

Learn how to programme (in Python)

Marion Weinzierl

Advanced Research Computing

[@arc_du](#)

July 7, 2020

Outline

Introduction

Basics

Getting Data in and out

Repetitions and Conditions

Functions

Materials used and recommended

- ▶ Python Wiki - Python for Non-Programmers
- ▶ How to think like a Computer Scientist
- ▶ A Whirlwind Tour of Python
- ▶ Software Carpentry - Programming with Python

Introduction

Course Objectives

By the end of this course you should know

- ▶ how a basic computer program is written and executed,
- ▶ what basic data types and control statements are,
- ▶ how to get and process user input and data,
- ▶ how to structure your code using functions,
- ▶ what can lead to your program not working, and what to do about it,
- ▶ where to find further resources to practice your Python programming.

Programming and Programming Languages

Why do we want to program?

Programming and Programming Languages

Programming means: make the computer do the work for you!

Programming and Programming Languages

Programming means: make the computer do the work for you!

- ▶ Do the maths
- ▶ Boring repetitions
- ▶ Too complicated/extensive tasks
- ▶ Big data sets
- ▶ ...

Programming and Programming Languages

Steps:

- ▶ Write your code in high-level programming language.
- ▶ Translate into low-level (machine/assembly) language.
- ▶ Execute program.

Programming and ~~Programming~~ Scripting Languages

Steps:

- ▶ Write your code in high-level programming language.
- ▶ Interpret code and execute directly

Programming and ~~Programming~~ Scripting Languages

Steps:

- ▶ Write your code in high-level programming language.
- ▶ Interpret code and execute directly

Beware: Oversimplification!

How do you start?

We go the easy way (so you can build it up from there):

- ▶ Choose Python.
- ▶ Skip the installation bit: [Jupyter Notebooks](#).
- ▶ HOWEVER: You have to type yourselves! Don't copy-paste (yet)!¹
- ▶ Have a play.

¹If you try to copy-paste from these slides, you will sometimes get a syntax error because of the characters used in the PDF.

Hello World!

Hello World! (in C++)

helloworld.cpp:

```
#include <iostream>

using namespace std;

int main() {
    cout << "Hello World!\n";
    return 0;
}
```

compile:

```
g++ -o helloworld helloworld.cpp
```

execute:

```
./helloworld
```

Hello World! (in Python)

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

Hello World!

```
name = "Marion"
```

```
print("Hello " + name + " !")
```


Hello World!

```
name = "Marion"
```

```
print("Hello " + name + " !")
```

```
mySum = 2+3
```

```
print("I can add: 2+3 = ", mySum)
```

Basics

Basic Data Types

- ▶ Strings: "Heinz", 'Banana', 'He said "Hello"'
- ▶ Integers: 1, 2, 3, 22222222, -777
- ▶ Floats: -1.2, 0.0, 2.7182
- ▶ Booleans: True, False

Basics: Variables

- ▶ “I reserve a space in memory for my data bit, and I call it by the name x ”
- ▶ Syntax: *name* = *value*

Examples

```
print( 'He said "Hello" ')
```

```
myString = 'He said "Hello" '
```

```
print( myString )
```

```
type( myString )
```

Examples

```
print(2+5)
```

```
print("2+5 = " + 2 + 5)
```

```
print("2+5 = " + str(2 + 5))
```

```
print("2+5 = ", 2 + 5)
```

Examples

```
type(true)
```

```
type(True)
```

```
1+True
```

```
type(1+True)
```

```
bool(True+False)
```

```
bool(True and False)
```

```
bool(True or False)
```

```
not(False)
```

Basic Operations

- ▶ String: concatenation with `+`
- ▶ Bool: `and`, `or`, `not`
- ▶ Numerical data: `+`, `-`, `*`, `/`, `%`, `**`, `abs`, ...
- ▶ Order of execution:
 1. `()`
 2. `**`
 3. `*`, `/`
 4. `+`, `-`
 5. Left-to-right (except exponentiation!)

⇒ Use parenthesis to make sure!

Basics: Comments (and Documentation)

```
# This is my programme to demonstrate how to  
# do simple calculations in Python.
```

```
myNumber = 2
```

```
myOtherNumber = myNumber+5
```

```
myNumber = myOtherNumber/2 # I have to divide  
# by 2 here, as the  
# results are  
# otherwise rubbish
```

```
print(myNumber)
```

Debugging and Types of Errors

- ▶ Errors in computer programs are called “bugs” for historic reasons.
- ▶ For complex projects, you will usually spend more time testing and debugging than writing code.
- ▶ Three types of errors:
 - Syntax errors - written the code wrongly
 - Semantic errors - written the wrong code
 - Runtime errors - something's wrong with the code (during execution)

Have a play!

You could try

- ▶ what happens if you add a float and an integer,
- ▶ what happens if you mix numbers and bools in arithmetic expressions,
- ▶ how setting parenthesis changes the result of a large arithmetic expression,
- ▶ to print statements that include variables of different data types,
- ▶ try to reproduce each of the error types,
- ▶ ...

