



12

Modules & Libraries

practical computing biologists

Lydia Danglot

3rd of february

HADDOCK • DUNN



Chapter

12



Modules & Libraries

Definitions:

- Python Standard Library
- Modules

Importing modules:

Buit-in modules from the standard library:

- Urllib module
- Operating system module
- Math module
- Random module
- Time module

Third-party modules

- Numpy
- Biopython

Making your own modules

Going further with Python

Python Standard Library :

http://docs.python.org/library

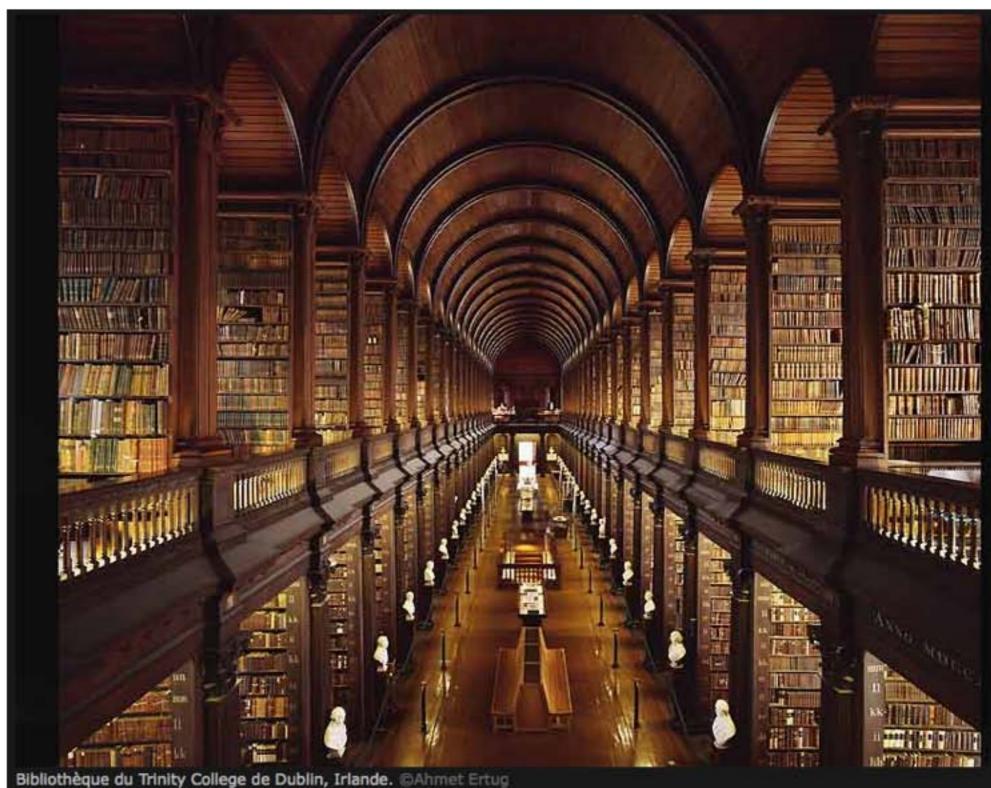


Contain all the built-in modules which can be used when coding Python.

All computer with Python have them already installed and ready to import.

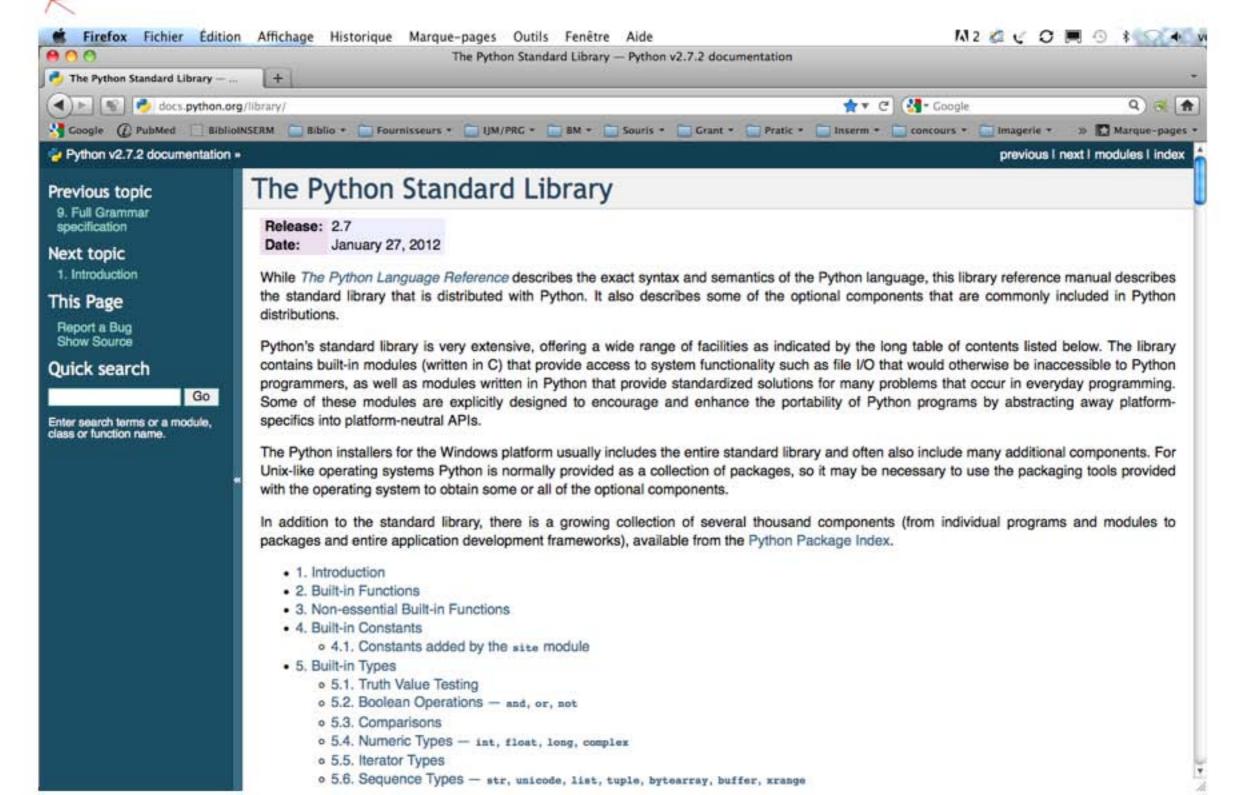
Exemple:

