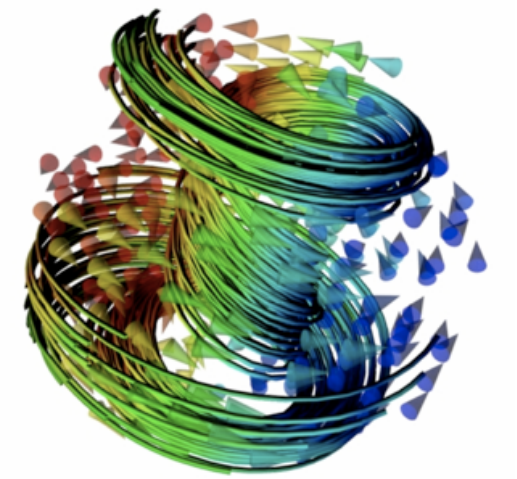
Introduction to

Python for Computational Science and Engineering

(A beginner's guide to Python 3)



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https://github.com/fangohr/introduction-to-python-for-computational-science-and-engineering

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1 Introduction

This text summarises a number of core ideas relevant to Computational Engineering and Scientific Computing using Python. The emphasis is on introducing some basic Python (programming) concepts that are relevant for numerical algorithms. The later chapters touch upon numerical libraries such as `numpy` and `scipy` each of which deserves much more space than provided here. We aim to enable the reader to learn independently how to use other functionality of these libraries using the available documentation (online and through the packages itself).

1.1 Computational Modelling

1.1.1 Introduction

Increasingly, processes and systems are researched or developed through computer simulations: new aircraft prototypes such as for the recent A380 are first designed and tested virtually through computer simulations. With the ever increasing computational power available through supercomputers, clusters of computers and even desktop and laptop machines, this trend is likely to continue.

Computer simulations are routinely used in fundamental research to help understand experimental measurements, and to replace – for example – growth and fabrication of expensive samples/-experiments where possible. In an industrial context, product and device design can often be done much more cost effectively if carried out virtually through simulation rather than through building and testing prototypes. This is in particular so in areas where samples are expensive such as nanoscience (where it is expensive to create small things) and aerospace industry (where it is expensive to build large things). There are also situations where certain experiments can only be carried out virtually (ranging from astrophysics to study of effects of large scale nuclear or chemical accidents). Computational modelling, including use of computational tools to post-process, analyse and visualise data, has been used in engineering, physics and chemistry for many decades but is becoming more important due to the cheap availability of computational resources. Computational Modelling is also starting to play a more important role in studies of biological systems, the economy, archeology, medicine, health care, and many other domains.

1.1.2 Computational Modelling

To study a process with a computer simulation we distinguish two steps: the first one is to develop a *model* of the real system. When studying the motion of a small object, such as a penny, say, under the influence of gravity, we may be able to ignore friction of air: our model — which might only consider the gravitational force and the penny's inertia, i.e. $a(t) = F/m = -9.81\mathrm{m/s}^2$ — is an approximation of the real system. The model will normally allow us to express the behaviour of the system (in some approximated form) through mathematical equations, which often involve ordinary differential equations (ODEs) or partial differential equatons (PDEs).

In the natural sciences such as physics, chemistry and related engineering, it is often not so difficult to find a suitable model, although the resulting equations tend to be very difficult to solve, and can in most cases not be solved analytically at all.

On the other hand, in subjects that are not as well described through a mathematical framework and depend on behaviour of objects whose actions are impossible to predict deterministically (such as humans), it is much more difficult to find a good model to describe reality. As a rule of thumb, in these disciplines the resulting equations are easier to solve, but they are harder to find and the validity of a model needs to be questioned much more. Typical examples are attempts to simulate the economy, the use of global resources, the behaviour of a panicking crowd, etc.

So far, we have just discussed the development of *models* to describe reality, and using these models does not necessarily involve any computers or numerical work at all. In fact, if a model's

equation can be solved analytically, then one should do this and write down the solution to the equation.

In practice, hardly any model equations of systems of interest can be solved analytically, and this is where the computer comes in: using numerical methods, we can at least study the model *for a particular set of boundary conditions*. For the example considered above, we may not be able to easily see from a numerical solution that the penny's velocity under the influence of gravity will change linearly with time (which we can read easily from the analytical solution that is available for this simple system: $v(t) = t \cdot 9.81\mathrm{m/s}^2 + v_0$)).

The numerical solution that can be computed using a computer would consist of data that shows how the velocity changes over time for a particular initial velocity $v0$ ($v0$ is a boundary condition here). The computer program would report a long lists of two numbers keeping the (i) value of time ti for which a particular (ii) value of the velocity vi has been computed. By plotting all vi against ti, or by fitting a curve through the data, we may be able to understand the trend from the data (which we can just see from the analytical solution of course).

It is clearly desirable to find an analytical solutions wherever possible but the number of problems where this is possible is small. Usually, the obtaining numerical result of a computer simulation is very useful (despite the shortcomings of the numerical results in comparison to an analytical expression) because it is the only possible way to study the system at all.

The name *computational modelling* derives from the two steps: (i) *modelling*, i.e. finding a model description of a real system, and (ii) solving the resulting model equations using *computational* methods because this is the only way the equations can be solved at all.

1.1.3 Programming to support computational modelling

A large number of packages exist that provide computational modelling capabilities. If these satisfy the research or design needs, and any data processing and visualisation is appropriately supported through existing tools, one can carry out computational modelling studies without any deeper programming knowledge.

In a research environment – both in academia and research on new products/ideas/... in industry – one often reaches a point where existing packages will not be able to perform a required simulation task, or where more can be learned from analysing existing data in news ways etc.

At that point, programming skills are required. It is also generally useful to have a broad understanding of the building blocks of software and basic ideas of software engineering as we use more and more devices that are software-controlled.

It is often forgotten that there is nothing the computer can do that we as humans cannot do. The computer can do it much faster, though, and also with making far fewer mistakes. There is thus no magic in computations a computer carries out: they could have been done by humans, and – in fact – were for many years (see for example Wikipedia entry on Human Computer).

Understanding how to build a computer simulation comes roughly down to: (i) finding the model (often this means finding the right equations), (ii) knowing how to solve these equations numerically, (ii) to implement the methods to compute these solutions (this is the programming bit).

1.2 Why Python for scientific computing?

The design focus on the Python language is on productivity and code readability, for example through:

- Interactive python console
- Very clear, readable syntax through whitespace indentation
- Strong introspection capabilities

- Full modularity, supporting hierarchical packages
- Exception-based error handling
- Dynamic data types & automatic memory management

As Python is an interpreted language, and it runs many times slower than compiled code, one might ask why anybody should consider such a 'slow' language for computer simulations?

There are two replies to this criticism:

1. *Implementation time versus execution time*: It is not the execution time alone that contributes to the cost of a computational project: one also needs to consider the cost of the development and maintenance work.

In the early days of scientific computing (say in the 1960/70/80), compute time was so expensive that it made perfect sense to invest many person months of a programmer's time to improve the performance of a calculation by a few percent.

Nowadays, however, the CPU cycles have become much cheaper than the programmer's time. For research codes which often run only a small number of times (before the researchers move on to the next problem), it may be economic to accept that the code runs only at 25% of the expected possible speed if this saves, say, a month of a researcher's (or programmers) time. For example: if the execution time of the piece of code is 10 hours, and one can predict that it will run about 100 times, then the total execution time is approximately 1000 hours. It would be great if this could be reduced to 25% and one could save 750 (CPU) hours. On the other hand, is an extra wait (about a month) and the cost of 750 CPU hours worth investing one month of a person's time [who could do something else while the calculation is running]? Often, the answer is not.

Code readability & maintenance - short code, fewer bugs: A related issue is that a research code is not only used for one project, but carries on to be used again and again, evolves, grows, bifurcates etc. In this case, it is often justified to invest more time to make the code fast. At the same time, a significant amount of programmer time will go into (i) introducing the required changes, (ii) testing them even before work on speed optimisation of the changed version can start. To be able to maintain, extend and modify a code in often unforeseen ways, it can only be helpful to use a language that is easy to read and of great expressive power.

2. *Well-written Python code can be very fast* if time critical parts in executed through compiled language.

Typically, less than 5% percent of the code base of a simulation project need more than 95% of the execution time. As long as these calculations are done very efficiently, one doesn't need to worry about all other parts of the code as the overall time their execution takes is insignificant.

The compute intense part of the program should to be tuned to reach optimal performance. Python offers a number of options.

- For example, the `numpy` Python extension provides a Python interface to the compiled and efficient LAPACK libraries that are the quasi-standard in numerical linear algebra. If the problems under study can be formulated such that eventually large systems of algebraic equations have to be solved, or eigenvalues computed, etc, then the compiled code in the LAPACK library can be used (through the Python-numpy package). At this stage, the calculations are carried out with the same performance of Fortran/C as it is essentially Fortran/C code that is used. Matlab, by the way, exploits exactly this: the Matlab scripting language is very slow (about 10 time slower than Python), but Matlab gains its power from delegating the matix operation to the compiled LAPACK libraries.

- Existing numerical C/Fortran libraries can be interfaced to be usable from within Python (using for example Swig, Boost.Python and Cython).
- Python can be extended through compiled languages if the computationally demanding part of the problem is algorithmically non-standard and no existing libraries can be used.

  Commonly used are C, Fortran and C++ to implement fast extensions.
- We list some tools that are used to use compiled code from Python:
  - ▷ The `scipy.weave` extension is useful if just a short expression needs to be expressed in C.
  - ▷ The Cython interface is growing in popularity to (i) semi-automatically declare variable types in Python code, to translate that code to C (automatically) and to then use the compiled C code from Python. Cython is also used to quickly wrap an existing C library with an interface so the C library can be used from Python.
  - ▷ Boost.Python is specialised for wrapping C++ code in Python.

The conclusion is that Python is "fast enough" for most computational tasks, and that its user friendly high-level language often makes up for reduced speed in comparison to compiled lower-level languages. Combining Python with tailor-written compiled code for the performance critical parts of the code, results in virtually optimal speed in most cases.

1.2.1 Optimisation strategies

We generally understand reduction of execution time when discussing "code optimisation" in the context of computational modelling, and we essentially like to carry out the required calculations as fast as possible. (Sometimes we need to reduce the amount of RAM, the amount of data input output to disk or the network.) At the same time, we need to make sure that we do not invest inappropriate amounts of programming time to achieve this speed up: as always there needs to be a balance between the programmers' time and the improvement we can gain from this.

1.2.2 Get it right first, then make it fast

To write fast code effectively, we note that the right order is to (i) first write a program that carries out the correct calculation. For this, choose a language/approach that allows you to *write the code quickly and make it work quickly* — regardless of execution speed. Then (ii) either change the program or re-write it from scratch in the same language to make the execution faster. During the process, keep comparing results with the slow version written first to make sure the optimisation does not introduce errors. (Once we are familiar with the concept of regression tests, they should be used here to compare the new and hopefully faster code with the original code.)

A common pattern in Python is to start writing pure Python code, then start using Python libraries that use compiled code internally (such as the fast arrays Numpy provides, and routines from scipy that go back to established numerical codes such as ODEPACK, LAPACK and others). If required, one can – after careful profiling – start to replace parts of the Python code with a compiled language such as C and Fortran to improve execution speed further (as discussed above).

1.2.3 Prototyping in Python

It turns out that – even if a particular code has to be written in, say, C++ – it is (often) more time efficient to prototype the code in Python, and once an appropriate design (and class structure) has been found, to translate the code to C++.

1.3 Literature

While this text starts with an introduction of (some aspects of) the basic Python programming language, you may find - depending on your prior experience - that you need to refer to secondary sources to fully understand some ideas.

We repeatedly refer to the following documents:

- Allen Downey, *Think Python*. Available online in html and pdf at http://www.greenteapress.com/thinkpython/thinkpython.html, or from Amazon.
- The Python documentation http://www.python.org/doc/, and:
- The Python tutorial (http://docs.python.org/tutorial/)

You may also find the following links useful:

- The `numpy` home page (http://numpy.scipy.org/)
- The `scipy` home page (http://scipy.org/)
- The `matplotlib` home page (http://matplotlib.sourceforge.net/).
- The Python style guide (http://www.python.org/dev/peps/pep-0008/

1.3.1 Recorded video lectures on Python for beginners

Do you like to listen/follow lectures? There is a series of 24 lectures titled *Introduction to Computer Science and Programming* delivered by Eric Grimsom and John Guttag from the MIT available at http://ocw.mit.edu/courses/electrical-engineering-and-computer-science/6-00-introduction-to-computer-science-and-programming-fall-2008/ This is aimed at students with little or no programming experience. It aims to provide students with an understanding of the role computation can play in solving problems. It also aims to help students, regardless of their major, to feel justifiably confident of their ability to write small programs that allow them to accomplish useful goals.

1.3.2 Python tutor mailing list

There is also a Python tutor mailing list (http://mail.python.org/mailman/listinfo/tutor) where beginners are welcome to ask questions regarding Python. Both using the archives and posting your own queries (or in fact helping others) may help with understanding the language. Use the normal mailing list etiquette (i.e. be polite, concise, etc). You may want to read http://www.catb.org/esr/faqs/smart-questions.html for some guidance on how to ask questions on mailing lists.

1.4 Python version

There are two version of the Python language out there: Python 2.x and Python 3.x. They are (slightly) different — the changes in Python 3.x were introduced to address shortcomings in the design of the language that were identified since Python's inception. A decision was made that some incompatibility should be accepted to achieve the higher goal of a better language for the future.

For scientific computation, it is crucial to make use of numerical libraries such as numpy, scipy and the plotting package matplotlib.

All of these are now available for Python 3, and we will use Python 3.x in this book.

However, there is a lot of code still in use that was written for Python 2, and it's useful to be aware of the differences. The most prominent example is that in Python 2.x, the `print` command is special, whereas in Python 3 it is an ordinary function. For example, in Python 2.7, we can write:

```
print "Hello World"
```

where as in Python 3, this would cause a SyntaxError. The right way to use `print` in Python 3 would be as a function, i.e.

[1]:
```
print("Hello World")
```

```
Hello World
```

See Section **??** for further details.

