

# Lezione 3

## Introduzione alla programmazione con Python

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## Quick introduction to Python and Biopython

Python: a great language for science

BioPython, NumPython, SciPython, and more

## Basic elements of programming

Expressions and types

Variables and assignment

Strings, escape chars and multiline strings

User input and formatted printing



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## Main references

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## Useful readings

- ▶ Chapman [2003]
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# Why Python ?

- ▶ It is free and well documented
- ▶ It runs everywhere
- ▶ It has a clean syntax
- ▶ It is relevant. Thousands of companies and academic research groups use it every day;
- ▶ It is well supported by tools



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# What is Python? Executive Summary

Extracted from [van Rossum, 2002]

Python is an interpreted, object-oriented, high-level programming language with dynamic semantics

- ▶ high-level data structures, with dynamic typing, make it very attractive for Rapid Application Development
- ▶ simple, easy to learn syntax emphasizes readability
- ▶ supports modules and packages, which encourages program modularity and code reuse
- ▶ available free for all major platforms



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# What is Python? increased productivity

Extracted from [van Rossum, 2002]

- ▶ Since there is no compilation step, the edit-test-debug cycle is incredibly fast
- ▶ Debugging Python programs is easy: a bug or bad input will never cause a segmentation fault
- ▶ Instead, when the interpreter discovers an error, it raises an exception
- ▶ When the program doesn't catch the exception, the interpreter prints a stack trace
- ▶ A source level debugger allows inspection of local and global variables, evaluation of arbitrary expressions, setting breakpoints, stepping through the code a line at a time, and so on
- ▶ The debugger is written in Python itself, testifying to Python's introspective power
- ▶ On the other hand, often the quickest way to debug a program is to add a few print statements to the source: the fast edit-test-debug cycle makes this simple approach very effective



# Comparing Python to Other Languages

Extracted from [van Rossum, 1997]

- ▶ [Campbell et al., 2009]
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# Installing

on Mac OS X and Windows

- ▶ The suggested book [Campbell et al., 2009] on Python programming is

Practical Programming:

An Introduction to Computer Science Using Python

- ▶ Basic install  
(Python + NumPy + Wing IDE 101)

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# Numerical Python

NumPy is the fundamental package needed for scientific computing with Python

It contains:

- ▶ a powerful N-dimensional array object
- ▶ sophisticated broadcasting functions
- ▶ basic linear algebra functions
- ▶ basic Fourier transforms
- ▶ sophisticated random number capabilities
- ▶ tools for integrating Fortran code.
- ▶ tools for integrating C/C++ code.

NumPy can also be used as an efficient multi-dimensional container of generic data. Arbitrary data-types can be defined.

This allows NumPy to seamlessly and speedily integrate with a wide variety of databases.



# Scientific Python

SciPy: Scientific Library for Python

- ▶ open-source software for mathematics, science, and engineering
- ▶ It is also the name of a popular conference on scientific programming with Python
- ▶ The SciPy library depends on NumPy
- ▶ The SciPy library provides many user-friendly and efficient numerical routines





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- ▶ Official source and binary releases of [NumPy and SciPy](#)
- ▶ A better alternative: [SciPy Superpack](#) for Python
- ▶ [Biology packages](#)
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Python tools for computational molecular biology

- ▶ **Biopython** is a set of freely available tools for biological computation written in Python
- ▶ It is a distributed collaborative effort to develop Python **libraries and applications**
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# Python comments

Comments are to clarify code and are not interpreted by Python

- ▶ Comments start with the *hash* character, #, and *extend to the end* of the line
- ▶ A comment may appear at the start of a line or following whitespace or code, but *not within a string* literal<sup>1</sup>

```
# this is the first comment
SPAM = 1          # and this is the second comment
                  # ... and now a third!
STRING = "#_This_is_not_a_comment."
```

---

<sup>1</sup>*Literal* ≡ according with the letter of the scriptures;  
expression that returns itself by evaluation.