- Regex (re)
- System (sy)
- Operating system (os)



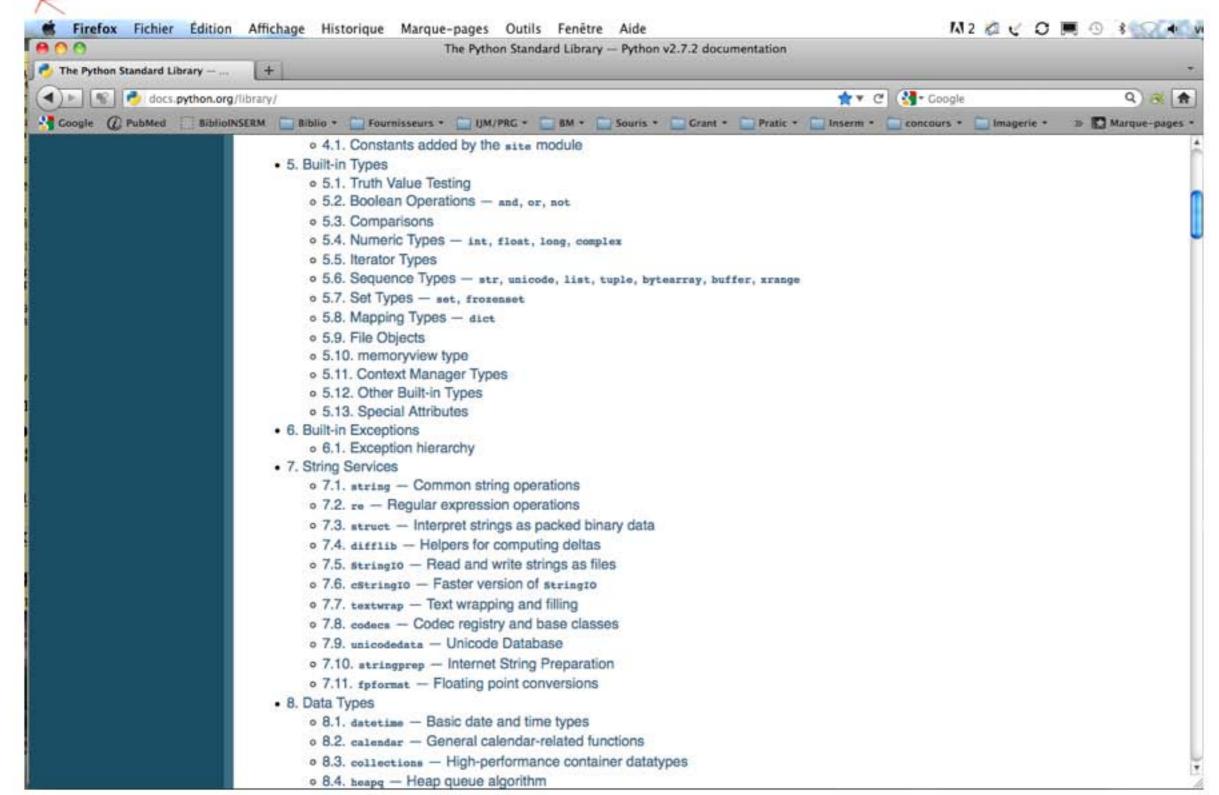
Python Standard Library :