Fortunately, the function notation (i.e. with the parantheses) is also allowed in Python 2.7, so our examples should execute in Python 3.x and Python 2.7. (There are other differences.)

1.5 These documents

This material has been converted from Latex to a set of Jupyter Notebooks, making it possible to interact with the examples. You can run any code block with an `In [ ]:` prompt by clicking on it and pressing shift-enter, or by clicking the button in the toolbar.

1.5.1 The `%%file` magic

We use some features in the notebook that are worth being aware of at this point: a cell starting with the special command `%%file FILENAME` will create (or override) a file with name `FILENAME` that contains the content that is shown in the cell below.

For example

[2]:
```
%%file hello.txt
This is the content of the file hello.txt
```

```
Writing hello.txt
```

To confirm the file has been written and contains, we use some Python commands (which you are not expected to understand at this point):

[3]:
```
with open("hello.txt") as f:
    print(f.read())
```

```
This is the content of the file hello.txt
```

1.5.2 The `!` to execute shell commands

If we want to run a shell command, we can type it and preceed it by the `!` character. Here is an example: first we create a file that contains a Python hello world program, then we execute it:

[4]:
```
%%file hello.py
print("Hello World")
```

```
Overwriting hello.py
```

[5]:
```
!python hello.py
```

```
Hello World
```

1.5.3 The #NBVAL tags

In some cells, you will find tags like `#NBVAL_SKIP`, `#NBVAL_IGNORE_OUTPUT` and `#NBVAL_RAISES_EXCEPTION`. You can ignore these.

(We use them to be able to automatically execute all notebooks to check that the output produced is the same as what is stored in the notebook. This is an advanced topic of testing, and you can read more about NBVAL at https://github.com/computationalmodelling/nbval).

See Section **??** for more information on Jupyter and other Python interfaces.

1.6 Your feedback

is desired. If you find anything wrong in this text, or have suggestions how to change or extend it, please feel free to contact Hans at `hans.fangohr@xfel.eu` .

If you find a URL that is not working (or pointing to the wrong material), please let Hans know as well. As the content of the Internet is changing rapidly, it is difficult to keep up with these changes without feedback.

2 A powerful calculator

2.1 Python prompt and Read-Eval-Print Loop (REPL)

Python is an *interpreted* language. We can collect sequences of commands into text files and save this to file as a *Python program*. It is convention that these files have the file extension ".py", for example `hello.py`.

We can also enter individual commands at the Python prompt which are immediately evaluated and carried out by the Python interpreter. This is very useful for the programmer/learner to understand how to use certain commands (often before one puts these commands together in a longer Python program). Python's role can be described as Reading the command, Evaluating it, Printing the evaluated value and repeating (Loop) the cycle – this is the origin of the REPL abbreviation.

Python comes with a basic terminal prompt; you may see examples from this with >>> marking the input:

```
>>> 2 + 2
4
```

We are using a more powerful REPL interface, the Jupyter Notebook. Blocks of code appear with an `In` prompt next to them:

[1]:
```
4 + 5
```

[1]:
```
9
```

To edit the code, click inside the code area. You should get a green border around it. To run it, press Shift-Enter.

2.2 Calculator

Basic operations such as addition (+), subtraction (-), multiplication (*), division (/) and exponentiation (**) work (mostly) as expected:

[2]:
```
10 + 10000
```

[2]:
```
10010
```

[3]:
```
42 - 1.5
```

[3]:
```
40.5
```

[4]:
```
47 * 11
```

[4]:
```
517
```

[5]:
```
10 / 0.5
```

[5]:
```
20.0
```

[6]:
```
2**2   # Exponentiation ('to the power of') is **, NOT ^
```

[6]:
```
4
```

[7]:
```
2**3
```

[7]:
```
8
```

[8]:
```
2**4
```

[8]:
```
16
```

[9]:
```
2 + 2
```

[9]:
```
4
```

[10]:
```
# This is a comment
2 + 2
```

[10]:
```
4
```

[11]:
```
2 + 2  # and a comment on the same line as code
```

[11]:
```
4
```

and, using the fact that $\sqrt[n]{x} = x^{1/n}$, we can compute the $\sqrt{3} = 1.732050\ldots$ using **:

[12]:
```
3**0.5
```

[12]:
```
1.7320508075688772
```

Parenthesis can be used for grouping:

[13]:
```
2 * 10 + 5
```

[13]:
```
25
```

[14]:
```
2 * (10 + 5)
```

[14]:
```
30
```

2.3 Integer division

In Python 3, division works as you'd expect:

[15]:
```
15/6
```

[15]:
```
2.5
```

In Python 2, however, `15/6` will give you `2`.

This phenomenon is known (in many programming languages, including C) as *integer division*: because we provide two integer numbers (`15` and `6`) to the division operator (`/`), the assumption is that we seek a return value of type integer. The mathematically correct answer is (the floating point number) 2.5. (numerical data types in Section **??**.)

The convention for integer division is to truncate the fractional digits and to return the integer part only (i.e. `2` in this example). It is also called "floor division".

2.3.1 How to avoid integer division

There are two ways to avoid the problem of integer division:

1. Use Python 3 style division: this is available even in Python 2 with a special import statement:

```
python    >>> from __future__ import division    >>> 15/6    2.5
```

   If you want to use the `from __future__ import division` feature in a python program, it would normally be included at the beginning of the file.

2. Alternatively, if we ensure that at least one number (numerator or denominator) is of type float (or complex), the division operator will return a floating point number. This can be done by writing `15.` instead of `15`, of by forcing conversion of the number to a float, i.e. use `float(15)` instead of `15`:

```
python    >>> 15./6    2.5    >>> float(15)/6    2.5    >>> 15/6.    2.5    >>>
15/float(6)    2.5    >>> 15./6.    2.5
```

   If we really want integer division, we can use `//`: `1//2` returns 0, in both Python 2 and 3.

2.3.2 Why should I care about this division problem?

Integer division can result in surprising bugs: suppose you are writing code to compute the mean value m=(x+y)/2 of two numbers x and y. The first attempt of writing this may read:

```
m = (x + y) / 2
```

Suppose this is tested with x=0.5,y=0.5, then the line above computes the correct answers m=0.5 (because`0.5 + 0.5 = 1.0`, i.e. a 1.0 is a floating point number, and thus `1.0/2` evaluates to `0.5`). Or we could use x=10,y=30, and because `10 + 30 = 40` and `40/2` evaluates to `20`, we get the correct answer m=20. However, if the integers x=0 and y=1 would come up, then the code returns m=0 (because `0 + 1 = 1` and `1/2` evaluates to `0`) whereas m=0.5 would have been the right answer.

We have many possibilities to change the line of code above to work safely, including these three versions:

```
m = (x + y) / 2.0
```

```
m = float(x + y) / 2
```

```
m = (x + y) * 0.5
```

This integer division behaviour is common amongst most programming languages (including the important ones C, C++ and Fortran), and it is important to be aware of the issue.

2.4 Mathematical functions

Because Python is a general purpose programming language, commonly used mathematical functions such as sin, cos, exp, log and many others are located in the mathematics module with name `math`. We can make use of this as soon as we *import* the math module:

[16]:
```
import math
math.exp(1.0)
```

[16]:
```
2.718281828459045
```

Using the `dir` function, we can see the directory of objects available in the math module:

[17]:
```
# NBVAL_IGNORE_OUTPUT
dir(math)
```

[17]:
```
['__doc__',
 '__file__',
 '__loader__',
 '__name__',
 '__package__',
 '__spec__',
 'acos',
 'acosh',
 'asin',
 'asinh',
 'atan',
 'atan2',
 'atanh',
 'ceil',
 'copysign',
 'cos',
 'cosh',
 'degrees',
 'e',
 'erf',
 'erfc',
 'exp',
 'expm1',
 'fabs',
 'factorial',
 'floor',
 'fmod',
 'frexp',
 'fsum',
 'gamma',
 'gcd',
 'hypot',
 'inf',
 'isclose',
 'isfinite',
 'isinf',
 'isnan',
```

```
 'ldexp',
 'lgamma',
 'log',
 'log10',
 'log1p',
 'log2',
 'modf',
 'nan',
 'pi',
 'pow',
 'radians',
 'sin',
 'sinh',
 'sqrt',
 'tan',
 'tanh',
 'tau',
 'trunc']
```

As usual, the `help` function can provide more information about the module (`help(math)`) on individual objects:

[18]:
```
# NBVAL_IGNORE_OUTPUT
help(math.exp)
```

```
Help on built-in function exp in module math:

exp(...)
    exp(x)

    Return e raised to the power of x.
```

The mathematics module defines to constants π and e:

[19]:
```
math.pi
```

[19]:
```
3.141592653589793
```

[20]:
```
math.e
```

[20]:
```
2.718281828459045
```

[21]:
```
math.cos(math.pi)
```

[21]:
```
-1.0
```

[22]:
```
math.log(math.e)
```

[22]:
```
1.0
```

2.5 Variables

A *variable* can be used to store a certain value or object. In Python, all numbers (and everything else, including functions, modules and files) are objects. A variable is created through assignement:

[23]:
```
x = 0.5
```

Once the variable x has been created through assignment of 0.5 in this example, we can make use of it:

[24]:
```
x*3
```

[24]:
```
1.5
```

[25]:
```
x**2
```

[25]:
```
0.25
```

[26]:
```
y = 111
y + 222
```

[26]:
```
333
```

A variable is overriden if a new value is assigned:

[27]:
```
y = 0.7
math.sin(y) ** 2 + math.cos(y) ** 2
```

[27]:
```
1.0
```

The equal sign ('=') is used to assign a value to a variable.

[28]:
```
width = 20
height = 5 * 9
width * height
```

[28]:
```
900
```

A value can be assigned to several variables simultaneously:

[29]:
```
x = y = z = 0  # initialise x, y and z with 0
x
```

[29]:
```
0
```

[30]:
```
y
```

[30]:
```
0
```

[31]:
```
z
```

[31]:
```
0
```

Variables must be created (assigned a value) before they can be used, or an error will occur:

[32]:
```
# NBVAL_RAISES_EXCEPTION
# try to access an undefined variable:
n
```

```
---------------------------------------------------------------------------

NameError                                 Traceback (most recent call last)

<ipython-input-32-a15a18dc7d7c> in <module>()
  1 # NBVAL_SKIP
  2 # try to access an undefined variable:
```

```
----> 3 n


    NameError: name 'n' is not defined
```

In interactive mode, the last printed expression is assigned to the variable `_`. This means that when you are using Python as a desk calculator, it is somewhat easier to continue calculations, for example:

[ ]:
```
tax = 12.5 / 100
price = 100.50
price * tax
```

[ ]:
```
price + _
```

This variable should be treated as read-only by the user. Don't explicitly assign a value to it — you would create an independent local variable with the same name masking the built-in variable with its magic behavior.

2.5.1 Terminology

Strictly speaking, the following happens when we write

[ ]:
```
x = 0.5
```

First, Python creates the object `0.5`. Everything in Python is an object, and so is the floating point number 0.5. This object is stored somewhere in memory. Next, Python *binds a name to the object*. The name is `x`, and we often refer casually to `x` as a variable, an object, or even the value 0.5. However, technically, `x` is a name that is bound to the object `0.5`. Another way to say this is that `x` is a reference to the object.

While it is often sufficient to think about assigning 0.5 to a variable x, there are situations where we need to remember what actually happens. In particular, when we pass references to objects to functions, we need to realise that the function may operate on the object (rather than a copy of the object). This is discussed in more detail in Section **??**.

2.6 Impossible equations

In computer programs we often find statements like

[ ]:
```
x = x + 1
```

If we read this as an equation as we are use to from mathematics, x=x+1 we could subtract x on both sides, to find that 0=1. We know this is not true, so something is wrong here.

The answer is that "equations" in computer codes are not equations but *assignments*. They always have to be read in the following way two-step way:

1. Evaluate the value on the right hand side of the equal sign
2. Assign this value to the variable name shown on the left hand side. (In Python: bind the name on the left hand side to the object shown on the right hand side.)

Some computer science literature uses the following notation to express assignments and to avoid the confusion with mathematical equations:

$$x \leftarrow x + 1$$

Let's apply our two-step rule to the assignment `x = x + 1` given above:

1. Evaluate the value on the right hand side of the equal sign: for this we need to know what the current value of `x` is. Let's assume `x` is currently `4`. In that case, the right hand side `x+1` evaluates to `5`.
2. Assign this value (i.e. `5`) to the variable name shown on the left hand side `x`.

Let's confirm with the Python prompt that this is the correct interpretation:

[ ]:
```
x = 4
x = x + 1
x
```

2.6.1 The += notation

Because it is a quite a common operation to increase a variable `x` by some fixed amount `c`, we can write

```
x += c
```

instead of

```
x = x + c
```

Our initial example above could thus have been written

[ ]:
```
x = 4
x += 1
x
```

The same operators are defined for multiplication with a constant (`*=`), subtraction of a constant (`-=`) and division by a constant (`/=`).

Note that the order of `+` and `=` matters:

[ ]:
```
x += 1
```

will increase the variable `x` by one where as

[ ]:
```
x =+ 1
```

will assign the value `+1` to the variable `x`.

3 Data Types and Data Structures

3.1 What type is it?

Python knows different data types. To find the type of a variable, use the `type()` function:

[1]:
```
a = 45
type(a)
```

[1]:
```
int
```

[2]:
```
b = 'This is a string'
type(b)
```

[2]:
```
str
```

[3]:
```
c = 2 + 1j
type(c)
```

[3]:
```
complex
```

[4]:
```
d = [1, 3, 56]
type(d)
```

[4]:
```
list
```

3.2 Numbers

Further information

- Informal introduction to numbers. Python tutorial, section 3.1.1
- Python Library Reference: formal overview of numeric types, http://docs.python.org/library/stdtypes.html#numeric-types-int-float-long-complex
- Think Python, Sec 2.1

The in-built numerical types are integers and floating point numbers (see Section **??**) and complex floating point numbers (Section **??**).

3.2.1 Integers

We have seen the use of integer numbers already in Section **??**. Be aware of integer division problems (Section **??**).

