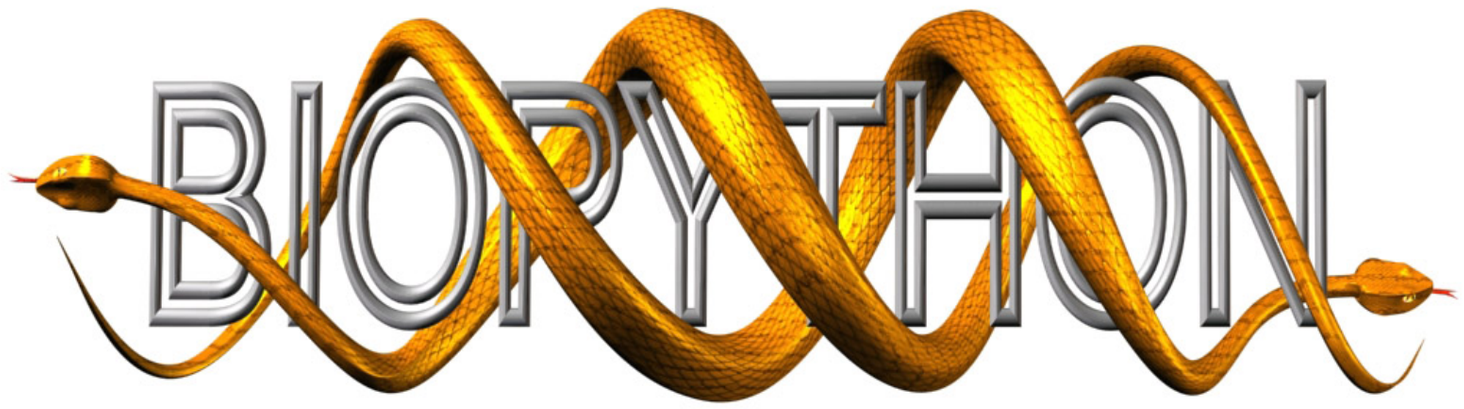
Packages and modules



Scipy, Numpy and Biopython

What are modules and packages?

Essentially just python code in other files.

Module: One file
(which usually contains many functions)

Package: Collection of many files(modules)

```
sound/                          Top-level package
      __init__.py               Initialize the sound package
      formats/                  Subpackage for file format conversions
              __init__.py
              wavread.py
              wavwrite.py
              aiffread.py
              aiffwrite.py
              auread.py
              auwrite.py
              ...
      effects/                  Subpackage for sound effects
              __init__.py
              echo.py
              surround.py
              reverse.py
              ...
      filters/                  Subpackage for filters
              __init__.py
              equalizer.py
              vocoder.py
              karaoke.py
              ...
```

```
from sound.effects import echo
```

```
echo.echofilter(input, output, delay=0.7, atten=4)
```

stdlib: packages included with python as default

A few useful stdlib modules (there are many more)

csv
tools fore manipulating plain text tables

re
regular expression (regex)

subprocess
allows you to spawn new processes, connect to their input/output/error pipes

math
mathematical functions

sys
access to some variables and functions used or maintained by the interpreter

datetime
supplies classes for manipulating dates and times

os
interact with the operating system

glob
finds all the pathnames matching a specified pattern according to the rules used by the Unix shell

urllib2
functions and classes which help in opening URLs

shutil
high-level operations on files and collections of files

random
pseudo-random number generators for various distributions

multiprocessing
parallelisation

all info on the stdlib modules is available at:
https://docs.python.org

Scipy Stack:

- Python
- NumPy
- SciPy library
- Matplotlib
- pandas
- SymPy

Easiest way to install:
Anaconda distribution

Download:
https://www.continuum.io/downloads

Packages included in Anaconda:
https://docs.continuum.io/anaconda/pkg-docs

- Array oriented computing
- 1D, 2D, 3D arrays
- Faster due to calculating in C (static array)
- Lots of data? Use this

>>> import numpy as np

```
>>> a = np.arange(6)                         # 1d array
>>> print(a)
[0 1 2 3 4 5]
>>>
>>> b = np.arange(12).reshape(4,3)           # 2d array
>>> print(b)
[[ 0  1  2]
 [ 3  4  5]
 [ 6  7  8]
 [ 9 10 11]]
>>>
>>> c = np.arange(24).reshape(2,3,4)         # 3d array
>>> print(c)
[[[ 0  1  2  3]
  [ 4  5  6  7]
  [ 8  9 10 11]]
 [[12 13 14 15]
  [16 17 18 19]
  [20 21 22 23]]]
```