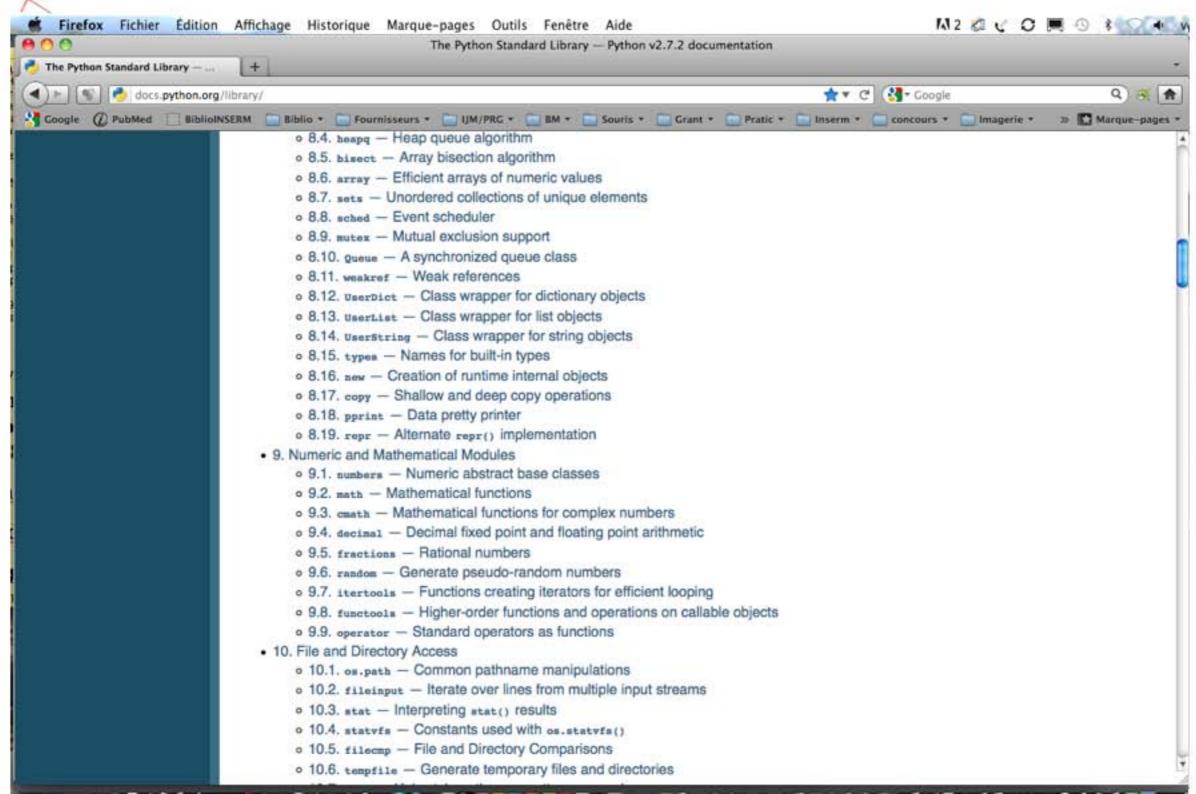
Python Standard Library :





Python Standard Library :





Python Standard Library :











Python Standard Library :

Contain all the built-in modules which can be used when coding Python.



Modules:

Pre-packaged of code that add functionality to the core language and simplify many tasks. Import modules only as needed: avoid the overcharge, avoid accumulation of function name that we don't need.

Buit-in modules from the standard library:

- Urllib module
- · Operating system module
- Math module
- Random module
- Time module

Third-party modules

- Numpy
- Biopython

Your own modules

Installed on your computer

To be installed ...

To be written ...



Operating system module (os):

Object/function

Modules and Libraries 219

TABLE 12.1 Some useful functions of the os module, along with their shell equivalents Module command Operation Shell equivalent

Module name

Module command	Operation	Shell equivalent
os.chdir('/Users/lucy/pcfb')	Change directory	cd ~/pcfb
os.getcwd()	Get current dir	pwd
os.listdir('.')	List directory	ls
glob.glob("*.txt")	Wildcard search for files (requires import glob)	ls *.txt
os.path.isfile('data.txt')	Does file exist?	
os.path.exists('/Users/lucy')	Does folder exist?	
os.rename('test.txt','test2.txt')	Rename file	mv test.txt test2.txt
os.popen('pwd','r').read()	Run a shell command and load the output into a variable	Any command; in this case pwd is shown

How to import modules?

