Introduction to Python

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Babraham Bioinformatics

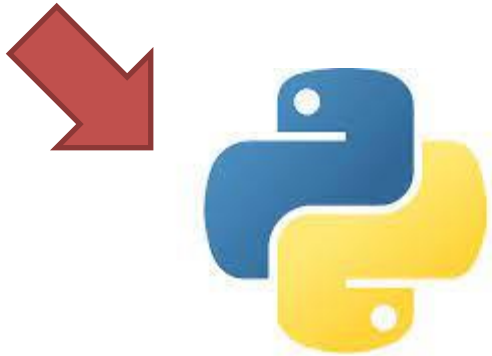
Setting up a Python Environment

Babraham Bioinformatics

Python is a ‘scripting’ language

```
#!/usr/bin/env python

print("I am a python program")
```

VS Code



python™

```
python
python.exe
python3
python3.exe
```

https://www.python.org/

```
C:\Introduction to Python>python example.py
I am a python program
```

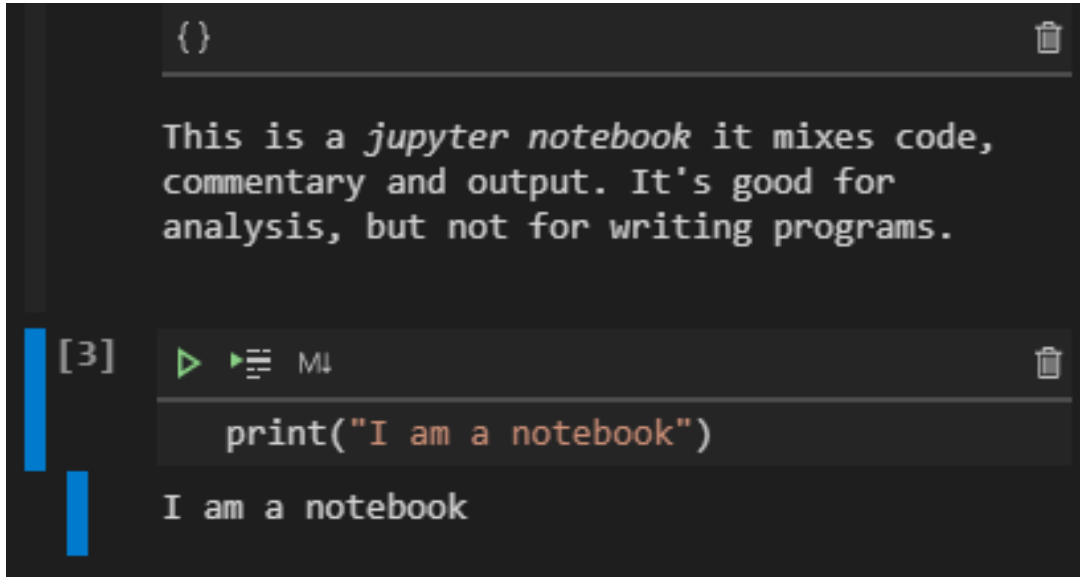
Different environments for writing python

```
#!/usr/bin/env python

print("I am a python program")
```

Scripted: code in text file, output in console

```
C:\Users\andrewss\>python
Python 3.9.1 (tags/v3.9.1:1e5d33e, Dec  7 2020,
17:08:21) [MSC v.1927 64 bit (AMD64)] on win32
Type "help", "copyright", "credits" or
"license" for more information.
>>>
>>> print("I am an interactive session")
I am an interactive session
>>>
```

Interactive: code and output in console



Notebook: code, commentary and output in a single file

Nexons

Introduction

Nexons is a program to quantitate RNA-Seq data from nanopore sequencing runs. It takes in a BAM file aligned with a suitable spliced aligner, and a GTF file of gene annotations from the genome to which the BAM file was aligned and creates a series of count tables from transcript or gene level matches with differing degress of confidence. It also generates QC reports to summarise the findings from each file.

https://github.com/s-andrews/nexons

SRA Downloader

SRAdownloader is a program which takes the annotation table from the SRA run selector tool and retrives the raw fastq files from either the ENA or NCBI databases for the selected samples, giving them meaningful names at the same time. It is designed to make it slightly less painful to get data out of GEO and the SRA.

https://github.com/s-andrews/sradownloader

Auto-Align

Automatic Nanopore Alignments

Introduction

The validation of sequencing constructs used to be performed using Sanger sequencing. More recently small scale Nanopore sequencing has been used instead, producing small fastq files from a single amplified PCR product, or plasmid.

This tool provides a simple way to align these small scale sequencing runs to a custom refernece sequence, most commonly the expected sequence of the construct.

https://github.com/s-andrews/autoalign

Splice Site Quantitation

This program implements a method for quantitating RNA-Seq data to produce a raw count matrix suitable for feeding into downstream analyses with programs such as DESeq2 or EdgeR.

What does the program do?

Rather than count all of the reads in your data this quantitation is based off the observed splice sites seen when matching the data to the reference genome. When you quantitate your BAM files you provide a GTF file with the details of your gene models and the program will count only reads which cross a known and annotated splice junction in the gene.

https://github.com/s-andrews/canonicalsplicecount

VDJ Replacement Circle Detection

The software here does the processing and analysis of VDJ-Seq amplicon data to detect non-canonical splicing events.

https://github.com/s-andrews/replacementcircles

Quantitation of Nonsense Mediated Decay

Nonsense Mediated Decay, or NMD for short, is a surveilance mechanims in cells which identifies and removes protein coding RNA molecules which contain a premature termination codon. Any transcript which contains splice junctions, and where the coding sequence within the transcript does not extend beyond the final splice junction is susceptible to degradation via this mechanism.

The `nmdquant` program aims to quantitate the level of nonsense mediated decay target transcripts within a set of RNA-Seq samples. It takes in BAM files of RNA-Seq data which have been mapped using a splicing aware mapper such as Hisat2 or STAR and produces counts of reads crossing all splice boundaries in a supplied GTF annotation file. The splice boundaries are annotated as to whether they are exclusively found in NMD target transcripts.

From the output of `nmdquant` you can visualise and analyse the levels of NMD in different samples.

https://github.com/s-andrews/nmdquant

codonuse - Efficient calculation of codon optimisation

Background

Although the genetic code contains redundancy, with the same amino acid often being able to be encoded by multiple codons, the distribution of tRNAs in an organism means that some codons are used more efficiently than others, and that by changing from an optimised to a non-optimised codon balance you can potentially modulate the rate at which a transcript is traslated.

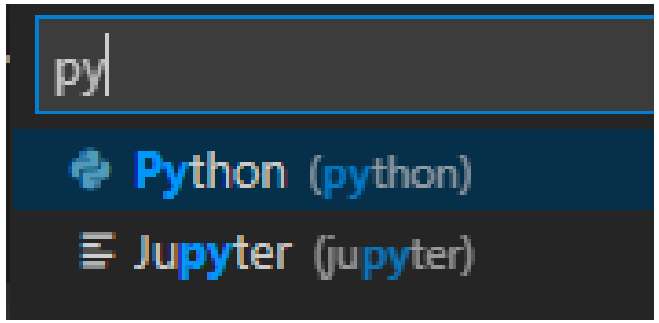
It is useful to have a method to quantitate the degree to which the codon usage for a particular sequence is optimised and that is what this program does. It uses the method described in https://bmcbioinformatics.biomedcentral.com/articles/10.1186/1471-2105-9-65 to produce a number of metrics to assess the optimisation of codon usage.

https://github.com/s-andrews/codonuse

Using VSCode to write a python script

- Install VSCode
- Install Python interpreter
- Open VSCode
  - File > New File

  - Select Python



  - File > SaveAs
    - Use a `.py` extension

Your first python program

```
#!python

my_name = "Simon"

print (my_name,"wrote his first python program")

print("He is very proud")
```

```
C:\>"C:/Program Files/Python39/python.exe" "c:/Introduction to Python/first_program.py"
Simon wrote his first python program
He is very proud
```

Python script basics

Where to find an interpreter

Comments use #

Series of python ‘statements’. One per line (generally). These are executed in order, from the top of the file to the bottom.

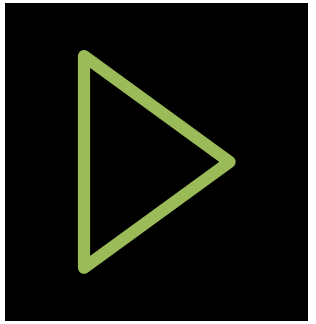
Your program finishes at the end of the file

```
#!python

# Create a variable with my name in it

my_name = "Simon"

print (my_name,"wrote his first python program")

print ("He is very proud")
```

Your turn..

- Copy the program below into VSCode and get it to run.

```
#!python

my_name = "Simon"

print (my_name,"wrote his first python program")

print("He is very proud")
```



Variables and Data Types

- A ‘variable’ is some data which you have given a name
- There are several different types of data structure
  - We’re starting with the ‘scalar’, a data type which holds a single value
- Python is a ‘dynamic’ but ‘strongly typed’ language
  - **Dynamic** = You don’t need to say what type of data a variable will hold when you create it (and you can change it at any time)
  - **Strongly typed** = Python tracks what type of data you have and changes its behaviour based on the type of the data

Creating a variable

- Variables are created or updated using the = operator
  - ‘Operator’ just means special symbol
  - Variable ‘types’ are determined by the data used
  - Python style guide says *"Variable names should be lowercase, with words separated by underscores as necessary to improve readability"*

```
x = 5         # x is an int (Integer, whole number)
x = 5.5       # x is a float (Floating point number, fractional)
x = True      # x is a bool (Boolean, logical True/False)
x = "Simon" # x is an str (String, piece of text)
```

```
x = input("What is your name? ") # Ask user for a str
```

Different ways to access functionality

- Operators
  - Special symbols to denote an operation (eg + * / etc)

```
5 + 10
```

- Functions
  - Named pieces of functionality into which data is passed

```
len("simon")
```

- Methods
  - Functions which are accessed via the data directly

```
"simon".upper()
```

Functions vs Methods

- Functions
  - Named pieces of code. All data (arguments) must be passed in to them. Accessed either in the core language or from packages

```
>>> len("Simon")
5
```

- Methods
  - Functions which are associated with a type of data (string, date etc). Called via the data, you don’t need to pass the data in to the method

```
>>> "Simon".upper()
'SIMON'
```

Functionality is linked to data type

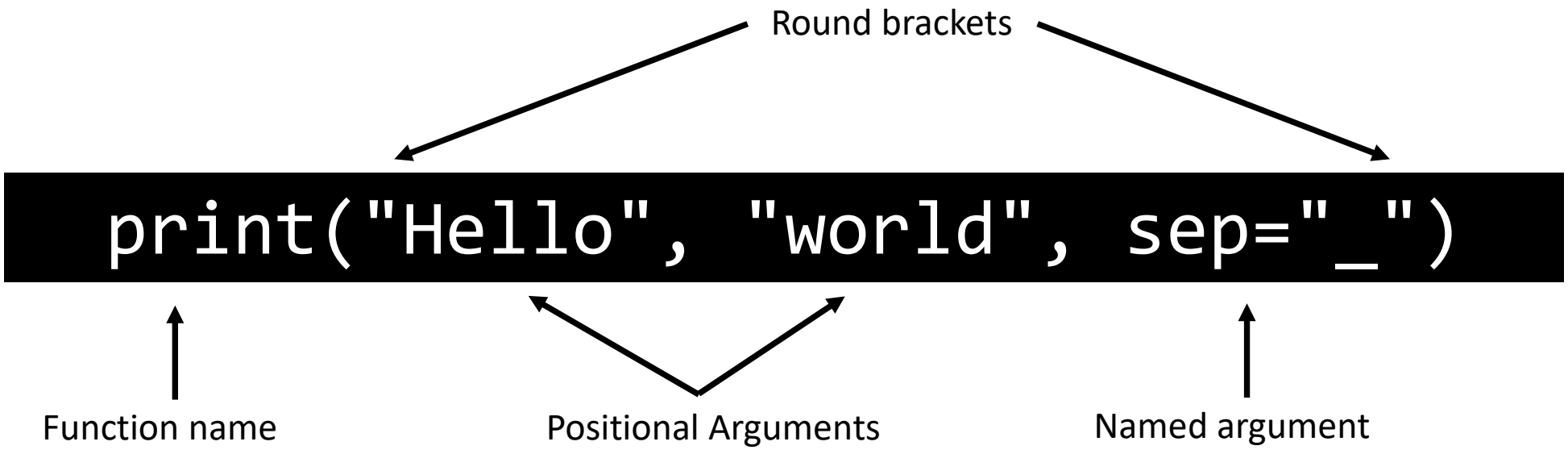
```
•  5  +  10       # 15
• "5" + "10"      # 510

• "5".upper()     # 5
•  5.upper()      # SyntaxError: invalid syntax

• float("5") + int("10") # 15
• str(5) + str(10)       # "510"
```