# Using Python as a calculator

including comments

```
>>> 2+2
4
>>> # This is a comment
... 2+2
4
>>> 2+2 # and a comment on the same line as code
4
>>> (50-5*6)/4
5
>>> # Integer division returns the floor:
... 7/3
2
>>> 7/-3
-3
```





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# Variables and assignment

- ▶ 3.4. Declaring variables<sup>2</sup>

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# Using Python as a Calculator

## Numbers

- ▶ The interpreter acts as a simple calculator: you can type an expression at it and it will write the value
- ▶ Expression syntax is straightforward: the operators  $+$ ,  $-$ ,  $*$  and  $/$  work just like in most other languages
- ▶ parentheses can be used for grouping

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## Numbers

- ▶ The equal sign ('=') is used to assign a value to a variable
- ▶ Afterwards, no result is displayed before the next interactive prompt:

```
>>> width = 20
>>> height = 5*9
>>> width * height
900
```





# Using Python as a Calculator

## Numbers

- ▶ A value can be assigned to several variables simultaneously:

```
>>> x = y = z = 0 # Zero x, y and z
>>> x
0
>>> y
0
>>> z
0
```



# Using Python as a Calculator

## Numbers

- ▶ Variables must be “defined” (assigned a value) before they can be used, or an error will occur:

```
>>> # try to access an undefined variable
... n
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
NameError: name 'n' is not defined
```



# Using Python as a Calculator

## Numbers

- ▶ There is full support for floating point
- ▶ operators with mixed type operands convert the integer operand to floating point

```
>>> 3 * 3.75 / 1.5  
7.5  
>>> 7.0 / 2  
3.5
```



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# Using Python as a Calculator

## Numbers

- ▶ Complex numbers are also supported
- ▶ imaginary numbers are written with a suffix of j or J
- ▶ Complex numbers with a nonzero real component are written as (real+imagj), or can be created with the `complex(real, imag)` function.

```
>>> 1j * 1J
(-1+0j)
>>> 1j * complex(0,1)
(-1+0j)
>>> 3+1j*3
(3+3j)
>>> (3+1j)*3
(9+3j)
>>> (1+2j)/(1+1j)
(1.5+0.5j)
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## Numbers

- ▶ Complex numbers are always represented as two floating point numbers, the real and imaginary part
- ▶ To extract these parts from a complex number  $z$ , use  $z.real$  and  $z.imag$ .

```
>>> a=1.5+0.5j
>>> a.real
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# Using Python as a Calculator

## Numbers

- ▶ The conversion functions to floating point and integer (`float()`, `int()` and `long()`) don't work for complex numbers
- ▶ there is no one correct way to convert a complex number to a real number
- ▶ Use `abs(z)` to get its magnitude (as a float) or `z.real` to get its real part.

```
>>> a=3.0+4.0j
>>> float(a)
Traceback (most recent call last):
  File "<stdin>", line 1, in ?
TypeError: can't convert complex to float; use abs(z)
>>> a.real
3.0
>>> a.imag
4.0
>>> abs(a) # sqrt(a.real**2 + a.imag**2)
5.0
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# Using Python as a Calculator

## Numbers

- ▶ 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

```
>>> tax = 12.5 / 100
>>> price = 100.50
>>> price * tax
12.5625
>>> price + _
113.0625
>>> round(_, 2)
113.06
>>>
```

- ▶ 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.





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Python: a great language for science

BioPython, NumPython, SciPython, and more

## Basic elements of programming

Expressions and types

Variables and assignment

**Strings, escape chars and multiline strings**

User input and formatted printing



# Strings

- ▶ Besides numbers, Python can also manipulate strings, which can be expressed in several ways
- ▶ They can be enclosed in single quotes or double quotes:

```
>>> 'spam eggs'
'spam eggs'
>>> 'doesn\'t'
"doesn't"
>>> "doesn't"
"doesn't"
>>> '"Yes," he said.'
'"Yes," he said.'
>>> "\"Yes,\" he said."
'"Yes," he said.'
>>> '"Isn\'t," she said.'
'"Isn\'t," she said.'
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# Strings

- ▶ String literals can span multiple lines in several ways
- ▶ Continuation lines can be used, with a backslash as the last character on the line indicating that the next line is a logical continuation of the line:

```
hello = "This is a rather long string containing\n\
several lines of text just as you would do in C.\n\
    Note that whitespace at the beginning of the line is\
significant."

print hello
```

- ▶ newlines still need to be embedded in the string using `\n`
- ▶ the newline following the trailing backslash is discarded
- ▶ This example would print the following:

