Introduction to Python

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1 Pre-session preparation

1.1 Installing Python

Complete the instructions in this first section before attending the first session.

We assume you are either using a Windows or Mac PC. If you are running Linux then you can probably work it out for yourself! A basic understanding of the terminal (mac) or command prompt (windows) is assumed. If not then Google a tutorial. We assume that you have not previously installed a Python 3 distribution to your system.

Download the Anaconda Python 3.6 distribution from `https://www.anaconda.com/download/`. This includes the Python language as well as useful libraries and tools. Install following the instructions and accepting default values.

Open a terminal window (mac) or command prompt (Windows). Navigate (using the "cd" command to navigate the file system) to an empty directory (I suggest somewhere in My Documents) where you want to store files generated in these lectures. Type:

```
jupyter notebook
```

After a few moments this should open a window in your internet browser. In the top right hand corner click "new" and under notebooks select Python 3. This should open a Jupyter (formerly known as Ipython) notebook. This is an interactive Python session where your code is input into "cells" on the page. Once you have written some code in a cell, press the "Shift" and "Return" keys simultaneously to execute the code in the cell.

To test your distribution has installed correctly type the following into a cell and execute it:

```
1 import numpy as np
2 print("Hello World")
```

```
> Hello World
```

In this tutorial, the numbered code on the light grey background is code that you should execute. Bold text is the expected output from that code. Text in `typewriter font` refers to a Python function. You should attempt all basic tasks in the text. If you find the tasks too simple or have previous experience try the optional advanced tasks for a greater challenge.

Ensure that this works correctly before attending the first session. If in doubt, collaborate with one of your colleagues also taking this course to get it working.

2 Basic Python structures

2.1 Basic Maths

You can just start typing maths into Python and it will do it.

```
1 1+2
```

```
> 3
```

Division in Python 3 gives a decimal answer as you would expect.

```
1 5/2
```

```
> 2.5
```

Beware the division operator in Python 2 (you should all be using Python 3!). The above would give an integer division and so return an answer of 2.

The symbol for power is a double star. A square root can be achieved by raising to the power of 1/2.

```
1 2**3
```

```
> 8
```

2.2 Variables

We can store values in variables. You can think of these as "buckets" which hold values. You can call variables anything you like as long as it starts with a letter and uses only alphanumeric characters or underscore. In addition it

is a very bad idea to use variable names that are reserved keywords elsewhere in Python such as `print`, `sum` or `list`. The `print` function prints things to the screen.

```
a = 6 + 3
print(a)
dead_parrot = "This parrot is no more! He has ceased to be!"
print(dead_parrot)
```

```
> 9
> This parrot is no more! He has ceased to be!
```

Variables have types. The main types you need to worry about are integers, floats (short for floating point numbers) and strings. Integers are whole numbers, floats are decimals and strings are text. Operations between floats and integers are permitted and the answer will be expressed as a float.

```
spam = 7
eggs = 0.5
food = spam+eggs
print(food)
```

```
> 7.5
```

Operations between strings and number types are generally not permitted since they make no sense.

```
song = "I'm a lumberjack and I'm OK" + 1
```

```
> TypeError                                 Traceback (most recent call last)
<ipython-input-47-84d795fdab55> in <module>()
----> 1 "I'm a lumberjack and I'm OK" + 1

TypeError: cannot concatenate 'str' and 'int' objects
```

Strings can be concatenated though using the plus symbol.

```
line_one = "I'm a lumberjack and I'm OK, "
line_two = "I work all night and I work all day"
song = line_one + line_two
print(song)
```

```
> "I'm a lumberjack and I'm OK, I work all night and I work all day"
```

2.3 Lists

Lists are a simple data structure that allow the storage of multiple values. Lists are designated by square brackets. Lists are just another type of variable, so as before you can name them anything you like as long as you follow the above variable naming rules.

```
numberlist = [1, 2, 5]
print(numberlist)
```

```
> [1, 2, 5]
```