• in the terminal :

```
LD:~ lydiadanglot$ python
Python 2.6.1 (r261:67515, Jun 24 2010, 21:47:49)
[GCC 4.2.1 (Apple Inc. build 5646)] on darwin
Type "help", "copyright", "credits" or "license" for more information.

>>> from (math) import *
>>> pi
3.1415926535897931
>>> sqrt(64)
8.0

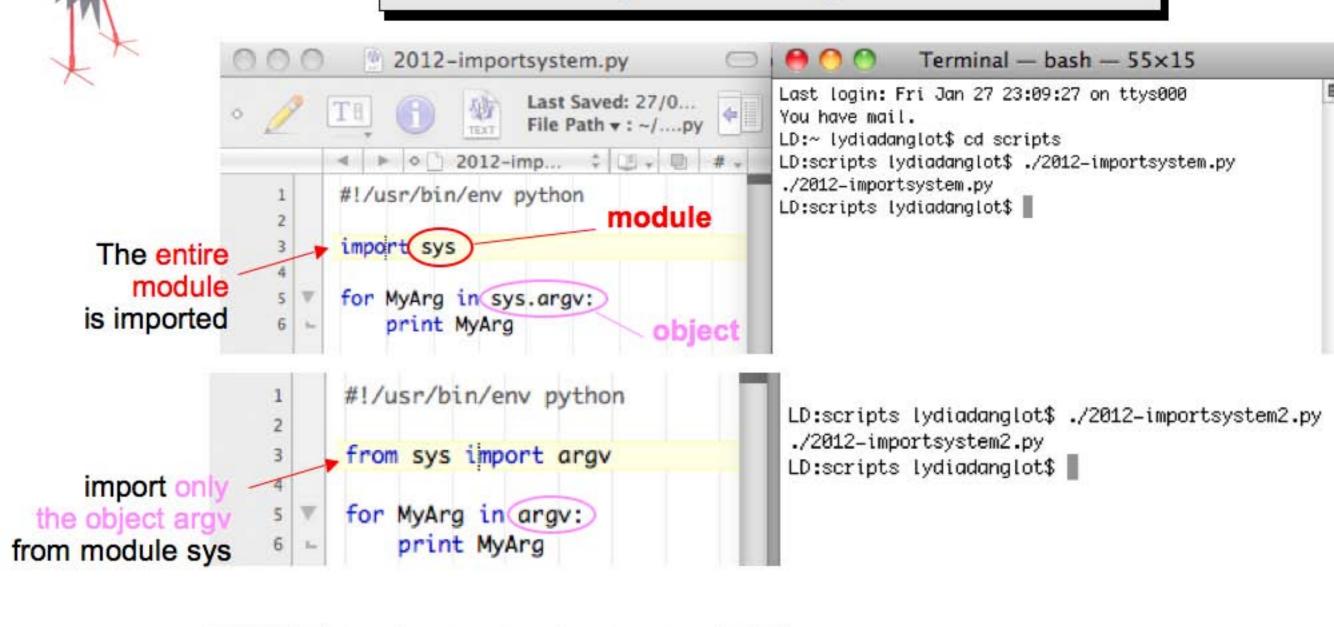
| Terminal — Python — 120×10
| Terminal — Py
```

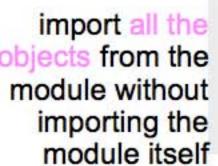
in the text editor :

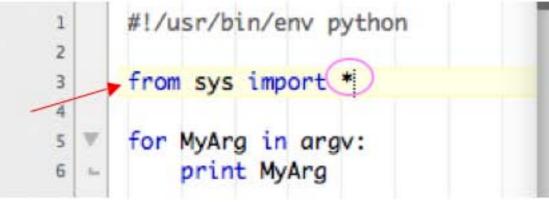
```
authors4.py
                        Last Saved: 28/01/12 16:26:17
                       File Path : ~/scripts/authors4.py
                                                                                            Documents

♦ ♦ ○ authors4.py ÷ (no symbol selected) ÷
                                                                                   o mauthors4.py
      #!/usr/bin/env bython
                                                                                        bootstrap.py
                                                                                        Exercices du 27-01-...
      import (random
                                                                                        filestoXYYY-skipline.py
                                                                                        LEDBlue.txt
      Casev = 4
      Steve = 6
                                                                                        LEDGreen.txt
      Possible = 10
      NumList = [
      Z = \Box
11
      print NumList
12
      print ['Casey', 'Steve'][Num == Steve]+' wins!!'
         Python # Unicode (UTF-8) # Unix (LF) # 163 / 24 / 13
3 7
```

