorea victoria:

PYTHON

```python
dna_sequence = (
    'ATGTCTAAAGGTGAAGAATTATTCACTGGTGTTGTCCCAATTTTGGTTGAATTAGATGGTGATGTTAATGGT'
    'CACAAATTTTCTGTCTCCGGTGAAGGTGAAGGTGATGCTACTTACGGTAAATTGACCTTAAAATTTATTTGT'
    'ACTACTGGTAAATTGCCAGTTCCATGGCCAACCTTAGTCACTACTTTCGGTTATGGTGTTCAATGTTTTGCT'
    'AGATACCCAGATCATATGAAACAACATGACTTTTTCAAGTCTGCCATGCCAGAAGGTTATGTTCAAGAAAGA'
    'ACTATTTTTTTCAAAGATGACGGTAACTACAAGACCAGAGCTGAAGTCAAGTTTGAAGGTGATACCTTAGTT'
    'AATAGAATCGAATTAAAAGGTATTGATTTTAAAGAAGATGGTAACATTTTAGGTCACAAATTGGAATACAAC'
    'TATAACTCTCACAATGTTTACATCATGGCTGACAAACAAAAGAATGGTATCAAAGTTAACTTCAAAATTAGA'
    'CACAACATTGAAGATGGTTCTGTTCAATTAGCTGACCATTATCAACAAAATACTCCAATTGGTGATGGTCCA'
    'GTCTTGTTACCAGACAACCATTACTTATCCACTCAATCTGCCTTATCCAAAGATCCAAACGAAAAGAGAGAC'
    'CACATGGTCTTGTTAGAATTTGTTACTGCTGCTGGTATTACCCATGGTATGGATGAATTGTACAAATAA'
)
```

Use the DNA sequence and the conversion table to:

1. Write a Python script to *transcribe* this sequence to mRNA as it occurs in a biological organism. That is, determine the complimentary DNA first, and use this to produce the mRNA sequence.

2. Use the following dictionary in a Python script to obtain the translation (protein sequence) of the Green Fluorescent Protein using the mRNA sequence you obtained.

PYTHON

```python
codon2aa = {
    "UUU": "F", "UUC": "F", "UUA": "L", "UUG": "L", "CUU": "L",
    "CUC": "L", "CUA": "L", "CUG": "L", "AUU": "I", "AUC": "I",
    "AUA": "I", "GUU": "V", "GUC": "V", "GUA": "V", "GUG": "V",
    "UCU": "S", "UCC": "S", "UCA": "S", "UCG": "S", "AGU": "S",
    "AGC": "S", "CCU": "P", "CCC": "P", "CCA": "P", "CCG": "P",
    "ACU": "T", "ACC": "T", "ACA": "T", "ACG": "T", "GCU": "A",
    "GCC": "A", "GCA": "A", "GCG": "A", "UAU": "Y", "UAC": "Y",
    "CAU": "H", "CAC": "H", "CAA": "Q", "CAG": "Q", "AAU": "N",
    "AAC": "N", "AAA": "K", "AAG": "K", "GAU": "D", "GAC": "D",
    "GAA": "E", "GAG": "E", "UGU": "C", "UGC": "C", "UGG": "W",
    "CGU": "R", "CGC": "R", "CGA": "R", "CGG": "R", "AGA": "R",
    "AGG": "R", "GGU": "G", "GGC": "G", "GGA": "G", "GGG": "G",
    "AUG": "<Met>", "UAA": "<STOP>", "UAG": "<STOP>", "UGA": "<STOP>"
}
```

Solution

KEY POINTS

- Dictionaries associate a set of *values* with a number of *keys*.
- *Keys* are used to access the values of a dictionary.
- Dictionaries are mutable.
- Nested dictionaries are constructed to organise data in a hierarchical fashion.
- Some of the useful methods to work with dictionaries are: `.items()`, `.get()`

Content from Functions

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OVERVIEW

Questions

- What are functions?
- How are functions created?
- What are optional arguments?