If we need to convert string containing an integer number to an integer we can use `int()` function:

[5]:
```
a = '34'        # a is a string containing the characters 3 and 4
x = int(a)      # x is in integer number
```

The function `int()` will also convert floating point numbers to integers:

[6]:
```
int(7.0)
```

[6]:
```
7
```

[7]:
```
int(7.9)
```

[7]:
```
7
```

Note than `int` will truncate any non-integer part of a floating point number. To `round` an floating point number to an integer, use the `round()` command:

[8]:
```
round(7.9)
```

[8]:
```
8
```

3.2.2 Integer limits

Integers in Python 3 are unlimited; Python will automatically assign more memory as needed as the numbers get bigger. This means we can calculate very large numbers with no special steps.

[9]:
```
35**42
```

[9]:
```
70934557307860443711736098025989133248003781773149967193603515625
```

In many other programming languages, such as C and FORTRAN, integers are a fixed size—most frequently 4 bytes, which allows 2^{32} different values—but different types are available with different sizes. For numbers that fit into these limits, calculations can be faster, but you may need to check that the numbers don't go beyond the limits. Calculating a number beyond the limits is called *integer overflow*, and may produce bizarre results.

Even in Python, we need to be aware of this when we use numpy (see Section **??**). Numpy uses integers with a fixed size, because it stores many of them together and needs to calculate with them efficiently. Numpy data types include a range of integer types named for their size, so e.g. `int16` is a 16-bit integer, with 2^{16} possible values.

Integer types can also be *signed* or *unsigned*. Signed integers allow positive or negative values, unsigned integers only allow positive ones. For instance:

- uint16 (unsigned) ranges from 0 to $2^{16} - 1$
- int16 (signed) ranges from -2^{15} to $2^{15} - 1$

3.2.3 Floating Point numbers

A string containing a floating point number can be converted into a floating point number using the `float()` command:

[10]:
```
a = '35.342'
b = float(a)
b
```

[10]:
```
35.342
```

[11]:
```
type(b)
```

[11]:
```
float
```

3.2.4 Complex numbers

Python (as Fortran and Matlab) has built-in complex numbers. Here are some examples how to use these:

[12]:
```
x = 1 + 3j
x
```

[12]:
```
(1+3j)
```

[13]:
```
abs(x)                # computes the absolute value
```

[13]:
```
3.1622776601683795
```

[14]:
```
x.imag
```

[14]:
```
3.0
```

[15]:
```
x.real
```

[15]:
```
1.0
```

[16]:
```
x * x
```

[16]:
```
(-8+6j)
```

[17]:
```
x * x.conjugate()
```

[17]:
```
(10+0j)
```

[18]:
```
3 * x
```

[18]:
```
(3+9j)
```

Note that if you want to perform more complicated operations (such as taking the square root, etc) you have to use the `cmath` module (Complex MATHematics):

[19]:
```
import cmath
cmath.sqrt(x)
```

[19]:
```
(1.442615274452683+1.0397782600555705j)
```

3.2.5 Functions applicable to all types of numbers

The `abs()` function returns the absolute value of a number (also called modulus):

[20]:
```
a = -45.463
abs(a)
```

[20]:
```
45.463
```

Note that `abs()` also works for complex numbers (see above).

3.3 Sequences

Strings, lists and tuples are *sequences*. They can be *indexed* and *sliced* in the same way.

Tuples and strings are "immutable" (which basically means we can't change individual elements within the tuple, and we cannot change individual characters within a string) whereas lists are "mutable" (*.i.e* we can change elements in a list.)

Sequences share the following operations

- `a[i]` returns i-th element of `a`
- `a[i:j]` returns elements i up to j-1
- `len(a)` returns number of elements in sequence
- `min(a)` returns smallest value in sequence
- `max(a)` returns largest value in sequence
- `x in a` returns `True` if `x` is element in `a`
- `a + b` concatenates `a` and `b`
- `n * a` creates `n` copies of sequence `a`

3.3.1 Sequence type 1: String

Further information

- Introduction to strings, Python tutorial 3.1.2

A string is a (immutable) sequence of characters. A string can be defined using single quotes:

[21]:
```
a = 'Hello World'
```

double quotes:

[22]:
```
a = "Hello World"
```

or triple quotes of either kind

[23]:
```
a = """Hello World"""
a = '''Hello World'''
```

The type of a string is `str` and the empty string is given by `""`:

[24]:
```
a = "Hello World"
type(a)
```

[24]:
```
str
```

[25]:
```
b = ""
type(b)
```

[25]:
```
str
```

[26]:
```
type("Hello World")
```

[26]:
```
str
```

[27]:
```
type("")
```

[27]:
```
str
```

The number of characters in a string (that is its *length*) can be obtained using the `len()`-function:

[28]:
```
a = "Hello Moon"
len(a)
```

[28]:
```
10
```

[29]:
```
a = 'test'
len(a)
```

[29]:
```
4
```

[30]:
```
len('another test')
```

[30]:
```
12
```

You can combine ("concatenate") two strings using the + operator:

[31]:
```
'Hello ' + 'World'
```

[31]:
```
'Hello World'
```

Strings have a number of useful methods, including for example `upper()` which returns the string in upper case:

[32]:
```
a = "This is a test sentence."
a.upper()
```

[32]:
```
'THIS IS A TEST SENTENCE.'
```

A list of available string methods can be found in the Python reference documentation. If a Python prompt is available, one should use the `dir` and `help` function to retrieve this information, *i.e.* `dir()` provides the list of methods, `help` can be used to learn about each method.

A particularly useful method is `split()` which converts a string into a list of strings:

[33]:
```
a = "This is a test sentence."
a.split()
```

[33]:
```
['This', 'is', 'a', 'test', 'sentence.']
```

The `split()` method will separate the string where it finds *white space*. White space means any character that is printed as white space, such as one space or several spaces or a tab.

By passing a separator character to the `split()` method, a string can split into different parts. Suppose, for example, we would like to obtain a list of complete sentences:

[34]:
```
a = "The dog is hungry. The cat is bored. The snake is awake."
a.split(".")
```

[34]:
```
['The dog is hungry', ' The cat is bored', ' The snake is awake', '']
```

The opposite string method to `split` is `join` which can be used as follows:

[35]:
```
a = "The dog is hungry. The cat is bored. The snake is awake."
s = a.split('.')
s
```

[35]:
```
['The dog is hungry', ' The cat is bored', ' The snake is awake', '']
```

[36]:
```
".".join(s)
```

[36]:
```
'The dog is hungry. The cat is bored. The snake is awake.'
```

[37]:
```
" STOP".join(s)
```

[37]:
```
'The dog is hungry STOP The cat is bored STOP The snake is awake STOP'
```

3.3.2 Sequence type 2: List

Further information

- Introduction to Lists, Python tutorial, section 3.1.4

A list is a sequence of objects. The objects can be of any type, for example integers:

[38]:
```
a = [34, 12, 54]
```

or strings:

[39]:
```
a = ['dog', 'cat', 'mouse']
```

An empty list is presented by `[]`:

[40]:
```
a = []
```

The type is `list`:

[41]:
```
type(a)
```

[41]:
```
list
```

[42]:
```
type([])
```

[42]:
```
list
```

As with strings, the number of elements in a list can be obtained using the `len()` function:

[43]:
```
a = ['dog', 'cat', 'mouse']
len(a)
```

[43]:
```
3
```

It is also possible to *mix* different types in the same list:

[44]:
```
a = [123, 'duck', -42, 17, 0, 'elephant']
```

In Python a list is an object. It is therefor possible for a list to contain other lists (because a list keeps a sequence of objects):

[45]:
```
a = [1, 4, 56, [5, 3, 1], 300, 400]
```

You can combine ("concatenate") two lists using the + operator:

[46]:
```
[3, 4, 5] + [34, 35, 100]
```

[46]:
```
[3, 4, 5, 34, 35, 100]
```

Or you can add one object to the end of a list using the `append()` method:

[47]:
```
a = [34, 56, 23]
a.append(42)
a
```

[47]:
```
[34, 56, 23, 42]
```

You can delete an object from a list by calling the `remove()` method and passing the object to delete. For example:

[48]:
```
a = [34, 56, 23, 42]
a.remove(56)
a
```

[48]:
```
[34, 23, 42]
```

The range() command A special type of list is frequently required (often together with `for-loops`) and therefor a command exists to generate that list: the `range(n)` command generates integers starting from 0 and going up to *but not including* n. Here are a few examples:

[49]:
```
list(range(3))
```

[49]:
```
[0, 1, 2]
```

[50]:
```
list(range(10))
```

[50]:
```
[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
```

This command is often used with for loops. For example, to print the numbers 02,12,22,32,...,102, the following program can be used:

[51]:
```
for i in range(11):
    print(i ** 2)
```

```
0
1
4
9
16
25
36
49
64
81
100
```

The range command takes an optional parameter for the beginning of the integer sequence (start) and another optional parameter for the step size. This is often written as `range([start],stop,[step])` where the arguments in square brackets (*i.e.* start and step) are optional. Here are some examples:

[52]:
```
list(range(3, 10))            # start=3
```

[52]:
```
[3, 4, 5, 6, 7, 8, 9]
```

[53]:
```
list(range(3, 10, 2))          # start=3, step=2
```

[53]:
```
[3, 5, 7, 9]
```

[54]:
```
list(range(10, 0, -1))         # start=10,step=-1
```

[54]:
```
[10, 9, 8, 7, 6, 5, 4, 3, 2, 1]
```

Why are we calling `list(range())`?

In Python 3, `range()` generates the numbers on demand. When you use `range()` in a for loop, this is more efficient, because it doesn't take up memory with a list of numbers. Passing it to `list()` forces it to generate all of its numbers, so we can see what it does.

To get the same efficient behaviour in Python 2, use `xrange()` instead of `range()`.

3.3.3 Sequence type 3: Tuples

A *tuple* is a (immutable) sequence of objects. Tuples are very similar in behaviour to lists with the exception that they cannot be modified (i.e. are immutable).

For example, the objects in a sequence can be of any type:

[55]:
```
a = (12, 13, 'dog')
a
```

[55]:
```
(12, 13, 'dog')
```

[56]:
```
a[0]
```

[56]:
```
12
```

The parentheses are not necessary to define a tuple: just a sequence of objects separated by commas is sufficient to define a tuple:

[57]:
```
a = 100, 200, 'duck'
a
```

[57]:
```
(100, 200, 'duck')
```

although it is good practice to include the paranthesis where it helps to show that tuple is defined.

Tuples can also be used to make two assignments at the same time:

[58]:
```
x, y = 10, 20
x
```

[58]:
```
10
```

[59]:
```
y
```

[59]:
```
20
```

This can be used to *swap* to objects within one line. For example

[60]:
```
x = 1
y = 2
x, y = y, x
x
```

[60]:
```
2
```

[61]:
```
y
```

[61]:
```
1
```

The empty tuple is given by `()`

[62]:
```
t = ()
len(t)
```

[62]:
```
0
```

[63]:
```
type(t)
```

[63]:
```
tuple
```

The notation for a tuple containing one value may seem a bit odd at first:

[64]:
```
t = (42,)
type(t)
```

[64]:
```
tuple
```

[65]:
```
len(t)
```

[65]:
```
1
```

The extra comma is required to distinguish `(42,)` from `(42)` where in the latter case the parenthesis would be read as defining operator precedence: `(42)` simplifies to `42` which is just a number:

[66]:
```
t = (42)
type(t)
```

[66]:
```
int
```

This example shows the immutability of a tuple:

[67]:
```
a = (12, 13, 'dog')
a[0]
```

[67]:
```
12
```

[68]:
```
# NBVAL_RAISES_EXCEPTION
a[0] = 1
```

```
---------------------------------------------------------------------------

TypeError                                 Traceback (most recent call last)

<ipython-input-68-fa35ffef1c7d> in <module>()
      1 # NBVAL_RAISES_EXCEPTION
----> 2 a[0] = 1


TypeError: 'tuple' object does not support item assignment
```

The immutability is the main difference between a tuple and a list (the latter being mutable). We should use tuples when we don't want the content to change.

Note that Python functions that return more than one value, return these in tuples (which makes sense because you don't want these values be changed).

3.3.4 Indexing sequences

Further information

- Introduction to strings and indexing in Python tutorial, section 3.1.2, the relevant section is starting after strings have been introduced.

Individual objects in lists can be accessed by using the index of the object and square brackets (`[` and `]`):

[69]:
```
a = ['dog', 'cat', 'mouse']
a[0]
```

[69]:
```
'dog'
```

[70]:
```
a[1]
```

[70]:
```
'cat'
```

[71]:
```
a[2]
```

[71]:
```
'mouse'
```

Note that Python (like C but unlike Fortran and unlike Matlab) starts counting indices from zero!

Python provides a handy shortcut to retrieve the last element in a list: for this one uses the index "-1" where the minus indicates that it is one element *from the back* of the list. Similarly, the index "-2" will return the 2nd last element:

[72]:
```
a = ['dog', 'cat', 'mouse']
a[-1]
```

[72]:
```
'mouse'
```

[73]:
```
a[-2]
```

[73]:
```
'cat'
```

If you prefer, you can think of the index `a[-1]` to be a shorthand notation for `a[len(a) - 1]`.

