Python Beginners Bootcamp

Universität Potsdam

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print("Hello world!")

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Logistics

- This course is a one week intensive course designed to teach basic Python programming for data analysis
- The course is aimed at complete beginners to Python or programming in general, those who know another language, or just those that want to brush up
- Each day will consist of two sessions: one from 10:00 13:00, and one from 14:00 17:00
- All sessions will take place here in room 0.087

Logistics

- Each session will be lecture style for ~45 mins, followed by hands on coding for the remaining time where I will be available to help
- Material is available on moodle, and you may use the computers here or your own personal laptop
- You are encouraged to work together with your neighbour, and to google things - <u>stackoverflow</u> is your friend (whilst ChatGPT can write code, you are encouraged not to use it whilst learning)
- This is the first time this course is being delivered, so please ask questions is something is unclear! We can slow things down as much as needed.

Course content

What this course will cover

- Basic shell usage
- Python basics: Variables, input/output, operators, data types
- Control flow: conditional statements, boolean logic, error handling
- Data structures: Lists, tuples, dictionaries, sets
- Loops & functions
- Important modules: matplotlib, numpy, scipy, astropy
- Conda and virtual environments

What this course won't cover

- Shell scripting
- Binary and computer memory allocation
- Linux system administration or remote access tools
- More advanced Python: classes, generators, lambda functions
- Graphical user interfaces or animations
- Git

This is a course in Python *for scientists* **not** computer programmers, so we will focus on the practical aspects of Python and not the nitty grtty details.

What is Python?

- Python is a high level, interpreted programming language
- As an interpreted language it is easy to run and does not require a separate compiler such as with C/C++
- It is known for its ease of use and clear syntax
- Python is widely used in the scientific community, particularly for data analysis
- Python lets you use packages and code written by others easily,
 so you can build powerful programs without starting from scratch

Pros of Python

- Easy to read and write, very intuitive and easily debugged
- Huge community and libraries available
- Versatile, used in many industries

Cons of Python

- Slower than compiled languages such as C/C++
- Can be inefficient with memory
- Dynamically changing libraries can lead to outdated code

Session 1: Using the Terminal

```
Natalie@mylinux:~$ pwd
/home/williams
Natalie@mylinux:~$ ls
mycode.py Documents
Natalie@mylinux:~$ mkdir Computing
Natalie@mylinux:~$ cd Computing
Natalie@mylinux:~/Computing$ touch mynotes.txt
```

The terminal

- Before we look at Python, we need to understand how to navigate our computer system using the terminal
- The terminal is a text based interface which allows us to interact with the computer
- This may seem unnecessary when we have a file explorer however using the terminal provides much more flexibility, and as
 you become proficient at coding it will become easier and
 necessary to use the terminal

Opening the terminal

Linux & macOS:

Search in applications for "Terminal"

Windows:

Search in applications for "Powershell" or "Windows Terminal" Download WSL (once) with

wsl --install

Open WSL from Powershell or Windows Terminal with

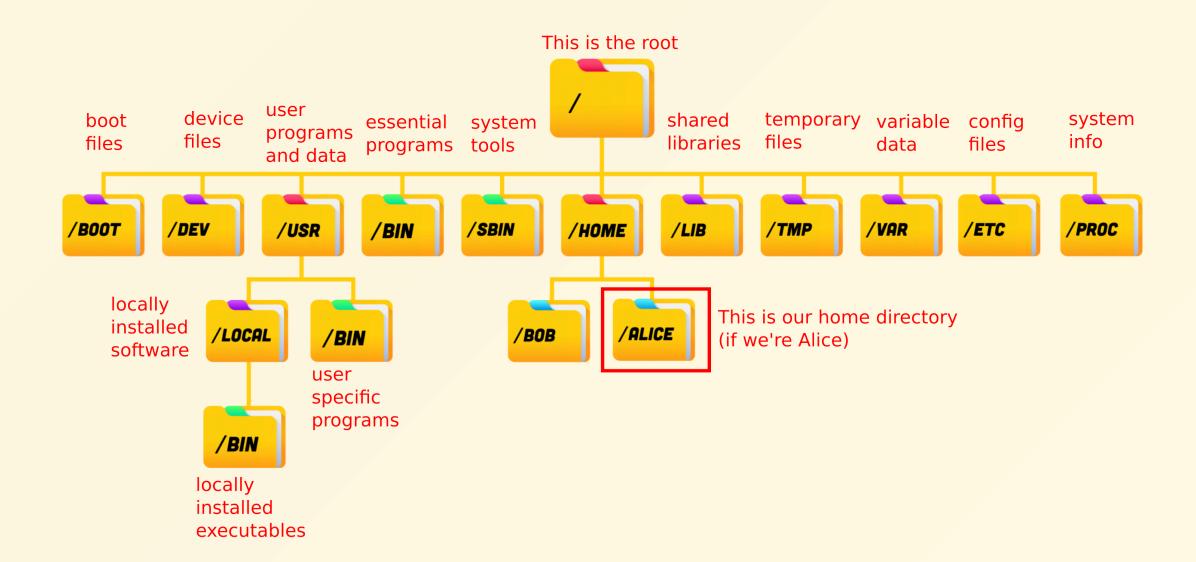
Where am I?

- When opening the terminal, we see the command line
- In the command line it shows user_name@computer_name:location\$

Natalie@mylinux:~\$

- We are in a location, our home **directory** (folder), denoted by ~.
- To check where you currently are in the file system, you can use the command pwd to print our current location (or path)

The file system



Commands

- We will explore some of the most useful commands that can be used on the command line and their functionality
- Each command may have many options, these can be listed for most commands by using man *command* or *command* --help

```
Natalie@mylinux:~$ pwd --help
```

Natalie@mylinux:~\$ man pwd

• **Top tip**: Use the up and down arrowkeys to cycle through previous commands rather than typing them out again

Looking around

• The contents of the location we are in can be viewed with ls

```
Natalie@mylinux:~$ ls
Documents mycode.py
```

- These file types are colour-coded as normal files, documents, and executable files.
- Hidden files (files/directories that start with . and are hidden from the user) can be shown with 1s -a

```
Natalie@mylinux:~$ ls -a
. .. .bashrc mycode.py Documents .jupyter .ssh
```

Looking around

• To view more details on the files we use ls -1 with form

```
permissions | # of hard links | Owner | Group | File size (bytes)| Last modified | Name
```

```
Natalie@mylinux:~$ ls -l
drwxr-xr-x 6 Natalie Natalie 4096 Feb 20 14:32 Documents
-rw-rw-r-- 1 Natalie Natalie 5 Mar 27 14:34 mycode.py
```

- Permissions are laid out as drwxrwxrwx where d directory, r read, w - write, x - execute for user, group and others users
- Permissions can be changed with chmod i.e., chmod u+x mycode.py

Moving around

To move to another directory from your current location use cd

```
Natalie@mylinux:~$ cd Documents
Natalie@mylinux:~/Documents$ ls
Computing myfile1.txt myfile2.txt
```

- Top tip: use tab to autocomplete file and directory names
- We denote one directory back with ..., and the current with ...

```
Natalie@mylinux:~/Documents$ cd ..
Natalie@mylinux:~$ cd .
Natalie@mylinux:~$
```

Moving around

- When only running cd, it takes you back to your home directory, this is the equivalent of cd ~
- We can pass relative paths from the current position

```
Natalie@mylinux:~$ cd Documents/Computing
Natalie@mylinux:~/Documents/Computing$ cd ../Computing
```

We can also pass absolute paths to anywhere on system

```
Natalie@mylinux:~$ cd /home/Natalie/Documents/Computing
Natalie@mylinux:~/Documents/Computing$ cd ~/Documents
Natalie@mylinux:~/Documents$ cd /usr/bin
```

Creating and deleting directories

• We make new directories using mkdir

```
Natalie@mylinux:~$ mkdir Masters
Natalie@mylinux:~$ ls
Documents Masters mycode.py
Natalie@mylinux:~$ cd Masters
Natalie@mylinux/Masters:~$
```

• Directories can be deleted with rm -r (only need rm for files)

```
Natalie@mylinux:~$ rm -r Masters
Natalie@mylinux:~$ ls
Documents mycode.py
```

Copying and moving files/directories

We can copy a file/directory using cp

```
Natalie@mylinux:~$ cp mycode.py ./Documents
Natalie@mylinux:~$ ls ./Documents
Computing mycode.py myfile1.txt myfile2.txt
Natalie@mylinux:~$ cp mycode.py mycode_copy.py
Natalie@mylinux:~$ ls
Documents mycode.py mycode_copy.py
```

• We can move/rename a file/directory with mv

```
Natalie@mylinux:~$ mv mycode.py ./Documents/Computing Natalie@mylinux:~$ mv mycode_copy.py mycode_renamed.py
```

Creating files and text editing

• We can create a new file with touch

```
Natalie@mylinux:~$ touch newfile.txt
Natalie@mylinux:~$ ls
Documents mycode.py newfile.txt
```

• We can also create a file using a text editor (emacs, nano, vim)

```
Natalie@mylinux:~$ vim newfile.txt
Natalie@mylinux:~$ emacs newfile.txt &
```

Here vim opens in the terminal, emacs in the background (with &)

Using vim

• We use vim as an example - after opening the file press i to start editing

```
This is my text file
--INSERT-- 1,1 All
```

- After finishing press esc and enter :wq to write and quit, or :q! to quit without saving and go back to the terminal
- Vim can be used to write Python files with, i.e. vim myscript.py

Session 2: Python basics

```
# Calculate adjusted travel time to the ISS

name = input("Astronaut name: ")
speed = int(input("Speed in km/s: "))
distance = 400
time = distance / speed

time += 2 # docking delay
print(f"ETA for {name[:3]}: {time}")
```

Installing python

Everything for this course is set up on the lab computers, however you can do the exercises on your personal laptops if you wish.

You will need to make sure Python is installed - you can download Python <u>here</u>.

All exercises will be done through jupyter notebooks - for now this is easiest done by downloading and launching <u>Anaconda navigator</u>.

How does Python run code?

- Python execute your code one line at a time, from top to bottom
- This means

```
This line runs first
Then this one
And so on...
```

- If there's an error on a line, Python **stops running**, and shows an error, reading no more code
- This makes it easy for us to debug code

Ways to run Python

On the terminal line by line

```
Natalie@mylinux:~$ python
>>> print('Hello world')
Hello world
```

• Through a prewritten python script (.py file) via the terminal

```
Natalie@mylinux:~$ python myscript.py
```

 Through an interactive development environment (Spyder, PyCharm, Visual Studio Code, Jupyter notebooks/lab)

Print

- The print() function displays output to the screen
- You can print text, numbers or variables
- Use quotes "" or " for text (strings)

```
print('Hello world!')
```

Output:

Hello world!