Example with sys module







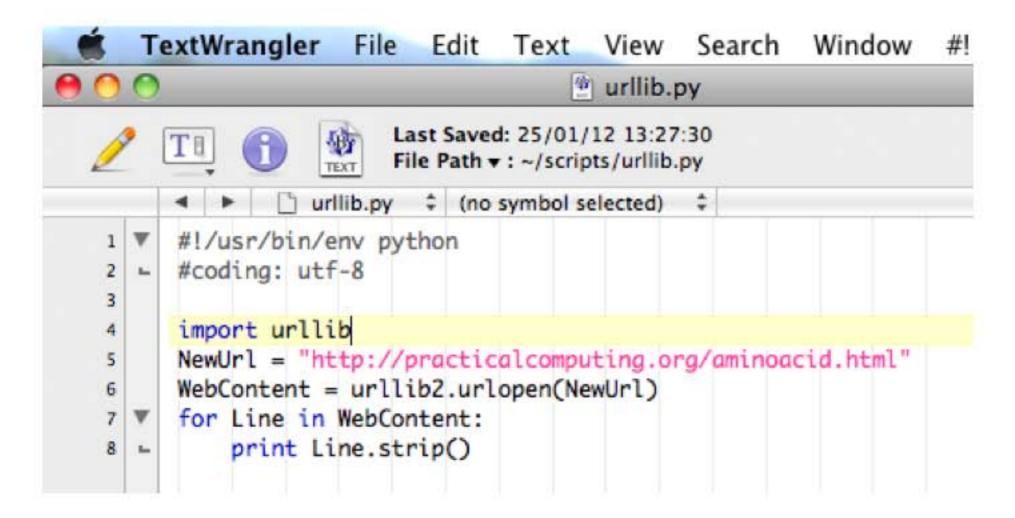
LD:scripts lydiadanglot\$./2012-importsystem3.py ./2012-importsystem3.py LD:scripts lydiadanglot\$





Url library module (urllib):

To download ressources directly from internet for use in Python program. Similar to the *curl* command (chapter 5).





html file open in text editor :

```
1 W
  <html><head>
2
  <meta http-equiv="content-type" content="text/html; charset=UTF-8"><title>AMINO
3 W
  <font face="Helvetica, Arial">
4 W
5 W
  6 W
  NameAbbreviationSingle-LetterMol Wt
7
  AlanineAlaA89.09
8
  ArginineArgR174.20
9
  AsparagineAsnN132.12
10
  Aspartic acidAspD133.10
11
  CysteineCysC121.15
12
  GlutamineGlnQ146.15
13
  Glutamic acidGluE147.13
14
  GlycineGlyc/td>Gc/td>75.07
15
  HistidineHisHc/td>155.16
16
  IsoleucineIleI131.17
17
  LeucineLeuLeu131.17
18
  \tr>\tysine\tys\td>\td>\td>
19
  MethionineMetMt/td>149.21
20
  21
  ProlinePro15.13
22
  SerineSer5105.09
23
  ThreonineThrT19.12
24
  TryptophanTrpXto>23
25
  TyrosineTyrY181.19
26
  ValineValVd>17.15
27
  28
  GapGap
29
  StopEnd*0.0
30
31
  32
  </font>
33
34
  </body></html>
```

LD:scripts lydiadanglot\$

00					
	NO ACIDS	+			
4 1- 8 :	practicalcomp	outing.org/amino	acid,html		
Google 🗧 P	ubMed Bibl	ioINSERM 📋 Bi	blio * 🔋		
Name	Abbreviation	Single-Letter	Mol Wi		
Alanine	Ala	A	89.09		
Arginine	Arg	R	174.20		
Asparagine	Asn	N	132.12		
Aspartic acid	Asp	D	133.10		
Cysteine	Cys	С	121.15		
Glutamine	Gln	Q	146.15		
Glutamic acid	Glu	E	147.13		
Glycine	Gly	G	75.07		
Histidine	His	Н	155.16		
Isoleucine	lle	1	131.17		
Leucine	Leu	L	131.17		
Lysine	Lys	K	146.19		
Methionine	Met	M	149.21		
Phenylalanine	Phe	F	165.19		
Proline	Pro	P	115.13		
Serine	Ser	S	105.09		
Threonine	Thr	T	119.12		
Tryptophan	Trp	W	204.23		
Tyrosine	Tyr	Y	181.19		
Valine	Val	V	117.15		
Unknown	Xaa	X	0.0		
Gap	Gap		0.0		
Stop	End	•	0.0		

```
#!/usr/bin/env python
| #coding: utf-8
| import urllib|
| NewUrl = "http://practicalcomputing.org/aminoacid.html"
| WebContent = urllib2.urlopen(NewUrl)
| for Line in WebContent:
| print Line.strip()
```

```
LD:scripts lydiadanglot$ ./2012-urllib.py
<html><head><title>AMINO ACIDS</title></head>
-dont face="Helvetica, Arial">
NameAbbreviationSingle-LetterMt
AlanineAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAlaAla<t
-tr>-td>Arginine-td>-td>Arg-td>-td>R-td>174.28-
-tr>-tdsGlutamine--tdsGln--tdsQ--tds-146.15-
dr>dr>dr>dr>dr>dr>dr>dr>dr>dr>dr>dr>dr>dr>dr>dr>dr>drdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdrdr</t
dro-ddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucineddoIsoleucine
ds/fethioninefd>fd>fd>fd>fd>fd>fd>fd>fd>fd
ctr>Pheny la lan inePhetd>F165.19
Threoninetd>Thre/td>Td>119.12
tr>TyrosineTyrY181.19
-tr>-td>Gop=/td>-td>Gop=/td>-td>-td>-td>-0.8</ra>
</fonts
</body>
</html>
```

the random module (random):

This module implements pseudo-random number generators for various distributions.