More NumPy examples

Modify arrays using vectors

```
import numpy as np

# We will add the vector v to each row of the matrix x,
# storing the result in the matrix y
x = np.array([[1,2,3], [4,5,6], [7,8,9], [10, 11, 12]])
v = np.array([1, 0, 1])
y = x + v  # Add v to each row of x using broadcasting
print y  # Prints "[[ 2  2  4]
         #          [ 5  5  7]
         #          [ 8  8 10]
         #          [11 11 13]]"
```

Modify arrays using indices

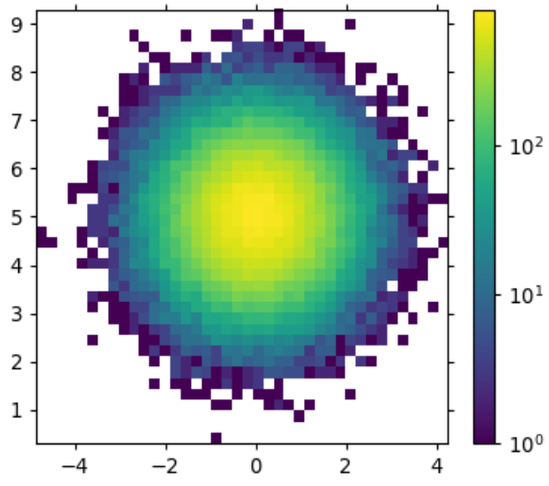
```
import numpy as np

# Create a new array from which we will select elements
a = np.array([[1,2,3], [4,5,6], [7,8,9], [10, 11, 12]])

print a  # prints "array([[ 1,  2,  3],
         #                [ 4,  5,  6],
         #                [ 7,  8,  9],
         #                [10, 11, 12]])"

# Create an array of indices
b = np.array([0, 2, 0, 1])

# Select one element from each row of a using the indices in b
print a[np.arange(4), b]  # Prints "[ 1  6  7 11]"

# Mutate one element from each row of a using the indices in b
a[np.arange(4), b] += 10

print a  # prints "array([[11,  2,  3],
         #                [ 4,  5, 16],
         #                [17,  8,  9],
         #                [10, 21, 12]])
```