Common Numeric Operators

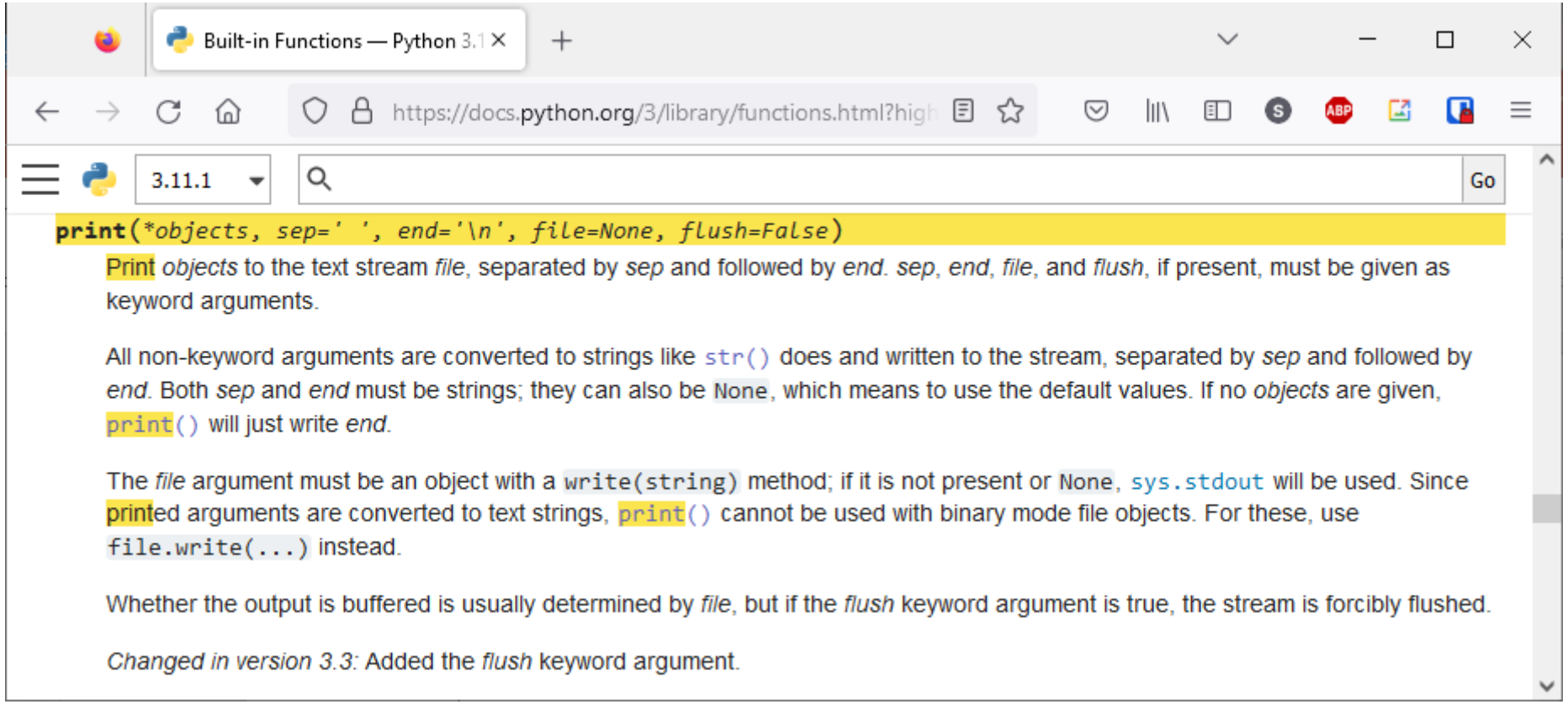
Operator	Action
+	Addition
-	Subtraction
*	Multiplication
/	Division
**	Raise to a power
//	Floor division
%	Modulo

```
5 + 10
23 - 56
10 * 4.5    # Can mix int/float
20 / 7      # Converts to float
2 ** 5
20 // 7     # Stays as int
20 % 7      # Calculates remainder
```

Running a function

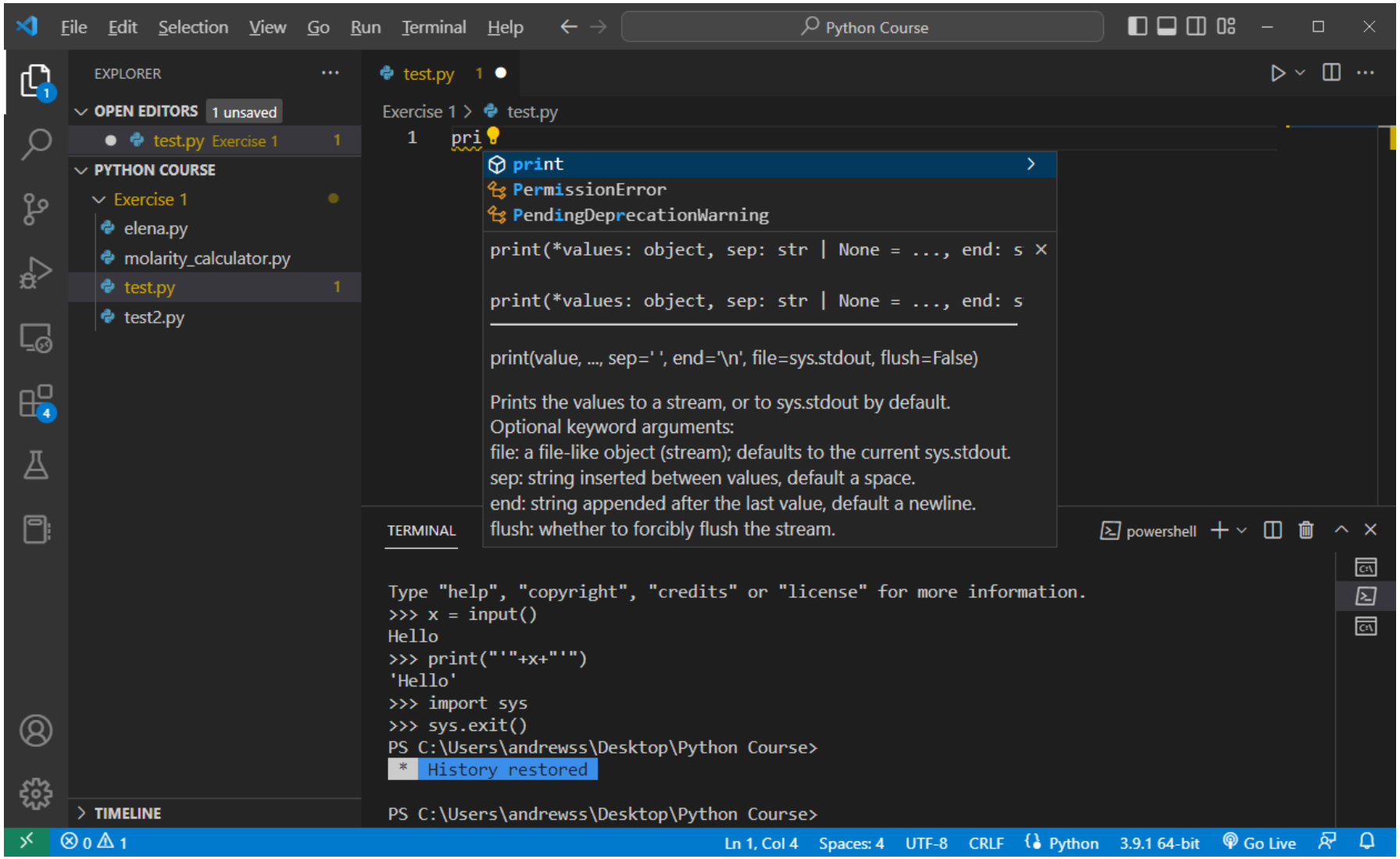


How to use a function?



https://docs.python.org/3/

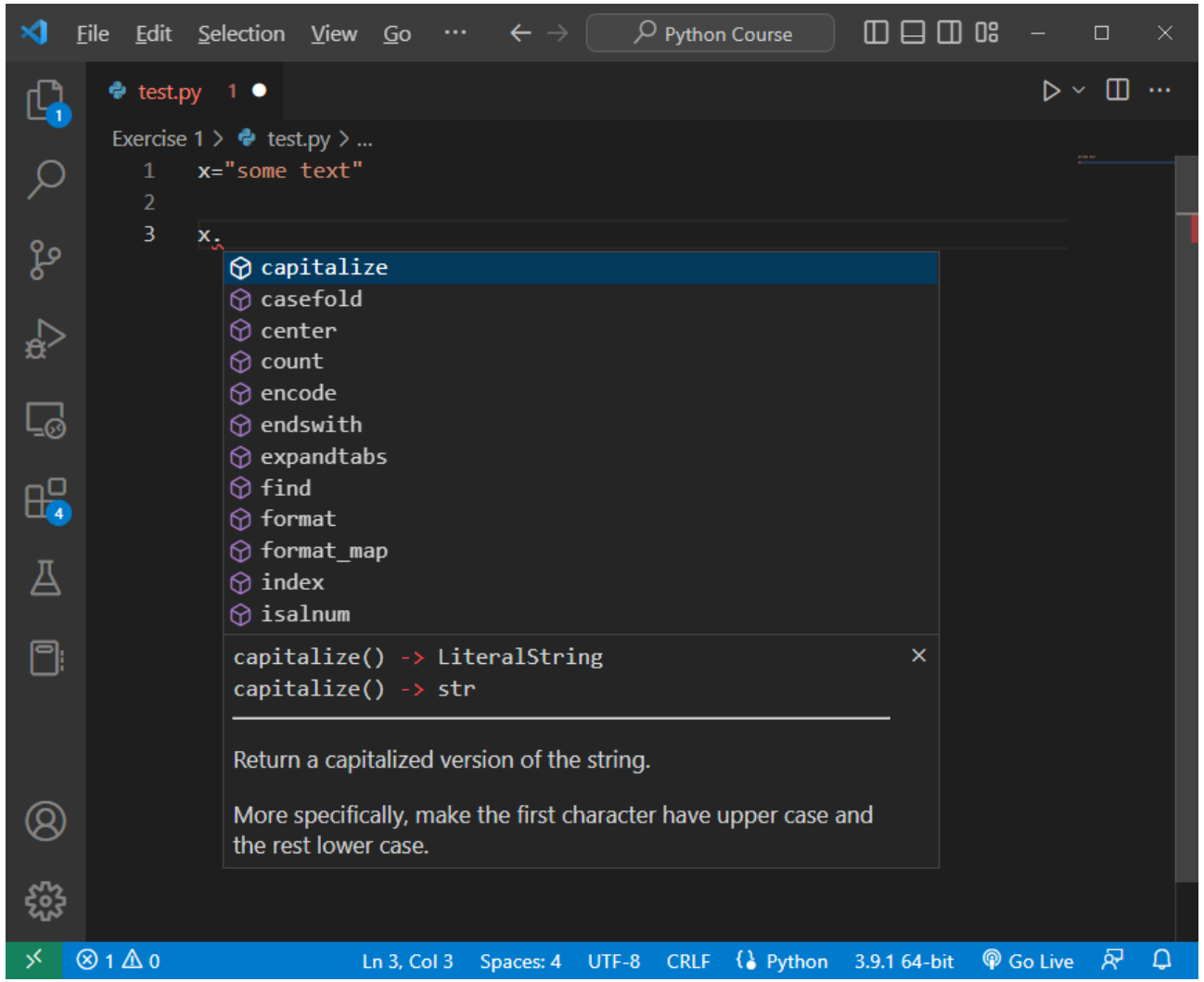
How to use a function?



