intro_Python

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1 A Introduction to Python for dummies...

This is part of the Python lecture given by Veronica Gomez Llanos and Christophe Morisset at IA-UNAM.

1.0.1 Using Python as a calculator

Using of "print" command is not necesary to obtain a result. Just type some operations and the result is obtain with ENTER.

Python likes the use of spaces to make scripts more readable

The art of writing good python code is described in the following document: http://legacy.python.org/dev/peps/pep-0008/

1.0.2 Assignments

Like any other langage, you can assign a value to a variable. This is done with = symbol:

```
In [5]: a = 4
```

A lot of operations can be performed on the variables. The most basics are for example:

```
In [6]: a
```

Some variable name are not available, they are reserved to python itself: and, as, assert, break, class, continue, def, del, elif, else, except, exec, finally, for, from, global, if, import, in, is, lambda, not, or, pass, print, raise, return, try, while, with, yield

```
In [10]: lambda_ = 2
    file = 3
```

1.0.3 Comments

Out[12]: 'This is a large comment\non multiple lines\nending as it started\n'

1.0.4 Types

The types used in Python are: integers, long integers, floats (double prec.), complexes, strings, booleans.

Double precision: machine dependent, generally between 10⁻-308 and 10⁻308, with 16 significant digits.

The function type gives the type of its argument:

```
In [13]: type(2)
Out[13]: int
In [14]: type(2.3)
Out[14]: float
In [15]: int(0.8) # truncating
Out[15]: O
In [16]: round(0.8765566777) # nearest, result is integer (was float with python 2.N)
Out[16]: 1
```

1.0.5 Complex numbers

```
In [17]: a = 1.5 + 0.5j
In [18]: a**2.
Out[18]: (2+1.5j)
In [19]: (1+2j)*(1-2j)
Out[19]: (5+0j)
In [20]: a.real
Out[20]: 1.5
In [21]: (a**3).imag
Out[21]: 3.25
In [22]: a.conjugate() # this is a function, it requieres ()
Out[22]: (1.5-0.5j)
1.0.6 Booleans
Comparison operators are <, >, <=, >=, !=
In [23]: 5 < 3
Out[23]: False
In [24]: a = 5
         b = 7
In [25]: b < a
Out[25]: False
In [26]: c = 2
In [27]: c < a < b
Out[27]: True
In [28]: a < b and b < c
Out[28]: False
In [29]: res = a < 7
         print(res, type(res))
```

```
True <class 'bool'>
In [30]: print(int(res))
         print(int(not res))
1
0
In [31]: not res is True
Out[31]: False
In [32]: a = True
         print(a)
True
1.0.7 Formating strings
In [33]: print("Hello world!")
Hello world!
In [34]: print('Hello world!')
Hello world!
In [35]: print("Hello I'm here") # ' inside ""
Hello I'm here
In [36]: # This is the old fashion way of formating outputs (C-style)
         a = 7.5
         b = 'tralala'
         c = 8.9e-33
         print('a = \%f, b = \%s, c = \%e' \% (a, b, c))
a = 7.500000, b = tralala, c = 8.900000e-33
In [37]: # The new way is using the format() method of the string object, and {} to define which
         print('a = {} \& b = {} \& c = {} \)'\'.format(a,b,c))
         print('a = \{0\}, b = \{1\}, c = \{2\}'.format(a**2,b,c))
         print('a = {:f}, b = {:20s}, c = {:15.3e}'.format(a,b,c))
a = 7.5 \& b = tralala \& c = 8.9e-33 \setminus
a = 56.25, b = tralala, c = 8.9e-33
                                       , c =
a = 7.500000, b = tralala
                                                    8.900e-33
```