You can fetch a single value from a list by subscripting the list with square brackets. You can fetch multiple values by asking for a range.

```
numberlist = [1, 2, 3, 4, 5, 6, 7]
print(numberlist[4])
print(numberlist[0:3])
```

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

Notice how the first command returns 5. This is because Python lists (and many things in programming) start counting at zero. This means asking for the zeroth element would return 1. The second command returns only three values. This is because the lower bound is inclusive but the upper bound is exclusive (for mostly the same reasons that things start counting at zero not one). The append command will add things onto the end of a list.

```
numberlist = [1, 2, 5]
numberlist.append(8)
print(numberlist)
```

```
> [1, 2, 5, 8]
```

The `range` function generates lists that are integer sequences between two specified numbers.

```
my_list = range(3, 6)
print(my_list)
```

```
> [3, 4, 5]
```

Note how the bounds of the `range` function work. As for list subscripting, the first value (3) is printed but not the last value (7).

2.4 User input

Somtimes it is useful to accept some user input while the program is running and operate on this input. This can be achieved with the input command.

```
person_name = input("What is your name?")
print("Hello " + person_name)
```

```
> Hello Arthur Pewty
```

Note that the input function always interprets the user's input as text. This means that if the input needs to be interpreted as a number then it should be converted explicitly to an integer or float using `int` or `float`

```
user_input_number = float(input("Enter a number of years: "))
print("Two more than your number is: ", user_input_number+2)
```

```
> Two more than your number is: 42.0
```

2.5 Flow control

2.5.1 If statements

Programs can only carry out very simple tasks if they do the same thing every time. If programs are able to make decisions based on values then this can make them much more powerful. The `if`' statement is the most simple of these flow control tools.

```
penguins = 4

if penguins < 10:
  print(penguins, " is less than 10.")
else:
  print(penguins, " is not less than 10.")
print("This is printed regardless of the value of penguins.")
```

```
> 4 is less than 10.
> This is printed regardless of the value of penguins.
```

Note how the program flow is controlled by the indentation. The `if` statement is evaluated and if True then the indented code is run and the else section is skipped. If the `if` statement is evaluated and is False, the indented code is skipped and the code beneath the else statement is run. After the `if` statement is fully evaluated the program flow returns to the next unindented statement. In this case the last sentence is always printed since it

is outside of the `if` statement. Also the if statement is finished by a colon. This indicates where the question finishes.

If you recall the discussion of types in section 2.2, you will notice that that the `print` function seems happy to combine a numeric and string type. This is because `print` is a special function which converts arguments to strings before printing them. It will only do this if the arguments are separated by a comma as above.

More complex questions can be asked by asking multiple times using the `elif` statement. The `elif` statement only executes if the previous statements have been False

```
1  num_penguins = 17
2
3  if num_penguins < 10:
4    print("You have too few penguins.")
5  elif num_penguins > 10:
6    print("That is quite a lot of penguins")
7  elif num_penguins == 10:
8    print("Just the right number of penguins")
9  else:
10   print("This statement should never be printed")
```

```
> That is quite a lot of penguins
```

As with the `if` statement, syntactically the `elif` and `elise` statements are finished with a colon (as are all flow control statments).

It is important to understand the distinction between comparions and assignment. Notice how on line 1 the assignment operator is one equals sign while on line 7 the comparison operator is two equals signs. The assignment assigns a value to a variable while the comparison operator is asking whether two values are equal.

Task 1. What happens if you change num_penguins?

Task 2. Write a program that takes two numbers from user input, stores them in two variables and then checks whether the numbers are equal. You should display a relvent message depending on whether or not they are equal.

Task 3. Write a program that asks for the users name, compliments them if it begins with the letter "P", insults them if the name is "Peter" and otherwise repeats the name back again.

Optional Advanced Task 1. Think about sanitising the user input

so that no possible user input can cause an error. Think about users inputting non-alphabetic characters and the case of the characters (PETER should be accepted).