Function	Result
randint(5,50)	Return a random integer, in this case between 5 and 50, inclusive
random.random()	Return a random fraction between 0 and 1
choice(['A',0,'B'])	Return a randomly chosen item from the list passed as a parameter
shuffle(MyList)	Randomly rearrange the items in MyList, in place
sample(MyList,10)	Return a sample of 10 items from MyList, without replacement



```
>>> random.randint(1, 10)
7

>>> random.random()
0.37444887175646646
>>> random.uniform(1, 10)
1.1800146073117523

>>> items = [1, 2, 3, 4, 5, 6, 7]
>>> random.shuffle(items)
>>> items
[7, 3, 2, 5, 6, 4, 1]

>>> random.sample([1, 2, 3, 4, 5], 3)
[4, 1, 5]
```

• the random module (random):

```
#!/usr/bin/env python
"""demo of bootstrapping via resample with replacement"""
import random
NumSamples = 100 # Number of resamplings to conduct
Bootstraps=[] # List to store the random lists
# for the demo, create a list of numbers 0 to 19
# normally these would be the original data
DataList = range(20)
# loop to perform repeated operations:
# Values of X and Y below are not used -- just counters
for X in range(NumSamples):
  # list comprehension in [] builds a list via sampling
  Resample = [random.choice(DataList) for Y in DataList]
  Bootstraps.append(Resample)
for Z in Bootstraps:
  print Z
```





the time module (time):



- time.asctime(): printable string version of the current date and time
 'Sun Jan 29 18:44:29 2012'
- time.time (): time in millisecond using computer clock
 1327859118.824008
- time.localtime(): list with the current time (year, month, day).
 time.struct_time(tm_year=2012, tm_mon=1,
 tm_mday=29, tm_hour=18, tm_min=46, tm_sec=3,
 tm_wday=6, tm_yday=29, tm_isdst=0)
- Help (time) or dir (time): for more options.

```
['__doc__', '__file__', '__name__', '__package__',
'accept2dyear', 'altzone', 'asctime', 'clock', 'ctime',
'daylight', 'gmtime', 'localtime', 'mktime', 'sleep', 'strftime',
'strptime', 'struct_time', 'time', 'timezone', 'tzname', 'tzset']
```



Chapter

12



Modules & Libraries

Definitions:

- Python Standard Library
- Modules

Importing modules:

Buit-in modules from the standard library:

- Urllib module
- Operating system module
- Math module
- Random module
- Time module

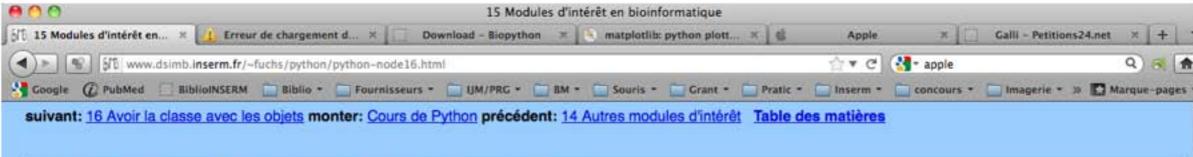
Third-party modules

- Numpy
- Biopython

Making your own modules

Going further with Python





15 Modules d'intérêt en bioinformatique

Nous allons voir dans cette section quelques modules très importants en bioinformatique. Le premier numpy permet notamment de manipuler des vecteurs et des matrices en Python. Le module biopython permet de travailler sur des données biologiques type séquence (nucléique et protéique) ou structure (fichier PDB). Le module matplotlib permet de dessiner des graphiques depuis Python. Enfin, le module rpy permet d'interfacer n'importe quelle fonction du puissant programme R.

Ces modules ne sont pas fournis avec le distribution Python de base (contrairement à tous les autres modules vus précédemment). Nous ne nous étendrons pas sur la manière de les installer. Consultez pour cela la documentation sur les sites internet des modules en question. Sachez cependant que ces modules existent dans la plupart des distributions Linux récentes.

Dans ce chapitre, nous vous montrererons quelques exemples d'utilisation de ces modules pour vous convaincre de leur pertinence.

15.1 Module numpy

Le module <u>numpy</u> est incontournable en bioinformatique. Il permet d'effectuer des calculs sur des vecteurs ou des matrices, élément par élément, via un nouveau type d'objet appelé <u>array</u>. Ce module contient des fonctions de base pour faire de l'algèbre linéaire, des transformées de Fourier ou encore des tirages de nombre aléatoire plus sophistiqués qu'avec le module <u>random</u>. Vous pourrez trouver les sources de numpy à cette <u>adresse</u>. Notez qu'il existe un autre module <u>scipy</u> que nous n'aborderons pas dans ce cours.