Much more on this here: https://docs.python.org/3/tutorial/inputoutput.html

1.0.8 Strings

```
In [38]: a = "this is a string"
In [39]: len(a)
Out[39]: 19
```

A lot of commands can operate on strings. Strings, like ANYTHING in python, are objects. Methods are run on objects by dots:

```
In [40]: a.upper()
Out[40]: 'THIS IS A
                       STRING'
In [41]: a.title()
Out[41]: 'This Is A
                       String'
In [42]: a.split()
Out[42]: ['this', 'is', 'a', 'string']
In [43]: a.split()[1]
Out[43]: 'is'
In [44]: a = "This is a string. With various sentences."
In [45]: a.split('.')
Out[45]: ['This is a string', ' With various sentences', '']
In [46]: a.split('.')[1].strip() # Here we define the character used to split. The default is sp
Out [46]: 'With various sentences'
In [47]: a = 'tra'
        b = 'la'
         print(' '.join((a,b,b)))
         print('-'.join((a,b,b)))
        print(''.join((a,b,b)))
        print(a+b+b)
         print(' '.join((a,b,b)).split())
        print(' & '.join((a,b,b)) + '\\\')
tra la la
tra-la-la
tralala
tralala
['tra', 'la', 'la']
tra & la & la\\
```

1.0.9 Containers: Tuples, Lists and Dictionaries

list: a collection of objects. May be of different types. It has an order.

```
In [48]: L = ['red', 'green', 'blue'] # squared brackets are used to define lists
In [49]: type(L) # Print the type of L
Out[49]: list
In [50]: L[1]
Out [50]: 'green'
In [51]: L[0] # indexes start at 0 !!!
Out[51]: 'red'
In [52]: L[-1] # last element
Out[52]: 'blue'
In [53]: L[-3]
Out [53]: 'red'
In [54]: L = L + ['black', 'white'] # addition symbol is used to agregate values to a list. See
In [55]: print(L)
['red', 'green', 'blue', 'black', 'white']
In [56]: L[1:3] \# L[start:stop] : elements if index i, where start <= i < stop !! stop not inclu
Out[56]: ['green', 'blue']
In [57]: L[2:] # boudaries can be omited
Out[57]: ['blue', 'black', 'white']
In [58]: L[-2:]
Out[58]: ['black', 'white']
In [59]: L[::2] # L[start:stop:step] every 2 elements
Out[59]: ['red', 'blue', 'white']
In [60]: L[::-1]
Out[60]: ['white', 'black', 'blue', 'green', 'red']
```

