# Lezione 4 Bioinformatica

Mauro Ceccanti<sup>‡</sup> e Alberto Paoluzzi<sup>†</sup>

†Dip. Informatica e Automazione – Università "Roma Tre" ‡Dip. Medicina Clinica – Università "La Sapienza"

#### Lecture 4: Python Overview

Installing Python
Using Python Interactively

Running Python Programs

Setting up Emacs for Python

Basics and Control Flow

Syntax, Variables and Namespaces

Python Data Structures

Basic Data Types

Container Data Structures

Files and Modules

Import statement

Documentation



#### Λ

#### Contents

#### Lecture 4: Python Overview

Installing Python
Using Python Interactively
Running Python Programs
Setting up Emacs for Python

Basics and Control Flow Syntax, Variables and Namespaces

Python Data Structures
Basic Data Types
Container Data Structures

Files and Modules
Import statement
Documentation

# **Installing Python**

- ► If you don't know which version to use, start with Python 2.6.3;
- more existing third party software is compatible with Python 2 than Python 3 right now.
- ► See the main Documentation page.

**Download Python** 





## Using Python Interactively

# Running Python Programs

- Most Python programmers write their programs to a plain file using a text editor.
- ► Instead of ending the file with a '.txt' suffix, Python programs usually end with '.py', like 'myprogram.py'.
- ► To execute the program file, type the following at a command prompt:

```
> python myprogram.py
```

- ▶ Unix-like systems allow you to add a "bang line" to your program.
- ➤ A "bang line" is a line that tells the computer where to find the interpreter.

```
#!/usr/bin/python
```

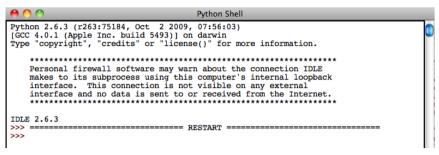
the execution in this case is direct (give execution rights to the file!)

```
> ./myprogram.py
```

## Using Python Interactively

Using Idle IDE

IDLE is an integrated development environment for Python, which is bundled in each release



- Multi-window text editor with syntax highlighting, autocompletion, smart indent and other.
- Python shell with syntax highlighting.
- Integrated debugger with stepping, persistent breakpoints, and call stack visibility



## **Running Python Programs**

#!/usr/bin/python

```
1. move to the file directory
2. verify file rights
3. add execution right
4. program execution

1. move to the file directory
2. cd dirname
3. ls -1 filename
4. chmod +x filename
6. /filename
```

```
host:~ pao> cd test
host:test pao> ls -l ciao.py
-rw-r--re-@ 1 paoluzzi staff 30 Oct 22 11:24 ciao.py
host:test pao> chmod +x ciao.py
host:test pao> ls -l ciao.py
-rwxr-xr-x@ 1 paoluzzi staff 30 Oct 22 11:24 ciao.py
host:test pao> ciao.py
host:test pao> /ciao.py
ciao
host:test pao>
```





#### Contents

#### Lecture 4: Python Overview

Installing Python
Using Python Interactively
Running Python Programs
Setting up Emacs for Python

#### Basics and Control Flow Syntax, Variables and Namespaces

Python Data Structures
Basic Data Types
Container Data Structures
Files and Modules
Import statement
Documentation

# Syntax, Variables and Namespaces

Python - Variable Types

#### **Basics and Control Flow**

Learning to program in Python

See also: Discover Python, Part 5: Programming in Python

#### Contents

#### Lecture 4: Python Overview

Installing Python
Using Python Interactively
Running Python Programs
Setting up Emacs for Python
Basics and Control Flow
Syntax, Variables and Namespaces

Python Data Structures
Basic Data Types
Container Data Structures

Files and Modules Import statement Documentation





## Python Data Structures

- Lists
- Tuples
- Dictionaries
- Sets

**Data Structures** 

#### Contents

#### Lecture 4: Python Overview

Installing Python
Using Python Interactively
Running Python Programs
Setting up Emacs for Python

Basics and Control Flow Syntax, Variables and Namespaces

Python Data Structures
Basic Data Types
Container Data Structures

Files and Modules Import statement Documentation

#### **Container Data Structures**

- ▶ In computer science, a container is a class, a data structure, or an abstract data type (ADT) whose instances are collections of other objects.
- ► In other words; They are used to store objects in an organized way following specific access rules.
- ► Generally, container classes are expected to implement methods to do the following:
  - create a new empty container (constructor),
  - report the number of objects it stores (size),
  - delete all the objects in the container (clear),
  - ▶ insert new objects into the container,
  - remove objects from it,
  - provide access to the stored objects.





#### Modules

From Python tutorial, see: 6. Modules See also: Importing Python Modules





#### File I/O

From Python tutorial, see: 7.2. Reading and Writing Files

# Λ

### Documentation

Source Documentation and Comments

# Import statement

See within the files: wireframe.py, pdb.py, and basic.py

```
To generate the wireframe of a protein.

Usage:
> python wireframe.py protein.pdb

"""

from pdb import *
```

```
import sys
import datetime
from basic import *
import FL06
```

```
Basic data and operations with amino acids and biomolecules.
"""

from numpy import array, reshape, transpose
```