2.5.2 For loops

For loops are a flow control tool that can be used to repeat a command multiple times by iterating over the members of a sequence.

```
list_of_numbers = []
for loop_number in [0, 1, 2, 3, 4]:
  list_of_numbers.append(7)
print(list_of_numbers)
```

```
> [7, 7, 7, 7, 7]
```

Task 4. What would happen if the `print` line was also indented?

Each time the for loop is evaluated the next value in the sequence is stored in the "loop_number" variable. This allows you to count

```
for loop_number in [3, 4, 5, 6]:
  print(loop_number)
```

```
> 3
> 4
> 5
> 6
```

Remember that the `range` function can be used to generate lists. This means that instead of

```
for loop_number in [3, 4, 5, 6]:
```

it is easier to use,

```
for loop_number in range(3, 7):
```

Task 5. Write a program that asks the user for a number n and prints the sum of the numbers 1 to n.

Task 6. Modify the previous program so it only sums odd numbers from 1 to n.

2.5.3 While loops

Sometimes it is useful to have a conditional loop. A while loop, repeats a process untill a condition is met.

```
secret_number = 4
user_number = 0

while secret_number != user_number:
  user_number = int(input("Guess my number by entering an integer
    between 1 and 10: "
  print("No, that's not it, guess again.")
print("Yes, that's it.")
```

```
 > Guess my number by entering an integer between 1 and 10:
>> 7
> No, that's not it, guess again.
> Guess my number by entering an integer between 1 and 10:
>> 4
> Yes, that's it.
```

The comparison operator != checks whether something is not equal. While the two values are not equal the loop will repeat. As soon as they are equal, the loop will exit and the next command will be printed.

Optional Advanced Task 2. How many integer prime numbers are there under 10,000? Hint: `https://en.wikipedia.org/wiki/Generating_primes`

2.6 Imports

Sometimes we want functions from another package that are not included in the basic Python set of functions. We can import these packages. Here we import the function `random` from the package `random` and then use it.

```
from random import random

print ("Your random number is: ", random())
```

```
> 0.29497908252
```

Packages only need to be imported once per session. This means that imports are usually done at the top of the Python script as the first thing that is done.

The random function prints a random decimal number between 0 and 1.

Task 7. Write a for loop that will print out a random number between 0 and 5, 5 times.

Task 8. Write a for loop that will print out a random integer number between 4 and 10 (including 4 and 10).

Task 9. Program a game of higher or lower. Generate a random integer between 1 and 100. Allow the user to inout a guess and tell them if the guess is too high or too low until they guess correctly.

2.7 Subroutines

Python has many built in functions like `input`, and `random`. You can tell they are functions as they take arguments (the bit in brackets after the function name). We can define our own functions called subroutines. When programs begin to get larger it can be convenient to split the program up into smaller subsections as this makes the logic of the program easier to follow and makes the code easier to maintain. A subroutine is a collection of code that is united under one title that can be "called" from elsewhere.

```
1 def hungarian_phrasebook():
2   print("My hovercraft is full of eels.")
3
4 for i in range(0, 2):
5   hungarian_phrasebook()
```

```
> My hovercraft is full of eels
> My hovercraft is full of eels
```

In this example lines 1 and 2 define the function. The code in the function does not run until it is called in line 4. When the program runs it first saves the function `hungarian_phrasebook` to memory and then begins executing the rest of the code on line 3.

While this does break up the code somewhat, the function is not very useful since it does exactly the same thing each time it is called. It would be much more useful if it could do different things depending on how we called it. This can be achieved by passing a value to the function called an argument.

```
1 def adding_six(input_value):
2   print(input_value + 6)
3
4 adding_six(3)
5 adding_six(14)
```

```
> 9
> 20
```

Here on line 1 we define the function `adding_six` to have the argument `input_value`, whenever this function is called it must be given an argument.