Comments

- Comments allow us to add text to our code which is not read by the code
- This allows us to explain what the code is doing, which is very useful for long and complex code
- You are highly encouraged to comment your code both for yourself looking back at code and anyone marking your code to understand what you did
- Comments are added by inserting a # followed by the comment

Variables

- Variables are names chosen by the coder to store values
- We assign values to variables with
- Variable names can include letters, numbers and underscores, but cannot start with a number or contain spaces
- Variables can be overwritten (be careful!)
- Multiple variables can be assigned at once

```
x = 5
y, z = x, 0.3
x = 2
print(x, y, z) # This will print: 2 5 0.3
```

Data Types

- There are several distinct data types we use in Python, including int (integers), float (decimals), string (text), bool (true/false)
- We can check the data type of a variable with type()

```
x = 5 # int -> integer
factor = 2.4 # float -> decimal
greeting = 'hello' # string -> text
mybool = True

y = 2. # this is a float = 2.0
a = 1.5e-3 # this is a float = 0.0015
print(type(greeting)) # Output -> <class 'string'>
```

Casting

 We can specify the data type we would like, and where allowed, convert between them

```
x, y, z = int(3), int(2.8), int('5') # x is 3, y is 2, z is 5

x, y, z = float(3), float(2.8), float('5') # x is 3.0, y is 2.8, z is 5.0

x, y, z = str('hello'), str(3), str(2.8) # x is 'hello', y is '3', z is '3.8'

x = 4.7
y = int(x) # y is 4
z = 'hello'
int(z) # raises ValueError -> letters cannot be converted to numbers
```

Operations

- Python is built in with simple operations
- These include add + , minus , times * , divide / , power ** , modulus (remainder) % and floor division //

```
x = 5

y = (6 - x)**2 / x # y is 0.2

z = y + x # z = 5.2
```

Note that during operations data types may be implicitly converted i.e. \times is implicitly converted from int to float in this last line

Assignment operators

- In this previous slide the variables are never altered (x stays 5,
 y stays 0.2 etc)
- Variables can be altered, this is commonly done with assignment operators which take the form *operator*=

```
x = 5

x +=3 # equivalent to x = x + 3, x is now 8

x *=2 # equivalent to x = x * 2, x is now 16

x //= 3 # equivalent to x = x // 3, x is now 5
```

Conditional Operators

- Conditional operators are used to compare values
- They return a **boolean** (data type bool) value True or False, which if treated as integers are equal to 1 and 0 respectively
- Examples include equal == , not equal != , greater than > , less than < , greater or equal to >= , less than or equal to <=

```
x, y = 5, 5.0
x == y # True -> implicitly converts x to a float to compare
x <= 10 # True
greeting, another_greeting = 'hello', 'hello '
greeting == another_greeting # False - how are they not the same?
a = x != greeting # a = True, we are allowed to compare different data types</pre>
```

Logical Operators

- Logical operators combine conditional operators
- These are and (returns True if both statements are true), or (returns True if one statement is true) and not (reverses the result, returns False if True and vice versa)

```
x, y = 2, 7
x < 5 and y > 5 # True
x >= 10 or y != 3 # True
not(x >= 10 and y != 3) # False
```

Indexing strings

• We can also use the + operator to concatenate strings

```
name, message = 'Natalie', 'Hello, '
greeting = message + name + '!'
print(greeting) # 'Hello, Natalie!'
```

- We use stringname[i] to index the i-th component of a string
- Important: In Python indexing starts a 0, not 1

```
print(name[0]) # first component -> 'N'
print(name[2]) # third component -> 't'
print(name[-1]) # last component -> 'e'
print(name[-3]) # third last component -> '1'
```

Slicing strings

• Slicing can be used to index multiple components of a string with notation stringname[start:stop:step] with defaults of start = 0, stop = -1 and step = 1

```
name = 'Natalie'
print(name[2:5]) # 3rd to 5th -> 'tal'
print(name[:5]) # 1st to 5th -> 'Natal'
print(name[5:]) # 5th to end -> 'ie'
print(name[1:6:2]) # every 2nd letter 2nd to 7th -> 'aai'
print(name[::3]) # every 3rd letter -> 'Nae'
```

• We can also use len to get the length of a string i.e. len(name)

Modifying strings

• Here is a selection of useful **methods** used to modify strings

```
x = ' Hello, World! '
print(x.upper()) # returns string in upper case -> ' HELLO, WORLD! '
print(x.lower()) # returns string in lower case -> ' hello, world! '
print(x.strip()) # removes whitespace -> 'Hello, World!'
print(x.replace('H', 'J')) # replaces one string with another -> ' Jello, World! '
print(x.split(',')) # returns a list of strings split by ',' -> '[' Hello', 'World! ']'
```

Formatting strings

- We can combine strings and numbers easily by using f-strings
- This requires f to be placed before the string, and number variables placed as {num}

```
num = 42
txt = f'The answer to Life, the Universe and Everything is {num}'
print(txt) # 'The answer to Life, the Universe and Everything is 42'
```

• Specify the number n of decimals to display x with x:.nf

```
pi = 3.14159265359
print(f'Pi is {pi:.2f}') # 'Pi is 3.14'
```

User input

• We use the function input to take an input from the user

```
name = input('Enter your name')
print(f'Hello {name}')
```

 Input always takes the input as a string, so if you require a number this needs to be manually converted

```
x = input('Enter a number')
print(x + 5) # returns TypeError: can only concatenate str (not "int") to str
x = int(input('Enter a number'))
print(x + 5) # returns expected value
```

Session 3: Lists, Tuples, Sets & Dictionaries

```
planets = ["Mercury", "Venus", "Earth"]
constellations = ("Orion", "Cassiopeia", "Lyra")
observatories = {"ALMA", "Keck", "VLT", "ALMA"}
galaxy = {"name": "Andromeda", "distance": 2.5}

planets.append("Mars")
print(constellations[1])
print(observatories)
print(galaxy["distance"])
```

Lists

• Lists are an **ordered**, **mutable** collection (can be changed after it has been created) denoted by square brackets

```
planets = ["Mercury", "Venus", "Earth"]
series = [2 , 8 , 3 , 4]
```

Lists can be indexed and sliced to obtain values

```
print(planets[2]) # 'Earth'
print(series[1:3]) # [8 , 4]
```

Changing and adding to lists

Lists can be changed using indexing

```
planets[1] = 'Mars'
print(planets) # ['Mercury' , 'Mars' , 'Earth']
```

We add single values to the end with the append method, inserted in specific positions with insert, and concantenate lists together with extend or +

```
planets.append('Jupiter')
planets.insert( 1 ,'Venus')
planets.extend(['Saturn', 'Neptune'])
print(planets) # ['Mercury' , 'Venus' , 'Mars' , 'Earth', 'Jupiter' , 'Saturn' , 'Neptune']
```

Removing from lists

• Items are removed by value with remove (removes first item of this value) and index with pop

```
planets.remove('Earth')
planets.pop(3)
print(planets) # ['Mercury' , 'Venus', 'Mars' , 'Saturn' , 'Neptune']
```

• Lists are mutable, so methods change them directly; string methods return new strings instead of changing the original.

```
mystring = 'Hello'
mystring[0] = 'J' # TypeError: 'str' object does not support item assignment
```

Lists properties

 Different data types can be combined in one list, and values can be repeated

```
mylist = ["banana", 4 , 1.8e-7 , "banana"]
```

Other useful functions (do not change the list) include

```
x = [2, 6, -3, 8]
print(len(x)) # length of list -> 4
print(sum(x)) # sum if numeric -> 16
print(min(x)) # minimum if numeric -> -3
print(max(x)) # maximum if numeric -> 8
```

Nested Lists

Lists can contain lists

```
matrix = [
  [1 , 2 , 3],
  [4 , 5 , 6],
  [7 , 8 , 9]
]
```

 This is a now a multidimensional object, and can be indexed as matrix[row][column]

```
print(matrix[1][2]) # 6
```

Tuples

 A tuple is a collection which is ordered and unchangeable, written with round brackets

```
planets = ("Mercury" , "Venus" , "Earth")
```

- We cannot change, add or remove items from a tuple
- Multiple entires with the same value are allowed

```
planets = ("Mercury" , "Venus" , "Earth" , "Venus")
```

Creating tuples

• Tuples can be created with one item but **must** contain a ,

```
planets = ("Earth") # NOT a tuple
planets = ("Earth",) # a tuple
```

Tuples can contain any and multiple data types

```
mytuple = ("Earth" , 5 , True , 3.46e5)
```

• len can still be used to obatain a tuple length

```
print(len(mytuple)) # 4
```

Accessing tuples

Values in tuples can still be indexed and sliced

```
planets = ("Mercury" , "Venus" , "Earth" , "Mars")
print(planets[2]) # "Earth"
print(planets[1:-1]) # ("Venus" , "Earth")
```

You can add a tuple to a tuple with +

```
x = ("Jupiter",)
planets += x
print(planets) # ("Mercury" , "Venus" , "Earth" , "Mars" , "Jupiter")
```

Unpacking tuples

Tuples can be **unpacked** to extract the individual values back into variables

```
planets = ("Mercury" , "Venus" , "Earth")
(planet1 , planet2 , planet3) = planets
print(planet1) # "Mercury"
```

Multiple variables can be unpacked with

```
(planet1 , *other_planets) = planets
print(other_planets) # ("Venus" , "Earth")
```

Sets

 A set is an unordered, unindexed collection denoted with curly brackets {}

```
planets = {"Mercury" , "Venus" , "Earth"}
print(planets) # {'Mercury', 'Earth', 'Venus'}
```

• Sets can contain all data types, but other collections, sets **do not** allow multiple entries with the same value

```
myset = {"Mercury" , "Venus" , "Earth" , "Mercury", 7.3 , 1 , True, False}
print(myset) # {False, 1, 'Earth', 'Mercury', 7.3, 'Venus'}
```

Acessing sets

- As they are unordered, sets cannot be indexed and can only be accessed by a loop (next session)
- We can use in / not in to check if an entry is in/not in a set

```
planets = {"Mercury" , "Venus" , "Earth"}
print("Earth" in planets) # True
print("Venus" not in planets) # False
```