- What makes functions so powerful?

Objectives

- Understand how to develop and utilise functions.
- Understanding different ways of creating functions.
- Explaining input arguments.
- Understanding the interconnectivity of functions.

Function to create a dictionary

Transcription Function

Covariance Function

This chapter assumes that you are familiar with the following concepts in Python:

PREREQUISITE

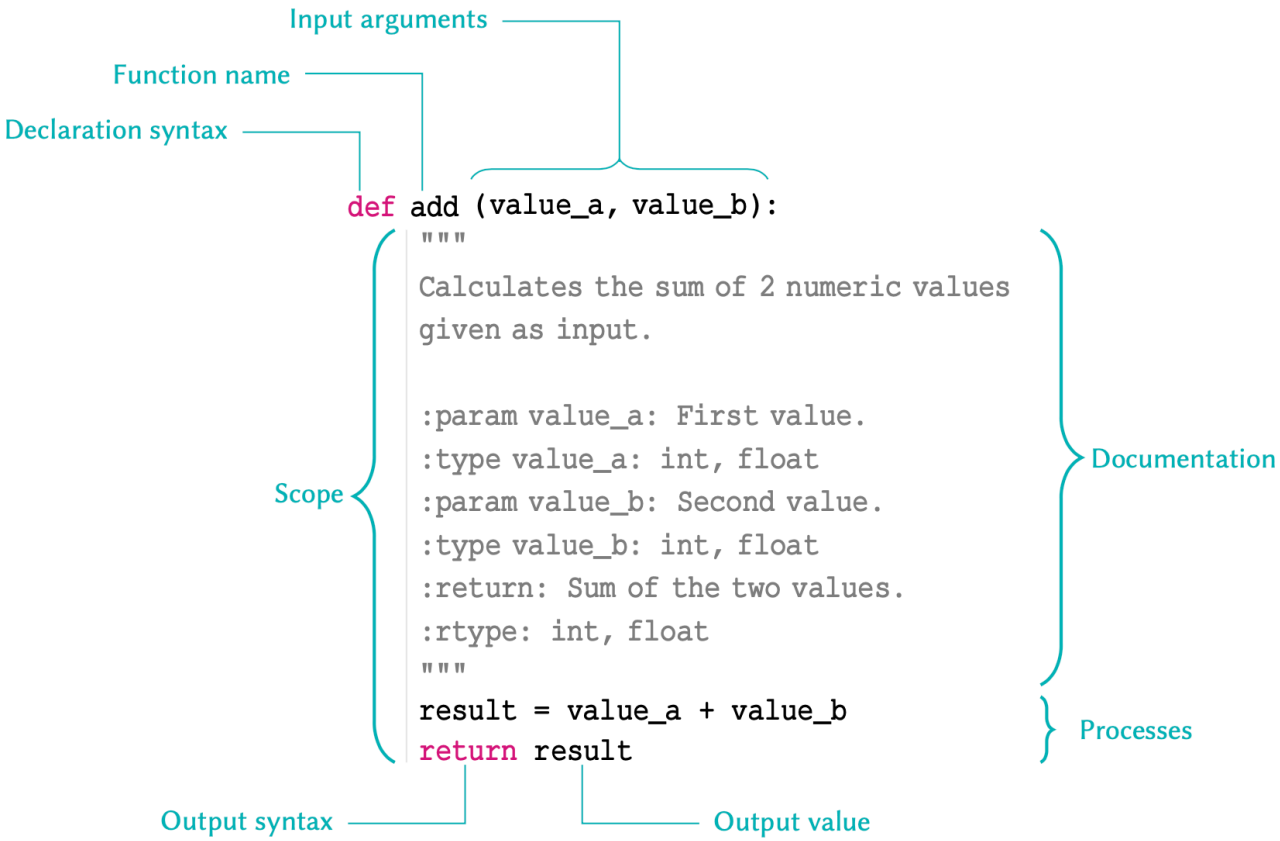
- Mathematical Operation
- Indentation Rule
- Conditional Statements
- Arrays
- Loops and Iterations

Functions

Defining Functions

In programming, functions are individual units or blocks of code that incorporate and perform specific tasks in a sequence defined and written by the programmer. As we learned in the first chapter (on outputs), a function usually takes in one or several variables or values, processes them, and produces a specific result. The variable(s) given to a function and those produced by it are referred to as *input arguments*, and *outputs* respectively.