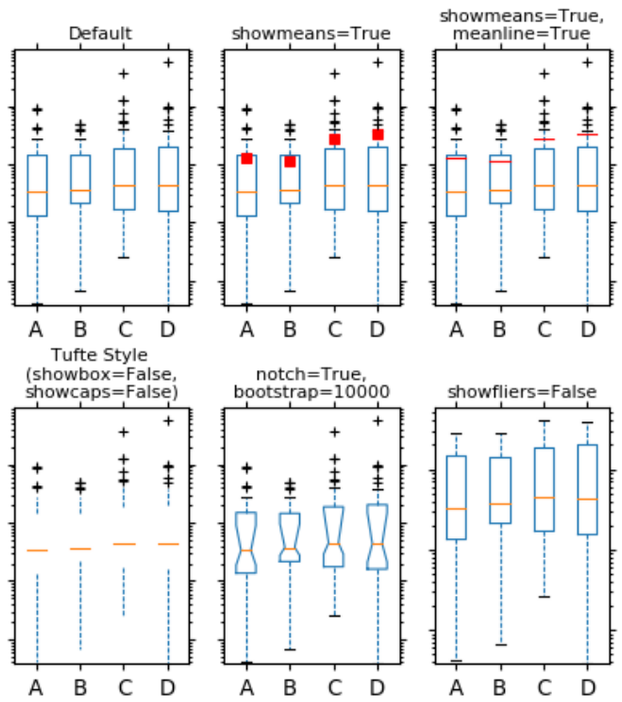
Array math

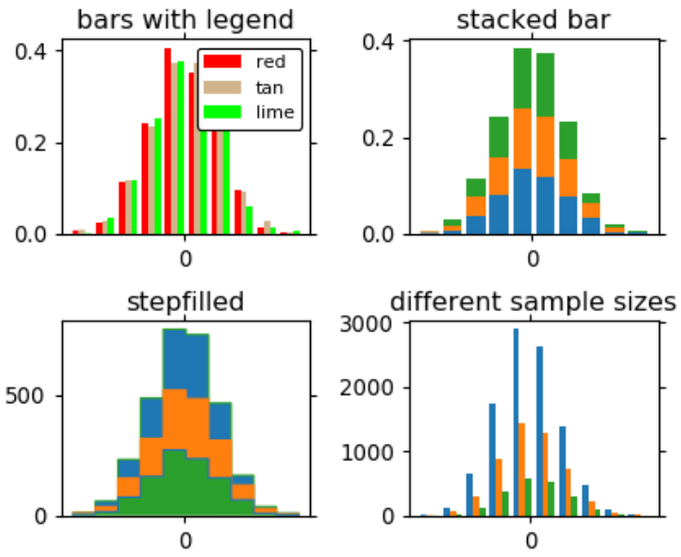
```
import numpy as np

x = np.array([[1,2],[3,4]], dtype=np.float64)
y = np.array([[5,6],[7,8]], dtype=np.float64)

# Elementwise sum; both produce the array
# [[ 6.0  8.0]
#  [10.0 12.0]]
print x + y
print np.add(x, y)

# Elementwise difference; both produce the array
# [[-4.0 -4.0]
#  [-4.0 -4.0]]
print x - y
print np.subtract(x, y)

# Elementwise product; both produce the array
# [[ 5.0 12.0]
#  [21.0 32.0]]
print x * y
print np.multiply(x, y)

# Elementwise division; both produce the array
# [[ 0.2         0.33333333]
#  [ 0.42857143  0.5       ]]
print x / y
print np.divide(x, y)

# Elementwise square root; produces the array
# [[ 1.          1.41421356]
#  [ 1.73205081  2.        ]]
print np.sqrt(x)
```

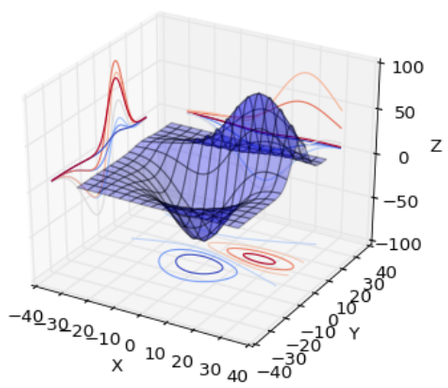
matplotlib

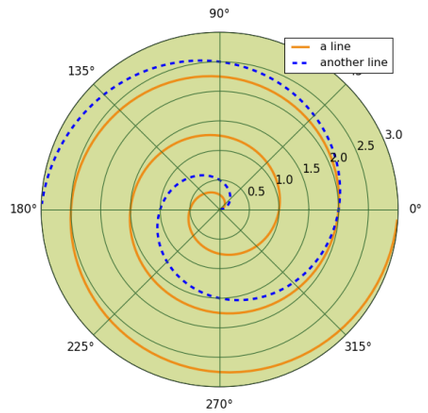
Turn your data into graphs!