This also means sets cannot be nested

Adding and removing from sets

 Set elements cannot be changed but sets can be added to with the add method

```
planets = {"Mercury" , "Venus" , "Earth"}
planets.add("Mars")
print(planets) # {"Mars" , "Mercury" , "Earth" , "Venus"}
```

• Items can be removed with either the remove or discard method

```
planets.remove("Venus")
planets.discard("Mars")
print(planets) # {"Mercury" , "Venus"}
```

Joining sets

• There are various method to join sets

```
planets1 = {"Mercury" , "Venus" , "Earth"}
planets2 = {"Venus" , "Earth" , "Mars"}
print(planets1.union(planets2))
# joins items from both sets -> {'Earth', 'Venus', 'Mercury', 'Mars'}
print(planets1.intersection(planets2))
# joins but keeps only duplicates -> {'Earth', 'Venus'}
print(planets1.difference(planets2))
# keeps itens in first set not in the second -> {'Mercury'}
print(planets1.symmetric_difference(planets2))
# keeps all except duplicates -> {'Mercury', 'Mars'}
```

Dictionaries

- Dictionaries are ordered, changeable collections
- Denoted with curly brackets with key: value pairs {key:value}

```
Mars = {
    "Radius": 3389.5,
    "Colour": "Red",
    "Temperature": -65 }
print(Mars) # {'Radius': 3389.5, 'Colour': 'Red', 'Temperature': -65}
```

• Since they are unordered, dictionaries cannot be indexed

```
print(Mars[0]) # KeyError: 0
```

Dictionaries

Duplicate entries will overwrite existing values

```
Mars = {
    "Radius": 3389.5,
    "Colour": "Red",
    "Temperature": -65,
    "Colour": "Blue" }
print(Mars) # {'Radius': 3389.5, 'Colour': 'Blue', 'Temperature': -65}
```

Dictionary keys can also be numbers

```
mydict = {0: 1}
print(mydict) # {0: 1}
```

Accessing dictionaries

• Items are accessed with dict_name["key_name"]

```
Mars = {
    "Radius": 3389.5,
    "Colour": "Red",
    "Temperature": -65 }
print(Mars["Colour"]) # 'Red'
```

• Key names can be listed with keys, and values with values

```
print(Mars.keys()) # dict_keys(['Radius', 'Colour', 'Temperature'])
print(Mars.values()) # dict_values([3389.5, 'Red', -65])
```

Editing dictionaries

Dictionaries can be added and changed with an assigment

```
Mars["Period"] = 687
Mars["Colour"] = "Blue"
print(Mars) # {'Radius': 3389.5, 'Colour': 'Blue', 'Temperature': -65, 'Period': 687}
```

• Entries can be deleted with the pop method

```
Mars.pop("Period")
print(Mars) # {'Radius': 3389.5, 'Colour': 'Blue' , 'Temperature': -65}
```

Editing dictionaries

• Dictionaries can be copied with the copy method

```
Mars_2 = Mars.copy()
```

You cannot copy dictionaries through assignement ie
 Mars_2 = Mars as any changes to one will change the other

Nested dictionaries

Dictionaries can be nested

```
planets = {
  "Mercury" : {
   "Radius" : 2439,
   "Mass" : 3.285e23 },
  "Venus" : {
   "Radius" : 6052,
   "Mass" : 4.867e24 },
  "Earth" : {
   "Radius" : 6378,
```

Nested dictionaries

 To access the items in a nested dictionary, use the key names moving outside in

```
print(planets["Venus"]["Radius"]) # 6052
```

• Again we can use len to get the length of a dictionary

```
print(len(Mars)) # 3
```

Property	List	Tuple	Set	Dictionary
Syntax	[1, 2, 3]	(1, 2, 3)	{1, 2, 3}	{"a": 1, "b": 2}
Ordered	Yes	Yes	No	Yes (Python 3.7+)
Indexed	Yes	Yes	No	By key
Mutable	Yes	No	Yes	Yes
Allows Duplicates	Yes	Yes	No	Keys: No Values: Yes

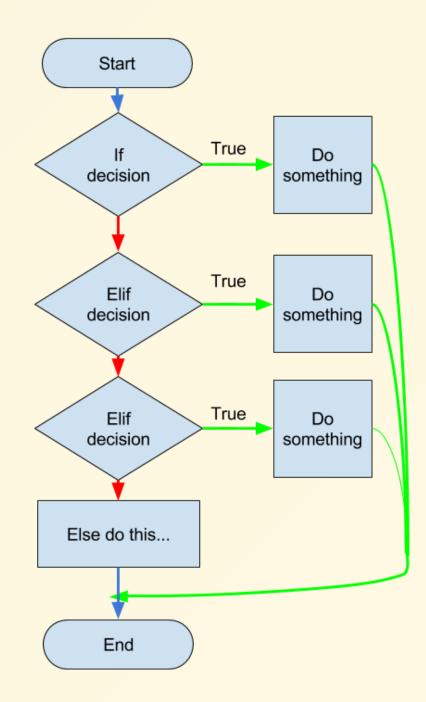
Session 4: Control Flow & Error Handling

```
numbers = [10, -5, 0, 23, -1]

for n in numbers:
    if n > 0:
        print(f"{n} is positive")
    elif n < 0:
        print(f"{n} is negative")
    else:
        print("Zero found")</pre>
```

We can combine the conditional statements we saw in session 2 (i.e. === , <, >) with if, elif and else statements to selectively evaluate blocks of code such as

```
if *some condition evaluates true *:
    *do something*
elif *some other condition evaluates true*:
    *do a different thing*
else:
    *do yet another different thing*
```



• If a statement evaluates to True, the indented code block is ran, and skipped otherwise

```
print(5 > 0) # True
print(5 == 6) # False

if 5 == 6:
    print('This is True') # This would not run as 5 == 6 is False
elif 5 > 3:
    print('This is True') # This would run as 5 > 3 is True
elif 5 == 5:
    print('This is True') # This would not run as the clause above was already fulfilled
else:
    print('Neither of these were True') # This would not run as one of the above was True
```

Aside: a note on indentation

- Notice that after the if / elif / else statements there is an indent
 - this is not style but necessary

```
x = 5
if x > 0:
    print('checking...') # this will run fine
    print('positive number') # both these lines are in the same code block and will run together
print('moving on...') # this will run regardless - outside of the if code block

if x > 0:
print('positive number') # This will raise an IndentationError
```

 We call the indented section a code block as it is a group of lines that are run together

• In a series of if, elif and else statements, if one is True, the rest are skipped

```
number = 8
if number > 5:
  print("Number is greater than 5")
elif number % 2 == 0:
  print("Number is even")
elif number > 10:
  print("Number is greater than 10")
else:
  print("Number is 5 or less and odd")
# prints only the first one -> Number is greater than 5
```

• Alternatively a series of only if statements, they are run separately

 We can use logical operators as well as conditional operators in our statements

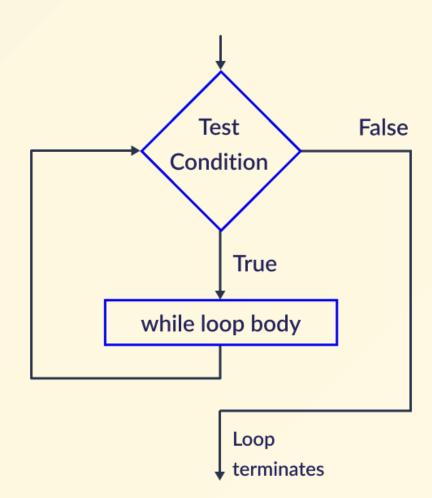
```
number = 5
if number % 2 == 0 and number > 10: # runs if both conditions evaluate to True
  print(f"{number} is even and greater than 10") # this does not run
elif number % 2 != 0 or number == 10: # runs if at least one condition evaluates to True
  print(f"{number} is either odd or exactly 10") # this runs
elif not number > 0:
  print(f"{number} is negative") # runs if condition is not True
else: # runs if neither of the above were fulfilled
  print(f"{number} does not match the above conditions") # this does not run
```

while loops

 while loops repeat a block of code whilst some condition is True

```
i = 1
while i < 10: # runs code block while this is True
  print(f'{i} is less than 10')
  i += 1</pre>
```

Warning: without proper care while loops can run infinitely! (cancel with a) terminal: Ctrl+C, b) jupyter: restart kernel)



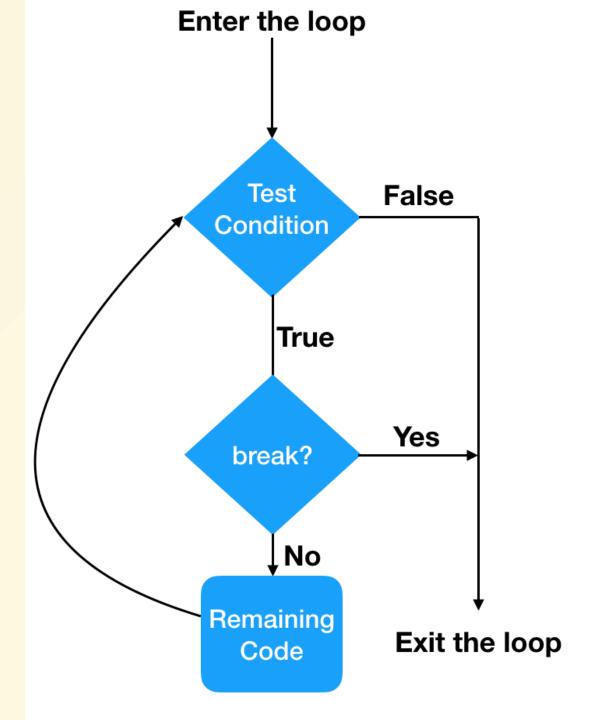
break statements

 We othean force the loop to end with a break statement

```
number = 1
while number <= 5:
  print(f"Number is: {number}")

if number == 3:
  print("Stopping the loop early!")
  break # exit the loop completely immediately
  print("That was a break!") # this will never run!

number += 1 # pay attention to indents
  # this runs outside of the if, but inside the while</pre>
```