There are different ways to create functions in Python. In the L2D, we will be using `def` to implement our functions. This is the simplest and most common method for declaring a function. The structure of a typical function defined using `def` is as follows:



REMEMBER

There are several points to remember relative to functions:

- The name of a function follows same principles as that of any other variable as discussed in variable names. The name must be in *lower-case* characters.
- The input arguments of a function — e.g. value_a and value_b in the above example; are essentially variables whose *scope* is the function. That is, they are *only* accessible *within* the function itself, and not from anywhere else in the code.
- Variables defined within a function, should *never* use the same name as variables defined outside of it; or they may override each other.
- A function declared using `def` should *always* be terminated with a `return` syntax. Any values or variables that follow `return` are regarded as the function's output.
- If we do not specify a return value, or fail to terminate a function using `return` altogether, the Python interpreter will automatically terminate that function with an implicit `return None`. Being an *implicit* process, this is generally regarded as a bad practice and should be avoided.

We implement functions to avoid repetition in our code. It is important that a function is *only* performing a very specific task, so that it can be context-independent. You should therefore avoid incorporating separable tasks inside a single function.

INTERESTING FACT

Functions are designed to perform specific tasks. That is why in the majority of cases, they are named using *verbs* — e.g. `add()` or `print()`. Verbs describe an action, a state, or an occurrence in the English language. Likewise, this type of nomenclature describes the action performed by a specific function. As we encourage with variable naming: sensible, short and descriptive names are best to consider, when naming a function.

Once you start creating functions for different purposes, you will eventually amass a library of ready-to-use functions which can individually address different needs. This is the primary principle of a popular programming paradigm known as functional programming.

So let us implement the example outline in the diagram:

PYTHON

```python
def add(value_a, value_b):
    """
    Calculates the sum of two numeric values
    given as inputs.

    :param value_a: First value.
    :type value_a: int, float
    :param value_b: Second value.
    :type value_b: int, float
    :return: Sum of the two values.
    :rtype: int, float
    """
    result = value_a + value_b
    return result
```

Once implemented, we can call and use the function we created. We can do so in the same way as we do with the *built-in* functions such as `max()` or `print()`:

PYTHON

```python
res = add(2, 5)

print(res)
```

OUTPUT

```
7
```

REMEMBER

When calling a function, we should always pass our *positional input arguments* in the order they are defined in the function definition: i.e. from left to right.

This is because in the case of *positional arguments*, as the name suggests, the Python interpreter relies on the *position* of each value to identify its *variable name* in the function signature. The function signature for our `add` function is as follows:

```
add(value_a, value_b)
```

So in the above example where we say add(2, 5), the value 2 is identified as the *input argument* for value_a, and not value_b. This happens automatically because in our function call, the value 2 is written in the first position: the position at which value_a is defined in our function declaration (signature).

Alternatively, we can use the name of each *input argument* to pass values onto them in any order. When we use the name of the *input argument* explicitly, we pass the values as *keyword arguments*. This is particularly useful in more complex functions where there are several *input arguments*.

Let us now use *keyword arguments* to pass values to our `add()` function:

PYTHON

```
res = add(value_a=2, value_b=5)

print(res)
```

OUTPUT

```
7
```

Now, even if we change the order of our arguments, the function would still be able to associate the values to the correct keyword argument:

PYTHON

```
res = add(value_b=2, value_a=5)

print(res)
```

OUTPUT

```
7
```

REMEMBER

Choose the order of your *input argument* wisely. This is important when your function can accept multiple *input arguments*.