Remember that strings (like lists) are also a sequence type and can be indexed in the same way:

[74]:
```
a = "Hello World!"
a[0]
```

[74]:
```
'H'
```

[75]:
```
a[1]
```

[75]:
```
'e'
```

[76]:
```
a[10]
```

[76]:
```
'd'
```

[77]:
```
a[-1]
```

[77]:
```
'!'
```

[78]:
```
a[-2]
```

[78]:
```
'd'
```

3.3.5 Slicing sequences

Further information

- Introduction to strings, indexing and slicing in Python tutorial, section 3.1.2

Slicing of sequences can be used to retrieve more than one element. For example:

[79]:
```
a = "Hello World!"
a[0:3]
```

[79]:
```
'Hel'
```

By writing `a[0:3]` we request the first 3 elements starting from element 0. Similarly:

[80]:
```
a[1:4]
```

[80]:
```
'ell'
```

[81]:
```
a[0:2]
```

[81]:
```
'He'
```

[82]:
```
a[0:6]
```

[82]:
```
'Hello '
```

We can use negative indices to refer to the end of the sequence:

[83]:
```
a[0:-1]
```

[83]:
```
'Hello World'
```

It is also possible to leave out the start or the end index and this will return all elements up to the beginning or the end of the sequence. Here are some examples to make this clearer:

[84]:
```
a = "Hello World!"
a[:5]
```

[84]:
```
'Hello'
```

[85]:
```
a[5:]
```

[85]:
```
' World!'
```

[86]:
```
a[-2:]
```

[86]:
```
'd!'
```

[87]:
```
a[:]
```

[87]:
```
'Hello World!'
```

Note that `a[:]` will generate a *copy* of `a`. The use of indices in slicing is by some people experienced as counter intuitive. If you feel uncomfortable with slicing, have a look at this quotation from the Python tutorial (section 3.1.2):

> The best way to remember how slices work is to think of the indices as pointing between characters, with the left edge of the first character numbered 0. Then the right edge of the last character of a string of 5 characters has index 5, for example:

```
+---+---+---+---+---+
| H | e | l | l | o |
+---+---+---+---+---+
```

```
 0   1   2   3   4   5   <-- use for SLICING
-5  -4  -3  -2  -1       <-- use for SLICING
                              from the end
```

The first row of numbers gives the position of the slicing indices 0...5 in the string; the second row gives the corresponding negative indices. The slice from i to j consists of all characters between the edges labelled i and j, respectively.

So the important statement is that for *slicing* we should think of indices pointing between characters.

For *indexing* it is better to think of the indices referring to characters. Here is a little graph summarising these rules:

```
  0   1   2   3   4    <-- use for INDEXING
 -5  -4  -3  -2  -1    <-- use for INDEXING
+---+---+---+---+---+          from the end
| H | e | l | l | o |
+---+---+---+---+---+
0   1   2   3   4   5  <-- use for SLICING
-5  -4  -3  -2  -1      <-- use for SLICING
                         from the end
```

If you are not sure what the right index is, it is always a good technique to play around with a small example at the Python prompt to test things before or while you write your program.

3.3.6 Dictionaries

Dictionaries are also called "associative arrays" and "hash tables". Dictionaries are *unordered* sets of *key-value pairs*.

An empty dictionary can be created using curly braces:

[88]:
```
d = {}
```

Keyword-value pairs can be added like this:

[89]:
```
d['today'] = '22 deg C'    # 'today' is the keyword
```

[90]:
```
d['yesterday'] = '19 deg C'
```

`d.keys()` returns a list of all keys:

[91]:
```
d.keys()
```

[91]:
```
dict_keys(['today', 'yesterday'])
```

We can retrieve values by using the keyword as the index:

[92]:
```
d['today']
```

[92]:
```
'22 deg C'
```

Other ways of populating a dictionary if the data is known at creation time are:

[93]:
```
d2 = {2:4, 3:9, 4:16, 5:25}
d2
```

[93]:
```
{2: 4, 3: 9, 4: 16, 5: 25}
```

[94]:
```
d3 = dict(a=1, b=2, c=3)
d3
```

[94]:
```
{'a': 1, 'b': 2, 'c': 3}
```

The function `dict()` creates an empty dictionary.

Other useful dictionary methods include `values()`, `items()` and `get()`. You can use `in` to check for the presence of values.

[95]:
```
d.values()
```

[95]:
```
dict_values(['22 deg C', '19 deg C'])
```

[96]:
```
d.items()
```

[96]:
```
dict_items([('today', '22 deg C'), ('yesterday', '19 deg C')])
```

[97]:
```
d.get('today','unknown')
```

[97]:
```
'22 deg C'
```

[98]:
```
d.get('tomorrow','unknown')
```

[98]:
```
'unknown'
```

[99]:
```
'today' in d
```

[99]:
```
True
```

[100]:
```
'tomorrow' in d
```

[100]:
```
False
```

The method `get(key,default)` will provide the value for a given `key` if that key exists, otherwise it will return the `default` object.

Here is a more complex example:

[101]:
```
# NBVAL_IGNORE_OUTPUT
order = {}         # create empty dictionary

#add orders as they come in
order['Peter'] = 'Pint of bitter'
order['Paul'] = 'Half pint of Hoegarden'
order['Mary'] = 'Gin Tonic'

#deliver order at bar
for person in order.keys():
    print(person, "requests", order[person])
```

```
Peter requests Pint of bitter
Paul requests Half pint of Hoegarden
Mary requests Gin Tonic
```

Some more technicalities:

- The keyword can be any (immutable) Python object. This includes:
  - ▷ numbers
  - ▷ strings

▷ tuples.

- dictionaries are very fast in retrieving values (when given the key)

An other example to demonstrate an advantage of using dictionaries over pairs of lists:

[102]:
```
# NBVAL_IGNORE_OUTPUT
dic = {}                          #create empty dictionary

dic["Hans"]   = "room 1033"       #fill dictionary
dic["Andy C"] = "room 1031"       #"Andy C" is key
dic["Ken"]    = "room 1027"       #"room 1027" is value

for key in dic.keys():
    print(key, "works in", dic[key])
```

```
Hans works in room 1033
Andy C works in room 1031
Ken works in room 1027
```

Without dictionary:

[103]:
```
people = ["Hans","Andy C","Ken"]
rooms  = ["room 1033","room 1031","room 1027"]

#possible inconsistency here since we have two lists
if not len( people ) == len( rooms ):
    raise RuntimeError("people and rooms differ in length")

for i in range( len( rooms ) ):
    print(people[i],"works in",rooms[i])
```

```
Hans works in room 1033
Andy C works in room 1031
Ken works in room 1027
```

3.4 Passing arguments to functions

This section contains some more advanced ideas and makes use of concepts that are only later introduced in this text. The section may be more easily accessible at a later stage.

When objects are passed to a function, Python always passes (the value of) the reference to the object to the function. Effectively this is calling a function by reference, although one could refer to it as calling by value (of the reference).

We review argument passing by value and reference before discussing the situation in Python in more detail.

3.4.1 Call by value

One might expect that if we pass an object by value to a function, that modifications of that value inside the function will not affect the object (because we don't pass the object itself, but only its value, which is a copy). Here is an example of this behaviour (in C):

```c
#include <stdio.h>

void pass_by_value(int m) {
  printf("in pass_by_value: received m=%d\n",m);
  m=42;
  printf("in pass_by_value: changed to m=%d\n",m);
}

int main(void) {
  int global_m = 1;
  printf("global_m=%d\n",global_m);
  pass_by_value(global_m);
  printf("global_m=%d\n",global_m);
  return 0;
}
```

together with the corresponding output:

```
global_m=1
in pass_by_value: received m=1
in pass_by_value: changed to m=42
global_m=1
```

The value 1 of the global variable `global_m` is not modified when the function `pass_by_value` changes its input argument to 42.

3.4.2 Call by reference

Calling a function by reference, on the other hand, means that the object given to a function is a reference to the object. This means that the function will see the same object as in the calling code (because they are referencing the same object: we can think of the reference as a pointer to the place in memory where the object is located). Any changes acting on the object inside the function, will then be visible in the object at the calling level (because the function does actually operate on the same object, not a copy of it).

Here is one example showing this using pointers in C:

```c
#include <stdio.h>

void pass_by_reference(int *m) {
  printf("in pass_by_reference: received m=%d\n",*m);
  *m=42;
  printf("in pass_by_reference: changed to m=%d\n",*m);
}

int main(void) {
  int global_m = 1;
  printf("global_m=%d\n",global_m);
  pass_by_reference(&global_m);
  printf("global_m=%d\n",global_m);
  return 0;
}
```

together with the corresponding output:

```
global_m=1
in pass_by_reference: received m=1
in pass_by_reference: changed to m=42
global_m=42
```

C++ provides the ability to pass arguments as references by adding an ampersand in front of the argument name in the function definition:

```
#include <stdio.h>

void pass_by_reference(int &m) {
  printf("in pass_by_reference: received m=%d\n",m);
  m=42;
  printf("in pass_by_reference: changed to m=%d\n",m);
}

int main(void) {
  int global_m = 1;
  printf("global_m=%d\n",global_m);
  pass_by_reference(global_m);
  printf("global_m=%d\n",global_m);
  return 0;
}
```

together with the corresponding output:

```
global_m=1
in pass_by_reference: received m=1
in pass_by_reference: changed to m=42
global_m=42
```

3.4.3 Argument passing in Python

In Python, objects are passed as the value of a reference (think pointer) to the object. Depending on the way the reference is used in the function and depending on the type of object it references, this can result in pass-by-reference behaviour (where any changes to the object received as a function argument, are immediately reflected in the calling level).

Here are three examples to discuss this. We start by passing a list to a function which iterates through all elements in the sequence and doubles the value of each element:

[104]:
```
def double_the_values(l):
    print("in double_the_values: l = %s" % l)
    for i in range(len(l)):
        l[i] = l[i] * 2
    print("in double_the_values: changed l to l = %s" % l)

l_global = [0, 1, 2, 3, 10]
print("In main: s=%s" % l_global)
double_the_values(l_global)
print("In main: s=%s" % l_global)
```

```
In main: s=[0, 1, 2, 3, 10]
in double_the_values: l = [0, 1, 2, 3, 10]
in double_the_values: changed l to l = [0, 2, 4, 6, 20]
In main: s=[0, 2, 4, 6, 20]
```

The variable `l` is a reference to the list object. The line `l[i] = l[i] * 2` first evaluates the right-hand side and reads the element with index `i`, then multiplies this by two. A reference to this new object is then stored in the list object `l` at position with index `i`. We have thus modified the list object, that is referenced through `l`.

The reference to the list object does never change: the line `l[i] = l[i] * 2` changes the elements `l[i]` of the list `l` but never changes the reference `l` for the list. Thus both the function and calling level are operating on the same object through the references `l` and `global_l`, respectively.

In contrast, here is an example where do not modify the elements of the list within the function: which produces this output:

[105]:
```
def double_the_list(l):
    print("in double_the_list: l = %s" % l)
    l = l + l
    print("in double_the_list: changed l to l = %s" % l)

l_global = "Hello"
print("In main: l=%s" % l_global)
double_the_list(l_global)
print("In main: l=%s" % l_global)
```

```
In main: l=Hello
in double_the_list: l = Hello
in double_the_list: changed l to l = HelloHello
In main: l=Hello
```

What happens here is that during the evaluation of `l = l + l` a new object is created that holds `l + l`, and that we then bind the name `l` to it. In the process, we lose the references to the list object `l` that was given to the function (and thus we do not change the list object given to the function).

Finally, let's look at which produces this output:

[106]:
```
def double_the_value(l):
    print("in double_the_value: l = %s" % l)
    l = 2 * l
    print("in double_the_values: changed l to l = %s" % l)

l_global = 42
print("In main: s=%s" % l_global)
double_the_value(l_global)
print("In main: s=%s" % l_global)
```

```
In main: s=42
in double_the_value: l = 42
in double_the_values: changed l to l = 84
In main: s=42
```

In this example, we also double the value (from 42 to 84) within the function. However, when we bind the object 84 to the python name `l` (that is the line `l = l * 2`) we have created a new object

(84), and we bind the new object to `l`. In the process, we lose the reference to the object 42 within the function. This does not affect the object 42 itself, nor the reference `l_global` to it.

In summary, Python's behaviour of passing arguments to a function may appear to vary (if we view it from the pass by value versus pass by reference point of view). However, it is always call by value, where the value is a reference to the object in question, and the behaviour can be explained through the same reasoning in every case.

3.4.4 Performance considerations

Call by value function calls require copying of the value before it is passed to the function. From a performance point of view (both execution time and memory requirements), this can be an expensive process if the value is large. (Imagine the value is a `numpy.array` object which could be several Megabytes or Gigabytes in size.)

One generally prefers call by reference for large data objects as in this case only a pointer to the data objects is passed, independent of the actual size of the object, and thus this is generally faster than call-by-value.

Python's approach of (effectively) calling by reference is thus efficient. However, we need to be careful that our function do not modify the data they have been given where this is undesired.

3.4.5 Inadvertent modification of data

Generally, a function should not modify the data given as input to it.

For example, the following code demonstrates the attempt to determine the maximum value of a list, and – inadvertently – modifies the list in the process:

[107]:
```
def mymax(s):  # demonstrating side effect
    if len(s) == 0:
        raise ValueError('mymax() arg is an empty sequence')
    elif len(s) == 1:
        return s[0]
    else:
        for i in range(1, len(s)):
            if s[i] < s[i - 1]:
                s[i] = s[i - 1]
        return s[len(s) - 1]

s = [-45, 3, 6, 2, -1]
print("in main before caling mymax(s): s=%s" % s)
print("mymax(s)=%s" % mymax(s))
print("in main after calling mymax(s): s=%s" % s)
```

```
in main before caling mymax(s): s=[-45, 3, 6, 2, -1]
mymax(s)=6
in main after calling mymax(s): s=[-45, 3, 6, 6, 6]
```

The user of the `mymax()` function would not expect that the input argument is modified when the function executes. We should generally avoid this. There are several ways to find better solutions to the given problem:

- In this particular case, we could use the Python in-built function `max()` to obtain the maximum value of a sequence.

- If we felt we need to stick to storing temporary values inside the list [this is actually not necessary], we could create a copy of the incoming list `s` first, and then proceed with the algorithm (see Section **??** on Copying objects).
- Use another algorithm which uses an extra temporary variable rather than abusing the list for this. For example:
- We could pass a tuple (instead of a list) to the function: a tuple is *immutable* and can thus never be modified (this would result in an exception being raised when the function tries to write to elements in the tuple).

3.4.6 Copying objects

Python provides the `id()` function which returns an integer number that is unique for each object. (In the current CPython implementation, this is the memory address.) We can use this to identify whether two objects are the same.