It is a common convention to use a function called main as the entry point of the code. This means that the code is run starting in main and then splits off into other subroutines. Note that you must remember to call main as seen in line 8. If you dont call main then Python will add all of the subroutines to its memory and then not run them and exit!

```
1 def adding_six(input_value):
2   print(input_value + 6)
3
4 def main():
5   for i in range(0, 2):
6     adding_six(i)
7
8 main()
```

```
> 6
> 7
```

You can stack as many subroutines as you like, subroutines can call other subroutines and so on. Be careful about how readable your code is though, if you have layers upon layers of subroutines it can be very complex to understand the program flow and there is probably a better way to structure the code.

Subroutines don't just have to print values. They can do some processing and then return the value to the main loop using the `return` function.

```
1 def adding_six(input_value):
2   return input_value + 6
3
4 def main():
5   number_list = [1, 2, 3, 4]
6
7   for i in range(0, len(number_list)):
8     number_list[i] = adding_six(number_list[i])
9   print(number_list)
10
11 main()
```

```
> [7, 8, 9, 10]
```

We pass each value of "number_list" into the subroutine `adding_six` which adds six and then returns the value to be put back into "number_list", replacing the original value.

Note the use of the `len` function inside `range`. `len` returns the number of elements in a list, in this case in combination with `range` it is an easy way to iterate through the whole list. There is an easier way though, as we saw earlier, Python treats lists as iterables which means that a for loop can refer to them directly,

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

for i in number_list:
  number_list[i] = number_list[i] * 2
print(numberlist)
```

```
> [2, 4, 6, 8]
```

With larger programs it can be convenient to split subroutines up into entirely different files. For example, if we have some simulation code to run a Monte Carlo simulation it would be sensible to split any analysis code off into a separate file. If we have a file called *main.py* and another file called *analysis.py* (in the same directory) containing the subroutine *do_analysis* then main.py might look like:

```
from analysis import do_analysis

def get_random_number()
  # Chosen by fair dice roll, guaranteed to be random
  return 4

def main()
  for counter in range(0, 100):
    test_number = get_random_number()
    do_analysis(test_number)

main()
```

By importing the file *analysis* in the first line, we can call any functions it contains as if they were in the same file.

While this may seem a little complex at first, it is vital to keep code organised as it grows. This will save a lot of time later down the line. Note the comment in one of the functions. By proceeding a line with a hash (#) we can insert text comments that are ignored by the Python processor. This aids in understanding the function of a particular piece of code. Commenting code is another important coding habit.

Task 10. Do the excercise in section 7.1.

Optional Advanced Task 3. Download a list of names from `https://angrypenguin.000webhostapp.com/sample_data3.txt`. Sort these names into alphabetical order. Give each name a value by summing the letter values in the name where A = 1, B = 2... Z = 26. Multiply the name value by the position of the name in the list to get a score for each name. What is the total sum of all of the name scores?

3 NumPy

3.1 NumPy arrays and vectorisation

Computers are fast but not infinitely fast. This means that while trivial calculations can be done using any method, more complex calculations such as simulations of hundreds or thousands of particles often need more care. Python is beautiful and easy to use but it is not the fastest programming language. This means that to do larger calculations we must take some consideration of the efficiency of the programming constructs that we use.

A very simple way to add 1 to each value in a list would be to step through the list and add 1 to each value.

```
from time import time

start_time = time()
long_list = range(0, 10000000)

for i in range(0, 10000000):
  long_list[i] = long_list[i] + 1
end_time = time()

print(end_time-start_time)
```

```
> 2.05770301819
```

Note the use of the time function in this example. This is a very simple way to assess the speed of code using the system clock. It is not the canonical way to measure performance but like many things in this short tutorial, it is simple and effective if not the best way to do it. If we think about it then that is fairly impressive, it has been through that loop 10,000,000 times in 2 seconds. But can we make it faster? One key concept in writing speedy

code is vectorisation, instead of a loop we want to apply the transformation to every element in the list simultaneously. Lets try that:

```
short_list = range(0, 5)
print(short_list)
short_list = short_list + 1
print(short_list)
```

```
> [0, 1, 2, 3, 4]
---------------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)
<ipython-input-9-5d83b7f97176> in <module>()
      3 print short_list
      4
----> 5 short_list = short_list + 1

TypeError: can only concatenate list (not "int") to list
```

Basic Python doesn't understand vectorisation. Instead of adding one to each element in the list it is trying to add the number 1 onto the end of the list. This is where NumPy (short for numerical Python) comes in. It is a library that adds data structures and functions suited to mathematical operations. A NumPy array looks like a list but has some subtle differences.