List of built in functions

abs()	delattr()	hash()	memoryview()	set()
all()	dict()	help()	min()	setattr()
any()	dir()	hex()	next()	slice()
ascii()	divmod()	id()	object()	sorted()
bin()	enumerate()	input()	oct()	staticmethod()
bool()	eval()	int()	open()	str()
breakpoint()	exec()	isinstance()	ord()	sum()
bytearray()	filter()	issubclass()	pow()	super()
bytes()	float()	iter()	print()	tuple()
callable()	format()	len()	property()	type()
chr()	frozenset()	list()	range()	vars()
classmethod()	getattr()	locals()	repr()	zip()
compile()	globals()	map()	reversed()	__import__()
complex()	hasattr()	max()	round()	

Finding methods in VSCode

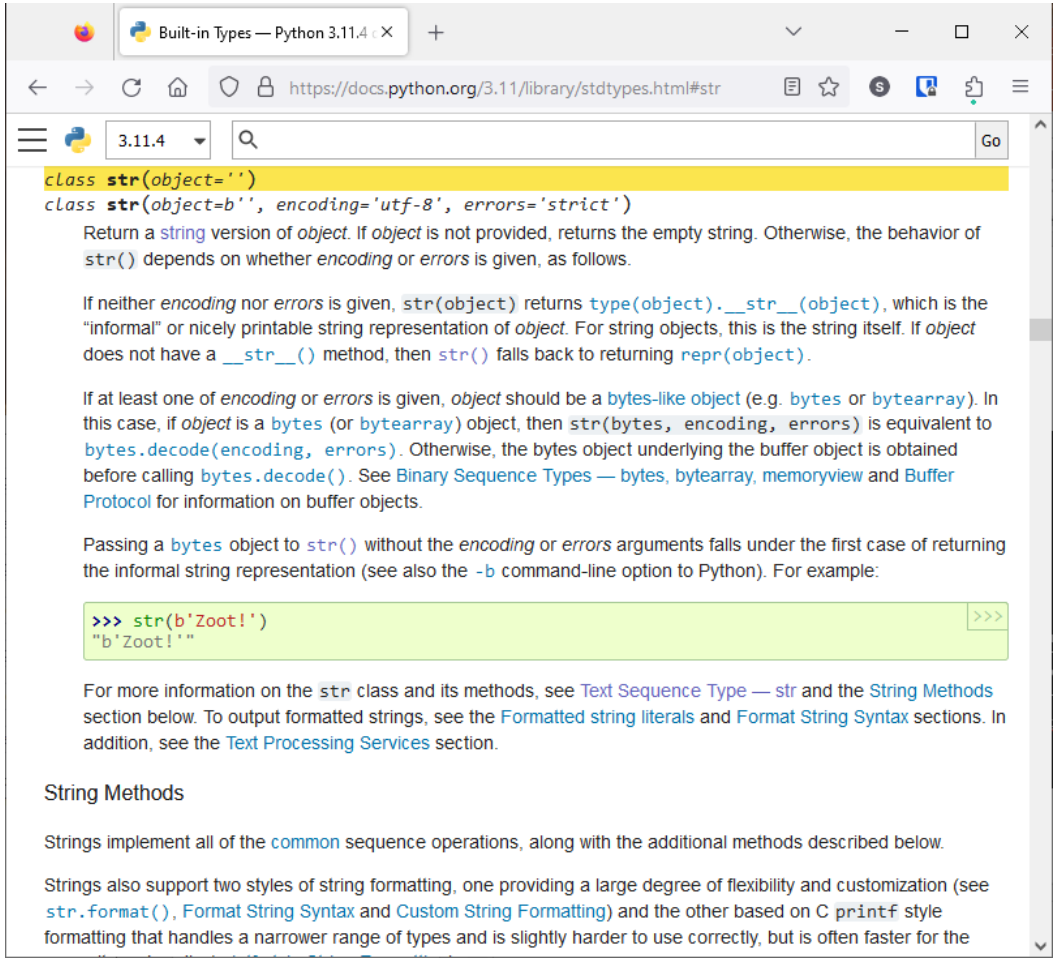


Click on the > for more details

Control + Space forces suggestions

Finding methods via data type (class)

```
>>> type("simon")
<class 'str'>

>>> help(str)
Help on class str in module builtins:

class str(object)
 |  str(object='') -> str
 |  str(bytes_or_buffer[, encoding[, errors]]) -> str
 |
 |  Create a new string object from the given object. If encoding or
 |  errors is specified, then the object must expose a data buffer
 |  that will be decoded using the given encoding and error handler.
 |  Otherwise, returns the result of object.__str__() (if defined)
 |  or repr(object).
 |  encoding defaults to sys.getdefaultencoding().
 |  errors defaults to 'strict'.
 |
 |  Methods defined here:
```



Your turn…

- Got to docs.python.org
- Find the help for the string class (called `str`)
- Have a look through the available methods
- What does the `title` method do?

- Can you write a small program which runs the `title` method on the string `"convert this to title"`

The python standard library

- Most functionality (functions / methods) is not in the core python language, but comes from extensions called 'packages'
- Python comes with an enormous collection of packages called the 'standard library' which are guaranteed to be present with any python installation
- Additional packages can be installed from the Python Package Index (pypi)

Text manipulation

`string` — Common string operations
`re` — Regular expression operations

Data Types

`datetime` — Basic date and time types
`zoneinfo` — IANA time zone support
`calendar` — General calendar-related functions
`array` — Efficient arrays of numeric values
`copy` — Shallow and deep copy operations
`pprint` — Data pretty printer
`graphlib` — Operate with graph-like structures

Numeric and Mathematical Modules

`math` — Mathematical functions
`random` — Generate pseudo-random numbers
`statistics` — Mathematical statistics functions

File and Directory Access

`os.path` — Common pathname manipulations
`stat` — Interpreting stat() results
`tempfile` — Generate temporary files and directories
`glob` — Unix style pathname pattern expansion
`shutil` — High-level file operations

Data Persistence

`pickle` — Python object serialization
`sqlite3` — DB-API 2.0 interface for SQLite databases

Data Compression and Archiving

`gzip` — Support for gzip files
`bz2` — Support for bzip2 compression
`zipfile` — Work with ZIP archives
`csv` — CSV File Reading and Writing

Generic Operating System Services

`os` — Miscellaneous operating system interfaces
`io` — Core tools for working with streams
`time` — Time access and conversions
`argparse` — Parser for command-line options

Internet Data Handling

`email` — An email and MIME handling package
`json` — JSON encoder and decoder

Graphical User Interfaces with Tk

`tkinter` — Python interface to Tcl/Tk

Software Packaging and Distribution

`distutils` — Building and installing Python modules
`venv` — Creation of virtual environments

Using functions from the standard library

Use functions via the package

```
import math
math.sqrt(10)

3.162277
```

Import individual functions

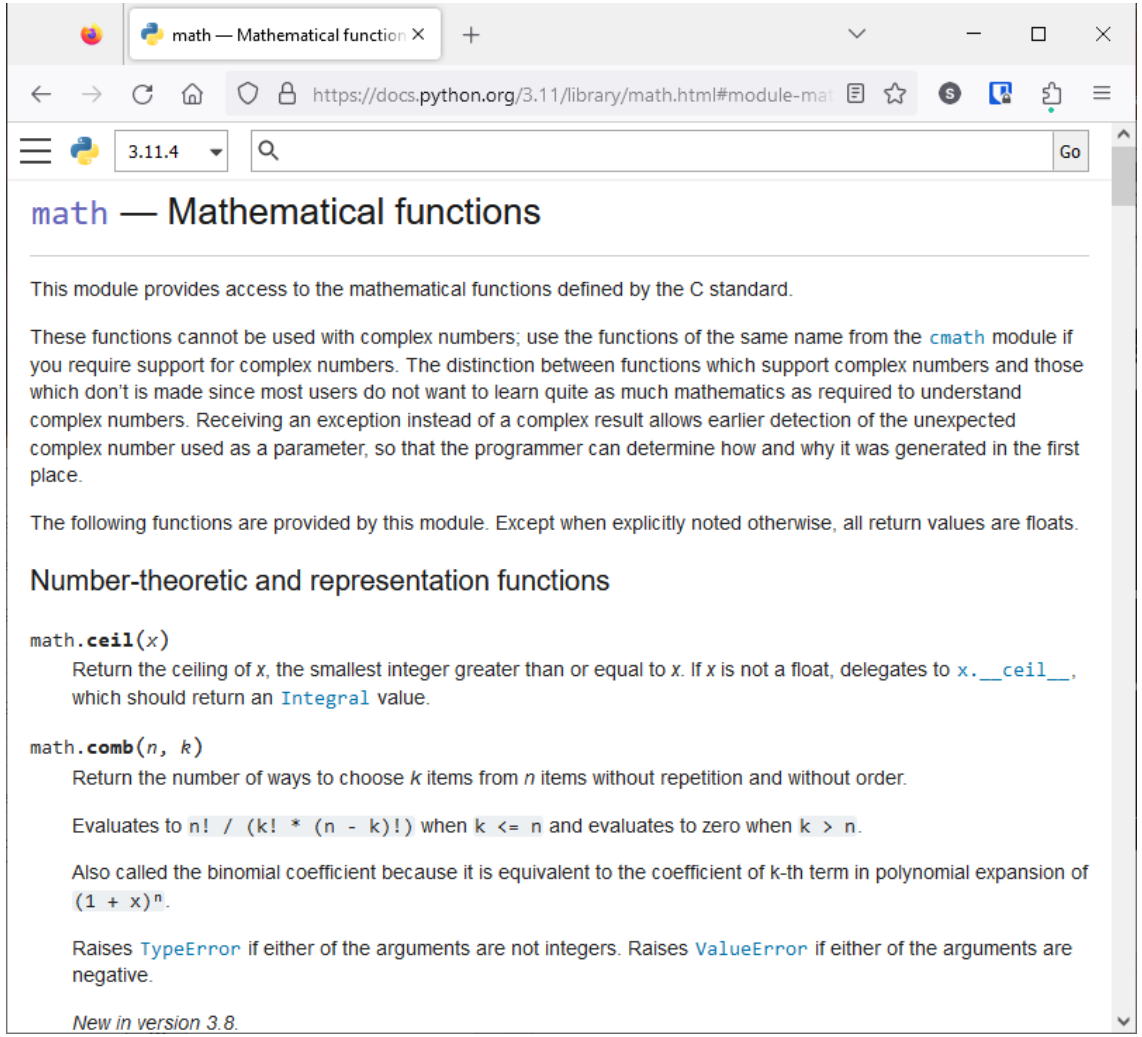
```
from math import sqrt
sqrt(10)

3.162277
```

```
import math as m
m.sqrt(10)

3.162277
```

```
from math import *
sqrt(10)

3.162277
```

Finding functions in a package

```
import math
help(math)

Help on built-in module math:

NAME
    math

DESCRIPTION
    This module provides access to the mathematical functions
    defined by the C standard.

FUNCTIONS
    acos(x, /)
        Return the arc cosine (measured in radians) of x.
        The result is between 0 and pi.

    acosh(x, /)
        Return the inverse hyperbolic cosine of x.

    asin(x, /)
        Return the arc sine (measured in radians) of x.
        The result is between -pi/2 and pi/2.
```



Also at: https://docs.python.org/3/library/math.html

Finding methods in a package

- Some packages define a new data type (class) and use that to call methods, rather than providing functions

```
CLASSES
    class Random(_random.Random)
     |  Random(x=None)
     |
     |  Random number generator base class used by bound module functions.
     |
     |  Used to instantiate instances of Random to get generators that don't
     |  share state.
...
     |  Methods defined here:
...
     |  choice(self, seq)
     |      Choose a random element from a non-empty sequence.
```

Also at: https://docs.python.org/3/library/random.html

The random package has both methods and functions

```
CLASSES
    class Random(_random.Random)
     |  Random(x=None)
     |
     |  randint(self, a, b)
     |    Return random integer in range [a, b], including
     |    both end points.
```

```
FUNCTIONS
    randint(a, b) method of Random instance
      Return random integer in range [a, b], including
      both end points.
```

Example of using random

```
import random

# Use a function
print(random.randint(0,10))

# Use a method
# Make an instance of the Random datatype (class)
generator = random.Random()
# Call a method on this variable
print(generator.randint(0,10))
```

Example Script

- Input a name
- Input an age in years

- Output the year in which they were born
- Output the number of days they've been alive

`time.gmtime([secs])`

Convert a time expressed in seconds since the epoch to a `struct_time` in UTC in which the dst flag is always zero. If *secs* is not provided or `None`, the current time as returned by `time()` is used. Fractions of a second are ignored. See above for a description of the `struct_time` object. See `calendar.timegm()` for the inverse of this function.

