Python for Scientists

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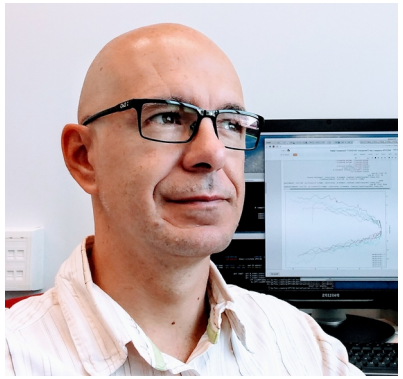
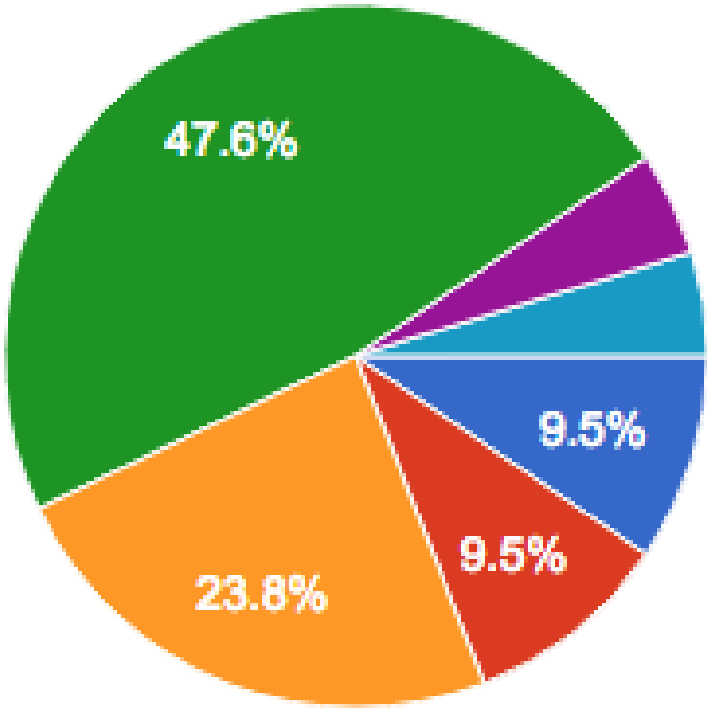


Us

- Researcher at the CSIC
- Computational biochemistry &biophysics
- Started with Fortran. Learnt some Perl, R, Mathematica
- But now mainly use Python
- Analysis of simulation
- Implementing new methods

- Ass. Professor at UB
- Computational Dynamics
- Started with Fortran. Learnt some PHP, Mathematica
- Use Fortran to generate results, Python to analyze and plot
- Analysis of simulations