```
import numpy as np
short_list = [0, 1, 2, 3, 4, 5]
print(short_list)
short_np_array = np.array(short_list)
print(short_np_array)
short_np_array = short_np_array + 1
print(short_np_array)
```

```
> [0, 1, 2, 3, 4, 5]
> [0 1 2 3 4]
> [1 2 3 4 5]
```

The NumPy function `array` generates a NumPy array. It can take a few diffferent types of input but in this case we passed it a regular Python list. This is a type of object like a Python list which holds a series of values. The only difference we see in the output that is printed is that while Python lists have commas seperating the values, a NumPy array doesn't. One of the big differences between lists and NumPy arrays underneath is that arrays allow vector operations. This means mathematical operations can be applied to the whole array simultaneously and quickly.

```
from time import time
```

```
import numpy as np

start_time = time()
long_np_array = np.arange(0, 10000000)

long_np_array = long_np_array + 1
end_time = time()

print(end_time-start_time)
```

```
> 0.0694818496704
```

Using NumPy arrays instead of lists provides an impressive speedup of nearly 30 times for this simple operation. There are many other useful functions in NumPy and a lot of them make use of the NumPy array as a basic data structure.

Task 11. Generate a large Python list of data and using a loop take the sqaure root of each element in the list. How does looping through a NumPy array compare speedwise? Finally use the np.sqrt function (Google for how to use it) to vectorise the operation. How much faster is this?

4 Reading and writing text files

4.1 Reading from files

The basic way to read in a text file is with the open function. This opens an iterable file object which can be iterated with a for loop to extract each line. For a simple data file with a single column of numbers, one approach might be

```
input_file = open("example_data_file.txt", 'r')
for line in input_file:
  data_list = data_list.append(float(line))
input_file.close()
```

There are a couple of interesting points here. Firstly, we open the file with the argument `'r'`. This means read mode, we can read data from the file but not write to it. Next, data is always read in as a string whether it is characters or digits. This means that to do mathematical operations on numerical data it must implicitly be converted to a float or int type. Be careful though, this is a forceful way of doing things and if the program tries

to convert a string into an integer then it will crash. This means that this method is only suitable for input files that we are sure are solely numeric. The next point is that we close the file object when we are finished reading from it. This is important as Python is connected to the file when the file object is open. If you don't disconnect then the file link may stay open in the background after Python finishes which may cause problems accessing the file later. Just like a fridge, you need to open the door before taking things in or out but must remember to close the door afterwards.

Task 12. Download a sample data file from: `https://angrypenguin.000webhostapp.com/sample_data1.txt`. Read the data in to Python and print the numbers to screen.

4.2 Writing to files

Writing to files is similar to reading from files but this time we have to open the file in write mode

```
my_calculated_data = [4, 5, 6, 7]
output_file = open("example_data_file.txt", 'w')
for number in my_calculated_data:
  output_file.write(str(my_calculated_data[number]) + "\n")
output_file.close()
```

Here the 'w' in the open file is opening `output_file` in write mode. This means that if the file does not exist on disk it will be created and if it already exists the file will be overwritten. If you want to write to a file that already exists then you need to open in write append mode, `'wa'`. Note again that file operations are done with strings so numbers have to be excplicitly converted before wiring to the file. But what is the ‘‘
`n"` at the end? This is the special character for a new line. This ensures that each of our numbers will be printed to a new line.

Reading and writing to files directly like this is good if the file you want to read or write has a very specific or complex format. These methods can also write combinations of numbers and strings which can be useful. However, most of the time our data analysis will just be done on grids of numbers. For this there is an easier way in NumPy.

Task 13. Read in the dataset from the last task, multiply each number by two and save it to a new text file.

4.3 NumPy loadtxt

Most likely whatever experiment or simulation we have done will have already written data to a file that can be read. Most simulations and some experimental equipment will allow you to output your data as a plain text file. There are many functions from different libraries that allow file reading but for simple text files of numbers `numpy.loadtxt` works well.