Suppose we want to define a 'division' function. It makes sense to assume that the first number passed to the function will be divided by the second number:

PYTHON

```python
def divide(a, b):
    return a / b
```

It is also much less likely for someone to use *keywords* to pass arguments to this function – that is, to say:

PYTHON

```python
result = divide(a=2, b=4)
```

than it is for them to use positional arguments (without any keywords), that is:

PYTHON

```python
result = divide(2, 4)
```

But if we use an arbitrary order, then we risk running into problems:

PYTHON

```python
def divide_bad(denominator, numerator):
    return numerator / denominator
```

In which case, our function would perform perfectly well if we use *keyword arguments*; however, if we rely on positional arguments and common sense, then the result of the division would be calculated incorrectly.

PYTHON

```python
result_a = divide_bad(numerator=2, denominator=4)
result_b = divide_bad(2, 4)

print(result_a == result_b)
```

OUTPUT

```
False
```

PRACTICE EXERCISE 1

Implement a function called find_tata that takes in one `str` argument called seq and looks for the TATA-box motif inside that sequence. Then:

- if found, the function should return the index for the TATA-box as output.
- if not found, the function should *explicitly* return `None`.

Example:

The function should behave, as follows:

```
sequence = 'GCAGTGTATAGTC'

res = find_tata(sequence)
```

Solution

PYTHON

```python
def find_tata(seq):
    tata_box = 'TATA'
    result = seq.find(tata_box)

    return result
```

Documentation

It is *essential* to write short, informative documentation for a functions that you are defining. There is no single *correct* way to document a code. However, as a general rule, a sufficiently informative documentation should tell us:

- what a function does;
- the names of the input arguments, and what type each argument should be;
- the output, and its type.

This documentation string is referred to as the *docstring*. It is always written inside triple quotation marks. The *docstring* must be implemented on the *very first line*, immediately following the declaration of the function, in order for it to be recognised as documentation:

PYTHON

```python
def add(value_a, value_b):
    """
    Calculates the sum of two numeric values
    given as inputs.

    :param value_a: First value.
    :type value_a: int, float
    :param value_b: Second value.
    :type value_b: int, float
    :return: Sum of the two values.
    :rtype: int, float
    """
    result = value_a + value_b
    return result
```

REMEMBER

You might feel as though you would remember what your own functions do. Assuming this is often naive, however, as it is easy to forget the specifics of a function that you have written; particularly if it is complex and accepts multiple arguments. Functions that we implement tend to perform specialist, and often complex, interconnected processes. Whilst you might remember what a specific function does for a few days after writing it, you will likely have trouble remembering the details in a matter of months. And that is not even considering details regarding the type of the input argument(s) and those of the output. In addition, programmers often share their work with other fellow programmers; be it within their team or in the wider context of a publication, or even for distribution *via* public repositories, as a community contribution. Whatever the reason, there is one golden rule: a function should not exist unless it is documented.

Writing the *docstring* on the first line is important. Once a function is documented, we can use `help()`, which is a built-in function in Python, to access the documentations as follows:

PYTHON

```python
help(add)
```

OUTPUT

```
Help on function add in module __main__:

add(value_a, value_b)
    Calculates the sum of two numeric values
    given as inputs.

    :param value_a: First value.
    :type value_a: int, float
    :param value_b: Second value.
    :type value_b: int, float
    :return: Sum of the two values.
    :rtype: int, float
```

For very simple functions – like the `add()` function that we implemented above, it is sufficient to simplify the docstring into something straightforward, and concise. This is because it is fairly obvious what are the input and output arguments are, and what their respective types

are/should be. For example:

PYTHON

```python
def add(value_a, value_b):
    """value_a + value_b -> number"""
    result = value_a + value_b
    return result
```

PYTHON

```python
help(add)
```

OUTPUT

```
Help on function add in module __main__:

add(value_a, value_b)
    value_a + value_b -> number
```

PRACTICE EXERCISE 2

Re-implement the function you defined in the previous Practice Exercise 1 with appropriate documentation.