Lists are mutable: their content can be modified.

```
In [61]: L[2] = 'yellow'
        L
Out[61]: ['red', 'green', 'yellow', 'black', 'white']
In [62]: L.append('pink') # append a value at the end
Out[62]: ['red', 'green', 'yellow', 'black', 'white', 'pink']
In [63]: L.insert(2, 'blue') #L.insert(index, object) -- insert object before index
        L
Out[63]: ['red', 'green', 'blue', 'yellow', 'black', 'white', 'pink']
In [64]: L.extend(['magenta', 'purple'])
Out[64]: ['red',
          'green',
          'blue',
          'yellow',
          'black',
          'white',
          'pink',
          'magenta',
          'purple']
In [65]: L.append(['magenta', 'azul'])
        L
Out[65]: ['red',
          'green',
          'blue',
          'yellow',
          'black',
          'white',
          'pink',
          'magenta',
          'purple',
          ['magenta', 'azul']]
In [66]: L.append(2)
        L
Out[66]: ['red',
          'green',
          'blue',
```

```
'yellow',
          'black',
          'white',
          'pink',
          'magenta',
          'purple',
          ['magenta', 'azul'],
          21
In [67]: L = L[::-1] # reverse order
Out[67]: [2,
          ['magenta', 'azul'],
          'purple',
          'magenta',
          'pink',
          'white',
          'black',
          'yellow',
          'blue',
          'green',
          'red']
In [68]: L2 = L[:-3] # cutting the last 3 elements
         print(L)
         print(L2)
[2, ['magenta', 'azul'], 'purple', 'magenta', 'pink', 'white', 'black', 'yellow', 'blue', 'green
[2, ['magenta', 'azul'], 'purple', 'magenta', 'pink', 'white', 'black', 'yellow']
In [69]: L[25] # Out of range leads to error
        IndexError
                                                   Traceback (most recent call last)
        <ipython-input-69-c16babb9288f> in <module>()
    ----> 1 L[25] # Out of range leads to error
        IndexError: list index out of range
In [70]: print(L)
        print(L[20:25]) # But NO ERROR when slicing.
         print(L[20:])
         print(L[2:20])
```

```
[2, ['magenta', 'azul'], 'purple', 'magenta', 'pink', 'white', 'black', 'yellow', 'blue', 'green
['purple', 'magenta', 'pink', 'white', 'black', 'yellow', 'blue', 'green', 'red']
In [71]: print(L.count('yellow'))
1
In [72]: L2 = L[2:20]
         L2.sort() # One can use TAB to look for the methods (functions that apply to an object)
        print(L2)
['black', 'blue', 'green', 'magenta', 'pink', 'purple', 'red', 'white', 'yellow']
In [73]: a = [1,2,3]
        b = [10, 20, 30]
In [74]: print(a+b) # may not be what you expected, but rather logical too
[1, 2, 3, 10, 20, 30]
In [75]: print(a*b) # Does NOT multiply element by element. Numpy will do this job.
        TypeError
                                                  Traceback (most recent call last)
        <ipython-input-75-ddfd21d938fe> in <module>()
    ----> 1 print(a*b) # Does NOT multiply element by element. Numpy will do this job.
        TypeError: can't multiply sequence by non-int of type 'list'
In [76]: L = range(4) # Create an interator. Notice the parameter is the number of elements, not
         print(L) # In python 2, that was a lit
        print(list(L))
range(0, 4)
[0, 1, 2, 3]
In [77]: L = range(2, 20, 2) # every 2 integer
```

print(L)

```
The types os the elements of a list are not always the same:
In [78]: L = [1, '1', 1.4]
Out[78]: [1, '1', 1.4]
   Remove the n+1-th element:
In [79]: L = list(range(0,20,2))
         print(L)
         del(L[5])
         print(L)
[0, 2, 4, 6, 8, 10, 12, 14, 16, 18]
[0, 2, 4, 6, 8, 12, 14, 16, 18]
   Slicing: extracting sub-list of a list
In [80]: a = [[1, 2, 3], [10, 20, 30], [100, 200, 300]] # Not a 2D table, but rather a table of
         print(a)
         print(a[0])
         print(a[1][1])
[[1, 2, 3], [10, 20, 30], [100, 200, 300]]
[1, 2, 3]
20
In [81]: print(a[1,1]) # Does NOT work
        TypeError
                                                    Traceback (most recent call last)
        <ipython-input-81-d8214b6adea8> in <module>()
    ---> 1 print(a[1,1]) # Does NOT work
        TypeError: list indices must be integers or slices, not tuple
In [82]: b = a[1]
         print(b)
```

range(2, 20, 2)

```
[10, 20, 30]
In [83]: b[1] = 999 \# Changing the value of a single element
         print(b)
[10, 999, 30]
In [84]: print(a) # Changing b changed a !!!
[[1, 2, 3], [10, 999, 30], [100, 200, 300]]
In [85]: b[1] is a[1][1]
Out[85]: True
In [86]: c = a[1][::] \# copy instead of slicing
         print(c)
         c[0] = 77777
         print(c)
         print(a)
[10, 999, 30]
[77777, 999, 30]
[[1, 2, 3], [10, 999, 30], [100, 200, 300]]
tuples: like lists, but inmutables
In [87]: T = (1,2,3)
         Т
Out[87]: (1, 2, 3)
In [88]: T2 = 1, 2, 3
         print(T2)
         type(T2)
(1, 2, 3)
Out[88]: tuple
In [89]: T[1]
Out[89]: 2
```