break statements

We can use break statements to exit an otherwise infinte loop

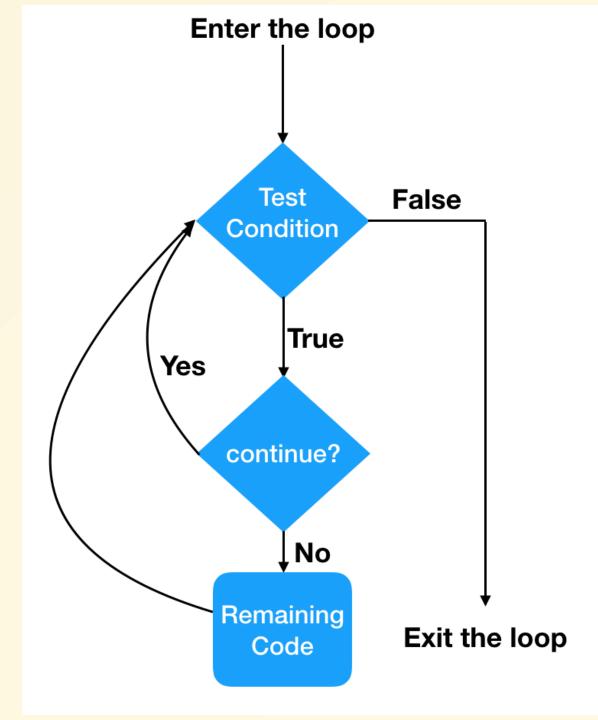
```
count = 0
while True: # this forms an infinite loop as it will always be True
  print(f"Loop number: {count}")
  count += 1

if count == 5:
   print("Reached 5, breaking the loop.")
   break # Exit the infinite loop
```

continue statements

 We can force a loop to skip the rest of it's block and return to the start with continue

```
i = 0
while i < 10:
    i += 1
    if i == 5:
        print(f'skipping 5!')
        continue
    print(i)</pre>
```



Exception handling

We can check for errors and deal with them before we run a line with try and except

```
try:
  num = int("hello") # trying to convert text to a number
except:
  print("Something went wrong!")
print("anyway...moving on!")
```

• Here if an error takes place in the try block, it triggers the except block, but the code still continues after

Exception handling

• We can combine this with a while loop to ensure the user inputs the correct data type for the problem

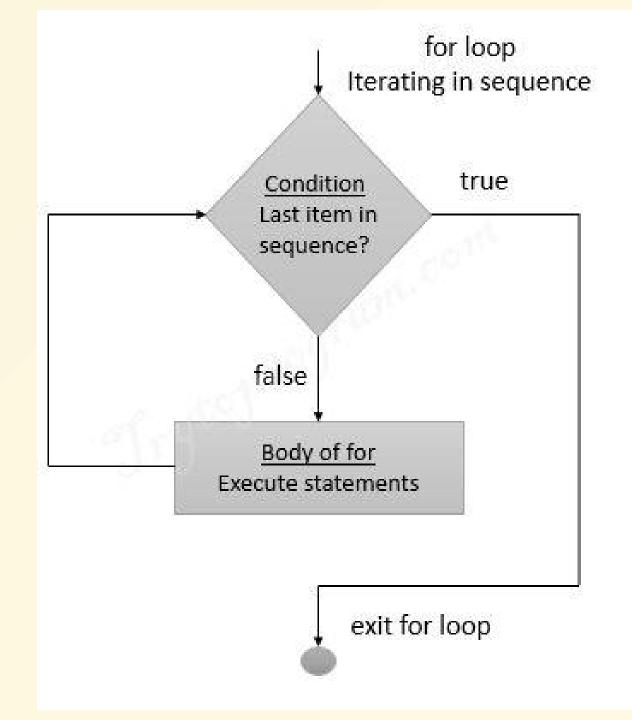
```
while True:
    try:
        number = int(input("Enter a number: ")) # Errors if string is given
        print(f"You entered: {number}")
        break # Exit the loop if input is valid
    except: # can also specify except ValueError for example
        print("Invalid input. Please enter a valid number.")
```

for loops

 We can loop over a sequence (i.e. list, tuple, dictionary, set, string) with a for loop

```
planets = ['Mercury', 'Venus', 'Mars']
for x in planets:
   print(x)
```

We have assigned a variable
 x to take on each value in
 the list per loop iteration



range

 When looping over consecutive numbers it is useful to create a list to loop over with the range function

```
for i in range(6): # range(6) = [0 , 1 , 2 , 3 , 4 , 5]
  print(i)

for i in range(2, 6): # range(2, 6) = [2 , 3 , 4 , 5]
  print(i)

for i in range(2, 12 , 3): # range(2, 12, 3) = [2 , 5 , 8 , 11]
  print(i)
```

Accessing index and variable

We can loop over the indexes of a collection by creating a list with range up to len of the collection

```
planets = ['Mercury' , 'Venus' , 'Earth' , 'Mars']
for i in range(len(planets)):
   print(f'planet {i}:{planets[i]}')
```

• Alternatively we can use enumerate which gives index and value

```
planets = ['Mercury' , 'Venus' , 'Earth' , 'Mars']
for i, planet_name in enumerate(planets):
   print(f'planet {i}:{planet_name}')
```

break and continue

• We can also use break and continue in for loops

```
for num in range(-10,10):
   if num < 0:
      continue # skip negative numbers

print(f"Checking number: {num}")

if num == 5:
   print("Found the number 5! Breaking the loop.")
   break</pre>
```

Nested for loops

• We can work in n dimensions by using n nested for loops

```
for i in range(1, 4): # Outer loop
  for j in range(1, 4): # Inner loop
    print(f"{i} x {j} = {i * j}") # loops through every combination of i and j
```

• This is particularly useful when indexing multidimensional objects

```
matrix = [[1, 2, 3],[4, 5, 6],[7, 8, 9]]

for i in range(len(matrix)):
    for j in range(len(matrix[i])):
        print(f"Value at ({i}, {j}) is {matrix[i][j]}")
```

Debugging code

- Coding can be very frustrating, and many times it isn't clear why the code doesnt work (or sometimes why it does...)
- The code may give a confusin or misleading error message, or it might run but give nonsensical answers (nan, inf)

```
def calculate_average_temperature(temps):
    total = 0
    count = 0
    for temp in temps:
        total += temp
    return total / count
temps = [5778, 9940, 3500]
print("Average temp:", calculate_average_temperature(temps)) # ZeroDivisionError
```

Debugging code

 Print statements are your friend - use them plentifully and throughout to track where the error comes in

```
def calculate_average_temperature(temps):
    total = 0
    count = 0
    for i, temp in enumerate(temps):
        print(f"Index {i}: temp = {temp}, total before adding = {total}, count before adding = {count}")
        total += temp
        print(f"Total after adding: {total}")
    print(f"Final total: {total}, final count: {count}")
    return total / count

temps = [5778, 9940, 3500]
print("Average temp:", calculate_average_temperature(temps))
```

Debugging code

 Print statements are your friend - use them plentifully and throughout to track where the error comes in

```
Index 0: temp = 5778, total before adding = 0, count before adding = 0
Total after adding: 5778
Index 1: temp = 9940, total before adding = 5778, count before adding = 0
Total after adding: 15718
Index 2: temp = 3500, total before adding = 15718, count before adding = 0
Total after adding: 19218
Final total: 19218, final count: 0
Traceback (most recent call last):
...
ZeroDivisionError: division by zero
```

Session 5: Functions

```
def luminosity(radius, temperature):
    Calculate the luminosity of a star using the Stefan-Boltzmann law.
    Parameters:
        radius (float): Radius of the star in meters (m).
        temperature (float): Surface temperature of the star in Kelvin (K).
    Returns:
        float: Luminosity in watts (W).
    sigma = 5.670374e-8 # Stefan-Boltzmann constant in W/m^2 \cdot K^4
    return 4 * 3.1416 * radius**2 * sigma * temperature**4
L = luminosity(6.96e8, 5778)
print(f"Luminosity: {luminosity(6.96e8, 5778):.2e} W")
```

Creating functions

- Functions are like a mini-program inside your code
- Functions take input arguments and return output arguments
- They can be used to reuse code without copy/pasting chunks
- Functions must be defined with def, the contents must be indented, and values may (not must) be returned with return

```
def greet(name): # def function_name(parameter1, parameter2)
    return f"Hello, {name}!" # return output_parameters

print(greet("Natalie")) # Output: Hello, Natalie!
print(greet("Nobody")) # Output: Hello, Nobody!
```

Function inputs

Functions can take a number of arguments of varying data types

```
def describe_planet(name, moons, mass):
    return f"{name} has {moons} moon(s) and a mass of {mass:.2e} kg."

print(describe_planet("Mars", 2, 6.39e23))
# Mars has 2 moon(s) and a mass of 6.39e+23 kg.
```

 When passing arguments to functions in this way, they must be in the correct order, these are called positional arguments

```
print(describe_planet(2, "Mars", 6.39e23))
# 2 has Mars moon(s) and a mass of 6.39e+23 kg.
```

Default Arguments

We can assign default values to a function that can be overwritten

```
def describe_star(name="Sun", temperature=5778):
   return f"{name} has a surface temperature of {temperature} K."
# Example usages
print(describe_star())
                                          # Uses both default values
# Sun has a surface temperature of 5778 K.
print(describe_star("Sirius")) # Overrides name, uses default temperature
# Sirius has a surface temperature of 5778 K.
print(describe_star("Betelgeuse", 3500)) # Overrides both
# Betelgeuse has a surface temperature of 3500 K.
```

Positional arguments and *args

 We can pass an unspecified number of positional arguments using *

```
def third_planet(*planets):
    print("The third planet is " + planets[2])
third_planet("Mercury", "Venus", "Earth", "Mars")
# The third planet is Earth
```

Keyword arguments and **kwargs

• **Keyword arguments**, unlike positional arguments, can be passed in any order

```
def describe_planet(name, moons, mass):
    return f"{name} has {moons} moon(s) and a mass of {mass:.2e} kg."
print(describe_planet(mass = 6.39e23, moons = 2, name = "Mars"))
# Mars has 2 moon(s) and a mass of 6.39e+23 \, kg.
```

Keyword arguments and **kwargs

 We can use **kwargs to pass an unspecified number of keyword arguments

```
def info(*args, **kwargs):
    print("Positional args:", args)
    print("Keyword args:", kwargs)
info("Mercury", "Venus", name="Earth", moons=1)
# Positional args: ('Mercury', 'Venus')
# Keyword args: {'name': 'Earth', 'moons': 1}
```

Docstrings

• Docstrings are a special kind of string placed right after the def line, which describes what a function does, its inputs and outputs

```
def greet(name):
    """

    Say hello to a person.
    Parameters:
        name (str): The person's name.
    Returns:
        str: A greeting message.
    """
    return f"Hello, {name}!"
```