Solution

PYTHON

```python
def find_tata(seq):
    """
    Finds the location of the TATA-box,
    if one exists, in a polynucleotide
    sequence.

    :param seq: Polynucleotide sequence.
    :type seq: str
    :return: Start of the TATA-box.
    :rtype: int
    """
    tata_box = 'TATA'
    result = seq.find(tata_box)

    return result
```

Optional arguments

We already know that most functions accept one or more input arguments. Sometimes a function does not need all of the arguments in order to perform a specific task.

Such an example that we have already worked with is `print()`. We already know that this function may be utilised to display text on the screen. However, we also know that if we use the `file` argument, it will behave differently in that it will write the text inside a file instead of

displaying it on the screen. Additionally, `print()` has other arguments such as `sep` or `end`, which have specific default values of ' ' (a single space) and \n (a linebreak) respectively.

REMEMBER

Input arguments that are necessary to call a specific function are referred to as *non-default arguments*. Those whose definition is not mandatory for a function to be called are known as *default* or *optional arguments*.

Optional arguments may *only* be defined *after* non-default arguments (if any). If this order is not respected, a `SyntaxError` will be raised.

ADVANCED TOPIC

The default value defined for *optional arguments* can theoretically be an instance of any type in Python. However, it is better and safer to only use *immutable* types (as demonstrated in Table) for default values. The rationale behind this principle is beyond the scope of this course, but you can read more about it in the official documentation.

In order to define functions with optional arguments, we need to assign a default value to them. Remember: input arguments are variables with a specific scope. As a result, we can treat our input argument as variables and assign them a value:

PYTHON

```python
def prepare_seq(seq, name, upper=False):
    """
    Prepares a sequence to be displayed.

    :param seq: Sequence
    :type seq: str
    :param name: Name of the sequence.
    :type name: str
    :param upper: Convert sequence to uppercase characters (default: False)
    :type upper: bool
    :return: Formatted string containing the sequence.
    :rtype: str
    """
    template = 'The sequence of {} is: {}'

    if not upper:
        response = template.format(name, seq)
    else:
        seq_upper = seq.upper()
        response = template.format(name, seq_upper)

    return response
```

Now if we don't explicitly define `upper` when calling `prepare_seq()`, its value is automatically considered to be `False`:

PYTHON

```python
sequence = 'TagCtGC'

prepped = prepare_seq(sequence, 'DNA')

print(prepped)
```

OUTPUT

```
The sequence of DNA is: TagCtGC
```

If we change the default value of `False` for `upper` and set to `True`, our sequence should be converted to upper case characters:

PYTHON

```python
prepped = prepare_seq(sequence, 'DNA', upper=True)

print(prepped)
```

OUTPUT

```
The sequence of DNA is: TAGCTGC
```

PRACTICE EXERCISE 3

Modify the function from the previous Practice Exercise 2 to accept an *optional argument* called `upper`, with a default value of `False`. Thereafter:

- if `upper` is `False`, then the function should perform as it already does (similar to the previous Practice Exercise 2);
- if `upper` is `True`, then the function should convert the sequence to contain only uppercase characters, before it looks for the TATA-box.

Do not forget to update the *docstring* of your function.

Solution

PYTHON

```python
def find_tata(seq, upper=False):
    """
    Finds the location of the TATA-box,
    if one exists, in a polynucleotide
    sequence.

    :param seq: Polynucleotide sequence.
    :type seq: str
    :param upper: Whether or not to
     homogenise the sequence
     to upper-case characters.
    :type upper: bool
    :return: Start of the TATA-box.
    :rtype: int
    """
    tata_box = 'TATA'

    if not upper:
        result = seq.find(tata_box)
    else:
        seq_prepped = seq.upper()
        result = seq_prepped.find(tata_box)

    return result
```

REMEMBER

It is not necessary to implement your functions in this way. It is, however, a common practice among programmers in any programming language. For this reason, you should be at least be familiar with the technique, as you will likely encounter it at some point.