tuples are unmutables

```
In [90]: T[1] = 3 # Does NOT work!
       ______
       TypeError
                                               Traceback (most recent call last)
       <ipython-input-90-6dd68cc28786> in <module>()
   ----> 1 T[1] = 3 # Does NOT work!
       TypeError: 'tuple' object does not support item assignment
Dictionnaries A dictionary is basically an efficient table that maps keys to values. It is an un-
ordered container
In [91]: D = {'Christophe': 12, 'Antonio': 15} # defined by {key : value}
In [92]: D['Christophe'] # access to a value by the key
Out[92]: 12
In [93]: D.keys() # list of the dictionary keys
Out[93]: dict_keys(['Christophe', 'Antonio'])
In [94]: D['Yilen'] = 16 # adding a new entry
In [95]: print(D)
{'Christophe': 12, 'Antonio': 15, 'Yilen': 16}
In [96]: print(D[0]) # use the keys to acces the elements. No order in dictionnary.
       KeyError
                                               Traceback (most recent call last)
       <ipython-input-96-035806c13f20> in <module>()
   ---> 1 print(D[0]) # use the keys to acces the elements. No order in dictionnary.
```

KeyError: 0

1.0.10 Blocks

S 32

```
Blocks are defined by indentation. Looks nice and no needs for end :-)
In [97]: for i in [1,2,3]: print(i) # compact way, not recomended.
1
2
3
In [98]: for cosa in [1,'ff',2]:
             print(cosa)
             print('end')
         print('final end') # end of the identation means end of the block
1
end
ff
end
2
end
final end
In [99]: # defining a dictionary:
         ATOMIC_MASS = {}
         ATOMIC_MASS['H'] = 1
         ATOMIC_MASS['He'] = 4
         ATOMIC_MASS['C'] = 12
         ATOMIC_MASS['N'] = 14
         ATOMIC_MASS['O'] = 16
         ATOMIC_MASS['Ne'] = 20
         ATOMIC_MASS['Ar'] = 40
         ATOMIC_MASS['S'] = 32
         ATOMIC_MASS['Si'] = 28
         ATOMIC_MASS['Fe'] = 55.8
         # Print the keys and values from the dictionary. As it is not ordered , they come as the
         for key in ATOMIC_MASS.keys():
             print(key, ATOMIC_MASS[key])
H 1
He 4
C 12
N 14
0 16
Ne 20
Ar 40
```

```
Si 28
Fe 55.8
```

```
In [100]: for key in sorted(ATOMIC_MASS): # sorting using the keys
              print('Element: {0:3s} Atomic Mass: {1}'.format(key, ATOMIC_MASS[key]))
Element: Ar
              Atomic Mass: 40
Element: C
              Atomic Mass: 12
Element: Fe
             Atomic Mass: 55.8
Element: H
             Atomic Mass: 1
Element: He
             Atomic Mass: 4
              Atomic Mass: 14
Element: N
Element: Ne
             Atomic Mass: 20
Element: 0
             Atomic Mass: 16
Element: S
              Atomic Mass: 32
              Atomic Mass: 28
Element: Si
```

a key parameter can be used to specify a function to be called on each list element prior to making comparisons. More in sorted function here: https://wiki.python.org/moin/HowTo/Sorting or here: http://www.pythoncentral.io/how-to-sort-a-list-tuple-or-object-with-sorted-in-python/

In [101]: for elem in sorted(ATOMIC_MASS, key = ATOMIC_MASS.get): # sorting using the values

```
print('Element: {0:3s} Atomic Mass: {1}'.format(elem, ATOMIC_MASS[elem]))
Element: H
              Atomic Mass: 1
Element: He
             Atomic Mass: 4
Element: C
             Atomic Mass: 12
Element: N
             Atomic Mass: 14
Element: 0
             Atomic Mass: 16
Element: Ne Atomic Mass: 20
             Atomic Mass: 28
Element: Si
Element: S
             Atomic Mass: 32
Element: Ar Atomic Mass: 40
Element: Fe
              Atomic Mass: 55.8
In [102]: for idx, elem in enumerate(sorted(ATOMIC_MASS, key = ATOMIC_MASS.get)): # adding an in
              print('{0:2} Element: {1:2s} Atomic Mass: {2:4.1f}'.format(idx+1, elem, ATOMIC_MA
 1 Element: H
                Atomic Mass: 1.0
 2 Element: He Atomic Mass:
                             4.0
 3 Element: C
                Atomic Mass: 12.0
 4 Element: N
                Atomic Mass: 14.0
 5 Element: 0
               Atomic Mass: 16.0
```