To copy a sequence object (including lists), we can slice it, *i.e.* if `a` is a list, then `a[:]` will return a copy of `a`. Here is a demonstration:

[108]:
```
a = list(range(10))
a
```

[108]:
```
[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
```

[109]:
```
b = a
b[0] = 42
a               # changing b changes a
```

[109]:
```
[42, 1, 2, 3, 4, 5, 6, 7, 8, 9]
```

[110]:
```
# NBVAL_IGNORE_OUTPUT
id(a)
```

[110]:
```
4446565320
```

[111]:
```
# NBVAL_IGNORE_OUTPUT
id(b)
```

[111]:
```
4446565320
```

[112]:
```
# NBVAL_IGNORE_OUTPUT
c = a[:]
id(c)           # c is a different object
```

[112]:
```
4444418824
```

[113]:
```
c[0] = 100
a               # changing c does not affect a
```

[113]:
```
[42, 1, 2, 3, 4, 5, 6, 7, 8, 9]
```

Python's standard library provides the `copy` module, which provides copy functions that can be used to create copies of objects. We could have used `import copy; c = copy.deepcopy(a)` instead of `c = a[:]`.

3.5 Equality and Identity/Sameness

A related question concerns the equality of objects.

3.5.1 Equality

The operators <, >, ==, >=, <=, and != compare the *values* of two objects. The objects need not have the same type. For example:

[114]:
```
a = 1.0; b = 1
type(a)
```

[114]:
```
float
```

[115]:
```
type(b)
```

[115]:
```
int
```

[116]:
```
a == b
```

[116]:
```
True
```

So the == operator checks whether the values of two objects are equal.

3.5.2 Identity / Sameness

To see check whether two objects `a` and `b` are the same (i.e. `a` and `b` are references to the same place in memory), we can use the `is` operator (continued from example above):

[117]:
```
a is b
```

[117]:
```
False
```

Of course they are different here, as they are not of the same type.

We can also ask the `id` function which, according to the documentation string in Python 2.7 "*Returns the identity of an object. This is guaranteed to be unique among simultaneously existing objects. (Hint: it's the object's memory address.)*"

[118]:
```
# NBVAL_IGNORE_OUTPUT
id(a)
```

[118]:
```
4446045984
```

[119]:
```
# NBVAL_IGNORE_OUTPUT
id(b)
```

[119]:
```
4406101840
```

which shows that `a` and `b` are stored in different places in memory.

3.5.3 Example: Equality and identity

We close with an example involving lists:

[120]:
```
x = [0, 1, 2]
y = x
x == y
```

[120]:
```
True
```

[121]:
```
x is y
```

[121]:
```
True
```

[122]:
```
# NBVAL_IGNORE_OUTPUT
id(x)
```

[122]:
```
4445528520
```

[123]:
```
# NBVAL_IGNORE_OUTPUT
id(y)
```

[123]:
```
4445528520
```

Here, `x` and `y` are references to the same piece of memory, they are thus identical and the `is` operator confirms this. The important point to remember is that line 2 (`y=x`) creates a new reference `y` to the same list object that `x` is a reference for.

Accordingly, we can change elements of `x`, and `y` will change simultaneously as both `x` and `y` refer to the same object:

[124]:
```
x
```

[124]:
```
[0, 1, 2]
```

[125]:
```
y
```

[125]:
```
[0, 1, 2]
```

[126]:
```
x is y
```

[126]:
```
True
```

[127]:
```
x[0] = 100
y
```

[127]:
```
[100, 1, 2]
```

[128]:
```
x
```

[128]:
```
[100, 1, 2]
```

In contrast, if we use `z=x[:]` (instead of `z=x`) to create a new name `z`, then the slicing operation `x[:]` will actually create a copy of the list `x`, and the new reference `z` will point to the copy. The *value* of `x` and `z` is equal, but `x` and `z` are not the same object (they are not identical):

[129]:
```
x
```

[129]:
```
[100, 1, 2]
```

[130]:
```
z = x[:]            # create copy of x before assigning to z
z == x              # same value
```

[130]:
```
True
```

[131]:
```
z is x              # are not the same object
```

[131]:
```
False
```

[132]:
```
# NBVAL_IGNORE_OUTPUT
id(z)               # confirm by looking at ids
```

[132]:
```
4446678088
```

[133]:
```
# NBVAL_IGNORE_OUTPUT
id(x)
```

[133]:
```
4445528520
```

[134]:
```
x
```

[134]:
```
[100, 1, 2]
```

[135]:
```
z
```

[135]:
```
[100, 1, 2]
```

Consequently, we can change x without changing z, for example (continued)

[136]:
```
x[0] = 42
x
```

[136]:
```
[42, 1, 2]
```

[137]:
```
z
```

[137]:
```
[100, 1, 2]
```

4 Introspection

A Python code can ask and answer questions about itself and the objects it is manipulating.

4.1 dir()

`dir()` is a built-in function which returns a list of all the names belonging to some namespace.

- If no arguments are passed to dir (i.e. `dir()`), it inspects the namespace in which it was called.
- If `dir` is given an argument (i.e. `dir(<object>)`, then it inspects the namespace of the object which it was passed.

For example:

[1]:
```
# NBVAL_IGNORE_OUTPUT
apples = ['Cox', 'Braeburn', 'Jazz']
dir(apples)
```

[1]:
```
['__add__',
 '__class__',
 '__contains__',
 '__delattr__',
 '__delitem__',
 '__dir__',
 '__doc__',
 '__eq__',
 '__format__',
 '__ge__',
 '__getattribute__',
 '__getitem__',
 '__gt__',
 '__hash__',
 '__iadd__',
 '__imul__',
 '__init__',
 '__init_subclass__',
 '__iter__',
```

```
 '__le__',
 '__len__',
 '__lt__',
 '__mul__',
 '__ne__',
 '__new__',
 '__reduce__',
 '__reduce_ex__',
 '__repr__',
 '__reversed__',
 '__rmul__',
 '__setattr__',
 '__setitem__',
 '__sizeof__',
 '__str__',
 '__subclasshook__',
 'append',
 'clear',
 'copy',
 'count',
 'extend',
 'index',
 'insert',
 'pop',
 'remove',
 'reverse',
 'sort']
```

[1]:
```
# NBVAL_IGNORE_OUTPUT
dir()
```

[1]:
```
['In',
 'Out',
 '_',
 '__',
 '___',
 '__builtin__',
 '__builtins__',
 '__doc__',
 '__loader__',
 '__name__',
 '__package__',
 '__spec__',
 '_dh',
 '_i',
 '_i1',
 '_ih',
 '_ii',
 '_iii',
 '_oh',
```

```
 '_sh',
 'exit',
 'get_ipython',
 'quit']
```

[3]:
```
# NBVAL_IGNORE_OUTPUT
name = "Peter"
dir(name)
```

[3]:
```
['__add__',
 '__class__',
 '__contains__',
 '__delattr__',
 '__dir__',
 '__doc__',
 '__eq__',
 '__format__',
 '__ge__',
 '__getattribute__',
 '__getitem__',
 '__getnewargs__',
 '__gt__',
 '__hash__',
 '__init__',
 '__init_subclass__',
 '__iter__',
 '__le__',
 '__len__',
 '__lt__',
 '__mod__',
 '__mul__',
 '__ne__',
 '__new__',
 '__reduce__',
 '__reduce_ex__',
 '__repr__',
 '__rmod__',
 '__rmul__',
 '__setattr__',
 '__sizeof__',
 '__str__',
 '__subclasshook__',
 'capitalize',
 'casefold',
 'center',
 'count',
 'encode',
 'endswith',
 'expandtabs',
 'find',
```

```
'format',
'format_map',
'index',
'isalnum',
'isalpha',
'isdecimal',
'isdigit',
'isidentifier',
'islower',
'isnumeric',
'isprintable',
'isspace',
'istitle',
'isupper',
'join',
'ljust',
'lower',
'lstrip',
'maketrans',
'partition',
'replace',
'rfind',
'rindex',
'rjust',
'rpartition',
'rsplit',
'rstrip',
'split',
'splitlines',
'startswith',
'strip',
'swapcase',
'title',
'translate',
'upper',
'zfill']
```

4.1.1 Magic names

You will find many names which both start and end with a double underscore (e.g. `__name__`). These are called magic names. Functions with magic names provide the implementation of particular python functionality.

For example, the application of the `str` to an object `a`, i.e. `str(a)`, will – internally – result in the method `a.__str__()` being called. This method `__str__` generally needs to return a string. The idea is that the `__str__()` method should be defined for all objects (including those that derive from new classes that a programmer may create) so that all objects (independent of their type or class) can be printed using the `str()` function. The actual conversion of some object `x` to the string is then done via the object specific method `x.__str__()`.

We can demonstrate this by creating a class `my_int` which inherits from the Python's integer base class, and overrides the `__str__` method. (It requires more Python knowledge than provided up to

this point in the text to be able to understand this example.)

[4]:
```
class my_int(int):
    """Inherited from int"""
    def __str__(self):
        """Tailored str representation of my int"""
        return "my_int: %s" % (int.__str__(self))

a = my_int(3)
b = int(4)             # equivalent to b = 4
print("a * b = ", a * b)
print("Type a = ", type(a), "str(a) = ", str(a))
print("Type b = ", type(b), "str(b) = ", str(b))
```

```
a * b =  12
Type a =  <class '__main__.my_int'> str(a) =  my_int: 3
Type b =  <class 'int'> str(b) =  4
```

Further Reading See Python documentation, Data Model

4.2 type

The `type(<object>)` command returns the type of an object:

[5]:
```
type(1)
```

[5]:
```
int
```

[6]:
```
type(1.0)
```

[6]:
```
float
```

[7]:
```
type("Python")
```

[7]:
```
str
```

[8]:
```
import math
type(math)
```

[8]:
```
module
```

[9]:
```
type(math.sin)
```

[9]:
```
builtin_function_or_method
```

4.3 isinstance

`isinstance(<object>, <typespec>)` returns True if the given object is an instance of the given type, or any of its superclasses. Use `help(isinstance)` for the full syntax.

[10]:
```
isinstance(2,int)
```

[10]:
```
True
```

[11]:
```
isinstance(2.,int)
```

[11]:
```
False
```

[12]:
```
isinstance(a,int)    # a is an instance of my_int
```

[12]:
```
True
```

[13]:
```
type(a)
```

[13]:
```
__main__.my_int
```

4.4 help

- The `help(<object>)` function will report the docstring (magic attritube with name `__doc__`) of the object that it is given, sometimes complemented with additional information. In the case of functions, `help` will also show the list of arguments that the function accepts (but it cannot provide the return value).
- `help()` starts an interactive help environment.
- It is common to use the `help` command a lot to remind oneself of the syntax and semantic of commands.

[14]:
```
help(isinstance)
```

```
Help on built-in function isinstance in module builtins:

isinstance(obj, class_or_tuple, /)
    Return whether an object is an instance of a class or of a subclass thereof.

    A tuple, as in ``isinstance(x, (A, B, ...))``, may be given as the target to
    check against. This is equivalent to ``isinstance(x, A) or isinstance(x, B)
    or ...`` etc.
```

[15]:
```
# NBVAL_IGNORE_OUTPUT
import math
help(math.sin)
```

```
Help on built-in function sin in module math:

sin(...)
    sin(x)

    Return the sine of x (measured in radians).
```

[16]:
```
# NBVAL_IGNORE_OUTPUT
help(math)
```

```
Help on module math:

NAME
    math
```

```
MODULE REFERENCE
    https://docs.python.org/3.6/library/math

    The following documentation is automatically generated from the Python
    source files.  It may be incomplete, incorrect or include features that
    are considered implementation detail and may vary between Python
    implementations.  When in doubt, consult the module reference at the
    location listed above.

DESCRIPTION
    This module is always available.  It provides access to the
    mathematical functions defined by the C standard.

FUNCTIONS
    acos(...)
        acos(x)

        Return the arc cosine (measured in radians) of x.

    acosh(...)
        acosh(x)

        Return the inverse hyperbolic cosine of x.

    asin(...)
        asin(x)

        Return the arc sine (measured in radians) of x.

    asinh(...)
        asinh(x)

        Return the inverse hyperbolic sine of x.

    atan(...)
        atan(x)

        Return the arc tangent (measured in radians) of x.

    atan2(...)
        atan2(y, x)

        Return the arc tangent (measured in radians) of y/x.
        Unlike atan(y/x), the signs of both x and y are considered.

    atanh(...)
        atanh(x)

        Return the inverse hyperbolic tangent of x.
```

```
    ceil(...)
        ceil(x)

        Return the ceiling of x as an Integral.
        This is the smallest integer >= x.

    copysign(...)
        copysign(x, y)

        Return a float with the magnitude (absolute value) of x but the sign
        of y. On platforms that support signed zeros, copysign(1.0, -0.0)
        returns -1.0.

    cos(...)
        cos(x)

        Return the cosine of x (measured in radians).

    cosh(...)
        cosh(x)

        Return the hyperbolic cosine of x.

    degrees(...)
        degrees(x)

        Convert angle x from radians to degrees.

    erf(...)
        erf(x)

        Error function at x.

    erfc(...)
        erfc(x)

        Complementary error function at x.

    exp(...)
        exp(x)

        Return e raised to the power of x.

    expm1(...)
        expm1(x)

        Return exp(x)-1.
        This function avoids the loss of precision involved in the direct
evaluation of exp(x)-1 for small x.
```

```
fabs(...)
    fabs(x)

    Return the absolute value of the float x.

factorial(...)
    factorial(x) -> Integral

    Find x!. Raise a ValueError if x is negative or non-integral.

floor(...)
    floor(x)

    Return the floor of x as an Integral.
    This is the largest integer <= x.

fmod(...)
    fmod(x, y)

    Return fmod(x, y), according to platform C.  x % y may differ.

frexp(...)
    frexp(x)

    Return the mantissa and exponent of x, as pair (m, e).
    m is a float and e is an int, such that x = m * 2.**e.
    If x is 0, m and e are both 0.  Else 0.5 <= abs(m) < 1.0.

fsum(...)
    fsum(iterable)

    Return an accurate floating point sum of values in the iterable.
    Assumes IEEE-754 floating point arithmetic.

gamma(...)
    gamma(x)

    Gamma function at x.

gcd(...)
    gcd(x, y) -> int
    greatest common divisor of x and y

hypot(...)
    hypot(x, y)

    Return the Euclidean distance, sqrt(x*x + y*y).

isclose(...)
```

```
        isclose(a, b, *, rel_tol=1e-09, abs_tol=0.0) -> bool

        Determine whether two floating point numbers are close in value.

           rel_tol
               maximum difference for being considered "close", relative to the
               magnitude of the input values
            abs_tol
               maximum difference for being considered "close", regardless of
the
               magnitude of the input values

        Return True if a is close in value to b, and False otherwise.

        For the values to be considered close, the difference between them
        must be smaller than at least one of the tolerances.

        -inf, inf and NaN behave similarly to the IEEE 754 Standard.  That
        is, NaN is not close to anything, even itself.  inf and -inf are
        only close to themselves.

    isfinite(...)
        isfinite(x) -> bool

        Return True if x is neither an infinity nor a NaN, and False otherwise.

    isinf(...)
        isinf(x) -> bool

        Return True if x is a positive or negative infinity, and False
otherwise.

    isnan(...)
        isnan(x) -> bool

        Return True if x is a NaN (not a number), and False otherwise.

    ldexp(...)
        ldexp(x, i)

        Return x * (2**i).

    lgamma(...)
        lgamma(x)

        Natural logarithm of absolute value of Gamma function at x.

    log(...)
        log(x[, base])
```

```
        Return the logarithm of x to the given base.
        If the base not specified, returns the natural logarithm (base e) of x.

    log10(...)
        log10(x)

        Return the base 10 logarithm of x.

    log1p(...)
        log1p(x)

        Return the natural logarithm of 1+x (base e).
        The result is computed in a way which is accurate for x near zero.

    log2(...)
        log2(x)

        Return the base 2 logarithm of x.

    modf(...)
        modf(x)

        Return the fractional and integer parts of x.  Both results carry the
sign
        of x and are floats.

    pow(...)
        pow(x, y)

        Return x**y (x to the power of y).

    radians(...)
        radians(x)

        Convert angle x from degrees to radians.

    sin(...)
        sin(x)

        Return the sine of x (measured in radians).

    sinh(...)
        sinh(x)

        Return the hyperbolic sine of x.

    sqrt(...)
        sqrt(x)

        Return the square root of x.
```

```
    tan(...)
        tan(x)

        Return the tangent of x (measured in radians).

    tanh(...)
        tanh(x)

        Return the hyperbolic tangent of x.

    trunc(...)
        trunc(x:Real) -> Integral

        Truncates x to the nearest Integral toward 0. Uses the __trunc__ magic
method.

DATA
    e = 2.718281828459045
    inf = inf
    nan = nan
    pi = 3.141592653589793
    tau = 6.283185307179586

FILE
    /Users/fangohr/anaconda3/lib/python3.6/lib-
dynload/math.cpython-36m-darwin.so
```