It is important to note that it is also possible to have more than one `return` in a function. This is useful when we need to account for different outcomes; such as the one we saw in the previous example with `prepare_seq()`.

This means that we can simplify the process as follows:

PYTHON

```python
def prepare_seq(seq, name, upper=False):
    """
    Prepares a sequence to be displayed.

    :param seq: Sequence
    :type seq: str
    :param name: Name of the sequence.
    :type name: str
    :param upper: Convert sequence to uppercase characters (default: False)
    :type upper: bool
    :return: Formated string containing the sequence.
    :rtype: str
    """
    template = 'The sequence of {} is: {}'

    if not upper:
        return template.format(name, seq)

    seq_upper = seq.upper()
    return template.format(name, seq_upper)
```

Notice that we got rid of response. Here is a description of what is happening:

- In this context, if the conditional statement holds — i.e. when `upper` is `False`— we enter the `if` block. In this case, we reach the first `return` statement. It is at this point, that function returns the corresponding results, and immediately terminates.
- Conversely, if the conditional statement does not hold — i.e. where `upper` is `True` — we skip the `if` block altogether and proceed. It is only then that we arrive at the second `return` statement where the alternative set of results are prepared.

This does not alter the functionality of the function, in any way. However, in complex functions which can be called repetitively (*e.g.* inside `for` loop), this technique may improve the performance of the function.

Now if we call our function, it will behave in exactly the same way as it did before:

PYTHON

```python
sequence = 'TagCtGC'

prepped = prepare_seq(sequence, 'DNA')

print(prepped)
```

OUTPUT

```
The sequence of DNA is: TagCtGC
```

PYTHON

```python
prepped = prepare_seq(sequence, 'DNA', upper=True)

print(prepped)
```

OUTPUT

```
The sequence of DNA is: TAGCTGC
```

Interconnectivity of functions

Functions can also call other functions. This is what makes them extremely powerful tools that may be utilised to address an unlimited number of problems.

This allows us to devise a network of functions that can all call each other to perform different tasks at different times. This network of functions can then collectively contribute to the production of a single, final answer.

REMEMBER

Functions should have specialist functionalities.They should ideally be written to perform one task, and one task only.

So in instances where more operations are required, it is advised not to write more code to execute these, into one function. This would defy the ethos of functional programming. Instead, consider writing more functions that contain less code, and perform more specialist functionalities.

EXAMPLE: A MINI TOOLBOX FOR STATISTICS

Suppose we want to calculate the variance of an array of numbers. This is a generalisable task, which means that we could, and should write a function that is able to calculate the variance of *any* array of numbers.

We start off by breaking down the process of calculating the variance, which we know is defined as follows:

$$\sigma^2 = \frac{\sum_{i=1}^{n}(x_i - \mu)^2}{n}$$

which breaks down into:

1. calculating the mean or μ,
2. using the mean to calculate the numerator,
3. dividing the numerator by the length of the array.

At least one of these processes is not unique to the calculation of variance; and that is the process by which we work out the *mean*. To that end, we should separate this calculation from our *variance* function, and define it independently:

PYTHON

```python
def mean(arr):
    """
    Calculates the mean of an array.

    :param arr: Array of numbers.
    :type arr: list, tuple, set
    :return: Mean of the values in the array.
    :rtype: float
    """
    summation = sum(arr)
    length = len(arr)

    result = summation / length

    return result
```

Now that we have function to calculate the *mean*, we can go ahead and write a function to calculate the variance; which itself relies on *mean*:

PYTHON

```python
def variance(arr):
    """
    Calculates the variance of an array.

    :param arr: Array of numbers.
    :type arr: list, tuple, set
    :return: Variance of the values in the array.
    :rtype: float
    """
    arr_mean = mean(arr)
    denominator = len(arr)

    numerator = 0

    for num in arr:
        numerator += (num - arr_mean) ** 2

    result = numerator / denominator

    return result
```

Now we have two functions, which can be used to calculate the *variance*, or the *mean*, for any array of numbers.

