

Introduction to Python

GBS 746-VT – Introduction to Scientific Computing

February 20th, 2014

Emidio Capriotti

<http://biofold.org/emidio>



**Biomolecules
Folding and
Disease**

Division of Informatics
Department of Pathology

UAB

THE UNIVERSITY OF
ALABAMA AT BIRMINGHAM



Python



- Python high-level programming language. Its design philosophy **emphasizes code readability**, and allows programmers to **express concepts in few lines** of code.
- Python is an **object-oriented** language supporting **imperative and functional** programming.
- **Object-oriented** programming that represents concepts as "objects" that have data fields (attributes) and associated procedures known as methods.
- Python implementation was started at the end of 1989 by *Guido van Rossum*. Python 2.0 was released in 2000, with new features including a **full garbage collector** and support for Unicode.

The interpreter

The interpreter can be accessed typing python in the shell

```
emidio-imac:data emidio$ python
Python 2.7.6 (default, Nov 23 2013, 23:57:52)
[GCC 4.2.1 Compatible Apple LLVM 5.0 (clang-500.2.79)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

To exit from the interpreter environment Ctrl+D or exit()

The interactive interpreter: ipython

```
emidio-imac:data emidio$ ipython-2.7
Python 2.7.6 (default, Nov 23 2013, 23:57:52)
Type "copyright", "credits" or "license" for more information.

IPython 0.13.1 -- An enhanced Interactive Python.
?                -> Introduction and overview of IPython's features.
%quickref        -> Quick reference.
help             -> Python's own help system.
object?         -> Details about 'object', use 'object??' for extra details.
```

```
In [1]:
```

Rules for naming variables

A variable name have to start with a letter start with a number

```
>>> 2name=True
File "<stdin>", line 1
  2name=True
    ^
SyntaxError: invalid syntax<type 'bool'>
```

A variable can not be one of the 31 python keyword

```
>>> print="Hello world"
File "<stdin>", line 1
  print="Hello world"
    ^
SyntaxError: invalid syntax
```

A variable can not contain illegal characters

```
>>> you*=1
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
NameError: name 'you' is not defined
```

Basic variable types

The simplest type of variable in programming is the boolean

```
>>> bit=True
>>> type(bit)
<type 'bool'>
```

The simplest numeric variable is integer

```
>>> inum=1
>>> type(inum)
<type 'int'>
```

More complex numeric variable is float

```
>>> fnum=1.5
>>> type(fnum)
<type 'float'>
```

In python character variable does not exist.

```
>>> text='Hello World'
>>> type(text)
<type 'str'>
```

String variables

In low level program languages the **string is not a basic variable**. It is actually a group of concatenated characters.

In programming languages such as fortran the length of a string is fix. **In python a string can assume any length** and it do not need to be declared.

Python provides built-in functions for dealing with string

```
>>> text="Hello world!"
>>> print len(text)
12
>>> print text[0]
H
>>> print text[-1]
!
>>> print text[2:5]
llo
```

Convert variable types

- In python variables are **not explicitly declared** and are defined instantiation.
- Variable **types can be converted**. This procedure is referred as variable casting.
- In python **changing the variable type** can be a **source of error**.

Few example about how to modify variable type

```
>>> fnum=5.6
>>> int(fnum)
5
>>> inum=4
>>> float(inum)
4.0
>>> text="1024"
>>> int(text)
1024
```

Standard operators

The standard operators for numeric variables are:

```
>>> 2+2
4
>>> 2-2
0
>>> 2*3
6
>>> 7/2
3
>>> 7%2
1
>>> 2**3
8
```

Some of these operators works also for strings

```
>>> 'a'+ 'b'
'ab'
>>> 2*'a'
'aa'
```


Function

Function is a set of statements to perform a task.

```
def name(list of variables):  
    statements
```

The function consists of **two parts: the header and the body.**

- The **header** contains the **name and the list of variables**
- The **body** contains the **set of statements and is indented**

The **order** of the statements **defines the flow of execution.**

A **function can not be called before** it has been **defined**

Example write a function that write a name.

```
>>> def print_name(name):  
...     print "My name is",name  
...  
>>> print_name('Emidio')  
My name is Emidio
```

Compose functions

Write the a function that calculate the square value of a given n

```
>>> def square(x):  
...     return x**2  
...  
>>> square(3)  
9
```

The function can composed and we can calculate

```
>>> square(square(3))  
81
```

Python as **built-in functions** such as:

<code>abs(x)</code>	- absolute value
<code>pow(x,n)</code>	- power $x**n$
<code>max(x,y)</code>	- maximum between x,y
<code>min(x,y)</code>	- minimum between x,y

Import function

Functions and variables can imported from a python script

Define the following polynomial functions in poly.py script

```
k=2

def square(x):
    return x**2

def cubic (x)
    return pow(x,3)
```

Import the functions square and cubic and variable k

```
>>> from poly import square, cubic, k
```

Calculate the value of $kx^3 - x^2$ with $x=2$

```
>>> x=2
>>> k*cubic(x)-square(x)
12
```

if and operators

Basic structure of if in python. Also elif can be used.

```
if (condition 1):
    do something 1
elif (condition 2):
    do something 2
else:
    do something 3
```

Standard operators are ==, !=, >, >=, <, <= that can be combined with **and, or, not**

Write a function that check names for length and first characters

```
>>> def check_name(name,name_len,letter):
...     if (len(name)>=name_len and name[0]==letter):
...         return True
...     else:
...         return False
...
>>> print chech_name('Goofy',5,'G')
True
```

for and while loops

Basic structure of the **for and while loop** in python.

```
for i in list:
    do something          # Indentation is needed

while (condition):
    do something          # Indentation is needed
```

Build a function that takes a text variable and print all the letters

```
>>> def print_for_letters(text):
...     for i in text:
...         print i

>>> def print_while_letters(text):
...     i=0
...     while i<len(text):
...         print text[i]
...         i+=1
```

Exercise 1

Write a function that takes in **input a string and a character** and find the position in the string that first match the character

Use the while loop

```
>>> def find(text, character):
...     i=0
...     while i<len(text)
...         if text[i]==character:
...             return i
...         else:
...             i+=1
...     return -1

>>> def find('Goofy','o')
1
```

The function find() returns same result

```
>>> 'Goofy'.find('o')
```

Important modules

The module sys

access to some variables used or maintained by the interpreter and to functions that interact strongly with the interpreter.

```
>>> import sys
>>> sys.argv[0]
```

The module math

provide standard mathematics functions

```
>>> import math
>>> math.pi
3.141592653589793

>>> math.sqrt(2)
>>> 1.4142135623730951
```

Exercise 2

Write the first python script to address the following problems

1. Count the number of vowels. The script takes in input a string and print the number of vowels
2. Write similar script that takes in input a string and a character and calculates the number matching characters.

Use the function `upper()` to compare string in uppercase

```
>>> text='abc'  
text.upper()  
ABC
```

Include `sys.argv[2]` variable to provide the character.

```
import sys  
sys.argv[2]
```