6 Element: Ne Atomic Mass: 20.0 7 Element: Si Atomic Mass: 28.0 8 Element: S Atomic Mass: 32.0

```
9 Element: Ar Atomic Mass: 40.0
10 Element: Fe Atomic Mass: 55.8
In [103]: for i in range(10):
              if i > 5:
                  print(i)
6
7
8
9
In [104]: for i in range(10):
              if i > 5:
                  print(i)
              else:
                  print('i lower than five')
          print('END')
i lower than five
7
8
9
END
```

Other commands are: if...elif...else AND while...

1.0.11 List and dictionnary comprehension

```
[0, 1, 4, 9]
In [107]: # The same is also used for dictionnaries
          D = \{ 'squared_{\{\}'} . format(k) : k**2 for k in range(10) \}
          print(D)
{'squared_0': 0, 'squared_1': 1, 'squared_2': 4, 'squared_3': 9, 'squared_4': 16, 'squared_5': 2
1.0.12 Functions, procedures
In [108]: def func1(x):
              print(x**3)
          func1(5)
125
In [109]: def func2(x,
                    y):
              Return the cube and the 4th power of the two parameters
              return(x**3, y**4)
          a = func2(3, 5)
          help(func2)
Help on function func2 in module __main__:
func2(x, y)
    Return the cube and the 4th power of the two parameters
In [110]: #func2() shift-TAB inside the parenthesis
          func2?
In [111]: print(a)
          print(func2(4, 6))
(27, 625)
(64, 1296)
In [112]: def func3(x, y, z, a=0, b=1):
              This function has 5 arguments, 2 of them have default values (then not mandatory)
```

```
11 11 11
              return a + b * (x**2 + y**2 + z**2)**0.5
          D = func3(3, 4, 5)
          print(D)
7.0710678118654755
In [113]: E = func3(3, 4, 5, 10, 100)
          print(E)
717.1067811865476
In [114]: F = func3(x=3, y=4, z=5, a=10, b=100)
          print(F)
717.1067811865476
In [115]: G = func3(3, 4, 5, a=10, 100) # ERROR!
          print(G)
          File "<ipython-input-115-7963f4c1b801>", line 1
        G = func3(3, 4, 5, a=10, 100) # ERROR!
    SyntaxError: positional argument follows keyword argument
In [116]: H = func3(3, 4, 5, a=10, b=100)
          print(H)
717.1067811865476
In [117]: I = func3(z=5, x=3, y=4, a=10, b=100) # quite risky!
          print(I)
717.1067811865476
   Lambda function is used to creat simple (single line) functions:
In [118]: J = lambda x, y, z: (x**2 + y**2 + z**2)**0.5
          J(1,2,3)
Out[118]: 3.7416573867739413
```

Changing the value of variable inside a routine Parameters to functions are references to objects, which are passed by value. When you pass a variable to a function, python passes the reference to the object to which the variable refers (the value). Not the variable itself. If the value is immutable, the function does not modify the caller's variable. If the value is mutable, the function may modify the caller's variable in-place, if a mutation of the variable is done (not if a new mutable value is assigned):

```
In [121]: def try_to_modify(x, y, z):
              x = 23
              y.append(22)
              z = [29] # new reference
                       IN THE ROUTINE')
              print('
              print(x)
              print(y)
              print(z)
          # The values of a, b and c are set
          a = 77
          b = [79]
          c = [78]
          print('
                    INIT')
          print(a)
          print(b)
          print(c)
          try_to_modify(a, b, c)
          print('
                    AFTER THE ROUTINE')
          print(a)
          print(b)
          print(c)
   INIT
77
[79]
[78]
```

```
IN THE ROUTINE
23
[79, 22]
[29]
   AFTER THE ROUTINE
77
[79, 22]
[78]
```