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# Strings

- ▶ strings can be surrounded in a pair of matching triple-quotes: `"""` or `'''`
- ▶ End of lines do not need to be escaped when using triple-quotes, but they will be included in the string

```
print """
Usage: thingy [OPTIONS]
    -h                Display this usage message
    -H hostname       Hostname to connect to
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- ▶ If we make the string literal a `r` string, sequences are not converted to newlines, but the backslash at the end of the line, and the newline character in the source, are both included in the string as data.
- ▶ Thus, the example:

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hello = r"This is a rather long string containing\n\  
several lines of text much as you would do in C."  
  
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# Strings

- ▶ Strings can be concatenated (glued together) with the + operator, and repeated with \*:

```
>>> word = 'Help' + 'A'  
>>> word  
'HelpA'  
>>> '<' + word*5 + '>'  
'<HelpAHelpAHelpAHelpAHelpA>'
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- ▶ Two string literals next to each other are automatically concatenated
- ▶ the first line above could also have been written word = 'Help' 'A'
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# Strings

Strings can be subscripted (indexed)

- ▶ the first character has index 0
- ▶ there is no separate character type
- ▶ a character is simply a string of size one
- ▶ substrings can be specified with the slice notation: two indices separated by a colon.

```
>>> word[4]
'A'
>>> word[0:2]
'He'
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- ▶ Slice indices have useful defaults
- ▶ an omitted first index defaults to zero
- ▶ an omitted second index defaults to the size of the string being sliced.

```
>>> word[:2]    # The first two characters
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>>> word[2:]   # Everything except the first two characters
'lpA'
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- ▶ Unlike a C string
- ▶ Python strings cannot be changed
- ▶ Assigning to an indexed position in the string results in an error:

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>>> word[0] = 'x'  
Traceback (most recent call last):  
  File "<stdin>", line 1, in ?  
TypeError: object does not support item assignment  
>>> word[:1] = 'Splat'  
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# Strings

- ▶ However, creating a new string with the combined content is easy and efficient:

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>>> 'x' + word[1:]  
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>>> 'Splat' + word[4:]  
'SplatA'
```

- ▶ Here,  $s[:i] + s[i:]$  equals  $s$ .

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>>> word[:2] + word[2:]  
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>>> word[:3] + word[3:]  
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# Strings

- ▶ Degenerate slice indices are handled gracefully:
- ▶ an index that is too large is replaced by the string size
- ▶ an upper bound smaller than the lower bound returns an empty string.

```
>>> word[1:100]
'elpA'
>>> word[10:]
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>>> word[2:1]
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- ▶ Indices may be negative numbers, to start counting from the right:

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>>> word[-1]      # The last character
'A'
>>> word[-2]     # The last-but-one character
'p'
>>> word[-2:]    # The last two characters
'pA'
>>> word[:-2]    # Everything except the last two characters
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```

- ▶ But note that -0 is really the same as 0, so it does not count from the right!

```
>>> word[-0]     # (since -0 equals 0)
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# Strings

- ▶ 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  $n$  characters has index  $n$
- ▶ The slice from  $i$  to  $j$  consists of all characters between the edges labeled  $i$  and  $j$

```
+---+---+---+---+---+
| H | e | l | p | A |
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0   1   2   3   4   5
-5  -4  -3  -2  -1
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# Strings

- ▶ For non-negative indices, the length of a slice is the difference of the indices
- ▶ if both are within bounds
- ▶ For example the length of `word[1:3]` is 2.

The built-in function `len()` returns the length of a string:

```
>>> s = 'supercalifragilisticexpialidocious'  
>>> len(s)  
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# Sequence Types

str, unicode, list, tuple, buffer, xrange

**strings** String literals are written in single or double quotes: 'xyzyzy', "frobozz".

**Unicode strings** specified using a preceding 'u' character: u'abc', u"def"

**lists** constructed with square brackets, separating items with commas: [a, b, c]

**tuples** Tuples are constructed by the comma operator (not within square brackets), with or without enclosing parentheses, but an empty tuple must have the enclosing parentheses, such as a, b, c or (). A single item tuple must have a trailing comma, such as (d,).

**buffers** created by calling the builtin function buffer(). They don't support concatenation or repetition

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