Docstrings

Where comments are there for the developer, doctrings are there for the user to make it clear the usage of a function. The docstring can be accessed with help(function_name) (anywhere) or function_name? (ipython/jupyter)

```
Signature: greet(name)
Docstring:
Say hello to a person.
Parameters:
    name (str): The person's name.

Returns:
    str: A greeting message.
Type: function
```

Global and local variables

- Global variables are set outside functions and used anywhere.
- Within a function, variables can be defined however these are local variables, and cannot be accessed outside the function

```
planet = "Earth" # Global variable

def describe():
    moon = "Moon" # Local variable
    print(f"{planet} has a natural satellite called {moon}.")

describe() # Earth has a natural satellite called Moon.
print(planet) # "Earth"
print(moon) # NameError: name 'moon' is not defined
```

Global and local variables

We can force a variable inside a function to be a global variable with global

```
planet = "Earth" # Global variable

def rename_planet():
    global planet
    planet = "Mars" # Modify the global variable
    print("Planet renamed inside function.")

rename_planet()
print("Planet is now:", planet)
```

• Using global is discouraged, it makes code hard to follow/debug

Loops within functions

Loops can be used freely within functions

```
def total_luminosity(luminosities):
    total = 0
    for L in luminosities:
        total += L
    return total

stars = [3.5e26, 1.2e27, 5.8e25] # Luminosities in watts
print(f"Total luminosity: {total_luminosity(stars):.2e} W")
# Total luminosity: 1.57e+27 W
```

Nested functions

• It is also possible to define a function within a function

```
def star_report(stars):
    print("Report start")
    def level(L):
        if L > 1e26:
          return "bright"
        else:
          return "dim"
    for star in stars:
        print(f"{star}: {level(stars[star])}")
stars = {"Sirius":2.5e27, "Alpha Cen":1.5e26, "Barnard":3e25}
star_report(stars) # Sirius: bright, Alpha Cen: bright, Barnard: dim
```

Classes

- Classes are a way to group data and their related functions (methods) into a single object
- We will not cover classes in detail scientific tasks can be done using functions and libraries
- However if you ever want to write your own library of code, most likely you would do so in a class
- Though we won't write classes often, we use them all the time
- Dictionaries, lists, tuples and sets are all examples of classes

Classes

- Classes are initialised using __init__, and after initialisation methods (class functions) within a class can be ran
- Classes are always initialised with self, which is a reference to the current object inside a class

```
class Star: # defining a class called 'Star'
    def __init__(self, name, temperature): # initialised with a name and temperature
        self.name = name # assigning the name to the object itself
        self.temperature = temperature # assigning the temperature to the object itself
    def report(self): # defining a method of the class
        return f"{self.name} has a temperature of {self.temperature} K."

sirius = Star("Sirius", 9940) # initialising the class
    print(sirius.report()) #running a class method
```

Classes

 In fact, many built-in types you've used — like lists and dictionaries — are already classes in Python

```
print(type([1, 2, 3]))  # <class 'list'>
print(type((1, 2, 3)))  # <class 'tuple'>
print(type({1, 2, 3}))  # <class 'set'>
print(type({"planet": "Mars", "moons": 2})) # <class 'dict'>

my_dict = {"planet": "Mars", "moons": 2}

# examples of dict methods
print(my_dict.keys())
print(my_dict.pop("moons"))
```

Session 6: Conda and Packages

```
Natalie@mylinux:~$ conda create -n myenv --python=3.13.0
Natalie@mylinux:~$ conda activate myenv
Natalie@mylinux:~$ conda install numpy
Natalie@mylinux:~$ conda install scipy==1.16.0
Natalie@mylinux:~$ conda update scipy
Natalie@mylinux:~$ conda env export > environment.yml
Natalie@mylinux:~$ conda deactivate
```

Packages

- Packages are pre-written codes we can utilise so we don't write everything from scratch
- Packages are installed on the command line with e.g. pip or conda

pip install numpy

conda install numpy

 We will use conda as it has the advantage of managing virtual environments which can be downloaded <u>here</u>

Virtual environments and conda

- Packages are installed by default in the global environment this can be problematic as different package versions can conflict with one another
- This can lead to broken dependencies (the packages that packages require to run) when updating libraries, and code that is not easily reproduced
- Instead virtual environments create a separate workspace for a Python project, with it's own Python version and it's own installed packages
- It can be thought of as a mini-computer for it's own job

Virtual environments and conda

We use virtual environments because

- We can isolate environments and keep packages between projects separate so they don't interfere with one another
- We can install exact versions of packages without affecting the system Python or other projects
- We can easily share environments so that other users can run your code with the same setup
- It is highly recommended to create a new environment for each coding project you create

Creating conda environments

• conda environments are created using the create command

```
(base) Natalie@mylinux:~$ conda create -n "myenv" python=3.12
```

The environment is created in ~/miniconda3/envs/ or ~/anaconda3/envs/, the paths are listed with

```
(base) Natalie@mylinux:~$ conda env list
```

Cloning and deleting conda environments

• Environments can be copied with the --clone flag

```
(base) Natalie@mylinux:~$ conda create --clone myenv -n myenv2
```

• Environments can be deleted with the remove command

```
(base) Natalie@mylinux:~$ conda env remove -n myenv2
```

Activating and deactivating environments

 To install packages in the environments or use it for a python script, it must first be activated

```
(base) Natalie@mylinux:~$ conda activate myenv
(myenv) Natalie@mylinux:~$
```

- Notice how base is now the name of our environment
- The environment can be deactivated with

```
(myenv) Natalie@mylinux:~$ conda deactivate
(base) Natalie@mylinux:~$
```

Installing packages

• Packages are installed with install, and updated with update

```
(myenv) Natalie@mylinux:~$ conda install numpy
(myenv) Natalie@mylinux:~$ conda update scipy
```

• If a package is unavailable in conda, it may be available with pip

```
(myenv) Natalie@mylinux:~$ pip install fastapi
```

• A list of the packages with their versions can be printed with list

```
(myenv) Natalie@mylinux:~$ conda list
```

Specifying package versions

Constraint type	Specification	Result
Fuzzy	numpy=1.11	1.11.0, 1.11.1, 1.11.2, 1.11.18 etc.
Exact	numpy==1.11	1.11.0
Greater than or equal to	numpy>=1.11	1.11.0 or higher
OR	numpy=1.11.1 1.11.3	1.11.1, 1.11.3
AND	numpy>=1.8,<2	1.8, 1.9, not 2.0

Exporting environments

• Environments can be exported to a .yaml file with

```
(base) Natalie@mylinux:~$ conda env export > environment.yml
```

• This can then be used to create a copy of the environment

```
(base) Natalie@mylinux:~$ conda env create -f myenv.yaml
```

 This is useful to share with others who can create a copy of your environment and run your code with the same dependancies

Virtual environments as jupyter kernels

• It's useful to be able to use our environment in a jupyter-lab session, which is done with the ipykernel package

```
(myenv) Natalie@mylinux:~$ conda install ipykernel
```

The environment can then be added with

```
(myenv) Natalie@mylinux:~$ python -m ipykernel install --user --name myenv --display-name "Python (myenv)"
```

• When jupyter is relaunched, the kernel for your environment should be available

Session 7: numpy

```
import numpy as np
data = np.loadtxt("luminosities.txt")
night1 = data[:, 1]
night2 = data[:, 2]
change = night2 - night1
mean_change = np.mean(change)
brightest = np.argmax(night2)
total_lum = np.sum(night2)
print(f"Mean change: {mean_change:.2e} W")
print(f"Brightest star ID: {int(data[brightest, 0])}")
print(f"Total luminosity (Night 2): {total_lum:.2e} W")
```

Importing packages

 Packages must be imported at the start of your python script to be used

```
import numpy
numpy.mean([3 , 7 , 3])
```

• For ease of use, packages can be imported with a shorter name

```
import numpy as np
np.mean([3 , 7 , 3])
```

Importing packages

• To save space you can import one function from a package

```
from numpy import mean
mean([3 , 7 , 3])
```

All functions from a library can be imported with * (not recommended - may overwrite functions - debugging headache)

```
from numpy import *
mean([3 , 7 , 3])
```

Importing packages

 Packages are just folders of code, if you want a function from deep within a subfolder, folders are seperated with

```
import numpy as np

matrix = [[1, 2], [3, 4]]
print(np.linalg.det(matrix))
```

```
from numpy.linalg import det as matrix_determinant

matrix = [[1, 2], [3, 4]]
print(matrix_determinant(matrix))
```

What is numpy?

- numpy (numerical Python) is a library used for working with arrays, and has many functions for linear algebra, fourier transforms and matrix operations
- numpy is widely used for data handling in Python, and is up to 50x faster than using lists for numerical problems (mostly C/C++ under the hood)
- numpy is open source, and new versions are released frequently
- <u>Documentation</u> of numpy is clear and useful

Arrays

• numpy works with arrays, which are multi-dimensional objects

• The dimensions of an array can be shown with shape

```
print(a0.shape, a1.shape, a2.shape, a3.shape)
# Output: () (3,) (2, 3) (2, 2, 3)
```

Creating arrays

 We can create arrays either manually as shown before, or with a variety of functions

```
zeros = np.zeros((3, 4)) # array of zeros (size 3x4)
ones = np.ones((2, 5)) # array of ones (size 2x5)
empty = np.empty((2, 3)) # empty array (uninitialized values, size 2x3)
full = np.full((3, 3), 7) # array filled with a specific value (e.g., 7), size 3x3
range_array = np.arange(10) # array with a range of values (0 to 9)
linspace = np.linspace(0, 1, 5) # linearly spaced array between 0 and 1 with 5 points
```

Reshaping arrays

• Use reshape to change shape (total size must stay the same), or flatten to reduce to 1D

Accessing arrays

• We can index and slice arrays using [] as we did with lists

```
arr = np.array([[10, 20, 30, 40],
                [50, 60, 70, 80],
                [90, 100,110,120]])
# Access element at row 1, column 2 (zero-indexed)
print(arr[1, 2]) # Output: 70
# Slice: get all rows, columns 1 to 3 (excluding 3)
print(arr[:, 1:3])
# Output:
# [[ 20 30]
  [ 60 70]
  [100 110]]
```