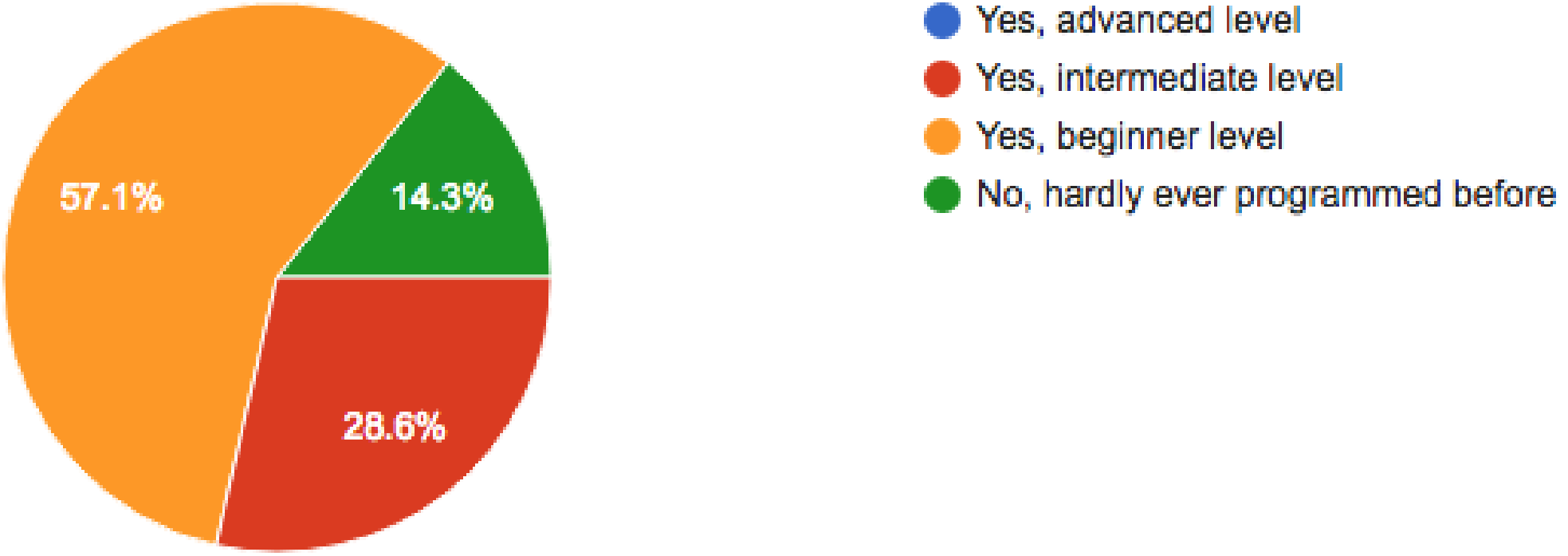
You UPDATE!



- Research Unit / Platform Director
- Experimental Research Unit / Platform technician
- Experimental Researcher
- Computational Researcher
- Experimental researcher currently focussed on physical modelling with Matlab
- Lab engineer

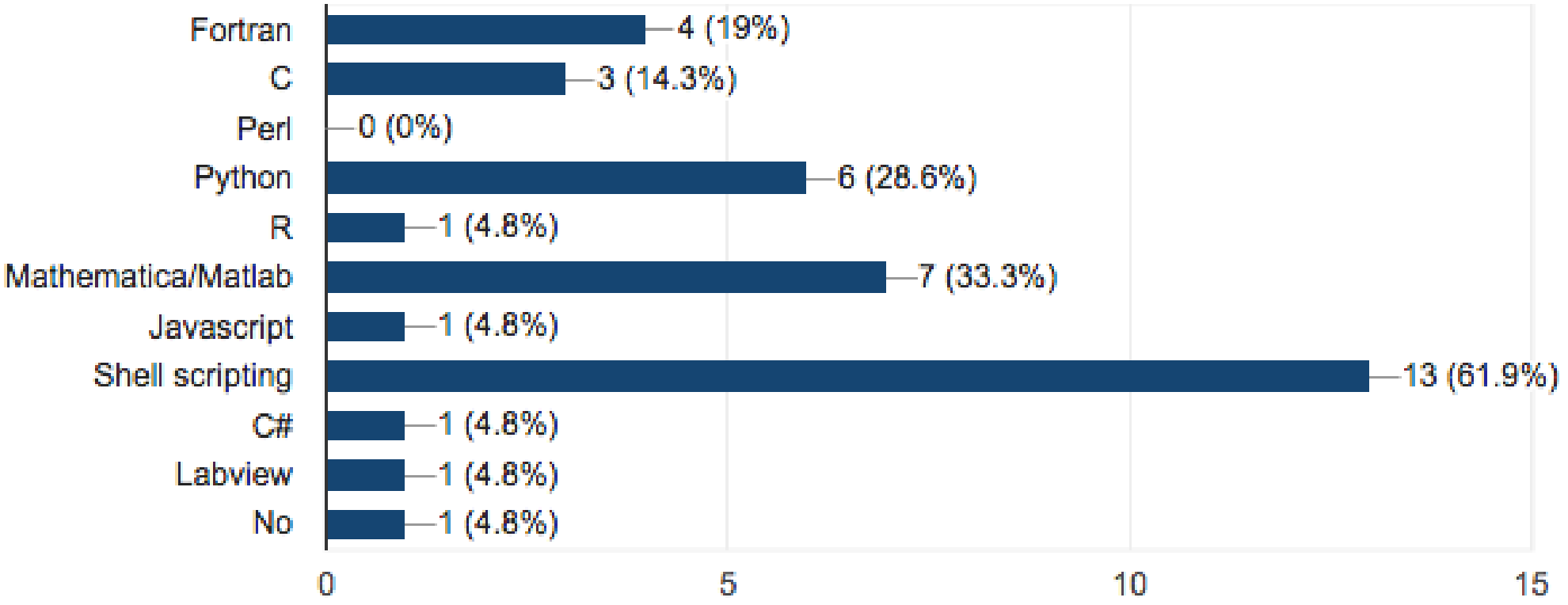
YouUPDATE!