Getting Data in and out

User Input

```
# Get some user input

x = input()

print(x)

type(x)    # This will be a string
           # if you don't convert it

# Get the user's name

name = input("What's your name?")

print("Hello " + name)
```

Reading and writing files

```
# Create a file object  
myFile = open("testfile.txt", "w")
```

Two things to note here:

- ▶ My object "myFile" is different from my file "testfile"!
- ▶ There are different modes:
 - read: r
 - (over-)write: w
 - append: a
 - read+write: w+ or r+

Reading and writing files

```
# Create a file object
myFile = open("testfile.txt", "w")

# Write – note special characters!
myFile.write("This is some text. \n \
And some more.")
myFile.write("\n\nI can also add numbers \
like this: %d %d \n" %(22, 333))

myFile.write(str(222))

# Don't forget to close the file
myFile.close();
```

see also [f-strings](#)

Reading and writing files

```
# Create a file object (this time for reading)  
myFile = open("testfile.txt", "r")  
  
# Read it and print it to screen  
print(myFile.read())  
  
# Try this:  
print(myFile.read(7))  
print(myFile.readline())  
print(myFile.readlines())  
  
# Don't forget to close the file  
myFile.close();
```


What do we have here?

```
myList = [1, 2, 3, 4, 5] # A list!  
  
print(myList)  
  
print(myList[3]) # Note: [] not ()  
  
print(myList[0]) # Start with 0!  
  
print(myList[-1]) # Go backwards  
  
print(myList[1:4]) # Include first ,  
                    # exclude last  
  
print(myList[:2]) # More slicing
```

Have a Play!

https://www.w3schools.com/python/python_lists.asp

For Arithmetic Operations Better: Arrays

```
import array as arr  
  
myList = [1, 2, 3, 4, 5]  
  
myArray = arr.array('i', myList)
```

Alternative import:

```
from array import *  
  
myList = [1, 2, 3, 4, 5]  
  
myArray = array('i', myList)
```

see also [numpy arrays](#), ([here a tutorial](#))

Repetitions and Conditions

While-Loop

```
mySum = 0
```

```
while mySum < 100:
```

```
    mySum = mySum + 3 # Mind the indentation!
```

```
print(mySum)
```

For-Loop

```
mySum = 0
```

```
for i in range(5): # i goes from 0 to 4
```

```
    mySum += i # mySum = mySum + i
```

```
print(mySum)
```

For-Loop

```
mySum = 0
```

```
i = 0
```

```
mySum = mySum + i
```

```
i = 1
```

```
mySum = mySum + i
```

```
i = 2
```

```
mySum = mySum + i
```

```
⋮
```

For-Loop – Real-Life Examples

```
for i in range(1, 100):
```

```
    filename = "myfile"+str(i)+".dat"
```

```
    #Do stuff with that file
```

```
for i in range(100):
```

```
    currentFile = myFileList[i]
```

```
    #Do stuff with that file
```

```
for myFile in myFileList:
```

```
    #Do stuff with that file
```


If-Statement

```
num1 = float(input(" Give me a number!"))
num2 = float(input(" Another number!"))

if num1 > num2:
    print("Your first number is bigger than \
          your second number.")
else:
    print("Your first number is not bigger \
          than your second number.")
```

(There will be some annoying whitespace if you type it like that, just remove the linebreaks and the whitespace in the messages in your code.)

Do we trust the user...?

```
try :  
    num1 = float(input(" Give me a number!"))  
    num2 = float(input(" Another number!"))  
    if num1 > num2:  
        print("Your first number is bigger than \  
            your second number.")  
    else :  
        print("Your first number is not bigger \  
            than your second number.")  
except :  
    print("This wasn't a valid input , \  
        I'm afraid.")
```

Have a play!

You could try

- ▶ writing numeric data into a file using a loop, and reading them into a list,
- ▶ defining a 2d list using a 'lists in a list' notation `[[...],[...]]` and try accessing its elements,
- ▶ doing nested loops,
- ▶ thinking about what type of errors *try-except* is able to catch (see slide 22),
- ▶ ...

Functions

Functions

We've seen functions (==useful code blocks that we need again and again, so we give them a name), for example *print*, *read(5)*, *open("testfile.txt", "w")*, etc.

⇒ Somewhere someone must have written some code for that...

Can we do that as well?

Functions

- ▶ Function Definition
- ▶ Arguments
- ▶ Return statement
- ▶ Function call
- ▶ Scope of variables

Functions

```
def myFunction(parameter1 , parameter2 ):  
    mySum = parameter1 + parameter2  
    return mySum
```

```
def anotherFunction(parameter):  
    print("Here you go: ", parameter)
```

```
myVar = myFunction(22, 55)
```

```
anotherFunction(myVar)
```

Functions

```
def myFunction(parameter1 , parameter2 ):
    mySum = parameter1 + parameter2
    return mySum
```

```
def anotherFunction(parameter):
    print("Here you go: ", parameter)
```

```
myVar = myFunction(22, 55)
```

```
anotherFunction(myVar)
```

Variables defined inside a function are only available in that function.

Functions

```
def myFunction(parameter1 , parameter2 ):
    mySum = parameter1 + parameter2
    return mySum
```

```
def anotherFunction(parameter):
    print("Here you go: ", parameter)
```

```
myVar = myFunction(22, 55)
```

```
anotherFunction(myVar)
```

Variables defined inside a function are only available in that function.

We should really give the functions and variables better names!

Advanced: Recursion

<https://realpython.com/python-thinking-recursively/>

Have a play!

You could try

- ▶ thinking about how to best name the variables and functions in the examples above, and why meaningful names are crucial,
- ▶ writing your own functions, and let one be called from within the other,
- ▶ writing a code that uses all that you have learned today,
- ▶ use the Python debugger to step through your code,
- ▶ ...

How to continue from here?

- ▶ Resources from the materials slide
- ▶ [Research Methods Cafe](#)
- ▶ Programmers are social!
- ▶ Please leave feedback:
https://bit.ly/arc_trainingfeedback