The `help` function needs to be given the name of an object (which must exist in the current name space). For example pyhelp(math.sqrt) will not work if the `math` module has not been imported before

[17]:
```
# NBVAL_IGNORE_OUTPUT
help(math.sqrt)
```

```
Help on built-in function sqrt in module math:

sqrt(...)
    sqrt(x)

    Return the square root of x.
```

[18]:
```
# NBVAL_IGNORE_OUTPUT
import math
help(math.sqrt)
```

```
Help on built-in function sqrt in module math:
```

```
sqrt(...)
    sqrt(x)

    Return the square root of x.
```

Instead of importing the module, we could also have given the *string* of `math.sqrt` to the help function, i.e.:

[19]:
```
# NBVAL_IGNORE_OUTPUT
help('math.sqrt')
```

```
Help on built-in function sqrt in math:

math.sqrt = sqrt(...)
    sqrt(x)

    Return the square root of x.
```

`help` is a function which gives information about the object which is passed as its argument. Most things in Python (classes, functions, modules, etc.) are objects, and therefor can be passed to help. There are, however, some things on which you might like to ask for help, which are not existing Python objects. In such cases it is often possible to pass a string containing the name of the thing or concept to help, for example

- `help(modules)` will generate a list of all modules which can be imported into the current interpreter. Note that help(modules) (note absence of quotes) will result in a NameError (unless you are unlucky enough to have a variable called modules floating around, in which case you will get help on whatever that variable happens to refer to.)
- `help(some_module)`, where some_module is a module which has not been imported yet (and therefor isn't an object yet), will give you that module's help information.
- `help(some_keyword)`: For example `and`, `if` or `print` (*i.e.* `help(and)`, `help(if)` and `help(print)`). These are special words recognized by Python: they are not objects and thus cannot be passed as arguments to help. Passing the name of the keyword as a string to help works, but only if you have Python's HTML documentation installed, and the interpreter has been made aware of its location by setting the environment variable PYTHONDOCS.

4.5 Docstrings

The command `help(<object>)` accesses the documentation strings of objects.

Any literal string apparing as the first item in the definition of a class, function, method or module, is taken to be its *docstring*.

`help` includes the docstring in the information it displays about the object.

In addition to the docstring it may display some other information, for example, in the case of functions, it displays the function's signature.

The docstring is stored in the object's `__doc__` attribute.

[20]:
```
# NBVAL_IGNORE_OUTPUT
help(math.sin)
```

```
Help on built-in function sin in module math:

sin(...)
    sin(x)

    Return the sine of x (measured in radians).
```

[21]:
```
# NBVAL_IGNORE_OUTPUT
print(math.sin.__doc__)
```

```
sin(x)

Return the sine of x (measured in radians).
```

For user-defined functions, classes, types, modules, ...), one should always provide a docstring. Documenting a user-provided function:

[22]:
```
def power2and3(x):
    """Returns the tuple (x**2, x**3)"""
    return x**2 ,x**3

power2and3(2)
```

[22]:
```
(4, 8)
```

[23]:
```
power2and3(4.5)
```

[23]:
```
(20.25, 91.125)
```

[24]:
```
power2and3(0+1j)
```

[24]:
```
((-1+0j), (-0-1j))
```

[25]:
```
help(power2and3)
```

```
Help on function power2and3 in module __main__:

power2and3(x)
    Returns the tuple (x**2, x**3)
```

[26]:
```
print(power2and3.__doc__)
```

```
Returns the tuple (x**2, x**3)
```

5 Input and Output

In this section, we describe printing, which includes the use of the `print` function, the old-style `%` format specifiers and the new style `{}` format specifiers.

5.1 Printing to standard output (normally the screen)

The `print` function is the most commonly used command to print information to the "standard output device" which is normally the screen.

There are two modes to use print.

5.1.1 Simple print

The easiest way to use the print command is to list the variables to be printed, separated by comma. Here are a few examples:

[1]:
```
a = 10
b = 'test text'
print(a)
```

```
10
```

[2]:
```
print(b)
```

```
test text
```

[3]:
```
print(a, b)
```

```
10 test text
```

[4]:
```
print("The answer is", a)
```

```
The answer is 10
```

[5]:
```
print("The answer is", a, "and the string contains", b)
```

```
The answer is 10 and the string contains test text
```

[6]:
```
print("The answer is", a, "and the string reads", b)
```

```
The answer is 10 and the string reads test text
```

Python adds a space between every object that is being printed.

Python prints a new line after every print call. To suppress that, use the `end=` parameter:

[7]:
```
print("Printing in line one", end='')
print("...still printing in line one.")
```

```
Printing in line one...still printing in line one.
```

5.1.2 Formatted printing

The more sophisticated way of formatting output uses a syntax very similar to Matlab's `fprintf` (and therefor also similar to C's `printf`).

The overall structure is that there is a string containing format specifiers, followed by a percentage sign and a tuple that contains the variables to be printed in place of the format specifiers.

[8]:
```
print("a = %d b = %d" % (10,20))
```

```
a = 10 b = 20
```

A string can contain format identifiers (such as `%f` to format as a float, `%d` to format as an integer, and `%s` to format as a string):

[9]:
```
from math import pi
print("Pi = %5.2f" % pi)
```

```
Pi =  3.14
```

[10]:
```
print("Pi = %10.3f" % pi)
```

```
Pi =      3.142
```

[11]:
```
print("Pi = %10.8f" % pi)
```

```
Pi = 3.14159265
```

[12]:
```
print("Pi = %d" % pi)
```

```
Pi = 3
```

The format specifier of type `%W.Df` means that a Float should be printed with a total Width of `W` characters and `D` digits behind the Decimal point. (This is identical to Matlab and C, for example.)

To print more than one object, provide multiple format specifiers and list several objects in the tuple:

[13]:
```
print("Pi = %f, 142*pi = %f and pi^2 = %f." % (pi,142*pi,pi**2))
```

```
Pi = 3.141593, 142*pi = 446.106157 and pi^2 = 9.869604.
```

Note that the conversion of a format specifier and a tuple of variables into string does not rely on the `print` command:

[14]:
```
from math import pi
"pi = %f" % pi
```

[14]:
```
'pi = 3.141593'
```

This means that we can convert objects into strings whereever we need, and we can decide to print the strings later – there is no need to couple the formatting closely to the code that does the printing.

Overview of commonly used format specifiers using the astronomical unit as an example:

[15]:
```
AU = 149597870700  # astronomical unit [m]
"%f" % AU          # line 1 in table
```

[15]:
```
'149597870700.000000'
```

specifier	style	Example output for AU
%f	floating point	149597870700.000000
%e	exponential notation	1.495979e+11
%g	shorter of %e or %f	1.49598e+11
%d	integer	149597870700
%s	str()	149597870700
%r	repr()	149597870700L

5.1.3 "str" and "__str__"

All objects in Python should provide a method `__str__` which returns a nice string representation of the object. This method `a.__str__()` is called when we apply the `str` function to object `a`:

[16]:
```
a = 3.14
a.__str__()
```

[16]:
```
'3.14'
```

[17]:
```
str(a)
```

[17]:
```
'3.14'
```

The `str` function is extremely convenient as it allows us to print more complicated objects, such as

[18]:
```
b = [3, 4.2, ['apple', 'banana'], (0, 1)]
str(b)
```

[18]:
```
"[3, 4.2, ['apple', 'banana'], (0, 1)]"
```

The way Python prints this is that it uses the `__str__` method of the list object. This will print the opening square bracket `[` and then call the `__str__` method of the first object, i.e. the integer 3. This will produce 3. Then the list object's `__str__` method prints the comma `,` and moves on to call the `__str__` method of the next element in the list (i.e. `4.2`) to print itself. This way any composite object can be represented as a string by asking the objects it holds to convert themselves to strings.

The string method of object `x` is called implicitly, when we

- use the "%s" format specifier to print `x`
- pass the object `x` directly to the print command:

[19]:
```
print(b)
```

```
[3, 4.2, ['apple', 'banana'], (0, 1)]
```

[20]:
```
print("%s" % b)
```

```
[3, 4.2, ['apple', 'banana'], (0, 1)]
```

5.1.4 "repr" and "__repr__"

A second function, `repr`, should convert a given object into a string presentation *so that this string can be used to re-created the object using the `eval` function*. The `repr` function will generally provide a more detailed string than `str`. Applying `repr` to the object `x` will attempt to call `x.__repr__()`.

[21]:
```
from math import pi as a1
str(a1)
```

[21]:
```
'3.141592653589793'
```

[22]:
```
repr(a1)
```

[22]:
```
'3.141592653589793'
```

[23]:
```
number_as_string = repr(a1)
a2 = eval(number_as_string)  # evaluate string
a2
```

[23]:
```
3.141592653589793
```

[24]:
```
a2-a1                    # -> repr is exact representation
```

[24]:
```
0.0
```

[25]:
```
a1-eval(repr(a1))
```

[25]:
```
0.0
```

[26]:
```
a1-eval(str(a1))         # -> str has lost a few digits
```

[26]:
```
0.0
```

We can convert an object to its `str()` or `repr` presentation using the format specifiers `%s` and`%r`, respectively.

[27]:
```
import math
"%s" % math.pi
```

[27]:
```
'3.141592653589793'
```

[28]:
```
"%r" % math.pi
```

[28]:
```
'3.141592653589793'
```

5.1.5 New-style string formatting

A new system of built-in formatting allows more flexibility for complex cases, at the cost of being a bit longer.

Basic ideas in examples:

[29]:
```
"{} needs {} pints".format('Peter', 4)     # insert values in order
```

[29]:
```
'Peter needs 4 pints'
```

[30]:
```
"{0} needs {1} pints".format('Peter', 4)   # index which element
```

[30]:
```
'Peter needs 4 pints'
```

[31]:
```
"{1} needs {0} pints".format('Peter', 4)
```

[31]:
```
'4 needs Peter pints'
```

[32]:
```
"{name} needs {number} pints".format(    # reference element to
    name='Peter',number=4)               # print by name
```

[32]:
```
'Peter needs 4 pints'
```

[33]:
```
"Pi is approximately {:f}.".format(math.pi)      # can use old-style format␣
↪options for float
```

[33]:
```
'Pi is approximately 3.141593.'
```

[34]:
```
"Pi is approximately {:.2f}.".format(math.pi)    # and precision
```

[34]:
```
'Pi is approximately 3.14.'
```

[35]:
```
"Pi is approximately {:6.2f}.".format(math.pi)   # and width
```

[35]:
```
'Pi is approximately   3.14.'
```

This is a powerful and elegant way of string formatting, which is gradually being used more.

Further information

- Examples http://docs.python.org/library/string.html#format-examples
- Python Enhancement Proposal 3101
- Python library String Formatting Operations
- Old string formatting
- Introduction to Fancier Output Formatting, Python tutorial, section 7.1

5.1.6 Changes from Python 2 to Python 3: `print`

One (maybe the most obvious) change going from Python 2 to Python 3 is that the `print` command loses its special status. In Python 2, we could print "Hello World" using:

```
print "Hello world"              # valid in Python 2.x
```

Effectively, we call the function `print` with the argument `Hello World`. All other functions in Python are called such that the argument is enclosed in parentheses, i.e.

[36]:
```
print("Hello World")              # valid in Python 3.x
```

```
Hello World
```

This is the new convention *required* in Python 3 (and *allowed* for recent version of Python 2.x.)