<u>scipy</u> est lui même basé sur <u>numpy</u>, mais il en étend considérablement les possibilités de ce dernier (e.g. statistiques, optimisation, intégration numérique, traitement du signal, traitement d'image, algorithmes génétiques, etc.).

15.1.1 Objets de type array

Les objets de type array correspondent à des tableaux à une ou plusieurs dimensions et permettent d'effectuer du calcul vectoriel. La fonction array () permet la conversion d'un objet séquentiel (type liste ou tuple) en un objet de type array. Voici un exemple simple de conversion d'une liste à une dimension en objet array :

```
>>> import numpy
>>> a = [1,2,3]
>>> numpy.array(1)
```





the numerical module (NumPy):

Limit of Python: inability to handle numerical matrix....

For example: no access to the second column of a two-dimension list of lists.

To any familiar with MATHLAB, Mathematica, or R, Numpy support for creating and accessing array objects:

The array object is a 2D table of numbers.





the numerical module (NumPy):

Thanks to numpy you can access a column of numbers.





the numerical module (NumPy):

```
>>> V = [1,1,3,5,6]

>>> median(V)

3

>>> mean(V)

3.200000

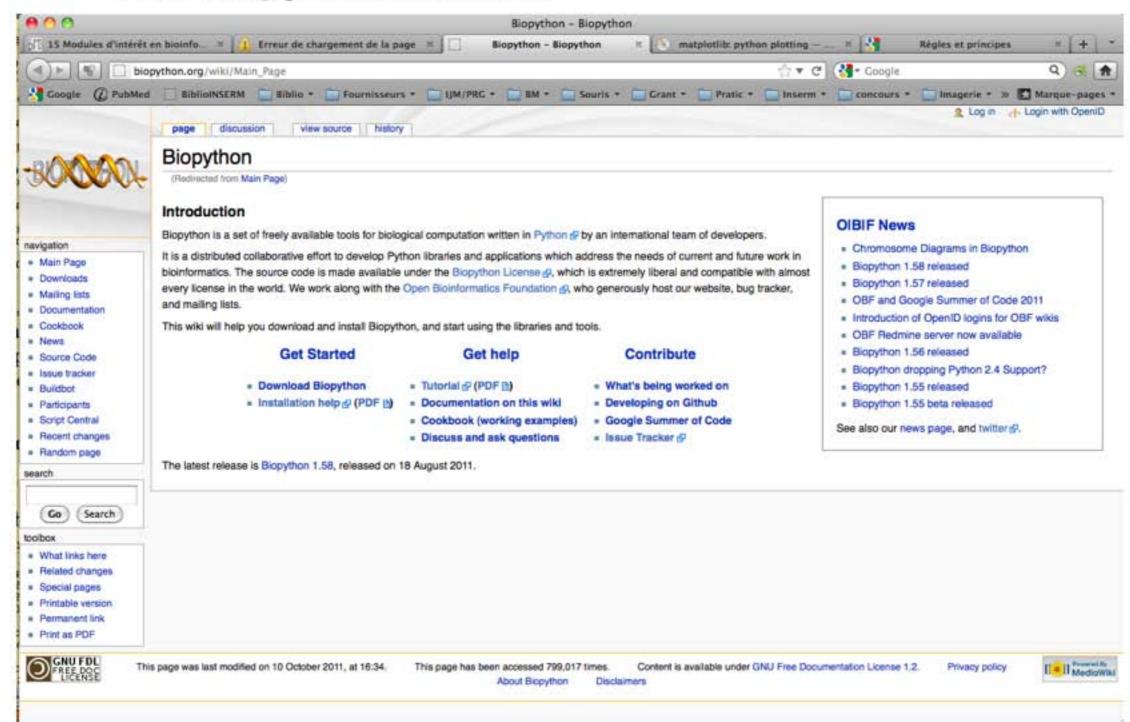
>>> max(V)

6

>>> min(V)
```



the Biopython module:





the Biopython module:

Download the biopython-1.58.zip on your computer.