- We're going to take some mathematical liberties ☺

class time.**struct_time**

The type of the time value sequence returned by `gmtime()`, `localtime()`, and `strptime()`. It is an object with a named tuple interface: values can be accessed by index and by attribute name. The following values are present:

Index	Attribute	Values
0	**tm_year**	(for example, 1993)
1	**tm_mon**	range [1, 12]
2	**tm_mday**	range [1, 31]
3	**tm_hour**	range [0, 23]
4	**tm_min**	range [0, 59]
5	**tm_sec**	range [0, 61]; see Note (2) in `strftime()`
6	**tm_wday**	range [0, 6]; Monday is 0
7	**tm_yday**	range [1, 366]
8	**tm_isdst**	0, 1 or -1; see below
N/A	**tm_zone**	abbreviation of timezone name
N/A	**tm_gmtoff**	offset east of UTC in seconds

```
#!C:\Program Files\Python39\python.exe

# A program to calculate someone's age
name = input("What is your name? ")
age = input("What is your age (in years)? ")

# Age starts as a string, so we need to convert it to be a number
age = int(age)

age_days = age * 365

# Import the time module so we can get the current year.
import time

year = time.gmtime().tm_year
born_in = year - age


print(name, "was borm in", born_in, "he is",age_days,"days old")
```

What went wrong?

```
#!python
age = input("What is your age? ")
age_in_days = age * 365

print("Your age is",age_in_days)
```

What is your age? 35
Your age is
353535353535353535353535353535353535353535353535353535353
535353535353535353535353535353535353535353535353535353535
353535353535353535353535353535353535353535353535353535353
535353535353535353535353535353535353535353535353535353535
353535353535353535353535353535353535353535353535353535353

What went wrong?

```
#!python
import math

root_two = sqrt(2)
```

```
Traceback (most recent call last):
  File "c:\Users\andrewss\test.py", line 4, in <module>
    root_two = sqrt(2)
               ^^^^
NameError: name 'sqrt' is not defined
```

What went wrong?

```python
#!python
number1 = input("What is the first number? ")
number2 = input("What is the second number? ")

float(number1)
float(number2)

print("The product is",(number1 * number2))
```

```
Traceback (most recent call last):
  File "c:\Users\andrewss\test.py", line 10, in <module>
    print("The product is",(number1 * number2))
                           ~~~~~~~~^~~~~~~~~~
TypeError: can't multiply sequence by non-int of type 'str'
```

What went wrong?

```
#!python
species = "homo sapiens"

species = species.capitalize

print(species)
```

```
<built-in method capitalize of str object at 0x0000026D99915170>
```

Exercise 1

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Python Data Structures

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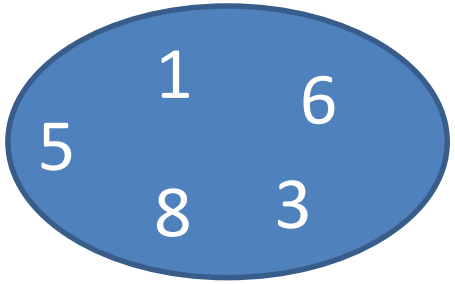
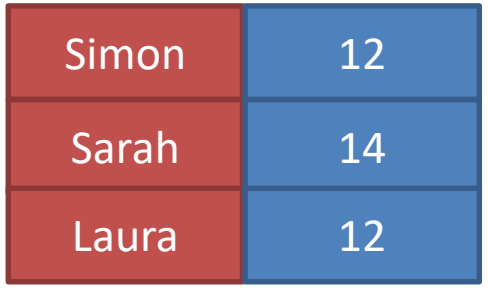
Python Data Structures

- Holds a single value
  - `scalar`
- Holds multiple ordered values
  - `list, tuple`
- Holds multiple, unique, unordered values
  - `set`
- Lookup table, keys and values
  - `dictionary`





Lists

- Modifiable structure to hold an ordered set of data
- Values can be anything, mixed types is allowed, but not great
- Lists can be created empty or with data in them
- You can add or remove data from a list, or extract subsets

```
empty_list = []

filled_list = [1,True,"simon"]
```

List Methods

- `append` - Add something to the end
- `clear` - Remove all content
- `count` - Count the instances of a specific value
- `extend` - join lists together
- `index` - find the position of a value
- `insert` - Add data anywhere in the list
- `pop` - Remove the last value
- `remove` - Remove a specific value
- `reverse` - Reverse the list
- `sort` - Order the list

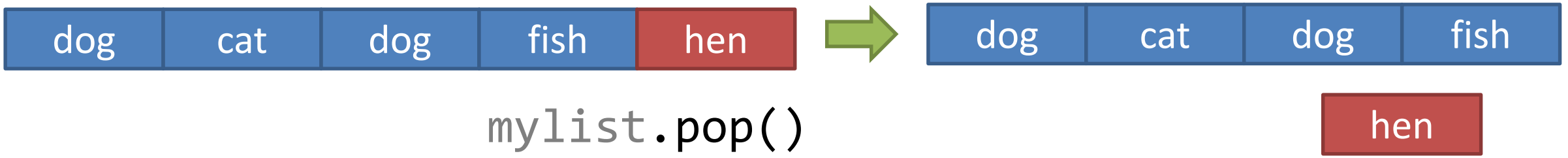
Note that these methods modify the list in place, they don't return anything.

List examples

```
my_list = ["dog","cat","gerbil"]            # dog cat gerbil

my_list.append("mouse")                     # dog cat gerbil mouse

my_list.extend(["cat","dog"])               # dog cat gerbil mouse cat dog

my_list.count("cat")                        # 2

my_list.remove("gerbil")                    # dog cat mouse cat dog

my_list.insert(2,"rat")                     # dog cat rat mouse cat dog

last_value = my_list.pop()                  # dog cat rat mouse cat

my_list.index("dog")                        # 0

my_list.reverse()                           # cat mouse rat cat dog

my_list.index("dog")                        # 4
```

List Questions


```
mylist.append("hen")
```




```
mylist.pop()
```

2 (number of dogs)

```
mylist.count("dog")
```

Accessing List Subsets

```
my_list[start:end:step]
```

- All positions start counting at 0 (everywhere in python)
  - Negative positions count back from the end of the list
  - Start is inclusive, end is exclusive

- You don’t have to supply all of the options
  - Later ones can just be omitted
  - Earlier ones can be omitted, but you still need the colons

Accessing List Subsets

my_list[start:end:step]

```
my_list = ["a","b","c","d","e","f","g","h"]

my_list[2]          # c
my_list[-2]         # g

my_list[0:5]        # a b c d e
my_list[:5]         # a b c d e

my_list[0:5:2]      # a c e

my_list[3:]         # d e f g h

my_list[::3]        # a d g
my_list[::-1]       # h g f e d c b a
```

Copying vs In-Place changes

- Python sometimes has two ways to do the same thing
  - Via a function or selection, returning a modified copy of the data
  - Via a method or replacement, changing the original copy of the data

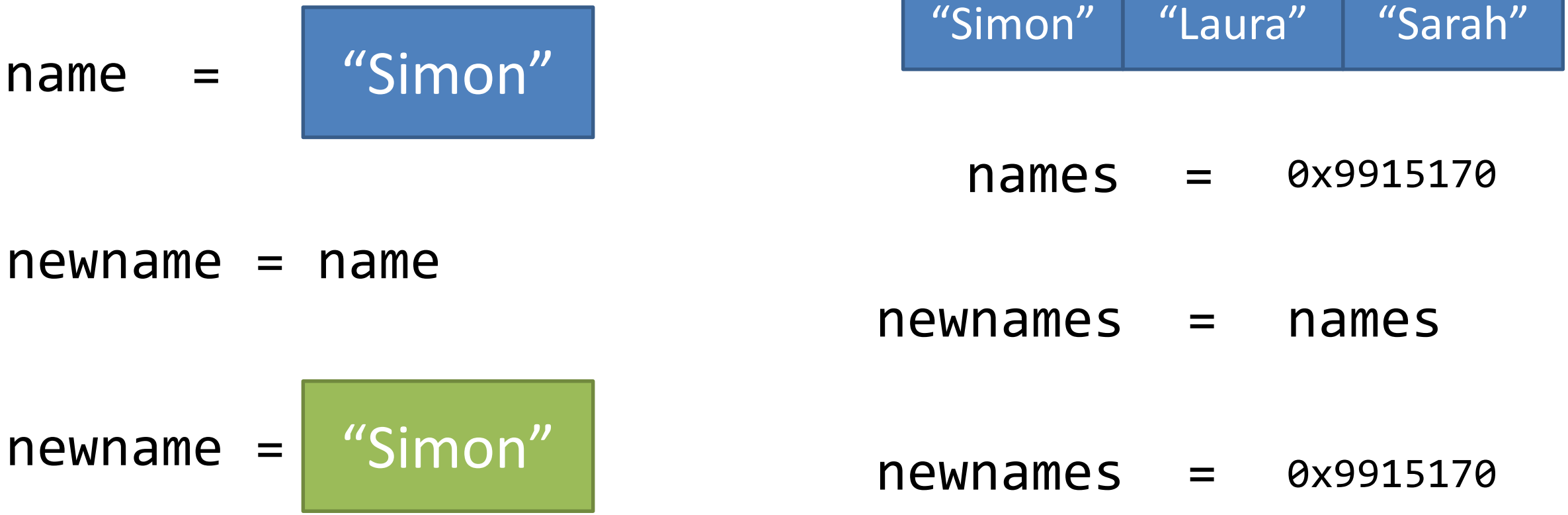
- All python data (other than scalars) are 'references', which means that copying can be unintuitive

Copying vs In-Place changes

```
sorted(my_list)     # Returns a sorted copy of my_list

my_list.sort()      # Returns nothing, but sorts my_list in place



reversed(my_list)   # Returns a reversed copy of my_list*
my_list[::-1]       # Returns a reversed copy of my_list

my_list.reverse()   # Returns nothing. Reverses my_list in place
```

* Technically it returns an iterator over a reversed version of `my_list`, but we haven't talked about those yet

References and Copying



References and Copying

```
my_list = ["dog","cat"]

my_copy = my_list

my_copy.append("mouse")

my_copy[-1]          # mouse
my_list[-1]          # ALSO mouse !!!
```

References and Copying

```
my_list = ["dog","cat","mouse"]

my_copy = my_list.copy()

my_copy[-1] = "gerbil"

# my_copy is       dog cat gerbil
# my_list is still dog cat mouse
```

The copy method only copies the first level of a list. For multi-level copies you need the `copy.deepcopy` function

Tuples

- Very similar to lists
  - Hold ordered sets of data
- Big difference is that tuples are 'immutable'
  - They can't be changed from the data they originally contain
- Most of the operations are the same as for lists
  - Selections return tuples rather than lists

Tuple examples

```
simple_tuple = (1,5,"fred") # Round brackets, not square
simple_tuple[:2]            # (1,5)

single_tuple = ("one",)     # Need trailing comma
```

Dictionaries

- The other big remaining data structure in core python
- Structured as a lookup table
  - **Key**: An index value (eg text or number) to look up by
  - **Value**: A data structure to link to that key

- Keys can be any immutable data type (strings, numbers or tuples)
- Keys must be unique
  - Values can be repeated under different keys

- Dictionaries are also ordered (they remember the order keys were added)*

* As of python v3.7 - before that they weren't

Dictionaries

```
# Creating dictionaries
empty_dict = {}                 # Curly brackets
populated_dict = {              # : between key and value
    "key1" : 10,                # , between value and next key
    "key2" : 20                 # Can also write on one line
}

# Retrieving values
populated_dict["key2"]      # Note SQUARE brackets to use

# Adding / replacing / removing values
empty_dict["simon"] = "Cambridge"      # Creates new key
populated_dict["key1"] = 1000          # Replaces old value
populated_dict.pop("key2")             # Removes (and returns)
```

Sets

- Sets are like dictionaries, but without values
- They hold a **unique** set of immutable keys
- They are very quick to look up what is (and isn't) in the set

- Sets are **NOT** ordered
  - There is an ordered-set package which provides this
  - It's not in the core package collection

Sets

```
# Creating a set
empty_set = set()                    # Must use a function, not {}
tree_set = {"oak","fir","ash"}       # No colons, just commas

# Adding / Removing
empty_set.add("simon")               # Fine if it's already there
tree_set.remove("fir")               # Get an error if it's not there

# Testing
"ash"   in tree_set   # True
"larch" in tree_set   # False
```

Which data structure for…

- Holding a single piece of data?
- Holding an ordered set of values which you need to change?
- Doing a lookup between a key and some associated data?
- Holding multiple values to see which you have seen before?