Everything we have learned about formatting strings using the percentage operator still works the same way:

[37]:
```
import math
a = math.pi
"my pi = %f" % a           # string formatting
```

[37]:
```
'my pi = 3.141593'
```

[38]:
```
print("my pi = %f" % a)    # valid print in 2.7 and 3.x
```

```
my pi = 3.141593
```

[39]:
```
"Short pi = %.2f, longer pi = %.12f." % (a, a)
```

[39]:
```
'Short pi = 3.14, longer pi = 3.141592653590.'
```

[40]:
```
print("Short pi = %.2f, longer pi = %.12f." % (a, a))
```

```
Short pi = 3.14, longer pi = 3.141592653590.
```

[41]:
```
print("Short pi = %.2f, longer pi = %.12f." % (a, a))
```

```
Short pi = 3.14, longer pi = 3.141592653590.
```

[42]:
```
# 1. Write a file
out_file = open("test.txt", "w")          #'w' stands for Writing
out_file.write("Writing text to file. This is the first line.\n"+\
               "And the second line.")
out_file.close()                          #close the file

# 2. Read a file
in_file = open("test.txt", "r")           #'r' stands for Reading
text = in_file.read()                     #read complete file into
                                          #string variable text
in_file.close()                           #close the file

# 3. Display data
print(text)
```

```
Writing text to file. This is the first line.
And the second line.
```

5.2 Reading and writing files

Here is a program that

1. writes some text to a file with name `test.txt`,
2. and then reads the text again and
3. prints it to the screen.

The data stored in the file `test.txt` is:

```
Writing text to file. This is the first line.
And the second line.
```

In more detail, you have opened a file with the `open` command, and assigned this open file object to the variable `out_file`. We have then written data to the file using the `out_file.write` method. Note that in the example above, we have given a string to the `write` method. We can, of course, use all the formatting that we have discussed before—see Section **??** and Section **??**. For example, to write this file with name table `table.txt` we can use this Python program It is good practice to `close()` files when we have finished reading and writing. If a Python program is left in a controlled way (i.e. not through a power cut or an unlikely bug deep in the Python language or the operating system) then it will close all open files as soon as the file objects are destroyed. However, closing them actively as soon as possible is better style.

5.2.1 File reading examples

We use a file named `myfile.txt` containing the following 3 lines of text for the examples below:

```
This is the first line.
This is the second line.
This is a third and last line.
```

[43]:
```
f = open('myfile.txt', 'w')
f.write('This is the first line.\n'
        'This is the second line.\n'
        'This is a third and last line.')
f.close()
```

fileobject.read() The `fileobject.read()` method reads the whole file, and returns it as one string (including new line characters).

[44]:
```
f = open('myfile.txt', 'r')
f.read()
```

[44]:
```
'This is the first line.\nThis is the second line.\nThis is a third and last
line.'
```

[45]:
```
f.close()
```

fileobject.readlines() The `fileobject.readlines()` method returns a list of strings, where each element of the list corresponds to one line in the string:

[46]:
```
f = open('myfile.txt', 'r')
f.readlines()
```

[46]:
```
['This is the first line.\n',
 'This is the second line.\n',
 'This is a third and last line.']
```

[47]:
```
f.close()
```

This is often used to iterate over the lines, and to do something with each line. For example:

[48]:
```
f = open('myfile.txt', 'r')
for line in f.readlines():
    print("%d characters" % len(line))
f.close()
```

```
24 characters
25 characters
30 characters
```

Note that this will read the complete file into a list of strings when the `readlines()` method is called. This is no problem if we know that the file is small and will fit into the machine's memory.

If so, we can also close the file before we process the data, i.e.:

[49]:
```
f = open('myfile.txt', 'r')
lines = f.readlines()
f.close()
```

```
for line in lines:
    print("%d characters" % len(line))
```

```
24 characters
25 characters
30 characters
```

Iterating over lines (file object) There is a neater possibility to read a file line by line which (i) will only read one line at a time (and is thus suitable for large files as well) and (ii) results in more compact code:

[50]:
```
f = open('myfile.txt', 'r')
for line in f:
    print("%d characters" % len(line))
f.close()
```

```
24 characters
25 characters
30 characters
```

Here, the file handler `f` acts as in iterator and will return the next line in every subsequent iteration of the for-loop until the end of the file is reached (and then the for-loop is terminated).

Further reading Methods of File objects, Tutorial, Section 7.2.1

6 Control Flow

6.1 Basics

For a given file with a python program, the python interpreter will start at the top and then process the file. We demonstrate this with a simple program, for example:

[1]:
```
def f(x):
    """function that computes and returns x*x"""
    return x * x

print("Main program starts here")
print("4 * 4 = %s" % f(4))
print("In last line of program -- bye")
```

```
Main program starts here
4 * 4 = 16
In last line of program -- bye
```

The basic rule is that commands in a file (or function or any sequence of commands) is processed from top to bottom. If several commands are given in the same line (separated by ;), then these are processed from left to right (although it is discouraged to have multiple statements per line to maintain good readability of the code.)

In this example, the interpreter starts at the top (line 1). It finds the `def` keyword and remembers for the future that the function `f` is defined here. (It will not yet execute the function body, i.e. line 3

– this only happens when we call the function.) The interpreter can see from the indentation where the body of the function stops: the indentation in line 5 is different from that of the first line in the function body (line2), and thus the function body has ended, and execution should carry on with that line. (Empty lines do not matter for this analysis.)

In line 5 the interpreter will print the output `Main program starts here`. Then line 6 is executed. This contains the expression `f(4)` which will call the function `f(x)` which is defined in line 1 where `x` will take the value `4`. [Actually `x` is a reference to the object `4`.] The function `f` is then executed and computes and returns `4*4` in line 3. This value `16` is used in line 6 to replace `f(4)` and then the string representation `%s` of the object 16 is printed as part of the print command in line 6.

The interpreter then moves on to line 7 before the program ends.

We will now learn about different possibilities to direct this control flow further.

6.1.1 Conditionals

The python values `True` and `False` are special inbuilt objects:

[2]:
```
a = True
print(a)
```

```
True
```

[3]:
```
type(a)
```

[3]:
```
bool
```

[4]:
```
b = False
print(b)
```

```
False
```

[5]:
```
type(b)
```

[5]:
```
bool
```

We can operate with these two logical values using boolean logic, for example the logical and operation (`and`):

[6]:
```
True and True          #logical and operation
```

[6]:
```
True
```

[7]:
```
True and False
```

[7]:
```
False
```

[8]:
```
False and True
```

[8]:
```
False
```

[9]:
```
True and True
```

[9]:
```
True
```

[10]:
```
c = a and b
print(c)
```

```
False
```

There is also logical or (`or`) and the negation (`not`):

[11]:
```
True or False
```

[11]:
```
True
```

[12]:
```
not True
```

[12]:
```
False
```

[13]:
```
not False
```

[13]:
```
True
```

[14]:
```
True and not False
```

[14]:
```
True
```

In computer code, we often need to evaluate some expression that is either true or false (sometimes called a "predicate"). For example:

[15]:
```
x = 30          # assign 30 to x
x > 15          # is x greater than 15
```

[15]:
```
True
```

[16]:
```
x > 42
```

[16]:
```
False
```

[17]:
```
x == 30         # is x the same as 30?
```

[17]:
```
True
```

[18]:
```
x == 42
```

[18]:
```
False
```

[19]:
```
not x == 42     # is x not the same as 42?
```

[19]:
```
True
```

[20]:
```
x != 42         # is x not the same as 42?
```

[20]:
```
True
```

[21]:
```
x > 30          # is x greater than 30?
```

[21]:
```
False
```

[22]:
```
x >= 30  # is x greater than or equal to 30?
```

[22]:
```
True
```

6.2 If-then-else

Further information

- Introduction to If-then in Python tutorial, section 4.1

The `if` statement allows conditional execution of code, for example:

[23]:
```
a = 34
if a > 0:
    print("a is positive")
```

```
a is positive
```

The if-statement can also have an `else` branch which is executed if the condition is wrong:

[24]:
```
a = 34
if a > 0:
    print("a is positive")
else:
    print("a is non-positive (i.e. negative or zero)")
```

```
a is positive
```

Finally, there is the `elif` (read as "else if") keyword that allows checking for several (exclusive) possibilities:

[25]:
```
a = 17
if a == 0:
    print("a is zero")
elif a < 0:
    print("a is negative")
else:
    print("a is positive")
```

```
a is positive
```

6.3 For loop

Further information

- Introduction to for-loops in Python tutorial, section 4.2

The `for`-loop allows to iterate over a sequence (this could be a string or a list, for example). Here is an example:

[26]:
```
for animal in ['dog','cat','mouse']:
    print(animal, animal.upper())
```

```
dog DOG
cat CAT
mouse MOUSE
```

Together with the `range()` command (Section **??**), one can iterate over increasing integers:

[27]:
```
for i in range(5,10):
    print(i)
```

```
5
6
7
8
9
```

6.4 While loop

The `while` keyword allows to repeat an operation while a condition is true. Suppose we'd like to know for how many years we have to keep 100 pounds on a savings account to reach 200 pounds simply due to annual payment of interest at a rate of 5%. Here is a program to compute that this will take 15 years:

[28]:
```
mymoney = 100          # in GBP
rate = 1.05            # 5% interest
years = 0
while mymoney < 200:   # repeat until 20 pounds reached
    mymoney = mymoney * rate
    years = years + 1
print('We need', years, 'years to reach', mymoney, 'pounds.')
```

```
We need 15 years to reach 207.89281794113688 pounds.
```

6.5 Relational operators (comparisons) in `if` and `while` statements

The general form of `if` statements and `while` loops is the same: following the keyword `if` or `while`, there is a *condition* followed by a colon. In the next line, a new (and thus indented!) block of commands starts that is executed if the condition is True).

For example, the condition could be equality of two variables `a1` and `a2` which is expressed as `a1==a2`:

[29]:
```
a1 = 42
a2 = 42
if a1 == a2:
    print("a1 and a2 are the same")
```

```
a1 and a2 are the same
```

Another example is to test whether `a1` and `a2` are not the same. For this, we have two possibilities. Option number 1 uses the *inequality operator* `!=`:

[30]:
```
if a1 != a2:
    print("a1 and a2 are different")
```

Option two uses the keyword `not` in front of the condition:

[31]:
```
if not a1 == a2:
    print("a1 and a2 are different")
```

Comparisons for "greater" (>), "smaller" (<) and "greater equal" (>=) and "smaller equal" (<=) are straightforward.

Finally, we can use the logical operators "`and`" and "`or`" to combine conditions:

[32]:
```
if a > 10 and b > 20:
    print("A is greater than 10 and b is greater than 20")
if a > 10 or b < -5:
    print("Either a is greater than 10, or "
          "b is smaller than -5, or both.")
```

```
Either a is greater than 10, or b is smaller than -5, or both.
```

Use the Python prompt to experiment with these comparisons and logical expressions. For example:

[33]:
```
T = -12.5
if T < -20:
    print("very cold")

if T < -10:
    print("quite cold")
```

```
quite cold
```

[34]:
```
T < -20
```

[34]:
```
False
```

[35]:
```
T < -10
```

[35]:
```
True
```

6.6 Exceptions

Even if a statement or expression is syntactically correct, it may cause an error when an attempt is made to execute it. Errors detected during execution are called *exceptions* and are not necessarily fatal: exceptions can be *caught* and dealt with within the program. Most exceptions are not handled by programs, however, and result in error messages as shown here

[36]:
```
# NBVAL_RAISES_EXCEPTION
10 * (1/0)
```

```
---------------------------------------------------------------------------
ZeroDivisionError                         Traceback (most recent call last)

<ipython-input-36-9ce172bd90a7> in <module>()
----> 1 10 * (1/0)


ZeroDivisionError: division by zero
```

[8]:
```
# NBVAL_RAISES_EXCEPTION
4 + spam*3
```

```
---------------------------------------------------------------------------
NameError                                 Traceback (most recent call last)

<ipython-input-8-dc7ecd1cc0aa> in <module>()
  1 # NBVAL_RAISES_EXCEPTION
```

```
----> 2 4 + spam*3


    NameError: name 'spam' is not defined
```

[9]:
```
# NBVAL_SKIP
'2' + 2
```

```
    ---------------------------------------------------------------------------

    TypeError                                 Traceback (most recent call last)

    <ipython-input-9-3e373c48d944> in <module>()
      1 # NBVAL_RAISES_EXCEPTION
----> 2 '2' + 2


    TypeError: must be str, not int
```

Schematic exception catching with all options

[6]:
```
try:
    # code body
    pass
except ArithmeticError:
    # what to do if arithmetic error
    pass
except IndexError as the_exception:
    # the_exception refers to the exeption in this block
    pass
except:
    # what to do for ANY other exception
    pass
else:  # optional
    # what to do if no exception raised
    pass

try:
    # code body
    pass
finally:
    # what to do ALWAYS
    pass
```

Starting with Python 2.5, you can use the with statement to simplify the writing of code for some predefined functions, in particular the open function to open files: see http://docs.python.org/tutorial/errors.html#predefined-clean-up-actions.

Example: We try to open a file that does not exist, and Python will raise an exception of type IOError which stands for Input Output Error:

[7]:
```
# NBVAL_RAISES_EXCEPTION
f = open("filenamethatdoesnotexist", "r")
```

```
---------------------------------------------------------------------------

FileNotFoundError                         Traceback (most recent call last)

<ipython-input-7-1fcefadfdaf6> in <module>()
      1 # NBVAL_RAISES_EXCEPTION
----> 2 f = open("filenamethatdoesnotexist", "r")


FileNotFoundError: [Errno 2] No such file or directory:␣
↪'filenamethatdoesnotexist'
```

If we were writing an application with a userinterface where the user has to type or select a filename, we would not want to application to stop if the file does not exist. Instead, we need to catch this exception and act accordingly (for example by informing the user that a file with this filename does not exist and ask whether they want to try another file name). Here is the skeleton for catching this exception:

[41]:
```
try:
    f = open("filenamethatdoesnotexist","r")
except IOError:
    print("Could not open that file")
```

```
Could not open that file
```

There is a lot more to be said about exceptions and their use in larger programs. Start reading Python Tutorial Chapter 8: Errors and Exceptions if you are interested.