Open the terminal:

```
host:~ lucy$ cd biopython-1.53
host:biopython-1.53 lucy$ python setup.py build
host:biopython-1.53 lucy$ sudo python setup.py install
```

Show the installBiopython.doc

```
THE LUMB COLUMN TO SERVICE AND ADDRESS OF THE PROPERTY OF THE
```

the Biopython module :

When the installation is done, enjoy the module in the terminal:

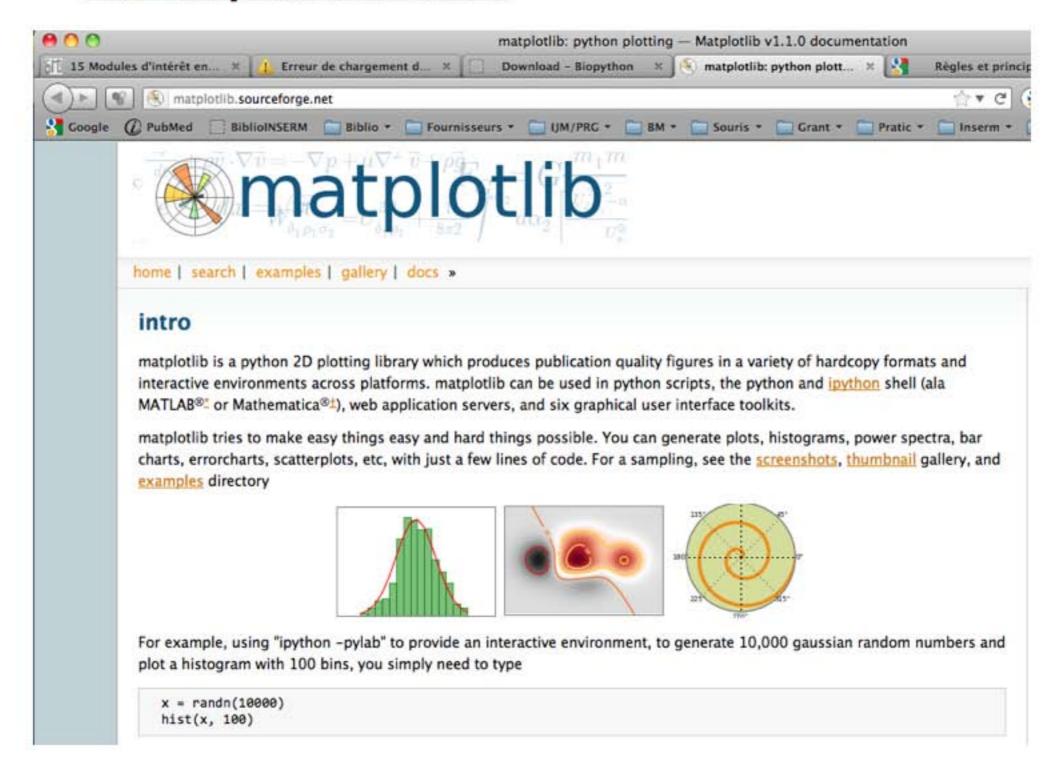
Define a sequence:

```
>>> import Bio
>>> from Bio.Seq import Seq
>>> from Bio.Alphabet import IUPAC
>>> ADN = Seq("ATATCGGCTATAGCATGCA", IUPAC.unambiguous_dna)
>>> ADN
Seq('ATATCGGCTATAGCATGCA', IUPACUnambiguousDNA())
```

```
>>> ADN.complement()
Seq('TATAGCCGATATCGTACGT', IUPACUnambiguousDNA())
>>> ADN.reverse_complement()
Seq('TGCATGCTATAGCCGATAT', IUPACUnambiguousDNA())
```

```
>>> ADN.translate()
Seq('ISAIAC', IUPACProtein())
```

the matplotlib module :





Chapter

12



Modules & Libraries

Definitions:

- Python Standard Library
- Modules

Importing modules:

Buit-in modules from the standard library:

- Urllib module
- Operating system module
- Math module
- Random module
- Time module

Third-party modules

- Numpy
- Biopython

Making your own modules

Going further with Python



Making your own modules

how to create them :

- In Chapter 10, we created a decimalat() function.
- Copy the def:block into a file
- You must define any variables you wish to be sent to it. You can set default values:

def bootstrap (DataList, Samples=10):

Save it in scripts folder as mymodules.py

how to import them :

from mymodules import *







Write a script describing the lottery draw: 5 balls taken among 50, with order and no replacement.

The chance number is taken among 10 balls. Use the random module.



LOTO: No replacement (= « sans remise »).



the random module (random):

This module implements pseudo-random number generators for various distributions.





Function	Result
randint(5,50)	Return a random integer, in this case between 5 and 50, inclusive
random.random()	Return a random fraction between 0 and 1
choice(['A',0,'B'])	Return a randomly chosen item from the list passed as a parameter
shuffle(MyList)	Randomly rearrange the items in MyList, in place
sample(MyList,10)	Return a sample of 10 items from MyList, without replacement



```
>>> random.randint(1, 10)
7

>>> random.random()
0.37444887175646646
>>> random.uniform(1, 10)
1.1800146073117523

>>> items = [1, 2, 3, 4, 5, 6, 7]
>>> random.shuffle(items)
>>> items
[7, 3, 2, 5, 6, 4, 1]

>>> random.sample([1, 2, 3, 4, 5], 3)
[4, 1, 5]
```