Which data structure?

```
x = [1,5,6,2,5]

x = {1,5,6,2,5}

x = {"Simon": 40, "Laura": 20}

x = ("bob","ana","may")

x["Simon"] = 5
```

Multi-level data structures

Simon	12
Sarah	14
Laura	12

Key is a scalar (string)
Value is a scalar (int)

Simon	5	8	5	7	
Sarah	4	2	1		
Laura	5	7	3	8	5

Key is a scalar (string)
Value is a list
List contains scalars (int)

Multi-Level Data

- Data structures can hold other data structures
- This is a simple way to create multi-level data structures

```
multi_list = []

multi_list.append([10,20,30])                # Note – append *not* extend
multi_list.append(["ten","twenty","thirty"])
multi_list.append(["X","XX","XXX"])

multi_list          # [[10, 20, 30], ['ten', 'twenty', 'thirty'], ['X', 'XX', 'XXX']]
multi_list[1]       # ['ten', 'twenty', 'thirty']
multi_list[1][2]    # 'thirty'
```

```python
#!python
existing_data = {
    "WT": [2,5,4,6],
    "KO": [8,6,9,12]
}

condition = input("Which condition? ")
value = float(input("What value? "))

existing_data[condition].append(value)

wt_count = len(existing_data["WT"])
ko_count = len(existing_data["KO"])

print ("There are",wt_count,"WT values:",existing_data["WT"])
print ("There are",ko_count,"KO values:",existing_data["KO"])

print("Latest WT value is",existing_data["WT"][-1])
print("Latest KO value is",existing_data["KO"][-1])
```

A dictionary:
Keys = strings
Values = List of integers

`existing_data[condition]` gets the correct list
append is a method on the list to add the new value

Exercise 2

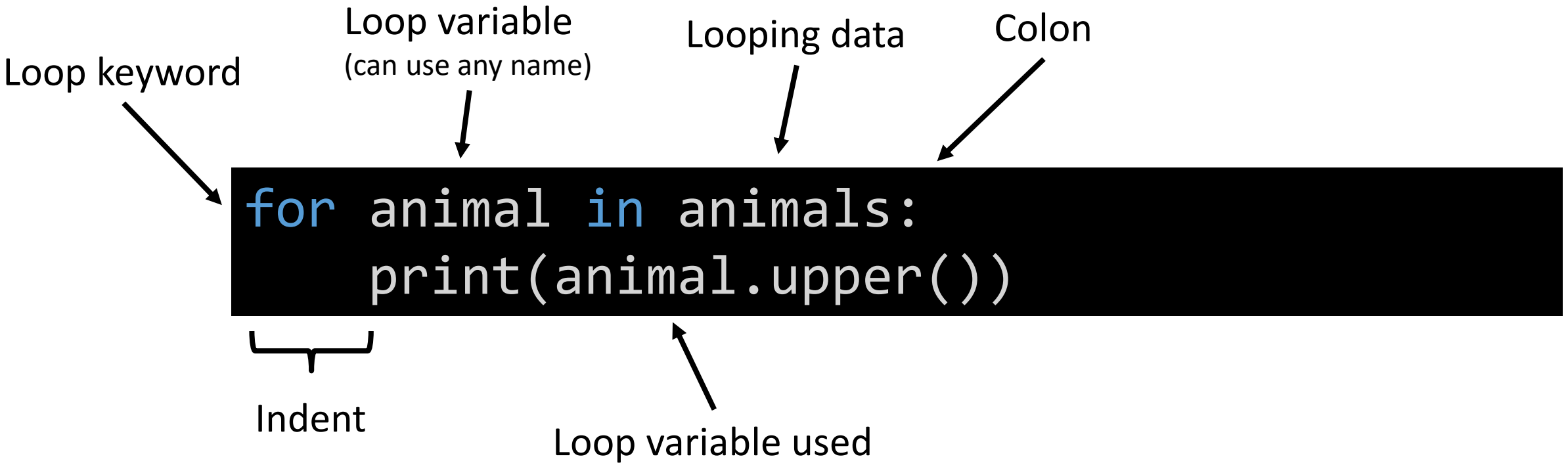
Babraham Bioinformatics

Iterators, Loops and Conditionals

Babraham Bioinformatics

Iteration over a list (or tuple, or set)

```
animals = ["dog","cat","mouse","elephant"]
```



Indenting code blocks

```
animals = ["dog","cat","mouse","elephant"]

for animal in animals:
    print(animal.lower())
    print(animal.upper())

print("Finished listing animals")
```

Block starts

Block finished

4 space indent

There must be at least 1 statement in a block. You can use `pass` as a way to make a dummy statement if you really need to.

Iterators

- Often you will iterate over a data set (list, dictionary etc)
- You can also iterate over a special function called an **iterator** which **dynamically** builds data for you to iterate over
- More efficient than building large lists, just to iterate over them

Ranges

- Simple and efficient way to loop over sets of integers

```
for i in range(5):              # 0, 1, 2, 3, 4
    print(i)

for i in range(5,10):           # 5, 6, 7, 8, 9
    print(i)

for i in range(5,16,2):         # 5, 7, 9, 11, 13, 15
    print(i)

for i in range(16,5,-2):        # 16, 14, 12, 10, 8, 6
    print(i)
```

Iterating over list indices (and values)

```
animals = ["dog","cat","mouse","elephant"]
```

```
for i in range(len(animals)):
    print(i, animals[i])
```

```
for i,animal in enumerate(animals):
    print(i, animal)
```

```
0 dog
1 cat
2 mouse
3 elephant
```

- `enumerate` makes an iterator of tuples (index, value) over a list
- `i,animal = (1,"dog")` is an easy way to extract tuple or list values into separate variables

Iterating over dictionaries

- Two options
  1. Iterate over the keys, and then use them to look up the values
  2. Iterate simultaneously over the keys and values

```
animal_dict = {"elephant":"big", "dog":"medium", "mouse":"small"}

for animal in animal_dict:                  # Iterates over the keys
    print(animal, animal_dict[animal])


for animal,size in animal_dict.items():# items() gives a (key,value) tuple
    print(animal, size)
```

Conditional Tests

- A way to have a block of code which runs under some circumstances but not others.
- Consists of a logical test followed by a code block which executes only if the test is 'true'
- Code blocks are indented in the same way that loop blocks were

What is 'true'

- Logical tests evaluate code to be 'true' or 'false', so what's true? Actually easier to say what's false.
  - The logical `False` value
  - A completely empty string
  - The `None` value
  - Empty lists, tuples and dictionaries
  - Any numerical zero value (`int` or `float`)

- Everything else is true

Constructing a logical test

```
test = False
another_test = True

if test:
    print("Answer 1")

elif another_test:
    print("Answer 2")

else:
    print("Answer 3")
```

Optional

You can have:

- One **`if`**
- Zero or more **`elif`**
- Zero or one **`else`**

Logical test operators

Operation	Meaning	Example
`<`	strictly less than	`5 < 6.5`
`<=`	less than or equal	`4 <= 4`
`>`	strictly greater than	`2.3 > 1.6`
`>=`	greater than or equal	`4.001 >= 4`
`==`	equal	`"simon" == "simon"`
`!=`	not equal	`4 != 4`
`is`	object identity	`[1,2] is [1,2]`
`is not`	negated object identity	`[1,2] is not [1,2]`

Logical tests on data structures

```
animals = ["dog","cat","mouse","elephant"]
animal_dict = {"elephant":"big", "dog":"medium", "mouse":"small"}

if "gerbil" in animals:                  # Works for lists, sets, tuples
    print("There's a gerbil there")
else:
    print("Sorry, no gerbils")

if "elephant" in animal_dict:            # Tests against the keys
    print("We know about elephants")

if "medium" in animal_dict.values(): # Tests against the values
    print("There's a medium animal")
```

Compound Tests

- You can use the operators **and** / **or** to link logical tests
- You can use **not** to invert the logic of a test

```
if "gerbil" not in animals:
    print("No gerbils here")


for animal,size in animal_dict.items():
    print(animal)
    if size=="big" and animal.startswith("e"):
        print("I bet it's an elephant")
```

`while` loops

- A way to execute a code block repeatedly until a logical test becomes false
- The logical test uses the same code as `if` statements
- Generally something within the loop needs to change the data used in the logical test
  - Otherwise the loop will run forever (an infinite loop)
  - There are ways to break out of a loop

while loops

```
I guessed 1
I guessed 4
I guessed 7
I guessed 1
I guessed 5
I stopped guessing
```


```python
#!python

import random

guessed_number = -1

while guessed_number != 5:
    guessed_number = random.randint(0,10)
    print("I guessed",guessed_number)

print("I stopped guessing")
```

```python
#!python
data = []

while True:             # An infinite loop
    answer = input("Enter data: ")

    if answer.strip() == "":
        break

    if not answer.isnumeric():      # Tests for integer
        print("Sorry, wasn't a number")
        continue

    data.append(int(answer))

mean = 0

for i in data:
    mean += i           # Shortcut for mean = mean + i

mean /= len(data)

print("The mean of",len(data),"observations was",mean)
```

Using `continue` and `break`

```python
#!python

data = {}
sample_count = 0

while sample_count < 10:
    sample_count += 1
    print("\n\nMeasurement",sample_count)
    sample = input("Sample Name: ")
    value = float(input("Data Value: "))

    if not sample in data:
        data[sample] = []

    data[sample].append(value)

for sample in data:
    data[sample].sort()
    print("Sample",sample,"had",len(data[sample]),"measures:",data[sample])
```

Exercise 3

Babraham Bioinformatics

String Processing

Babraham Bioinformatics

Creating Strings

```
text_single = 'simple single quotes'  # No real difference
                                      # between single and quotes
text_double = "simple double quotes"  # double quotes

text_escaped = 'It\'s tricky writing apostrophes'

text_special = 'header1\theader2\ndata1\tdata2\n' # Newlines / tabs

text_multi = """I can write
over several
lines
"""
```

Testing Strings

- `isalnum()` Are all characters in the string letters or numbers
- `isalpha()` Are all characters in the string letters
- `isascii()` Are all the characters standard ASCII (no extended characters)
- `isdecimal()`
- `isdigit()` Test for numbers (plus varying extended characters)
- `isnumeric()`
- `islower()` Is it lowercase
- `isupper()` Is it uppercase
- `istitle()` Is it title case (initial capital)
- `isprintable()` All characters are printable (not carriage returns etc)
- `isspace()` All characters are spaces/tabs

Splitting and Joining

- Convert between lists/tuples and delimited strings

```
text_delim = "Jan_Feb_Mar_Apr_May"

months = text_delim.split("_")                  # [Jan Feb Mar Apr May]

new_delim = ":".join(months)                    # Jan:Feb:Mar:Apr:May

",".join(["one",2,"three",4])                   # Fails, can't join int
",".join(["one",str(2),"three",str(4)])         # Works, but ugly!
```

Strings as tuples

- Behind the scenes strings are stored as a tuple of letters
- You can use the list/tuple subsetting syntax on strings

```
big = "arabidopsis"

small = big[-6:]                    # dopsis
small = big[::-1]                   # sispodibara

if "bido" in big:
    print("Found substring")        # Works
```

String Operators

- Strings can be 'added' or 'multiplied'

```
text1 = "join"
text2 = 'me'

text_joined = text1 + text2           # joinme
text_joined = "can't" + "mix" + 100   # Fails, can't add int
text_joined = "can" + "mix" + str(100)# Works

text_multi = text1 * 4                # joinjoinjoinjoin
```

Building strings with data (the ugly way)

```
sample = "WT"
count = 23
total_count = 101

print("Sample",sample,"comprised",count/total_count,"of all measures")

message = "Sample "+sample+" comprised "+str(count/total_count)+" of all measures"

# Sample WT comprised 0.2277227722772273 of all measures
```

- Multiple additions
- Type conversion
- Too much numeric precision

Format Strings (f-strings)

- Regular strings, prepended by `f` eg `f"Hello"`
- Embed variables / code directly in strings
- Works with all data types without conversion
- Provides numeric formatting

Only works on python >3.7

Format Strings (f-strings)

```
year = 1983
name = "Simon"
kids = ["Fred","Ethel"]

print(f"{name} was born in {year} and has {kids}")

# Simon was born in 1983 and has ['Fred', 'Ethel']

print(f"{name} was born in {year} and has {' & '.join(kids)}")

# Simon was born in 1983 and has Fred & Ethel
```

Number formatting in f-strings

```
{data:<20,.2f}
{data:[align][width][delimiter].[precision]}
```

- Align is < (left) > (right) ^ (center)
- Width is number of characters
- Delimiter is 1000s separator (normally , or _)
- Precision is number+letter
  - f is fixed decimal places
  - g is significant figures

`{data:<20.2f}` Occupy 20 spaces, align left show 2 decimal places

`{data:,.3g}` Take what space you need. Add commas. Show 3 sig figs

Number formatting in f-strings

```
fnum = 19876.12345

print(f"Simple={fnum}")                 # Simple=19876.12345

print(f"Decimal Places={fnum:.2f}")     # Decimal Places=19876.12

print(f"SigFigs={fnum:.3g}")            # SigFigs=1.99e+04

print(f"Commify={fnum:,.0f}")           # Commify=19,876

print(f"FixWidthR='{fnum:>15}'")        # FixWidthR='    19876.12345'

print(f"FixWidthC='{fnum:^15}'")        # FixWidthC='  19876.12345  '
```

Complex Matching

- Simple literal string matching can be achieved using either `in` or methods such as `index` or `find`
- More complex, ambiguous patterns can be found using methods from the `re` (regular expression) package - part of the standard library
- Regular expressions are used in many languages and are the same in all of them.