Remember that testing a function is inherent to successful design. So let's test our functions

PYTHON

```python
numbers = [1, 5, 0, 14.2, -23.344, 945.23, 3.5e-2]
```

PYTHON

```python
numbers_mean = mean(numbers)

print(numbers_mean)
```

OUTPUT

```
134.58871428571427
```

PYTHON

```python
numbers_variance = variance(numbers)

print(numbers_variance)
```

OUTPUT

```
109633.35462420408
```

Now that we have a function to calculate the *variance*, we can easily proceed to calculate the *standard deviation*, as well.

The standard deviation is calculated from the square root of variance. We can easily implement this in a new function as follows:

PYTHON

```python
def stan_dev(arr):
    """
    Calculates the standard deviation of an array.

    :param arr: Array of numbers.
    :type arr: list, tuple, set
    :return: Standard deviation of the values in the array.
    :rtype: float
    """
    from math import sqrt

    var = variance(arr)

    result = sqrt(var)

    return result
```

Now let's see how it works, in practice:

PYTHON

```python
numbers_std = stan_dev(numbers)

print(numbers_std)
```

OUTPUT

```
331.1092789762982
```

PRACTICE EXERCISE 4

Write a function that — given an array of any values — produces a dictionary containing the values within the array as *keys*, and the count of those values in the original array (their frequencies), as *values*.

Example:

For the following array:

PYTHON

```python
values = [1, 1.3, 1, 1, 5, 5, 1.3, 'text', 'text', 'something']
```

the function should return the above dictionary:

Suggestion: You can add this as a new tool to the statistics mini toolbox.

Solution

PYTHON

```python
def count_values(arr):
    """
    Converts an array into a dictionary of
    the unique members (as keys) and their
    counts (as values).

    :param arr: Array containing repeated
                members.
    :type arr: list, tuple
    :return: Dictionary of unique members
                         with counts.
    :rtype: dict
    """
    unique = set(arr)
    arr_list = list(arr)

    result = dict()

    for num in unique:
        result[num] = arr_list.count(num)

    return result
```

Exercises

END OF CHAPTER EXERCISES

Write a function with the following features:

- Call the function `get_basic_stats()` and let it take one input argument which may contain any number of input arrays, *e.g.* a tuple of arrays.
- Using a for loop, for each of the arrays calculate the mean and the variance for each of the arrays using the functions 'mean' and 'variance', given above, *i.e.* call these functions from within the function `get_basic_stats()`.
- Calculate the standard deviation for each array as the square root of the variance. You will have to import the function `sqrt` from module `math`.
- Return a single array containing (in that order) the mean, the variance and the standard deviation for each array.

To test the function, combine three arrays in a tuple as follows:

PYTHON

```python
my_arrays = (
    [1, 2, 3, 4, 5],
    [7, 7, 7, 7],
    [1.0, 0.9, 1.2, 1.12, 0.95, 0.76],
)
```

Call the function `get_basic_stats()` with this tuple as an argument, and write the output to a variable. Display the results in the following form:

```
STD of array' index, ':' STD
```

The result for the above arrays should be:

```
STD of array 0 :  1.4142135623730951
STD of array 1 :  0.0
STD of array 2 :  0.14357537702854514
```

Solution

KEY POINTS

- Functions can help to make repetitive tasks efficient, allowing the passing of values into whole blocks of code, with a simple function call.
- Keyword `def` is used to write a function.
- Optional arguments do not require prior definition.
- The potential interconnectivity of functions can make them very powerful.