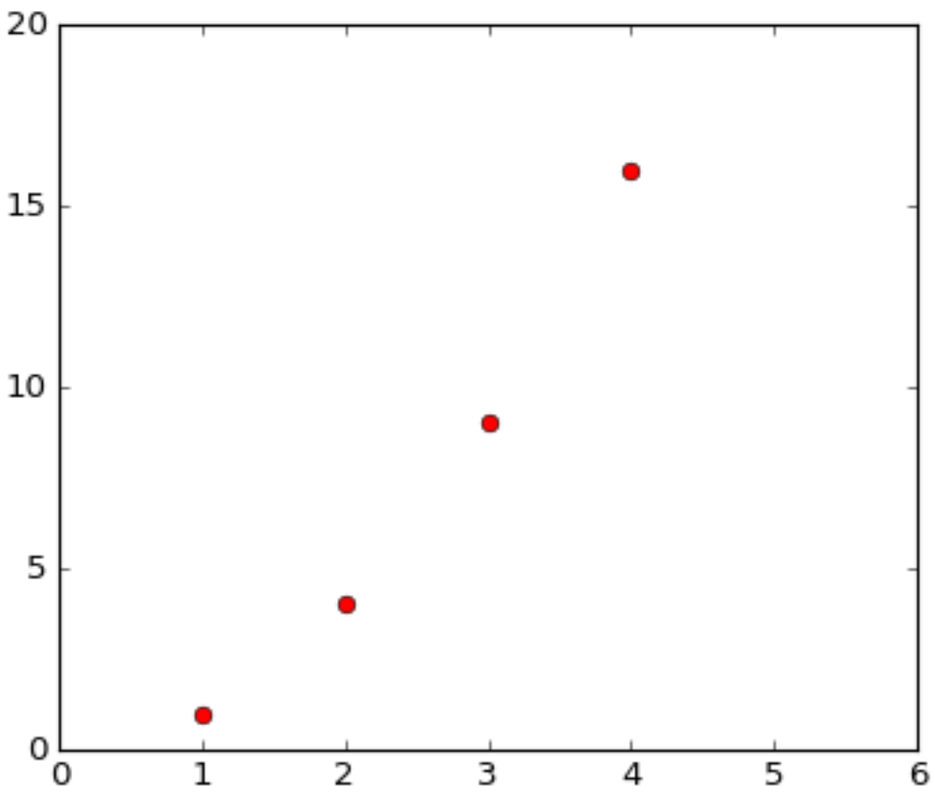




http://matplotlib.org/users/beginner.html

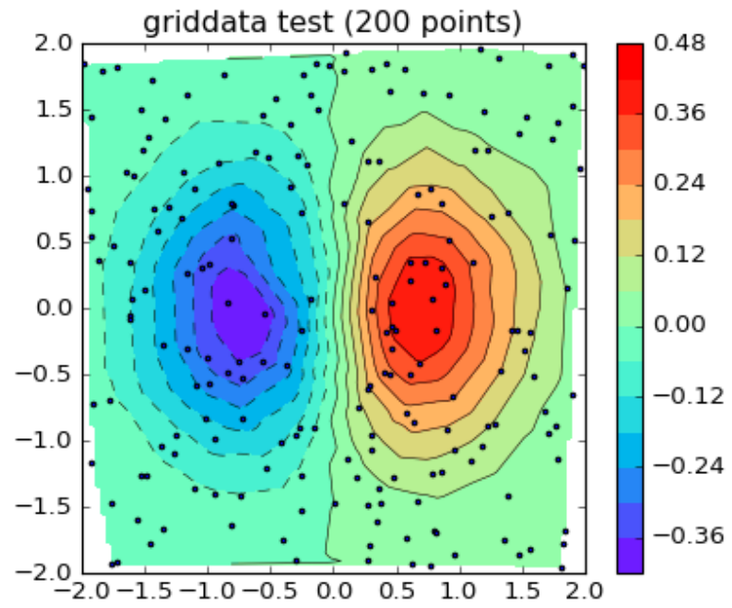
matplotlib

Simple




```
import matplotlib.pyplot as plt
plt.plot([1,2,3,4], [1,4,9,16], 'ro')
plt.axis([0, 6, 0, 20])
plt.show()
```

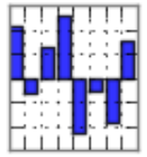
Less simple

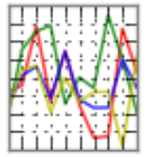


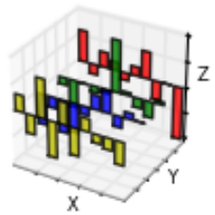

```
from numpy.random import uniform, seed
from matplotlib.mlab import griddata
import matplotlib.pyplot as plt
import numpy as np
# make up data.
#npts = int(raw_input('enter # of random points to plot:'))
seed(0)
npts = 200
x = uniform(-2, 2, npts)
y = uniform(-2, 2, npts)
z = x*np.exp(-x**2 - y**2)
# define grid.
xi = np.linspace(-2.1, 2.1, 100)
yi = np.linspace(-2.1, 2.1, 200)
# grid the data.
zi = griddata(x, y, z, xi, yi, interp='linear')
# contour the gridded data, plotting dots at the nonuniform data points.
CS = plt.contour(xi, yi, zi, 15, linewidths=0.5, colors='k')
CS = plt.contourf(xi, yi, zi, 15, cmap=plt.cm.rainbow,
                  vmax=abs(zi).max(), vmin=-abs(zi).max())
plt.colorbar()  # draw colorbar
# plot data points.
plt.scatter(x, y, marker='o', c='b', s=5, zorder=10)
plt.xlim(-2, 2)
plt.ylim(-2, 2)
plt.title('griddata test (%d points)' % npts)
plt.show()
```

pandas

$$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$$







Table/database treatment (similar to SQL)

```
In [6]: dates = pd.date_range('20130101', periods=6)

In [7]: dates
Out[7]:
DatetimeIndex(['2013-01-01', '2013-01-02', '2013-01-03', '2013-01-04',
               '2013-01-05', '2013-01-06'],
              dtype='datetime64[ns]', freq='D')

In [8]: df = pd.DataFrame(np.random.randn(6,4), index=dates, columns=list('ABCD'))

In [9]: df
Out[9]:
                   A         B         C         D
2013-01-01  0.469112 -0.282863 -1.509059 -1.135632
2013-01-02  1.212112 -0.173215  0.119209 -1.044236
2013-01-03 -0.861849 -2.104569 -0.494929  1.071804
2013-01-04  0.721555 -0.706771 -1.039575  0.271860
2013-01-05 -0.424972  0.567020  0.276232 -1.087401
2013-01-06 -0.673690  0.113648 -1.478427  0.524988
```