Common methods from `re`

- `re.findall` Find all matches to a pattern. Return a list of hit text
- `re.search` Find the first match to a pattern. Return a hit object
- `re.finditer` Find all matches to a pattern. Return a hit object iterator
- `re.split` Like `str.split` but using a pattern not literal text
- `re.sub` Find and replace based on a pattern

Constructing Patterns

- Patterns are strings, but containing special characters
- Special characters allow for ambiguity in the pattern

`.`	Anything
`[ade]`	Set of allowed characters
`|`	Either/or. Surrounded by () if ambiguous
`*`	Zero or more
`+`	One or more
`?`	None or one
`{}`	Specific number of occurrences, exact or {min,max}
`^`	Starts with
`$`	Ends with
`\`	Way to escape a special character you want to use literally
`()`	Capture group, used to capture part of a match for later use

Pattern Examples

`b.b`	b [anything] b
`^ga*t`	starts with g, then any number of a then t
`tata+$`	tat then one or more a at the end of the string
`c[aeiou]{4}`	c then exactly 4 vowels
`\.txt$`	.txt at the end of a string
`lane([0123456789])\.fq`	lane then a captured number then .fq
`file\.(fq|fastq)`	File dot fq or fastq

Character group shortcuts in regular expressions

- Certain groups of characters are so common there is a shortcut

`\d`	Digits (0-9)
`\D`	Non-digits
`\s`	Any whitespace (spaces or tabs)
`\S`	Any non-whitespace
`\w`	Any word character (letters, numbers and underscore)
`\W`	Any non-word character

- Eg: `lane([0123456789])\.fq` could be `lane(\d)\.fq`

Finding matches

```
import re

text="From sample 1535 we counted 712 colonies on 12 plates"

hits = re.findall("\d+",text)
print(hits)                                  # ['1535','712','12'] - always strings

no_hits = re.findall("bacteria",text)
print(no_hits)                               # [] Empty list

if re.findall("\d+",text):                   # Works because a populated list is
    print("There were numbers")              # true but and empty list is false

if not re.findall("bacteria",text):
    print("No bateria here")
```

Capturing parts of matches

- Using the search function allows you to use capture groups
  - Any part of the regex surrounded in round brackets
  - Can have multiple captures in the same regex

```
import re

text="From sample 1535 we counted 712 colonies on 12 plates"

hits = re.search("(\d+) colonies.* (\d+) plates",text)
```

  - Sample number and plate number will be captured

Capturing parts of matches

- From the hit object which is returned by `re.search` or `re.finditer`
  - `span()` is the position of the whole match, 2 element tuple, start, end
  - `groups()` is a tuple of data in the capture groups

```
import re

text="From sample 1535 we counted 712 colonies on 12 plates"

hits = re.search("(\d+) colonies.* (\d+) plates",text)

if hits is not None: # Tests whether there was a match
    print(f"Matched between {hits.span()[0]} and {hits.span()[1]}")
    print(f"Colonies={hits.groups()[0]} Plates={hits.groups()[1]}")

# Matched between 28 and 53
# Colonies=712 Plates=12
```

Find and Replace

- Use the `re.sub` function to replace a match
  - Regex for what to match
  - Replace with a string

```
import re

text="From sample 1535 we counted 712 colonies on 12 plates"

new_text = re.sub("sample \d+","sample 1234", text)
print(new_text)

# From sample 1234 we counted 712 colonies on 12 plates
```

```python
#!python
import re

hisat_text = """HISAT2 summary stats:
        Total reads: 77188721
                Aligned 0 time: 8862035 (11.48%)
                Aligned 1 time: 60127229 (77.90%)
                Aligned >1 times: 8199457 (10.62%)
        Overall alignment rate: 88.52%
"""
stats = {}
lines = hisat_text.split("\n")

for line in lines:
    if line.isspace():
        continue

    if "Total reads" in line:
        stats["total"] = line.split(":")[1]

    elif line.strip().startswith("Aligned"):
        hits = re.search("Aligned\s+(\S+)\s+times?:\s+(\d+)",line)

        if hits is None:
            print(f"Couldn't match expected pattern in {line}")
            continue

        stats[hits.groups()[0]] = hits.groups()[1]

for stat in stats:
    print(f"{stat} had value {stats[stat]}")
```

Exercise 4

Babraham Bioinformatics

Reading and Writing Files

Babraham Bioinformatics

Constructing File Paths

- A File paths is a string of folder / file name separated by a delimiter (usually /)
- On windows you often see `\` used to separate path elements, but behind the scenes it always appears as /
  - `"c:/Users/andrewss/python/example.py"`
- Traditionally a mix of `os`, `os.path`, `glob` and `shutils` packages were used to deal with paths
- These have largely been supplanted by the `pathlib` package

Using `pathlib`

- The `pathlib` package defines the `Path` data type

- Once you create a `Path` you can call methods on it
  - Constructing / joining paths
  - Testing paths
  - Listing files / folders
  - Creating / deleting files or folders

Using File Paths

- Construct a starting path using `Path("location")`

```
from pathlib import Path

mypath = Path("C:/Users/andrewss/Desktop")
```

Joining File Paths

- Start from a base path and add a file name to the end
- Can use / as a shortcut for `joinpath`

```
from pathlib import Path

base_path = Path("C:/Users/andrewss/Desktop")

final_path = base_path.joinpath("data.txt")
# C:\Users\andrewss\Desktop\data.txt

final_path = base_path / "data.txt"
# Also works
```

Path sections

C:/Program Files/Python39/python.exe

```
p.drive   "C:"
p.parent  Path('C:/Program Files/Python39')
p.name    "python.exe"
p.stem    "python"
p.suffix  ".exe"
str(p)    "C:/Program Files/Python39/python.exe"
```

Useful `Path` methods

- `p.exists()` — Does this path exist
- `p.is_file()` — Is this a file (not a dir)
- `p.is_dir()` — Is this a directory (not a file)

- `p.stat()` — Get statistics about the path
  - `p.stat().st_size` — The size (in bytes)
  - `p.stat().st_mtime` — When it was last modified (epoch seconds)
  - `p.stat().st_atime` — When it was last accessed (epoch seconds)*

*Not guaranteed to work on every filesystem

Reading Text Files

- The standard process for reading a text file is:

1. Construct the path to the file
2. Check the path exists
3. Open a 'stream' to the file - a variable from which data can be read
4. Read the data line by line in a loop
5. Close the stream

Full Read Example

```
from pathlib import Path
import sys

file_path = Path("C:/Users/andrewss/Python Intro Data/babraham_citations.txt")

if not file_path.exists():
    print(f"Couldn't find {file_path}", file=sys.stderr)
    sys.exit(1)

file_stream = open(file_path, "rt", encoding="UTF-8")

for line in file_stream:
    line = line.strip()
    if "Nat" in line:
        print(line)

file_stream.close()
```

Check file

Report problem

Create a stream

Read from stream

Close stream

Simpler reads using `with`

```
from pathlib import Path
import sys

file_path = Path("C:/Users/andrewss/Python Intro Data/babraham_citations.txt")

with open(file_path, "rt", encoding="UTF-8") as file_stream:

    for line in file_stream:
        line = line.strip()
        if "Nat" in line:
            print(line)
```

Clarifications: Text File Encodings

```
with open(file_path, "rt", encoding="UTF-8") as file_stream:
```

```
UnicodeDecodeError: 'charmap' codec can't decode byte 0x81 in position 4326:
character maps to <undefined>
```

- Text files are just files of numeric values decoded into symbols
- Original text file encoding was ASCII
  - ASCII can't represent many characters eg © ã α etc.
  - Several different schemes, 'Latin-1', 'cp1252' etc.
  - UTF-8 is now taking over and should be used
  - On OSX and Linux UTF-8 is the default encoding, but not windows

Error Reporting

```
if not file_path.exists():
    print(f"Couldn't find {file_path}", file=sys.stderr)
    sys.exit(1)
```

- All OSs have two types of output
  - `sys.stdout` Standard output for expected output
  - `sys.stderr` Standard error for errors, warnings or progress

- You can exit your program early using `sys.exit()`
  - The exit value should be 0 if the program exited normally
  - Non zero exit means there was a problem (error)

Using Exceptions (Errors)

- Exceptions are a more robust way of reporting and dealing with problems
- They will construct messages and code traces to allow debugging
- Exceptions can be 'caught' so you can deal with them internally
- There is a generic Exception but also more specific ones

```
+-- Exception
      +-- ArithmeticError
      |    +-- FloatingPointError
      |    +-- OverflowError
      |    +-- ZeroDivisionError
      +-- AssertionError
      +-- AttributeError
      +-- LookupError
      |    +-- IndexError
      |    +-- KeyError
      +-- NameError
      +-- OSError
      |    +-- FileExistsError
      |    +-- FileNotFoundError
      |    +-- NotADirectoryError
      |    +-- PermissionError
      |    +-- TimeoutError
      +-- SystemError
      +-- TypeError
      +-- ValueError
```

Using Exceptions (Errors)

```
if not file_path.exists():
    raise FileNotFoundError(f"Couldn't find {file_path}")
```

```
try:
    with open(file_name, "rt", encoding="UTF-8") as file_stream:

        for line in file_stream:
            line = line.strip()
            if "Nat" in line:
                print(line)

except Exception as ex:
    print("Oops it went wrong, never mind")
    print(ex)
```

Writing to text files

```
out_path = base_path.joinpath("interesting_genes.txt")

with open(out_path,"wt", encoding="utf8") as out:
    out.write("nanog")              # write doesn't automatically
    out.write("\n")                 # add a newline.

    print("brca2", file=out)        # print does
```

- File open modes
  - `rt` = read as text (default)
  - `rb` = read binary (ie non-text)
  - `wt` = write as text (and delete any existing content)
  - `wb` = write binary (and delete any existing content)
  - `a` = append to existing content

File Reading Packages

- `csv` - parses comma separated value files
- `gzip` - reads gzip compressed data
- zipfile - read data from zip files
- tarfile - read data from tar files
- `pysam` - reads SAM or BAM files (not in standard library)
- openpyxl - reads xlsx/xslm Excel files (not in standard library)

Listing Files

- Simple
  - Use the `iterdir` method of a directory Path
- Filtered
  - Use the `glob` method with a pattern containing a `*` (eg `*.txt`)
- Recursive
  - Use the `rglob` method instead of `glob`

```python
#!python
from pathlib import Path

base = Path("C:/Users/andrewss/git")

for d in base.iterdir():
    if d.is_dir():
        print(f"Found repository {d.name}")


for f in (base/"aws_training_images").glob("*.sh"):
    print(f"Found shell script {f.name}")


html_count = 0

for _ in base.rglob("*html"):
    html_count += 1

print(f"Found {html_count} HTML files")
```

Creating Directories

- Create a Path to a location which doesn't exist
- Call the `mkdir` method
  - Set `parents=True` if you want to create several directories

```
new_path = Path("C:/Users/andrewss/Data/Output/")

if not new_path.exists():
    new_path.mkdir(parents=True)
```

Deleting Files

- The `unlink` method of `Path` will remove files or empty directories
  - Be careful - files are not recycled, just deleted

- It won't recursively delete directories and data
  - You can use `shutil.rmtree` for this if you're **really** sure

```python
#!python
from pathlib import Path
import gzip
import re

base_path = Path("C:/Users/andrewss/Desktop/Introduction to Python/Python Intro Data")
polya_lengths = {}

with gzip.open(base_path/"example.fq.gz", mode="rt", encoding="UTF-8") as fq:
    for line in fq:
        if line.startswith("@SRR"):
            sequence = fq.readline()
            max_a = 0
            for polya in re.findall("A+",sequence):
                if len(polya) > max_a:
                    max_a = len(polya)

            if not max_a in polya_lengths:
                polya_lengths[max_a] = 0

            polya_lengths[max_a] += 1


with open(base_path/"palengths.txt","w") as out:
    for palength in sorted(polya_lengths.keys()):
        print(f"{palength}\t{polya_lengths[palength]}", file=out)
```

Exercise 5

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Writing Functions and Larger Scripts

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Better Code Structure

- When your scripts get larger
  - Split the code into modular chunks (functions)
  - Share code between scripts
  - Add some documentation
  - Parse command line options
  - Write tests

- Functions help with
  - Code readability
  - Code maintainability and testing
  - Code reuse