6.6.1 Raising Exceptions

Raising exception is also referred to as 'throwing an exception'.

Possibilities of raising an Exception

- `raise OverflowError`
- `raise OverflowError, Bath is full` (Old style, now discouraged)
- `raise OverflowError(Bath is full)`
- `e = OverflowError(Bath is full); raise e`

Exception hierarchy The standard exceptions are organized in an inheritance hierarchy e.g. OverflowError is a subclass of ArithmeticError (not BathroomError); this can be seen when looking at `help(exceptions)` for example.

You can derive your own exceptions from any of the standard ones. It is good style to have each module define its own base exception.

6.6.2 Creating our own exceptions

- You can and should derive your own exceptions from the built-in Exception.
- To see what built-in exceptions exist, look in the module exceptions (try `help(exceptions)`), or go to http://docs.python.org/library/exceptions.html#bltin-exceptions.

6.6.3 LBYL vs EAFP

- LBYL (Look Before You Leap) vs
- EAFP (Easer to ask forgiveness than permission)

[42]:
```
numerator = 7
denominator = 0
```

Example for LBYL:

[43]:
```
if denominator == 0:
    print("Oops")
else:
    print(numerator/denominator)
```

```
Oops
```

Easier to Ask for Forgiveness than Permission:

[44]:
```
try:
    print(numerator/denominator)
except ZeroDivisionError:
    print("Oops")
```

```
Oops
```

The Python documentation says about EAFP:

> Easier to ask for forgiveness than permission. This common Python coding style assumes the existence of valid keys or attributes and catches exceptions if the assumption proves false. This clean and fast style is characterized by the presence of many try and except statements. The technique contrasts with the LBYL style common to many other languages such as C.

Source: http://docs.python.org/glossary.html#term-eafp
The Python documentation says about LBYL:

> Look before you leap. This coding style explicitly tests for pre-conditions before making calls or lookups. This style contrasts with the EAFP approach and is characterized by the presence of many if statements.
>
> In a multi-threaded environment, the LBYL approach can risk introducing a race condition between "the looking" and "the leaping". For example, the code, if key in mapping: return mapping[key] can fail if another thread removes key from mapping after the test, but before the lookup. This issue can be solved with locks or by using the EAFP approach.

Source: http://docs.python.org/glossary.html#term-lbyl
EAFP is the Pythonic way.

7 Functions and modules

7.1 Introduction

Functions allow us to group a number of statements into a logical block. We communicate with a function through a clearly defined interface, providing certain parameters to the function, and receiving some information back. Apart from this interface, we generally do not how exactly a function does the work to obtain the value it returns

For example the function `math.sqrt`: we do not know how exactly it computes the square root, but we know about the interface: if we pass x into the function, it will return (an approximation of) $sqrtx$.

This abstraction is a useful thing: it is a common technique in engineering to break down a system into smaller (black-box) components that all work together through well defined interfaces, but which do not need to know about the internal realisations of each other's functionality. In fact, not having to care about these implementation details can help to have a clearer view of the system composed of many of these components.

Functions provide the basic building blocks of functionality in larger programs (and computer simulations), and help to control the inherent complexity of the process.

We can group functions together into a Python module (see Section **??**), and in this way create our own libraries of functionality.

7.2 Using functions

The word "function" has different meanings in mathematics and programming. In programming it refers to a named sequence of operations that perform a computation. For example, the function `sqrt()` which is defined in the `math` module computes the square root of a given value:

[1]:
```
from math import sqrt
sqrt(4)
```

[1]:
```
2.0
```

The value we pass to the function `sqrt` is 4 in this example. This value is called the *argument* of the function. A function may have more than one argument.

The function returns the value 2.0 (the result of its computation) to the "calling context". This value is called the *return value* of the function.

It is common to say that a function *takes* an argument and *returns* a result or return value.

Common confusion about printing and returning values It is a common beginner's mistake to confuse the *printing* of values with *returning* values. In the following example it is hard to see whether the function `math.sin` returns a value or whether it prints the value:

[2]:
```
import math
math.sin(2)
```

[2]:
```
0.9092974268256817
```

We import the `math` module, and call the `math.sin` function with an argument of `2`. The `math.sin(2)` call will actually *return* the value `0.909...` not print it. However, because we have not assigned the return value to a variable, the Python prompt will print the returned object.

The following alternative sequence works only if the value is returned:

[3]:
```
x = math.sin(2)
print(x)
```

```
0.9092974268256817
```

The return value of the function call `math.sin(2)` is assigned to the variable `x`, and `x` is printed in the next line.

Generally, functions should execute "silently" (i.e. not print anything) and report the result of their computation through the return value.

Part of the confusion about printed versus return values at the Python prompt comes from the Python prompt printing (a representation) of returned objects *if* the returned objects are not assigned. Generally, seeing the returned objects is exactly what we want (as we normally care about the returned object), just when learning Python this may cause mild confusion about functions returning values or printing values.

Further information

- Think Python has a gentle introduction to functions (on which the previous paragraph is based) in chapter 3 (Functions) and chapter 6 (Fruitful functions).

7.3 Defining functions

The generic format of a function definitions:

```
def my_function(arg1, arg2, ..., argn):
    """Optional docstring."""

    # Implementation of the function

    return result  # optional

#this is not part of the function
some_command
```

Allen Downey's terminology (in his book Think Python) of fruitful and fruitless functions distinguishes between functions that return a value, and those that do not return a value. The distinction refers to whether a function provides a return value (=fruitful) or whether the function does not explicitly return a value (=fruitless). If a function does not make use of the `return` statement, we tend to say that the function returns nothing (whereas in reality in will always return the `None` object when it terminates – even if the `return` statement is missing).

For example, the function `greeting` will print "Hello World" when called (and is fruitless as it does not return a value).

[4]:
```
def greeting():
    print("Hello World!")
```

If we call that function:

[5]:
```
greeting()
```

```
Hello World!
```

it prints "Hello World" to stdout, as we would expect. If we assign the return value of the function to a variable `x`, we can inspect it subsequently:

[6]:
```
x = greeting()
```

```
Hello World!
```

[7]:
```
print(x)
```

```
None
```

and find that the `greeting` function has indeed returned the `None` object.

Another example for a function that does not return any value (that means there is no `return` keyword in the function) would be:

[8]:
```
def printpluses(n):
    print(n * "+")
```

Generally, functions that return values are more useful as these can be used to assemble code (maybe as another function) by combining them cleverly. Let's look at some examples of functions that do return a value.

Suppose we need to define a function that computes the square of a given variable. The function source could be:

[9]:
```
def square(x):
    return x * x
```

The keyword `def` tells Python that we are *defining* a function at that point. The function takes one argument (`x`). The function returns `x*x` which is of course x^2. Here is the listing of a file that shows how the function can be defined and used: (note that the numbers on the left are line numbers and are not part of the program)

[10]:
```
def square(x):
    return x * x

for i in range(5):
    i_squared = square(i)
    print(i, '*', i, '=', i_squared)
```

```
0 * 0 = 0
1 * 1 = 1
2 * 2 = 4
3 * 3 = 9
4 * 4 = 16
```

It is worth mentioning that lines 1 and 2 define the square function whereas lines 4 to 6 are the main program.

We can define functions that take more than one argument:

[11]:
```
import math

def hypot(x, y):
    return math.sqrt(x * x + y * y)
```

It is also possible to return more than one argument. Here is an example of a function that converts a given string into all characters uppercase and all characters lowercase and returns the two versions. We have included the main program to show how this function can be called:

[12]:
```
def upperAndLower(string):
    return string.upper(), string.lower()

testword = 'Banana'
```

```
uppercase, lowercase = upperAndLower(testword)

print(testword, 'in lowercase:', lowercase,
      'and in uppercase', uppercase)
```

```
Banana in lowercase: banana and in uppercase BANANA
```

We can define multiple Python functions in one file. Here is an example with two functions:

[13]:
```
def returnstars( n ):
    return n * '*'

def print_centred_in_stars( string ):
    linelength = 46
    starstring = returnstars((linelength - len(string)) // 2)

    print(starstring + string + starstring)

print_centred_in_stars('Hello world!')
```

```
**********Hello world!**********
```

Further reading

- Python Tutorial: Section 4.6 Defining Functions

7.4 Default values and optional parameters

Python allows to define *default* values for function parameters. Here is an example: This program will print the following output when executed: So how does it work? The function `print_mult_table` takes two arguments: `n` and `upto`. The first argument `n` is a "normal" variable. The second argument `upto` has a default value of 10. In other words: should the user of this function only provide one argument, then this provides the value for `n` and `upto` will default to 10. If two arguments are provided, the first one will be for `n` and the second for `upto` (as shown in the code example above).

7.5 Modules

Modules

- Group together functionality
- Provide namespaces
- Python's standard library contains a vast collection of modules - "Batteries Included"
- Try `help(modules)`
- Means of extending Python

7.5.1 Importing modules

[14]:
```
import math
```

This will introduce the name `math` into the namespace in which the import command was issued. The names within the `math` module will not appear in the enclosing namespace: they must be accessed through the name `math`. For example: `math.sin`.

[15]:
```
import math, cmath
```

More than one module can be imported in the same statement, although the Python Style Guide recommends not to do this. Instead, we should write

[16]:
```
import math
import cmath

import math as mathematics
```

The name by which the module is known locally can be different from its "official" name. Typical uses of this are

- To avoid name clashes with existing names
- To change the name to something more manageable. For example `import SimpleHTTPServer as shs`. This is discouraged for production code (as longer meaningful names make programs far more understandable than short cryptic ones), but for interactively testing out ideas, being able to use a short synonym can make your life much easier. Given that (imported) modules are first class objects, you can, of course, simply do `shs = SimpleHTTPServer` in order to obtain the more easily typable handle on the module.

[17]:
```
from math import sin
```

This will import the `sin` function from the `math` module, but it will not introduce the name math into the current namespace. It will only introduce the name `sin` into the current namespace. It is possible to pull in more than one name from the module in one go:

[18]:
```
from math import sin, cos
```

Finally, let's look at this notation:

[19]:
```
from math import *
```

Once again, this does not introduce the name math into the current namespace. It does however introduce *all public names* of the math module into the current namespace. Broadly speaking, it is a bad idea to do this:

- Lots of new names will be dumped into the current namespace.
- Are you sure they will not clobber any names already present?
- It will be very difficult to trace where these names came from
- Having said that, some modules (including ones in the standard library, recommend that they be imported in this way). Use with caution!
- This is fine for interactive quick and dirty testing or small calculations.

7.5.2 Creating modules

A module is in principle nothing else than a python file. We create an example of a module file which is saved in `module1.py`:

"'

[20]:
```
%%file module1.py
def someusefulfunction():
    pass

print("My name is", __name__)
```

```
Overwriting module1.py
```

We can execute this (module) file as a normal python program (for example `python module1.py`):

[21]:
```
!python3 module1.py
```

```
My name is __main__
```

We note that the Python magic variable `__name__` takes the value `__main__` if the program file `module1.py` is executed.

On the other hand, we can *import* `module1.py` in another file (which could have the name `prog.py`), for example like this:

[22]:
```
import module1            #in file prog.py
```

```
My name is module1
```

When Python comes across the `import module1` statement in `prog.py`, it looks for the file `module1.py` in the current working directory (and if it can't find it there in all the directories in `sys.path`) and opens the file `module1.py`. While parsing the file `module1.py` from top to bottom, it will add any function definitions in this file into the `module1` name space in the calling context (that is the main program in `prog.py`). It this example, there is only the function `someusefulfunction`. Once the import process is completed, we can make use of `module1.someusefulfunction` in `prog.py`. If Python comes across statements other than function (and class) definitions while importing `module1.py`, it carries those out immediately. In this case, it will thus come across the statement `print(My name is, __name__)`.

Note the difference to the output if we *import* `module1.py` rather than executing it on its own: `__name__` inside a module takes the value of the module name if the file is imported.

7.5.3 Use of ___name___

In summary,

- `__name__` is `__main__` if the module file is run on its own
- `__name__` is the name of the module (i.e. the module filename without the `.py` suffix) if the module file is imported.

We can therefor use the following `if` statement in `module1.py` to write code that is *only run* when the module is executed on its own: This is useful to keep test programs or demonstrations of the abilities of a module in this "conditional" main program. It is common practice for any module files to have such a conditional main program which demonstrates its capabilities.

7.5.4 Example 1

The next example shows a main program for the another file `vectools.py` that is used to demonstrate the capabilities of the functions defined in that file:

[23]:
```
%%file vectools.py
from __future__ import division
import math

import numpy as N


def norm(x):
    """returns the magnitude of a vector x"""
    return math.sqrt(sum(x ** 2))


def unitvector(x):
    """returns a unit vector x/|x|. x needs to be a numpy array."""
    xnorm = norm(x)
    if xnorm == 0:
        raise ValueError("Can't normalise vector with length 0")
    return x / norm(x)


if __name__ == "__main__":
    #a little demo of how the functions in this module can be used:
    x1 = N.array([0, 1, 2])
    print("The norm of " + str(x1) + " is " + str(norm(x1)) + ".")
    print("The unitvector in direction of " + str(x1) + " is " \
        + str(unitvector(x1)) + ".")
```

```
Overwriting vectools.py
```

If this file is executed using `python vectools.py`, then `__name__==__main__` is true, and the output reads

[24]:
```
!python3 vectools.py
```

```
The norm of [0 1 2] is 2.23606797749979.
The unitvector in direction of [0 1 2] is [0.         0.4472136  0.89442719].
```

If this file is imported (i.e. used as a module) into another python file or the python prompt or in the Jupyter Notebook, then `__name__==__main__` is false, and that statement block will not be executed.

This is quite a common way to conditionally execute code in files providing library-like functions. The code that is executed if the file is run on its own, often consists of a series of tests (to check that the file's functions carry out the right operations – *regression tests* or *unit tests*), or some examples of how the library functions in the file can be used.

7.5.5 Example 2

Even if a Python program is not intended to be used as a module file, it is good practice to always use a conditional main program:

- often, it turns out later that functions in the file can be reused (and saves work then)