http://pandas.pydata.org/pandas-docs/stable/10min.html#min

- Symbolic mathematics
- Useful for algebraic equations

http://docs.sympy.org/latest/tutorial/

Modify equations

```
>>> import sympy
>>> x, y = sympy.symbols(‘x y')
>>> expr = x + 2*y
>>> expr
```

$$x+2y$$

```
>>> expr - x
```

$$2y$$

```
>>> expanded_expr = expand(x*expr)
>>> expanded_expr
```

$$x^2+2xy$$

```
>>> factor(expanded_expr)
```

$$x(x+2y)$$

IP[y]: IPython
Interactive Computing

An extended interactive shell.

Functionality includes:

- Tab auto-completion
- Magic commands (%)
- Shell commands (!)
  ex. “files = !ls”
- Configuration & aliases

command	description
?	Introduction and overview of IPython’s features.
%quickref	Quick reference.
help	Python’s own help system.
object?	Details about ‘object’, use ‘object??’ for extra details.

- Designed specifically with biology data in mind
- Lots of modules that work with sequences
- Parsing!

http://biopython.org

Seq object:

```
>>> from Bio.Seq import Seq
>>> my_seq = Seq("AGTACACTGGT")
>>> my_seq
Seq('AGTACACTGGT', Alphabet())
>>> print(my_seq)
AGTACACTGGT
>>> my_seq.complement()
Seq('TCATGTGACCA', Alphabet())
>>> my_seq.reverse_complement()
Seq('ACCAGTGTACT', Alphabet())
```

Transcribing, translating, rev/comp

```
>>> from Bio.Seq import Seq
>>> from Bio.Alphabet import IUPAC
>>> coding_dna
Seq('ATGGCCATTGTAATGGGCCGCTGAAAGGGTGCCCGATAG', IUPACUnambiguousDNA())
>>> messenger_rna = coding_dna.transcribe()
>>> messenger_rna
Seq('AUGGCCAUUGUAAUGGGCCGCUGAAAGGGUGCCCGAUAG', IUPACUnambiguousRNA())
>>> coding_dna.reverse_complement().transcribe()
Seq('CUAUCGGGCACCCUUUCAGCGGCCCAUUACAAUGGCCAU', IUPACUnambiguousRNA())
>>> coding_dna.translate()
Seq('MAIVMGR*KGAR*', HasStopCodon(IUPACProtein(), '*'))
```

More BIOPYTHON examples

Parsing a fasta file

```
from Bio import SeqIO
for seq_record in SeqIO.parse("/home/xalmal/SSQXT-19_S5_L001_R1_001.fasta", "fasta"):
    print(seq_record.id)
    print(repr(seq_record.seq))
    print(len(seq_record))
```

Web BLASTn:

```
>>> from Bio.Blast import NCBIWWW
>>> fasta_string = open(“your_sequences.fasta").read()
>>> result_handle = NCBIWWW.qblast("blastn", "nt", fasta_string)
>>> result_handle.read()
```

Local BLASTn:

```
>>> from Bio.Blast.Applications import NcbiblastxCommandline
>>> blastx_cline = NcbiblastxCommandline(query="opuntia.fasta", db="nr",
                   evalue=0.001, outfmt=5, out="opuntia.xml")
```

Installing python packages

Windows

1. Install `setuptools`:

```
curl https://bootstrap.pypa.io/ez_setup.py | python
```

2. Install `pip`:

```
curl https://bootstrap.pypa.io/get-pip.py | python
```

OS X

It's Easy (On Mac):

1. Install easy_install

```
curl https://bootstrap.pypa.io/ez_setup.py -o - | sudo python
```

2. Install pip

```
sudo easy_install pip
```

3. Now, you could install external modules. For example

```
pip install regex   # This is only an example for installing other modules
```

share improve this answer

edited Nov 4 '15 at 0:13 — Kevin Guan — 10.4k ● 9 ● 23 ● 47

answered Mar 21 '15 at 22:12 — Pavan — 870 ● 1 ● 6 ● 11

GNU/Linux

From source (download tarball)
or via package handler
(apt-get/rpm/yum)
get pip and continue from there

Anaconda: conda install <package>
(conda install pip -> pip install <package>)

Summary

Numpy:	Calculations on data
matplotlib:	Graphs
pandas:	Tables
SymPy:	Equations
IPython:	Useful coding tool
Biopython:	Sequence handling

These slides can be found at:
https://github.com/alvaralmstedt/Tutorials/blob/master/numpy_scipy_biopython.pdf