Vectorised operations

numpy allows vectorised operations unlike lists, making operations faster with less lines

```
numbers = [1, 2, 3, 4, 5] # example with lists
squares = []
for n in numbers:
    squares.append(n**2)
print(squares) # [1, 4, 9, 16, 25]
```

```
numbers = np.array([1, 2, 3, 4, 5]) # example with numpy
squares = numbers ** 2
print(squares) # [ 1  4  9 16 25]
```

Masking

 Masking allows us to select/edit elements from an array based on a condition through booleans

```
temps = np.array([273, 280, 290, 250, 300, 310])
print(temps > 280) # [False False True False True]
hot_temps = temps[temps > 280]
print(hot_temps) # [290 300 310]
moderate_temps = temps[(temps > 260) & (temps < 300)]</pre>
print(moderate_temps) # [273 280 290]
temps[temps < 275] = 275
print(temps) # [275 280 290 275 300 310]
```

numpy constants

• numpy has <u>constants</u> built in

```
np.e # Euler's constant
np.pi # pi
np.inf # Infinity
np.nan # Not a number
```

• The constants module gives more extensive constants in SI units

```
np.constants.Boltzmann # Boltzmann constant
np.constants.Planck # Planck constant
np.constants.g # Gravitational constant
np.constants.c # Speed of light
```

numpy mathematical functions

• numpy has many functions, here are some of the most useful

```
# Trigonometic and hyperbolic functions
np.sin(x) np.cos(x) np.tan(x) np.sinh(x) np.cosh(x) np.tanh(x)
# Rounding functions
np.round(x) np.floor(x) np.ceil(x)
# Sums & products
np.prod(x) np.sum(x) np.cumprod(x) np.cumsum(x)
# Exponents, logarithms (log is natural by default) and absolute
np.exp(x) np.log(x) np.log10(x) np.abs(x)
# Statistics
np.mean(x) np.std(x) np.median(x) np.sqrt(x)
# Other useful functions (argmin/argmax give the index of the min/max value)
np.max(x) np.argmax(x) np.min(x) np.argmin(x)
```

Using numpy functions

- Where applicable these functions work for arrays with various dimensions
- It might be useful to only apply a function to one dimension, which we can do with the axis argument

numpy.random

• numpy also has a module to generate (pseudo) random numbers

```
from numpy import random
random.seed(12345) # seed random numbers for reproducability
x = random.randint(100) # a random integer between 0 and 100
x = random.randint(100, size = (3,5)) # a 2D array with 3 x 5 random integers
x = random.rand() # a random float between 0 and 1
x = random.rand(3,5) \# a 2D array with 3 x 5 random floats between 0 and 1
x = random.choice([3,5,7,2]) # returns a random value from the array supplied
x = random.normal(loc = 1, scale = 2, size = (2,3)) # a random normal distribution
# of size 2x3 with mean at 1 and standard deviation of 2
```

numpy matrices and linalg

numpy has useful functions for matrices within the linalg module

```
A = np.array([[2, 4], [5, -6]])
B = np.array([[9, -3], [3, 6]])
sum = A + B # element wise addition
prod = A.dot(B) # matrix multiplication (* is element wise multiplication)
transpose = A.T # transpose
inverse = np.linalg.inv(A) # inverse
det = np.linalg.det(A) # determinant
trace = np.linalg.trace(A) # trace of matrix
eigenvalues, eigenvectors = np.linalg.eig(A) # eigenvalues and eigenvectors
norm = np.linalg.norm(A) # norm of matrix
```

numpy truth value testing

• numpy has functions any and all to test the values within arrays, which tests is all values are True or any values are True and outputs a boolean

```
arr = np.array([10, 25, 60, 150])
print(np.all(arr > 0)) # Output -> True
print(np.any(arr > 200)) # Output -> False
```

numpy array contents testing

• There are also functions to test the individual contents of an array

```
arr = np.array([3.5, np.nan, np.inf, -np.inf, 0.0, -2.1])

print(np.isnan(arr)) # check for NANs
# Output -> [False True False False False False]

print(np.isfinite(arr)) # check for finite numbers
# Output -> [ True False False False True True]

print(np.isinf(arr)) # check for infinate numbers
# Output -> [False False True True False False]
```

Fourier transforms with numpy

• The fft module provides simple functions to perform Fast Fourier Transforms (FFT) and their inverse (IFFT)

```
t = np.linspace(0, 1, 500) # time array
freq = 5 # frequency in Hz
signal = np.sin(2 * np.pi * freq * t) # Sine wave sin(2πft)

## Perform FFT
fft_result = np.fft.fft(signal)
# Compute frequencies
freqs = np.fft.fftfreq(len(t), d=(t[1] - t[0]))
# Perform IFFT, keeping real part
reconstructed_signal = np.fft.ifft(fft_result).real
```

Saving and loading files with numpy

numpy provides functions to save and load data files in .csv and .txt formats

```
arr = np.array([[1.1, 2.2], [3.3, 4.4]])
np.savetxt('array.txt', arr) # Save as plain text
np.savetxt('array.csv', arr, delimiter=',') # Save as CSV

loaded_txt = np.loadtxt('array.txt')
loaded_csv = np.loadtxt('array.csv', delimiter=',')
```

• The delimiter argument declares what separates values

Session 8: matplotlib

```
import matplotlib.pyplot as plt
x = [i \text{ for } i \text{ in } range(-10, 11)]
y = [i**2 for i in x]
plt.plot(x, y, color='orange')
plt.title("Parabola: y = x^2")
plt.xlabel("x")
plt.ylabel("y")
plt.grid(True)
plt.show()
```

What is matplotlib?

- matplotlib is a package that can create static, animated and interactive visualizations
- It is widely used in data science and scientific computing
- matplotlib is highly customisable, meaning clear, publication quality plots can be produced
- It is commonly imported with

import matplotlib.pyplot as plt

• .pyplot is the user interface used to create (mostly) static plots

Line plots

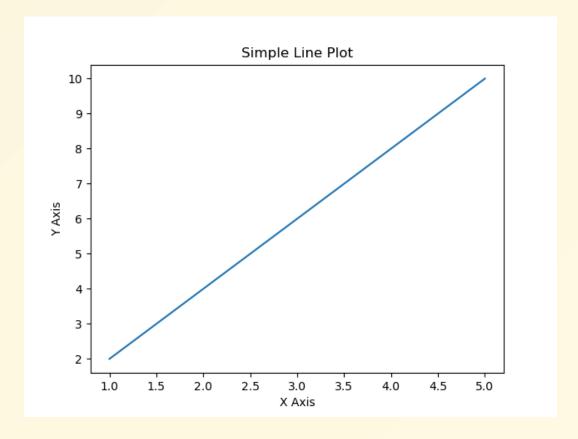
Line plots are simple made
 with plt.plot provided x and
 y have the same shape

```
x = [1, 2, 3, 4, 5] # X data
y = [2, 4, 6, 8, 10] # Y data

plt.plot(x, y) # Plotting

plt.xlabel('X Axis') # X axis label
plt.ylabel('Y Axis') # Y axis label
plt.title('Simple Line Plot') # Title

plt.show() # Displays plot
```



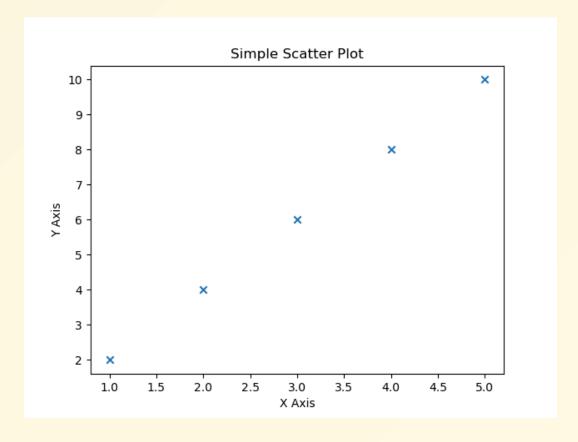
Scatter plots

Scatter plots are the same, but with plt.scatter, marker options can be found here (defaults to 'o')

```
plt.scatter(x, y, marker = 'x')

plt.xlabel('X Axis')
plt.ylabel('Y Axis')
plt.title('Simple Scatter Plot')

plt.show()
```



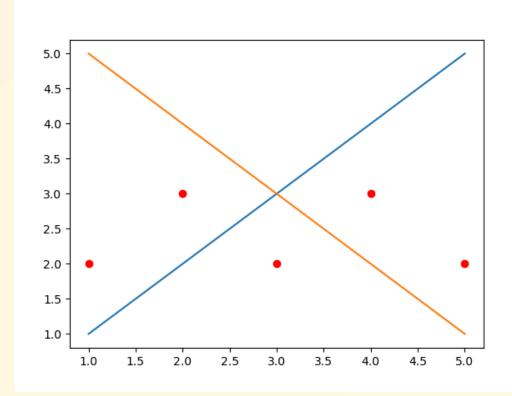
Plotting multiple datasets

 Multple datasets can be plotted, with a legend if desired

```
x = [1, 2, 3, 4, 5] # X data
y1 = [1, 2, 3, 4, 5] # Dataset 1
y2 = [5, 4, 3, 2, 1] # Dataset 2
y3 = [2, 3, 2, 3, 2] # Dataset 3

plt.plot(x, y1, label='Line 1')
plt.plot(x, y2, label='Line 2')
plt.scatter(x, y3, color='red', label='Scatter')

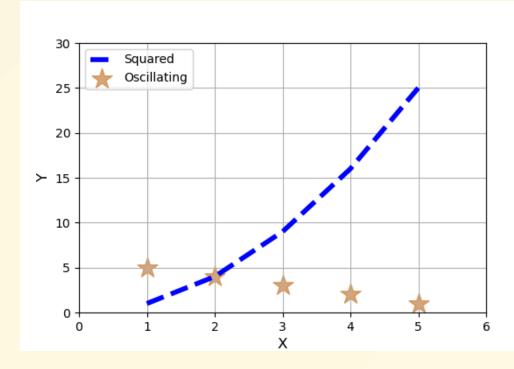
plt.legend() # Add legend using label args
plt.show()
```