Writing functions

```
def calculate_gc(sequence):
    total = len(sequence)
    gc = sequence.count("G") + sequence.count("C")

    percent = 100*(gc/total)

    return percent

seq = "GATTCGATAGCTAG"
gc = calculate_gc(seq)
print(f"The GC content of {seq} is {gc:.1f}")
# The GC content of GATTCGATAGCTAG is 42.9
```

Functions are processed in order

Use

Declaration

```
seq = "GATTCGATAGCTAG"
gc = calculate_gc(seq)
print(f"The GC content of {seq} is {gc:.1f}")


def calculate_gc(sequence):
    total = len(sequence)
    gc = sequence.count("G") + sequence.count("C")

    percent = 100*(gc/total)

    return percent
```

```
Traceback (most recent call last):
  File "c:\Users\andrewss\Intro_Python\functions.py", line 3, in <module>
    gc = calculate_gc(seq)
NameError: name 'calculate_gc' is not defined
```

Putting everything into a function

```
seq = "GATTCGATAGCTAG"
gc = calculate_gc(seq)
print(f"The GC content of {seq} is {gc:.1f}")


def calculate_gc(sequence):
    total = len(sequence)
    gc = sequence.count("G") + sequence.count("C")

    percent = 100*(gc/total)

    return percent
```

Scripts can be packages too

script.py

```python
import sequtils

def main():
    seq = "GATTCGATAGCTAG"
    gplusc = sequtils.calculate_gc(seq)
    print(f"The GC content of {seq} is {gplusc:.1f}")


main()
```

sequtils.py

```python
def calculate_gc(sequence):
    total = len(sequence)
    gc = sequence.count("G") + sequence.count("C")

    percent = 100*(gc/total)

    return percent
```

Am I a script, or am I a package?

script2.py

```
import script1

gc = script1.calculate_gc("GGG")
print(f"Script2 calculated {gc}")
```

```
The GC content of GATGCTAG is 50.0
Script2 calculated 100.0
```

Being able to simply reuse functions from other scripts is great, but how do we stop the 'script' part of script1 from running when it's being used as a package?

script1.py

```
def main():
    seq = "GATGCTAG"
    gplusc = calculate_gc(seq)
    print(f"The GC content of {seq} is {gplusc:.1f}")

def calculate_gc(sequence):
    total = len(sequence)
    gc = sequence.count("G") + sequence.count("C")

    percent = 100*(gc/total)
    return percent

main()
```

The `__name__` special variable

- When a script is executed directly then `__name__` has a value of `"__main__"`
- When a script is executed because it's called by being imported into another script `__name__` is set to the script name
- We can change our behaviour depending on the value of `__name__`

Variables surrounded by double underscores are designed for mostly internal use, and are created automatically. Sometimes they are useful to use directly.

Standard Script Structure

```
#!/usr/bin/env python

def main():
    pass

def myfunction():
    pass

def myotherfunction():
    pass

if __name__ == "__main__":
    main()
```

Code for this scripts direct functionality goes in here

These functions can be used from main or can be used in other scripts if this file has been imported into them.

The `main()` function only runs when the script is directly executed

Adding Documentation

- Simple function documentation can be added as a string immediately below the function definition

```
def calculate_gc(sequence):
    """Calculates the GC content of an
    uppercase sequence string"""
    total = len(sequence)
    gc = sequence.count("G") + sequence.count("C")

    percent = 100*(gc/total)

    return percent
```

```
>>> import sequtils
>>> help(sequtils.calculate_gc)
Help on function calculate_gc in module
sequtils:

calculate_gc(sequence)
    Calculates the GC content of an
    uppercase sequence string
```

Encapsulation and Scoping

- Functions should be self contained
  - They shouldn't rely on the presence of variables outside the function
  - They should only send data back via a return statement
  - It's OK to create new variables within the function but these won't affect the global environment

- It is possible to affect a global variable in a function, but it requires extra code

Encapsulation and Scoping

```
message = "Original value"

def changeme():
    new_message = "Changed message"
    message = new_message
    print(f"Inside, message is {message}")


print(f"Outside, message was {message}")
changeme()
print(f"Outside, message is {message}")
```

```
Outside, message was Original value
Inside, message is Changed message
Outside, message is Original value
```

If we try to use message at the start of the changeme function we'd get:

```
UnboundLocalError: local variable
'message' referenced before
assignment
```

Accessing global variables

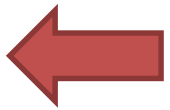
- Global variables are generally a bad idea and you should minimise their use
  - Variables scoped within the `main()` function and passed to other functions as needed are preferred
- There are times they can be useful though
- To access them in a function you need to use the global keyword

Accessing global variables

```
message = "Original value"

def changeme():
    global message
    print(f"Inside, message was {message}")
    new_message = "Changed message"
    message = new_message
    print(f"Inside, message is {message}")


print(f"Outside, message was {message}")
changeme()
print(f"Outside, message is {message}")
```



Says we're importing the message variable from the global environment

```
Outside, message was Original value
Inside, message was Original value
Inside, message is Changed message
Outside, message is Changed message
```

Command Line Options

- You can make your script more flexible by using command line arguments to change options, or the data to process

```
myscript.py cutoff=20 file=data1.csv
```

- Anything written after the script is put into a list accessed via `sys.argv`

Using `sys.argv` directly

```
import sys
def main():
    for i,v in enumerate(sys.argv):
        print(f"{i} was {v}")

if __name__=="__main__":
    main()
```

```
>python argv.py cutoff=20 data=data1.csv
0 was argv.py
1 was cutoff=20
2 was data=data1.csv
```

More robust command lines with argparse

```
import argparse

def main():
    options = parse_arguments()

    print(f"Cutoff is {options.cutoff} data file is {options.data}")

def parse_arguments():
    parser = argparse.ArgumentParser(description="Analyse my data")

    parser.add_argument("--cutoff", help="The cutoff to use for the analysis", default=20, type=int)
    parser.add_argument("data", help="The data file to process", type=str)

    return parser.parse_args()

if __name__ == "__main__":
    main()
```

More robust command lines with argparse

```
usage: commandline.py [-h] [--cutoff CUTOFF] data

Analyse my data

positional arguments:
  data                  The data file to process

optional arguments:
  -h, --help            show this help message and exit
  --cutoff CUTOFF       The cutoff to use for the analysis
```

More robust command lines with argparse

```
commandline.py somefile.csv
Cutoff is 20 data file is somefile.csv


commandline.py --cutoff 26 test.csv
Cutoff is 26 data file is test.csv


commandline.py --cutoff=26
usage: commandline.py [-h] [--cutoff CUTOFF] data
commandline.py: error: the following arguments are required: data


commandline.py --cutoff=no test.csv
usage: commandline.py [-h] [--cutoff CUTOFF] data
commandline.py: error: argument --cutoff: invalid int value: 'no'
```

Testing your code

- Adding tests to your code is a good way to ensure the functionality you're developing is working correctly
- You don't need anything else, but the `pytest` framework makes running tests somewhat easier
- Some people advocate 'test driven development', basically you write the tests first, and then write code until all of the tests pass

The `pytest` framework

- Not part of the standard library, so need to install with pip
- Looks for files called `test_*.py` or `*_test.py`
- Runs `test_` functions within these files containing `assert` statements
  - Asserts are statements containing a test, which produce an exception if the test result is not `True`
- Reports on the success of the tests

```python
def calculate_gc(sequence):
    """Calculates the GC content of an
    uppercase sequence string"""
    total = len(sequence)
    gc = sequence.count("G") + sequence.count("C")

    percent = 100*(gc/total)

    return percent

def reverse_complement(sequence):
    """Calculates the reverse complement of
    an uppercase sequence string"""

    rev = sequence[::-1]
    revcomp = rev.translate(
        str.maketrans("GATC","CTAG")
    )

    return revcomp
```

```python
import sequtils

def test_gc():
    seq = "GATC"
    assert(
        sequtils.calculate_gc(seq)==50
    )


def test_revcomp():
    seq = "GGAT"
    assert(
        sequtils.reverse_complement(seq)=="ATCC"
    )
```

```
python -m pytest
======================== test session starts ========================
platform win32 -- Python 3.9.1, pytest-6.2.4, py-1.10.0, pluggy-0.13.1
rootdir: C:\Users\andrewss\Desktop\Introduction to Python
collected 2 items

test_sequtils.py ..                                            [100%]

========================= 2 passed in 0.06s =========================
```

Exercise 6

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Using external resources

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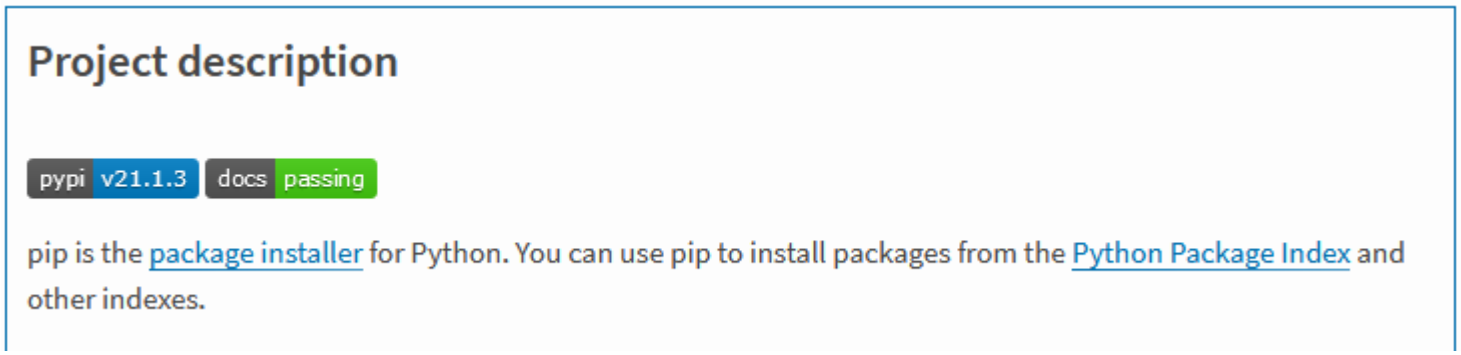
Installing Additional Packages



sys.path

```
>>> import sys
>>> sys.path
['', 'C:/Program Files/Python39/python39.zip', 'C:/Program Files/Python39/DLLs',
'C:/Program Files/Python39/lib', 'C:/Program Files/Python39',
'C:/Users/andrewss/AppData/Roaming/Python/Python39/site-packages',
'C:/Users/andrewss/AppData/Roaming/Python/Python39/site-packages/win32',
'C:/Users/andrewss/AppData/Roaming/Python/Python39/site-packages/win32/lib',
'C:/Users/andrewss/AppData/Roaming/Python/Python39/site-packages/Pythonwin',
'C:/Program Files/Python39/lib/site-packages']
```

- Packages are search for in the order of `sys.path`
- Stops at the first hit
- Some will be admin only, others are user-writeable

Installing with pip

```
pip install …
python -m pip install …

pip install biopython
pip install --user biopython
pip install --upgrade biopython
pip uninstall biopython
```

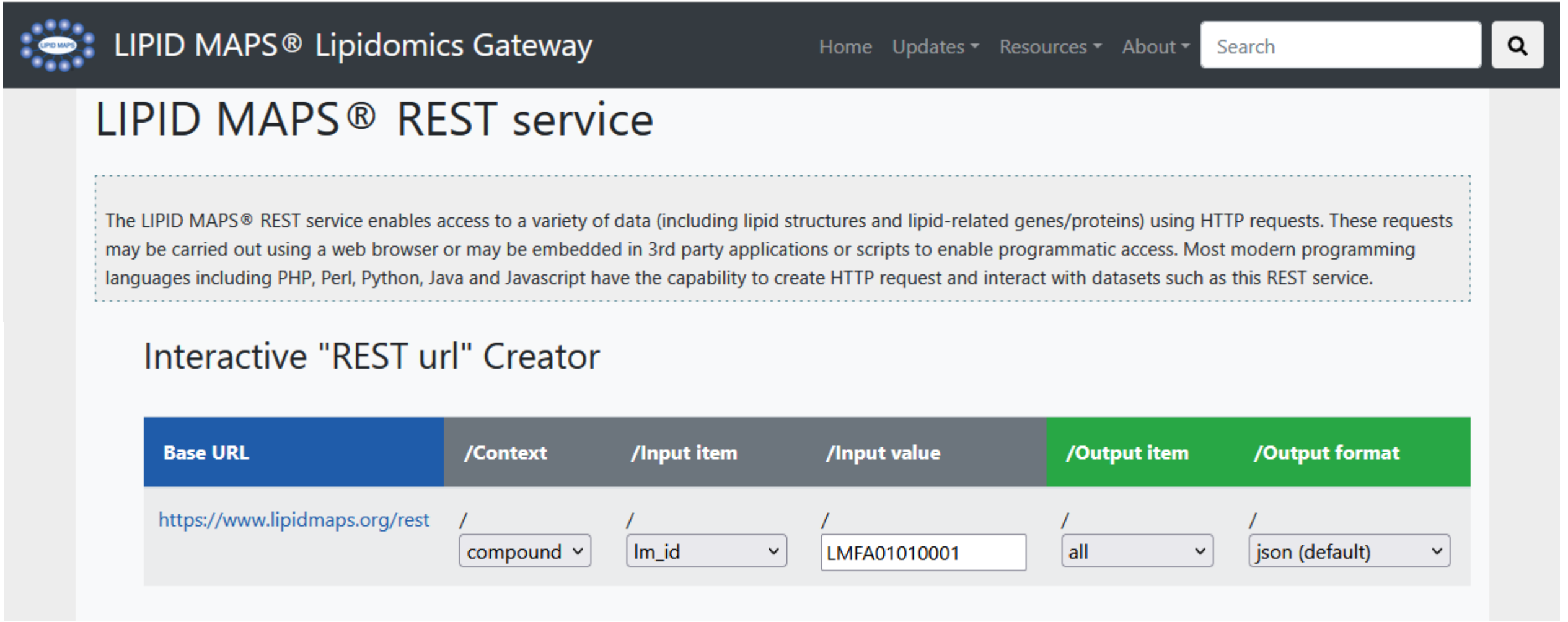
Virtual Environments

```
python -m venv mynewproject

source mynewproject/bin/activate  [Linux/Mac]
.\mynewproject\Scripts\activate   [Windows]

deactivate
```