```
x_data, y_data = np.loadtxt("example_input_data.txt", skiprows=1,
    unpack=True)
plt.plot(x_data, y_data)
plt.show()
```

Task 14. Download a sample data file from `https://angrypenguin.000webhostapp.com/sample_data2.txt`. Read in this data using loadtxt and print it to the screen.

`numpy.loadtxt` is a fairly basic way of reading in data files. It will only read in square grids of data and will struggle if there are data points missing. Notice how we use the skipline command to skip the tiltle line in the file. Try without the skipline parameter and see what happens. The unpack parameter is also important, this reads the first column into the first variable and the second column into the second variable we specified. Without the unpack parameter the data would be read into the first vairbale in as 2 column array.

Since `loadtxt` reads the data into a NumPy array it also accepts only numbers as input. If you need to read in a mixture of text and numbers this is probably better done with a Python list and a basic file read loop. If you have numerical data with a more complex layout such as missing values then `numpy.genfromtxt` is a more complex but flexible file reading function.

4.4 NumPy savetxt

In the same way as before, if you just havbe a simple numpy array of data, you can quickly save to a text file with NumPy savetxt,

```
my_clever_data = np.array([[2, 3], [4, 5], [6, 7]])

np.savetxt("output.txt", my_clever_data)
```

`numpy.loadtxt` is a fairly basic way of reading in data files. It will only read in square grids of data and will struggle if there are data points missing. Notice how we use the skipline command to skip the tiltle line in the file. Try

without the skipline parameter and see what happens. The unpack parameter is also important, this reads the first column into the first variable and the second column into the second variable we specified. Without the unpack parameter the data would be read into the first vairbale in as 2 column array.

Since `loadtxt` reads the data into a NumPy array it also accepts only numbers as input. If you need to read in a mixture of text and numbers this is probably better done with a Python list and a basic file read loop. If you have numerical data with a more complex layout such as missing values then `numpy.genfromtxt` is a more complex but flexible file reading function.

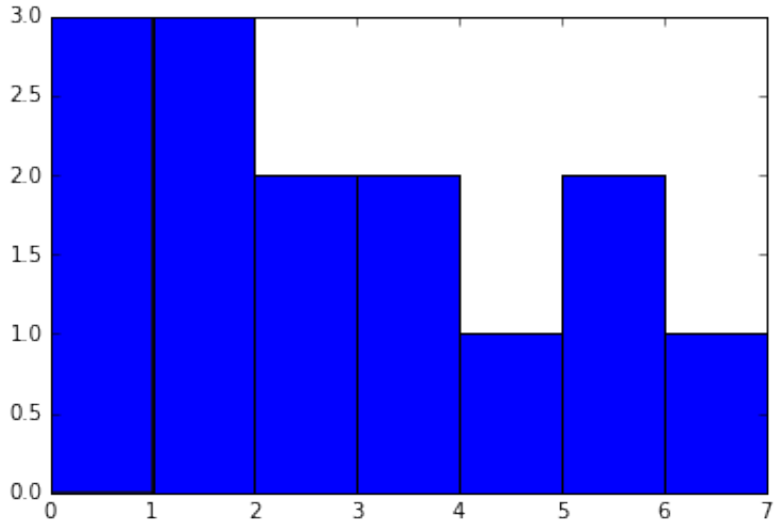
Task 15. Using the input from the previous exercise, read in the data using loadtxt, multiply by 4 and print to a file using numysavetxt. Check the savetxt documentation for how to save a title line before the data.

5 Matplotlib

5.1 Histograms

There is a very powerful package called matplotlib that provides functions for plotting graphs. Matplotlib is used across academia for producing publication quality figures. At first it might seem like a lot of effort to learn an entirely new script based method for plotting compared to sommething like Excel but it is worth it. Matplotlib graphs look much better than Excel ones, they are much more customisable and more powerful. In addition, once you have a nice set of temlates set up you can use them all through your academic career, slightly modifying them to suit whatever data you have.