Aesthetics

 There are many customisable options, e.g. <u>colour options</u>

```
x = [1, 2, 3, 4, 5]
y1 = [i**2 for i in x]
y2 = [5, 10, 5, 10, 5]
plt.figure(figsize=(6, 4)) Creates new figure
plt.plot(x, y1, label='Squared', ls = '--', c='blue', lw = 4)
# ls:linestyle, c:color, lw:linewidth, s:size, alpha:opacity
plt.scatter(x, y2, label='0scillating',
            s=300, marker = '*', c='peru', alpha=0.7)
plt.xlabel('X', fontsize = 12)
plt.ylabel('Y', fontsize = 12)
plt.grid(True) # Add a grid
plt.legend()
plt.xlim(∅, 6) # Set custom X limits
plt.ylim(0, 30) # Set custom Y limits
plt.savefig('flashy_plot.png') # Save as a png
plt.show()
```



rcParams for global plot styling

• If you would like to change the aesthetics for all plots without editing the settings individually, you can set the rcParams

```
plt.rcParams.update({
    'font.size': 14,
    'axes.titlesize': 18,
    'axes.labelcolor': 'darkblue',
    'figure.figsize': (6, 4)
})
```

• This changes the matplotlib defaults - they can be reset with

```
plt.rcdefaults()
```

Histograms

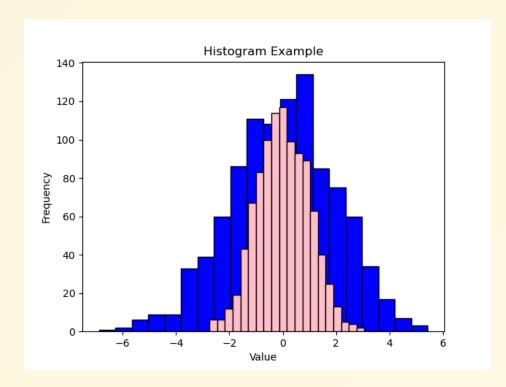
Histograms are plotted as shown

```
import numpy as np

data1 = np.random.normal(loc=0, scale=2, size=1000)

data2 = np.random.normal(loc=0, scale=1, size=1000)

plt.hist(data1, bins=20, color='blue', edgecolor='black')
plt.hist(data2, bins=20, color='pink', edgecolor='black')
plt.title('Histogram Example')
plt.xlabel('Value')
plt.ylabel('Frequency')
plt.show()
```

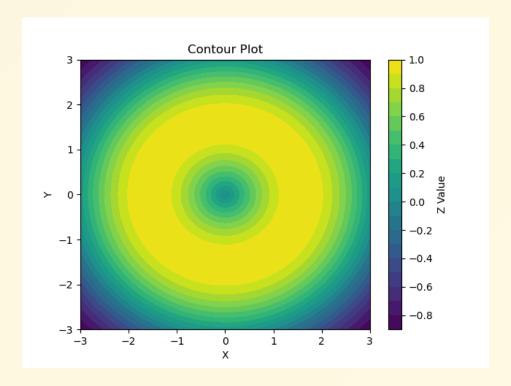


Contour plots

 Contour plots come with a range of colormaps

```
x = np.linspace(-3, 3, 1000)
y = np.linspace(-3, 3, 1000)
X, Y = np.meshgrid(x, y) # Coordinate grids from 1D arrays
Z = np.sin(np.sqrt(X**2 + Y**2))

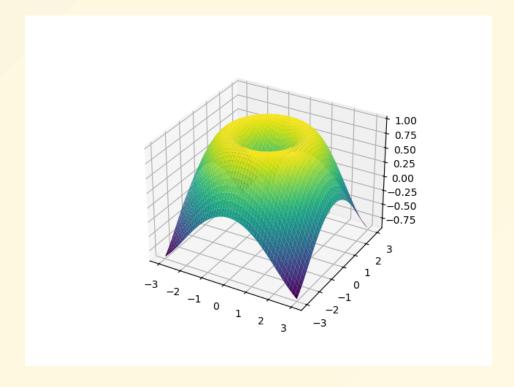
plt.contourf(X, Y, Z, levels=20, cmap='viridis')
plt.colorbar(label='Z Value') # Plots colorbar
plt.title('Contour Plot')
plt.xlabel('X')
plt.ylabel('Y')
plt.show()
```



3D plots

 Instead of a contour plot a 3D plot can also be made

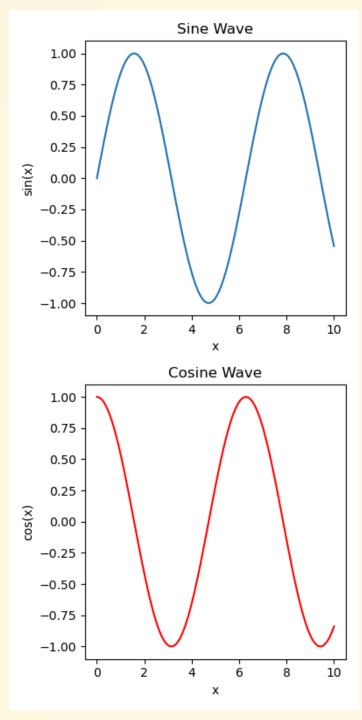
```
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')
ax.plot_surface(X, Y, Z, cmap='viridis')
plt.show()
```



Subplots

Multiple plots can be in the same figure

```
x = np.linspace(0, 10, 100)
fig, axs = plt.subplots(2, 1, figsize=(4, 8)) # 2 rows, 1 column
# First plot: sine wave
axs[0].plot(x, np.sin(x), 'b')
axs[0].set_title('Sine Wave') # now e.g. set_title, not title
axs[0].set_xlabel('x')
axs[0].set_ylabel('sin(x)')
# Second plot: cosine wave
axs[1].plot(x, np.cos(x), 'r')
axs[1].set_title('Cosine Wave')
axs[1].set_xlabel('x')
axs[1].set_ylabel('cos(x)')
plt.tight_layout() # Adjust spacing for subplots
plt.show()
```



Session 9: scipy and astropy

```
from astropy.coordinates import SkyCoord
from astropy import units as u
from scipy.optimize import root
def angular_distance(theta):
    c1 = SkyCoord(ra=10*u.degree, dec=20*u.degree)
    c2 = SkyCoord(ra=theta[0]*u.degree, dec=25*u.degree)
    return (c1.separation(c2).degree - 5)**2
sol = root(angular_distance, [10])
print(f"RA for 5° separation: {sol.x[0]:.3f} degrees")
```

What is scipy?

- scipy is a package that builds on numpy, extending its capabilites and adding more sophisticated routines for data analysis
- Routines commonly used include those for optimization, integration, interpolation, linear algebra, statistics etc
- scipy is widely used in scientific computing and data analysis

scipy.optimise: Minimising functions

• The function minimize can be used to minimise a chosen function with an initial guess

```
from scipy.optimize import minimize # often scipy functions are purpose imported
# otherwise it is common to use `import scipy as sp`

def f(x, a, b): # Define a function to minimize
    return (x - a)**2 + b

a, b = 2, 3
x0 = 0 # Initial guess
result = minimize(f, x0, args=(a, b)) # takes function, initial guess, any additional args

print("Minimum value:", result.fun) # Output -> Minimum value: 3.0
print("At x =", result.x[0]) # Output -> At x = 1.99999998937739
```

scipy.optimise: Root Solving

We can also find the roots of functions with root

```
from scipy.optimize import root

def g(x): # Define a function to find the root of
    return x**2 - 9

x0 = 2 # Initial guess

sol = root(g, x0)

print("Root found at:", sol.x) # Output -> Root found at: [3.]
print("Function value at root:", g(sol.x)) # Function value at root: [-7.63833441e-14]
```

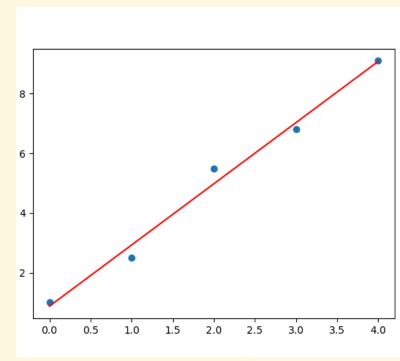
scipy.optimise: Curve fitting

 Given some data, we can fit it to a function with curve_fit

```
def model(x, a, b): # Define our model
    return a * x + b

x = np.array([0, 1, 2, 3, 4])
y = np.array([1.0, 2.5, 5.5, 6.8, 9.1])

p, c = curve_fit(model, x, y) # p: parameters, c: covariance
e = np.sqrt(np.diag(c)) # e: error
print(f"a = {p[0]:.2f} ± {e[0]:.2f}, b = {p[1]:.2f} ± {e[1]:.2f}")
# Output -> Fitted parameters: a=2.05, b=0.88
plt.scatter(x, y)
plt.plot(x, model(x, *p), 'r-')
plt.show()
```



scipy.integrate: Integration

Functions can be integrated between bounds with quad

```
from scipy.integrate import quad

def f(x): # Define the function to integrate
    return np.sin(x)

result, error = quad(f, 0, np.pi) # Integrate from 0 to pi

print(f"Integral result: {result}") # Output -> Integral result: 2.0
print(f"Estimated error: {error}") # Output -> Estimated error: 2.220446049250313e-14
```