Variables from outside (from a level above) are known:

```
In [122]: a = 5
          def test_a(x):
              print(a*x)
          test_a(5)
          a = 10
          test_a(5)
          print(a)
25
50
10
In [123]: # This works even if a2 is not known when defining the function:
          def test_a2(x):
             print(a2*x)
          a2 = 10
          test_a2(5)
50
```

Variables from inside are unknown outside:

5

NameError

Traceback (most recent call last)

```
<ipython-input-124-edf2e6190ece> in <module>()
              print(g2)
         4 test_g2()
   ---> 5 print(g2)
       NameError: name 'g2' is not defined
Global variable is known outside:
In [125]: def test_g3():
            global g3
            g3 = 5
            print(g3)
         test_g3()
         print(g3)
Recursivity
In [126]: def fact(n):
            if n <= 0:
                return 1
            return n*fact(n-1)
         print(fact(5))
         print(fact(8))
         print(fact(50))
120
40320
1.0.13 Scripting
In [127]: %%writefile ex1.py
         #!/usr/bin/env python
         # -*- coding: utf-8 -*-
         def f1(x):
             11 11 11
             This is an example of a function, that returns x^2
             - parameter: x
             11 11 11
```

5 5

return x**2

```
Overwriting ex1.py
```

```
In [128]: #We have created a script named ex1.py, to see inside the script we use:
    !cat ex1.py

#!/usr/bin/env python
# -*- coding: utf-8 -*-
def f1(x):
    """
    This is an example of a function, that returns x^2
    - parameter: x
    """
    return x**2
```

The first two lines of the ex1.py script are used to: tell the computer that this is python code, and to use special characters, respectively.

There are different ways to use the functions defined in a script

1.0.14 Importing libraries

Not all the power of python is available when we call (i)python. Some additional libraries (included in the python package, or as additional packages, like numpy) can be imported to increase the capacities of python. This is the case of the math library:

```
In [134]: print(sin(3.))
        NameError
                                                  Traceback (most recent call last)
        <ipython-input-134-3774d5a0e3c9> in <module>()
    ---> 1 print(sin(3.))
        NameError: name 'sin' is not defined
In [135]: import math
          print(math.sin(3.))
0.1411200080598672
In [136]: # This displays the help of the math library
          math?
In [137]: # This imports all the elements of the library in the current domain name (IS NOT A GO
          from math import *
          sin(3.)
Out[137]: 0.1411200080598672
In [138]: # One can look at the contents of a library with dir:
         print(dir(math))
['__doc__', '__file__', '__loader__', '__name__', '__package__', '__spec__', 'acos', 'acosh', 'a
In [139]: # The help command is used to have information on a given function:
          help(math.sin)
Help on built-in function sin in module math:
sin(...)
    sin(x)
    Return the sine of x (measured in radians).
```

```
In [140]: help(log)
Help on built-in function log in module math:
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.
In [141]: print(math.pi)
3.141592653589793
In [142]: math.pi = 2.71
In [143]: print(math.pi)
2.71
In [144]: import math
In [145]: math.pi
Out[145]: 2.71
In [149]: # In python 3 you need to import reload, in python 2 is included
          from importlib import reload
In [150]: reload(math)
Out[150]: <module 'math' from '/home/vero/anaconda2/envs/ipy3/lib/python3.6/lib-dynload/math.cpy
In [151]: # In python 2 the value is reset, in python 3 this is not the case!!!!
         math.pi
Out[151]: 2.71
In [152]: from math import pi as pa
In [153]: pa
Out[153]: 2.71
In [154]: math = 2
          math.pi
```