```
1 import matplotlib.pyplot as plt
2 %matplotlib inline
3
4 listofnumbers=[0.2, 0.3, 0.4, 1.2, 1.7, 1.9, 2.2, 2.5, 3.1, 3.4,
      4.6, 5.1, 5.6, 6.0, 7.4, 7.4, 7.6]
5 plt.hist(listofnumbers, bins=[0, 1, 2, 3, 4, 5, 6, 7])
6 plt.show()
```



First we import the matplotlib library, then the command `%matplotlib inline` tells Jupyter Notebook to plot the graphs in the workbook rather than opening them in another window. Again you only need this command once per session so it is common to put it at the top with the import commands. Then we generate a list of numbers and plot them as a histogram.

Task 16. What does the bins argument do? What happens if you leave it out entirely?

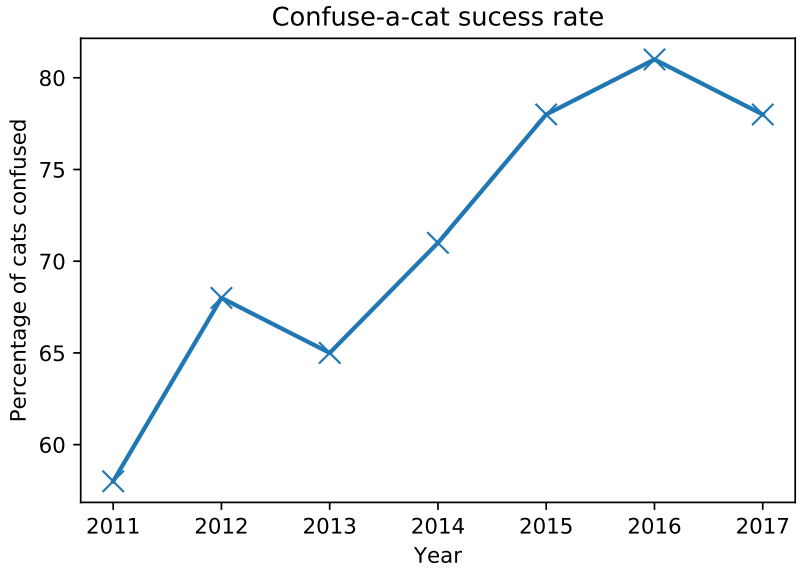
Task 17. Generate 1000 random numbers between 0 and 10 using a for loop and append them to a list. Plot a histogram of this list.

Task 18. Complete excercsie 7.2.

5.2 Line Plots

Line plots are very similar to histograms,z