• Also dblquad and tplquad for double and triple integration

scipy.integrate: Integration

• For discrete data we can use the trapezium rule trapz or Simpson's rule simps

```
from scipy.integrate import trapezoid

x = np.linspace(0, np.pi, 50)
y = np.sin(x) + 0.1 * np.random.normal(size=x.size) # sine with noise

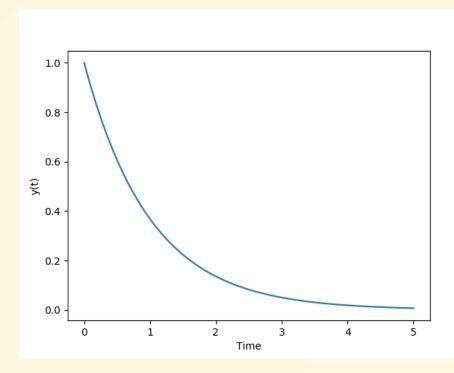
# Compute integral using trapezoidal rule
integral = trapezoid(y, x)

print(f"Approximate integral (trapz): {integral}")
# Output -> Approximate integral (trapz): 2.0623877389171197
```

scipy.integrate: ODEs

• odeint solves a series of first order ODEs: here $\frac{dy}{dx} = -y$

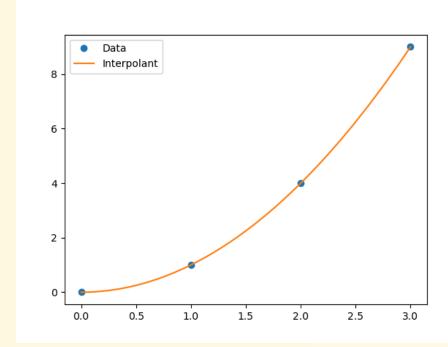
```
from scipy.integrate import odeint
def dydt(y, t): # Function for first order ODE
    return -y
t = np.linspace(0, 5, 100) # Time array
y0 = 1 \# Initial condition at t[0] = 0
y = odeint(dydt, y0, t)
plt.plot(t, y)
plt.xlabel('Time'); plt.ylabel('y(t)')
plt.show()
```



scipy.interpolation

 We can interpolate between data points with interp1d

```
from scipy.interpolate import interp1d
x = [0, 1, 2, 3]
y = [0, 1, 4, 9]
f = interp1d(x, y, kind='cubic') # linear by default
x_new = np.linspace(0, 3, 100)
plt.plot(x, y, 'o', label='Data')
plt.plot(x_new, f(x_new), '-', label='Interpolant')
plt.legend()
plt.show()
```



scipy.linalg

• Systems of linear equations can be solved using solve, in this example

$$3x + y = 9; \quad x + 2y = 8$$

```
from scipy.linalg import solve

A = np.array([[3, 1], [1, 2]])
b = np.array([9, 8])

x = solve(A, b)
print(x)
```

scipy.stats

Large amount of probability distributions and statistic <u>functions</u>

```
from scipy.stats import norm, binom, poisson, uniform, skew, kurtosis

# Generate random samples
data_norm = norm.rvs(loc=0, scale=1, size=1000) # Normal samples
data_binom = binom.rvs(n=10, p=0.5, size=1000) # Binomial samples
data_poisson = poisson.rvs(mu=3, size=1000) # Poisson samples
data_uniform = uniform.rvs(loc=0, scale=10, size=1000) # Uniform samples

# Descriptive statistics on normal data
print("Skewness:", skew(data_norm)) # Output -> Skewness: -0.07371307787886548
print("Kurtosis:", kurtosis(data_norm)) # Output -> Kurtosis: -0.02523185483204493
print("Uniform PDF at 5:", uniform.pdf(5, loc=0, scale=10)) # Output -> Uniform PDF at 5: 0.1
```

What is astropy?

- astropy is a specialised library for astronomical data and calculations
- This includes units and quantities, time and date conversions, coordiante and frame transformations
- Widely used by astronomers for research and data analysis

astropy.units

• The units module uses built in units to enable automatic unit conversion and dimensional analysis

```
from astropy import units as u
distance = 10 * u.meter
time = 5 * u.second
speed = distance / time
print(speed) # Output -> 2.0 m / s
print(speed.to(u.km / u.hour)) # Convert units , Output -> 7.2 km / h
print((3 * u.meter) * (4 * u.meter)) # Combine units for area, Output -> 12.0 m2
```

astropy.time

Automatic conversions for time are supported in Time

```
from astropy.time import Time

# Create a Time object in UTC
t = Time('2025-07-30 12:00:00', scale='utc')

# Convert to Julian Date (JD)
print("Julian Date:", t.jd) # Output -> Julian Date: 2460887.0

# Convert to Modified Julian Date (MJD)
print("Modified Julian Date:", t.mjd) # Output -> Modified Julian Date: 60886.5
```

astropy.coordinates

 Routines for coordinate transformations are built in, here we convert from altitude-azimuth to right ascention-declination

```
from astropy.coordinates import SkyCoord, AltAz, EarthLocation

loc = EarthLocation(lat=51.48*u.deg, lon=0*u.deg) # Observer location
time = Time('2025-07-30 22:00:00') # Time of observation
altaz = AltAz(alt=45*u.deg, az=130*u.deg, location=loc, obstime=time)
c = SkyCoord(altaz).icrs # Conversion

print(f"RA: {c.ra.degree:.2f}, Dec: {c.dec.degree:.2f}")
# Output -> RA: 312.72, Dec: 15.58
```

astropy.io

 In astronomy FITS files are common, and can be handled with fits

```
from astropy.io import fits

data = np.random.rand(100, 100) # Create some dummy image data

fits.writeto('example.fits', data) # Write to a FITS file

hdul = fits.open('example.fits') # Read from the FITS file
hdul.close()
```

astropy.cosmology

Routines for cosmological conversions and calculations

```
from astropy.cosmology import Planck18 as cosmo #
z = 1.5 # redshift
dl = cosmo.luminosity_distance(z)
da = cosmo.angular_diameter_distance(z)
age = cosmo.age(z)
print(f"Luminosity distance: {dl:.2f}")
# Output -> Luminosity distance: 11192.99 Mpc
print(f"Angular diameter distance: {da:.2f}")
# Output -> Angular diameter distance: 1790.88 Mpc
print(f"Age of Universe at z={z}: {age:.2f}")
# Output -> Age of Universe at z=1.5: 4.27 Gyr
```

Session 10: Using Git

```
git clone https://github.com/user/repo.git
cd repo
git checkout -b new-feature
git add analysis.py
git commit -m "Add analysis script"
git push origin new-feature
git checkout master
git merge new-feature
```

What is Git?

- Git is a version control system used to track changes in code and collaborate with others
- It allows you to save and back up versions of your project, undo mistakes and restore earlier versions, collaborate with others without overwriting each other's work
- Largest platforms used are GitHub and GitLab
- To take part in the exercise for this session you will need to make a <u>GitHub</u> account (free)

Setting up Git

- Git should be pre-installed on most machines, you can check this with git --version and install if needed
- Once you have an account and git is installed you can set up your identity (this only needs done once)

```
git config --global user.name "Your Name"
git config --global user.email "you@example.com"
```

Authenticating Git

 Authentication is set up through adding an SSH key. On your machine, navigate to ~/.ssh/ and create an ssh key

```
cd ~/.ssh
ssh-keygen
```

- After working thorugh the options (name of key, password you can leave password blank) you can copy the contents the .pub version to GitHub → Settings → SSH Keys
- Never share the contents of your private ssh key (without the .pub)

Starting a Git project

1. Start locally from scratch

• In an existing folder run

git init

- This creates a local git repo for tracking files. For local use only, you're done.
- To connect to GitHub, first create a repo on GitHub, then link it:

git remote add origin https://github.com/yourusername/your-repo.git

Starting a Git project

2. Start on GitHub from scratch

• You can also create an empty new repository on Github which you can then *clone* (copy) to your local computer (GitHub will give you the link to paste), e.g.

git clone https://github.com/yourname/my-project.git

• This will create a folder called my-project, so make sure you call this where you want the project folder to be, then you can start working in it

Cloning a Git project

- If working with collaborators, or wanting to use some custom code public on GitHub, you will need to clone their repository
- This is identical to before, there should be the clone link on the repository GitHub page i.e.

git clone git@github.com:NatalieW96/Python-Bootcamp.git

 You can edit this repository locally, and if you have permissions commit and push changes - without permissions you can fork the repository (see bonus exercise)

Adding and commiting

• Just because files are in a repository locally does not mean they are on the git - they need manually added or *staged* to the *staging area*

git add filename

 Once you have added all the files you would like to track, we commit the changes - this stores a current snapshot of your code locally on your machine

Pushing

• If we want to back up our changes to store on GitHub, for future use or for others to use we can now push the commit to the GitHub remote. On your first push to a branch use command

```
git push -u origin master
```

• This is setting your repo to the default master branch. After this when pushing in the future you can simply use

git push

Pulling

• To update our local repository with changes from GitHub, use

git pull

 Always git pull before making new changes or pushing changes to avoid conflicts

Checking Status

 To view staged (ready to commit), unstaged (modified), and untracked (new) files

```
git status
```

To see what is unstaged

```
git diff
```

To see what is staged but not committed

```
git diff --staged
```

Undoing changes

 You can undo unstaged changes to a file (revert to the last commit) with

```
git restore filename
```

You can unstage a file, but keep the changes locally with

```
git reset filename
```

• Undo the last commit, keep changes (--hard removes changes)

```
git reset --soft HEAD~1
```

Reverting to a past commit

Previous commits can be viewed with

git log

To temporarily view old code in a past state

git checkout <commit-hash>

Going back to the current code is then

git checkout master

Reverting to a past commit

• If you want to undo changes without erasing history

```
git revert <commit-hash>
```

- This creates a new commit, undoing the commit
- To fully rewind to a previous commit, deleting all changes since

```
git reset --hard <commit-hash>
git push --force
```

This deletes changes for all collaborators - use with caution!

Deleting files from git

To delete a file both locally and from git/GitHub

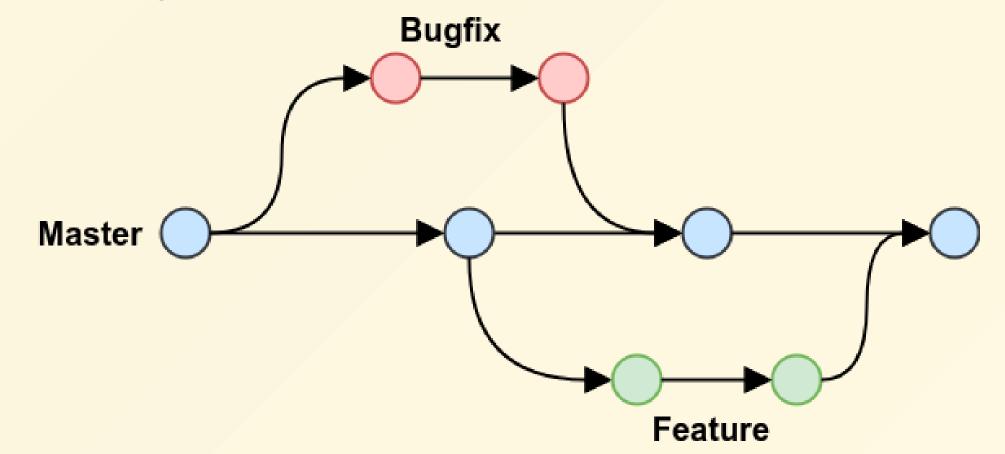
```
git rm filename
git commit -m "Remove filename"
git push
```

• To delete a file from git/GitHub but keep it locally

```
git rm --cached filename
```

Branches

 Branches allow you to work on new features/experiment without affecting the master code



Branches

View all branches with

git branch

Create a new branch and switch to it with

git branch new-feature
git checkout new-feature

When you want to merge the branch back into the master code

```
git checkout master
git merge new-feature
```