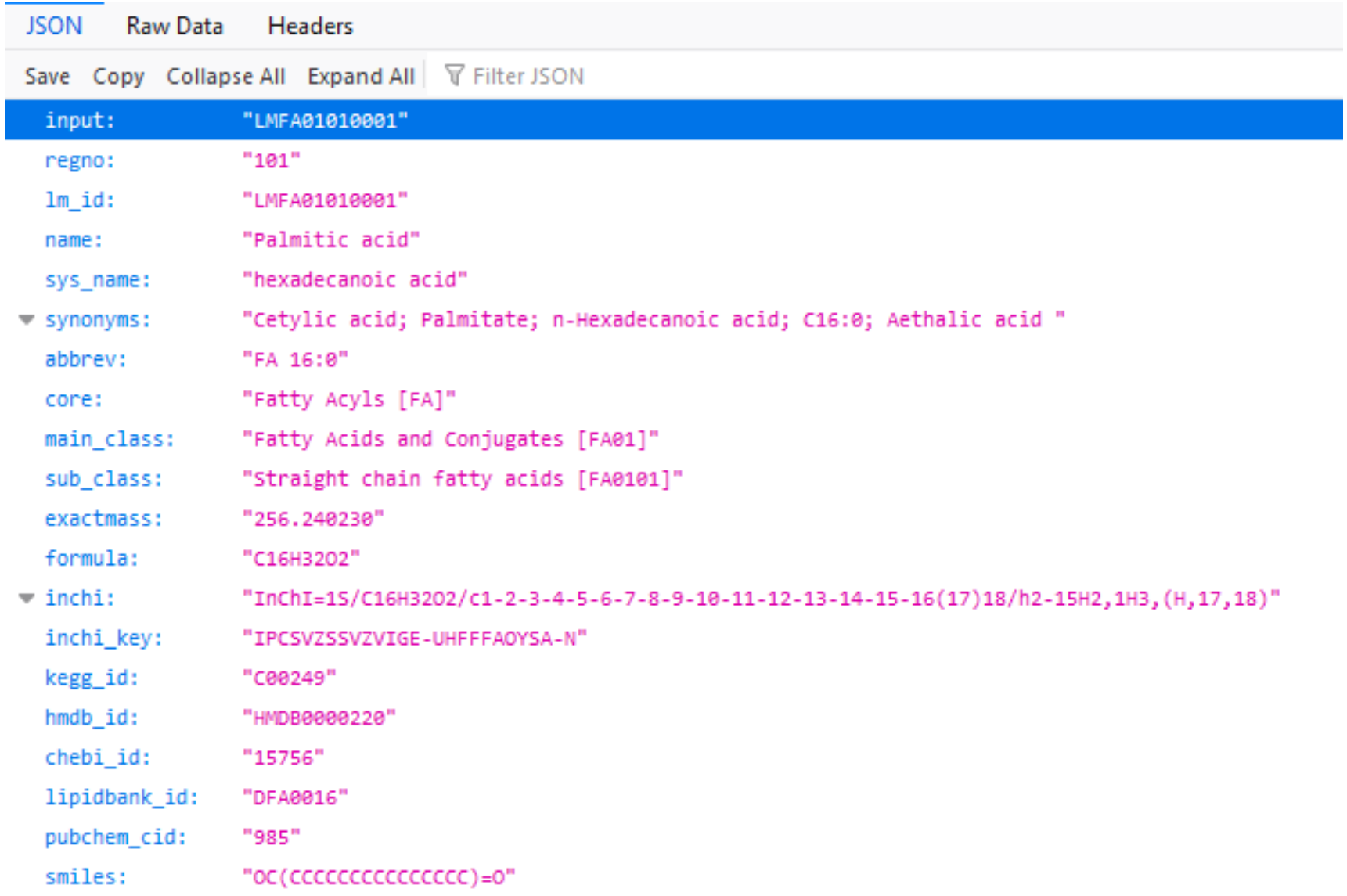
Getting data from REST APIs

- Many data sources offer a simple way to pull information from an online resource, called a REST API
- These are accessed by a structured URL defining the data required
- Data is normally returned in JSON format which can be easily parsed by python

REST Example



https://www.lipidmaps.org/rest/compound/lm_id/LMFA01010001/all/json



JSON - JavaScript Object Notation

- Simple text format
- Composed of lists and dictionaries
- Easily transposed into equivalent python data structures

- The `json` package is part of the standard library
  - Create json from list/dictionary `json.dumps`
  - Create list/dictionary from text json `json.loads`

Reading web data using `requests`

- Convenient package for reading data from the web
- Supports HTTP HTTPS and FTP URLs

```python
import requests

def main():
    lmid= "LMFA01010001"
    json_data = fetch_lm_json(lmid)

    print(f"LMID {lmid} is {json_data['name']} and has mass {float(json_data['exactmass']):.2f}")


def fetch_lm_json(lmid):
    answer = requests.get(f"https://www.lipidmaps.org/rest/compound/lm_id/{lmid}/all/json")
    return answer.json()

if __name__=="__main__":
    main()
```

More complex requests

g:Profiler

g:Profiler API

g:Profiler requests are generally made as POST requests with a JSON body and they return JSON output.

g:GOSt

URL: https://biit.cs.ut.ee/gprofiler/api/gost/profile/
METHOD: POST
PARAMETERS:

organism

ID of species to be queried. List of possible ID-s can be seen at the organisms list page.

```
organism:"hsapiens"
```

query

List of genes to be queried. Can be a list of strings or a dictionary of lists if multiple queries are submitted simultaneously.

```
query:["CASQ2", "CASQ1", "GSTO1", "DMD", "GSTM2"]
```

```
query:{
                first_query:["CASQ2", "CASQ1", "GSTO1", "DMD", "GSTM2"],
                second_query:["MLXIPL","SMARCB1","PIH1D1","SMARCA4","AGER"]
                }
```

g:GOSt query result fields

These are the result fields for most simple queries.

name
Term name.

description
Term description if available. If not available, repeats the term name.

native
Term ID in its native namespace. For non-GO terms, the ID is prefixed with the datasource abbreviation.

parents
List of native IDs that are hierarchically above the term. For non-hierarchical datasources, points to artificial root node if applicable.

p_value
Hypergeometric p-value after correction for multiple testing.

goshv
Internal g:Profiler numeric ID. Unique for the term. Not consistent across data updates.

significant
Indicator for statistically significant results.

https://biit.cs.ut.ee/gprofiler/page/apis

More complex requests

```
#!/usr/bin/env python3
import requests

def main():
    genes = "ENSG00000007171,ENSG00000141367,etc".split(",")
    request = {
        "organism": "hsapiens",
        "query": genes,
        "sources":[],
        "user_threshold":0.01
    }

    result = requests.post("https://biit.cs.ut.ee/gprofiler/api/gost/profile/", json=request)

    for hit in result.json()["result"]:
        print(f"{hit['name']}\t{hit['p_value']:.3f}")

if __name__ == "__main__":
    main()
```

More complex results

```
>python.exe gprofiler.py

clathrin binding        0.000
clathrin-coated vesicle 0.000
clathrin-coated vesicle membrane        0.000
coated vesicle  0.000
regulation of leukocyte mediated immunity       0.000
Formation of annular gap junctions      0.000
coated vesicle membrane 0.000
Gap junction degradation        0.000
leukocyte mediated cytotoxicity 0.000
clathrin-coated endocytic vesicle       0.000
regulation of immune system process     0.001
vesicle 0.001
receptor-mediated endocytosis   0.002
regulation of leukocyte mediated cytotoxicity   0.002
```

Running external programs from python

- The `subprocess` package provides the `Popen` and `run` functions which have options for the most common variations
  - Launch a process and wait for it to complete and check the exit code
  - Launch a process and collect output from STDOUT or STDERR
  - Launch a process and forget about it (later check exit if you like)

Main `subprocess` options

- Arguments
  - Can be a single string of program plus arguments, need `shell=True` for this
    - `“program.sh cutoff 20 threads 3 data.fq.gz”`
  - Can be a list of separate command components, doesn't need shell
    - `[“program.sh” , ”cutoff” , ”20” , ”threads” , ”3” , ”data.fq.gz”]`

- Check (for `subprocess.run`)
  - `check=False` (default) returns a result which you can query to see if it worked
  - `check=True` raises an Exception if the process exits in an error state

- Output
  - `stdout` and `stderr` can either be left to print to the screen, or sent to a pipe where they can be read like a file
  - If you're reading text from `stdout/stderr` then set `encoding` so it appears as text

```python
import subprocess

# Start a process and wait for it to complete
print("Starting notepad")
exit_status = subprocess.run("c:/Windows/system32/notepad.exe")
print(f"Notepad finished {exit_status}")


# Start a process and forget about it
print("Starting forgotten notepad")
subprocess.Popen("c:/Windows/system32/notepad.exe")
print(f"Notepad running")


# Start a process and collect data from it
print("Starting collected process")
with subprocess.Popen(
    "c:/Windows/system32/ipconfig.exe",
    stdout=subprocess.PIPE,
    encoding="UTF-8"
    ) as running_proc:

    for line in running_proc.stdout:
        print(f"Found line {line.strip()}")
```

Start and wait
Check exit code

Start and forget
No exit check

Start and collect stdout output as a stream

Use `with` so you don't have to manually clean up process or streams

Additional little tricks
(if we have time…)

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List Comprehension

- A useful shortcut for performing the same operation on all members of a list

```
data = [1,2,3,4,5]
print("\t".join(data))
```

```
 print("\t".join(data))
TypeError: sequence item 0: expected str instance, int found
```

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

fixed_data = []
for d in data:
    fixed_data.append(str(d))

print("\t".join(fixed_data))
```

```
1	2	3	4	5
```

List Comprehension

```
data = [1,2,3,4,5]
fixed_data = [str(x) for x in data]
print("\t".join(fixed_data))
print("\t".join( [str(x) for x in data] ))
```

```
# Filtering
print("\t".join(  [str(x) for x in data if x>3]  ))

# Conditional Transformation
print("\t".join(  ["odd" if x%2 else "even" for x in data]  ))
```

Debugging

- Python has a built in debugger which you can use to help sort out problems in your code

- You can start the debugger at any point in your code by inserting a call to the `breakpoint()` function (python 3.7+)
  - Good for logic errors

- You can enter the debugger instead of crashing by running
  `python3 -m pdb crashing_program.py`
  - Good for tracing the cause of crashes

Debugging

```
def print_lines(file):

    line_number = 1

    for line in file:
        line_number += 1
        if line_number == 10:
            breakpoint()
            break

        print(line)

    print("Finished")
```

```
Line 1
Line 2
Line 3
Line 4
Line 5
Line 6
Line 7
Line 8
Finished
```

```
Line 7
Line 8
> c:\users\andrewss\debugger.py(12)print_lines()
-> break
(Pdb)
```

Debugger commands

- Print the value of an expression (often just a variable)

```
(Pdb) p line
'Line 9'
```

- Step to the next line of code

```
(Pdb) s
> c:\users\andrewss\debugger.py(16)print_lines()
-> print("Finished")
```

- Allow the program to continue to the next breakpoint (or end)

```
(Pdb) c
Finished
```