

Lezione 4

Bioinformatica

Mauro Ceccanti[‡] e Alberto Paoluzzi[†]

[†]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



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;

Download Python



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.

Download Python



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

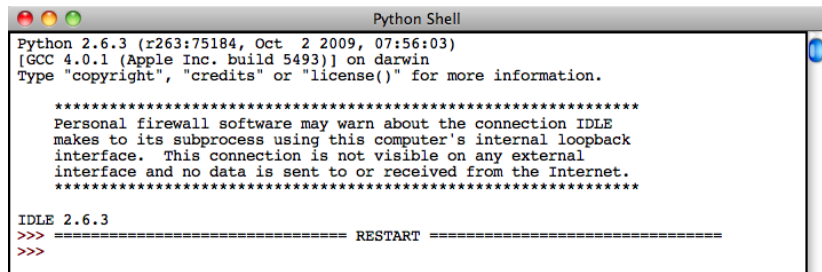
```
1 baruc3:~> python
2 Python 2.6.3 (r263:75184, Oct  2 2009, 07:56:03)
3 [GCC 4.0.1 (Apple Inc. build 5493)] on darwin
4 Type "help", "copyright", "credits" or "license" for
   more information.
5 >>> 2 + 2
6 4
7 >>> 3*(4 + 2))
8     File "<stdin>", line 1
9         3*(4 + 2))
10             ^
11 SyntaxError: invalid syntax
12 >>> 3 * (4 + 2)
13 18
14 >>>
```



Using Python Interactively

Using Idle IDE

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



```
Python 2.6.3 (r263:75184, Oct  2 2009, 07:56:03)
[GCC 4.0.1 (Apple Inc. build 5493)] on darwin
Type "copyright", "credits" or "license()" for more information.

*****
Personal firewall software may warn about the connection IDLE
makes to its subprocess using this computer's internal loopback
interface.  This connection is not visible on any external
interface and no data is sent to or received from the Internet.
*****

IDLE 2.6.3
>>> ===== RESTART =====
>>>
>>>
```

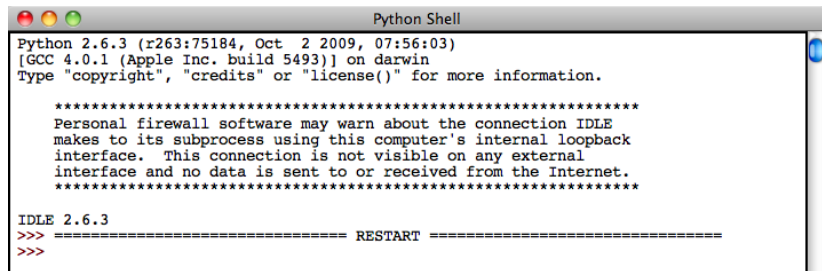
- ▶ Multi-window text editor with syntax highlighting, autocompletion, smart indent and other.



Using Python Interactively

Using Idle IDE

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



```
Python 2.6.3 (r263:75184, Oct 2 2009, 07:56:03)
[GCC 4.0.1 (Apple Inc. build 5493)] on darwin
Type "copyright", "credits" or "license()" for more information.

*****
Personal firewall software may warn about the connection IDLE
makes to its subprocess using this computer's internal loopback
interface. This connection is not visible on any external
interface and no data is sent to or received from the Internet.
*****

IDLE 2.6.3
>>> ===== RESTART =====
>>>
```

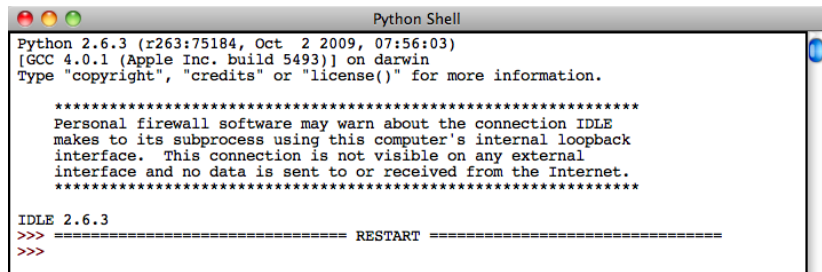
- ▶ Multi-window text editor with syntax highlighting, autocompletion, smart indent and other.
- ▶ Python shell with syntax highlighting.



Using Python Interactively

Using Idle IDE

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



```
Python 2.6.3 (r263:75184, Oct 2 2009, 07:56:03)
[GCC 4.0.1 (Apple Inc. build 5493)] on darwin
Type "copyright", "credits" or "license()" for more information.

*****
Personal firewall software may warn about the connection IDLE
makes to its subprocess using this computer's internal loopback
interface. This connection is not visible on any external
interface and no data is sent to or received from the Internet.
*****

IDLE 2.6.3
>>> ===== RESTART =====
>>>
```

- ▶ 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

- ▶ Most Python programmers write their programs to a plain file using a text editor.



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'.



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:

```
1 > python myprogram.py
```



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:

```
1 > python myprogram.py
```

- ▶ Unix-like systems allow you to add a "bang line" to your program.



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:

```
1 > 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.

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



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:

```
1 > 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.

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

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

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



Running Python Programs

```
1 #!/usr/bin/python
2 print "ciao"
```

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

```
cd dirname
ls -l filename
chmod +x filename
./filename
```

```
1 host:~ pao> cd test
2 host:test pao> ls -l ciao.py
3 -rw-r--r--@ 1 paoluzzi  staff  30 Oct 22 11:24 ciao.py
4 host:test pao> chmod +x ciao.py
5 host:test pao> ls -l ciao.py
6 -rwxr-xr-x@ 1 paoluzzi  staff  30 Oct 22 11:24 ciao.py
7 host:test pao> ciao.py
8 host:test pao> ./ciao.py
9 ciao
10 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

Basics and Control Flow

Learning to program in Python

See also: [Discover Python, Part 5: Programming in Python](#)



Syntax, Variables and Namespaces

Python - Variable Types

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

Data Structures



Python Data Structures

- ▶ Lists
- ▶ Tuples

Data Structures

Python Data Structures

- ▶ Lists
- ▶ Tuples
- ▶ Dictionaries

Data Structures



Python Data Structures

- ▶ Lists
- ▶ Tuples
- ▶ Dictionaries
- ▶ Sets

Data Structures



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.



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.



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:



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),



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),



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),



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,



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,



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.



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

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](#)



Import statement

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

```
1 """  
2 To generate the wireframe of a protein.  
3 Usage:  
4 > python wireframe.py protein.pdb  
5 """  
6 from pdb import *
```

```
1 import sys  
2 import datetime  
3 from basic import *  
4 import FL06
```

```
1 """  
2 Basic data and operations with amino acids and  
3 biomolecules.  
4 """  
5 from numpy import array, reshape, transpose
```



Documentation

Source Documentation and Comments