```
x_data=[2011, 2012, 2013, 2014, 2015, 2016, 2017]
y_data=[58, 68, 65, 71, 78, 81, 78 ]
plt.plot(x_data, y_data, linestyle = "-", marker = "x",
    markersize=10, linewidth=2)
plt.title("Confuse-a-cat sucess rate")
plt.xlabel("Year")
plt.ylabel("Percentage of cats confused")
plt.savefig("confuseacat.pdf")
plt.show()
```



You can read the full specification for the plot function online: `https://matplotlib.org/api/pyplot_api.html#matplotlib.pyplot.plot`. This gives detials about the marker and line types and other things linke how to change the line and marker colours.

Task 19. Adjust the axis range of the graph so it shows the percentage axis from 0 to 100. Google something like "matplotlib axis range example" to find the correct syntax.

Googling things is a very important skill that needs practice. There is always more than one way to do a simple task like this so have a look at a few different ones and see what works best. Beware that some of the examples you will find are hard to understand, inefficent or just wrong! You need to distinguish betweeen these and pick out the right commands for your task.

6 Fitting Data

Fitting data is easy in something like Origin but this is a poor approach if you have to fit 100 datasets.

7 Exercises

7.1 Lennard-Jones potential

The Lennard-Jones potential is a model potential to describe the pair interaction between two atoms as a function of their separation,

$$u_{LJ}(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right] \tag{1}$$

where r is the interparticle separation, ϵ is the well depth and σ is the separation where the interaction strength zero. For atomic Argon, $\epsilon = 3.4 * ^{-10}$ m and $\sigma = 1.65 * 10^{-21}$J.

Write a function which returns the interaction energy of two argon atoms as a function of their separation.

7.2 Calculation of pi

Some processes can be modelled using random numbers. One of the simplest examples of this is finding the value of pi. Pi is the ratio of a circle's radius to its circumference. Equivalently we can say that Pi is the ratio of the area of an inscribed circle of a square to the area of the square. This is illustrared in Fig. 1.

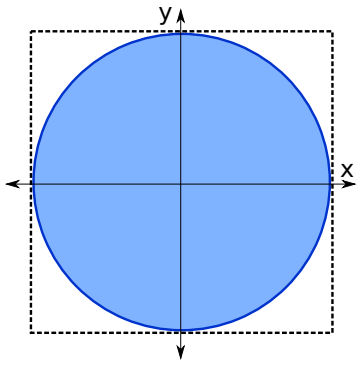


Figure 1: The blue circle is inscribed in the black dashed square.

If we pick a series of random points inside the square then some will fall inside the circle and some will fall outside. The ratio of these two quantities

will tell us the relative areas of the two shapes. From this it follows that we can calculate pi using this method.

How can we tell if a random point is inside the circle or not? Pythagorus' theorem tells us the hypotenuse of a right angled triangle. For a circle radius 1 we know that a point is inside the circle if:

$$\sqrt{a^2 + b^2} < -1, \tag{2}$$

where a and b are the side lengths of the triangle. Since the circle is symmetric, we don't need the whole thing, just a quarter will do. This makes the generation of random numbers easier since we can generate numbers between 0 and 1 to put random coordinates inside a box of side length 1. This scheme is shown in Fig. 2

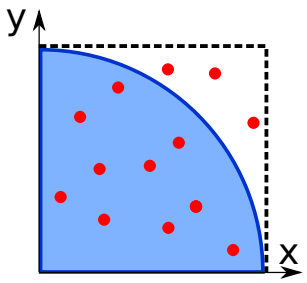


Figure 2: If we pick random points on the figure some will fall outside the circle and some inside. The ratio of the two allows us to find pi.

Using all of the above techniques, calculate pi using random numbers. Try using 100, 1000, 10,000 or more random samples, how does this affect the error? If you calculate pi 1000 times and plot a histogram of these values, what sort of distribution would you expect the values to follow and why? What is the nature of the relationship between number of samples and distribution width? If you find this task too hard, there are some hints in Appendix A. Try not to look at them unless you are really stuck. Learning (of programming in particular) works much better if you got through the process of problem solving rather than just reading the answer. The hints in Appendix A are graded in terms of difficulty. The first hint gives you a little help and the subsequent hints more help.

A Stochastic determination of pi hints

A.1 Hint 1

Try writing out an algorithm in pseudocode. This means writing out a series of logical steps in simple words first without worrying about the exact programming syntax. For a simple loop this might look something like:

```
import needed_libraries

total = 0

for loop from 1 to 10
  add loop value to my total
print the total to the screen
```

Once you have got the basic program flow sorted, you can then convert your pseudocode to valid Python.

A.2 Hint 2

This is a basic pseudocode example of the algorithm.

```
import needed_libraries

num_inside=0
num_interations = 1000
x_coord = 0
y_coord = 0

for loop from 0 to numiterations
  set x_coord using random number
  set y_coord using random number
  check distance of random coord from center
  if distance <= 1 then
    increment num_inside by 1

my_pi = 4* ratio of inside to outside
print my_pi
```