- Previous experience with programming



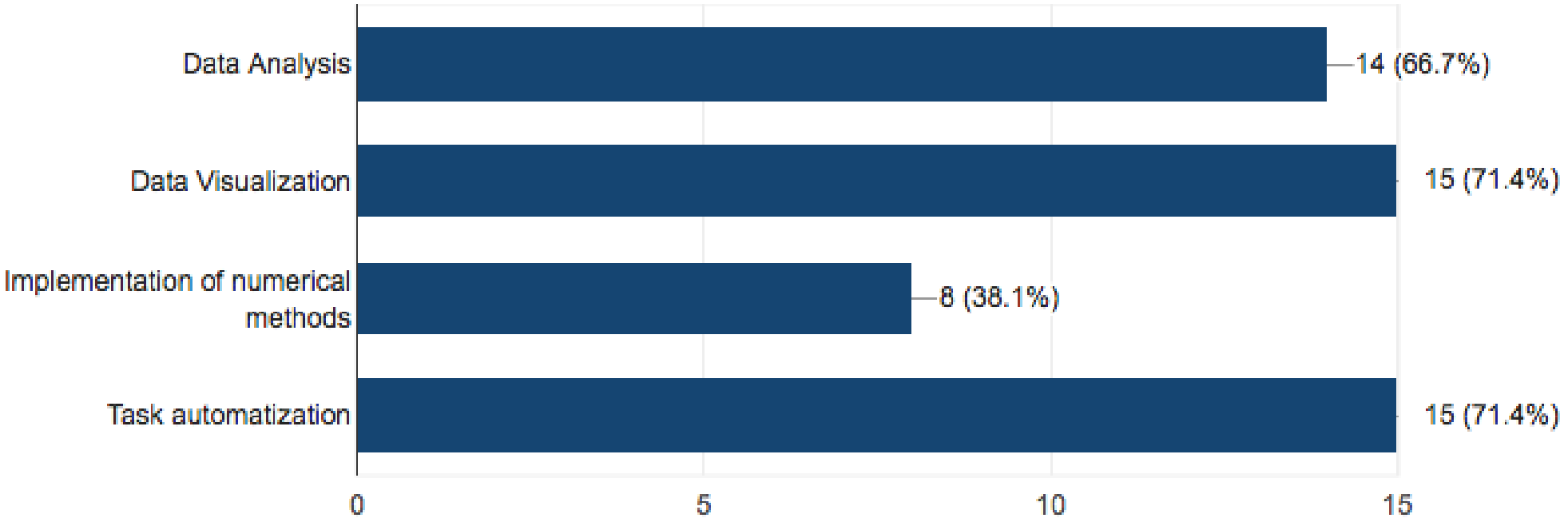
You UPDATE!

- Previous experience with programming



You UPDATE!

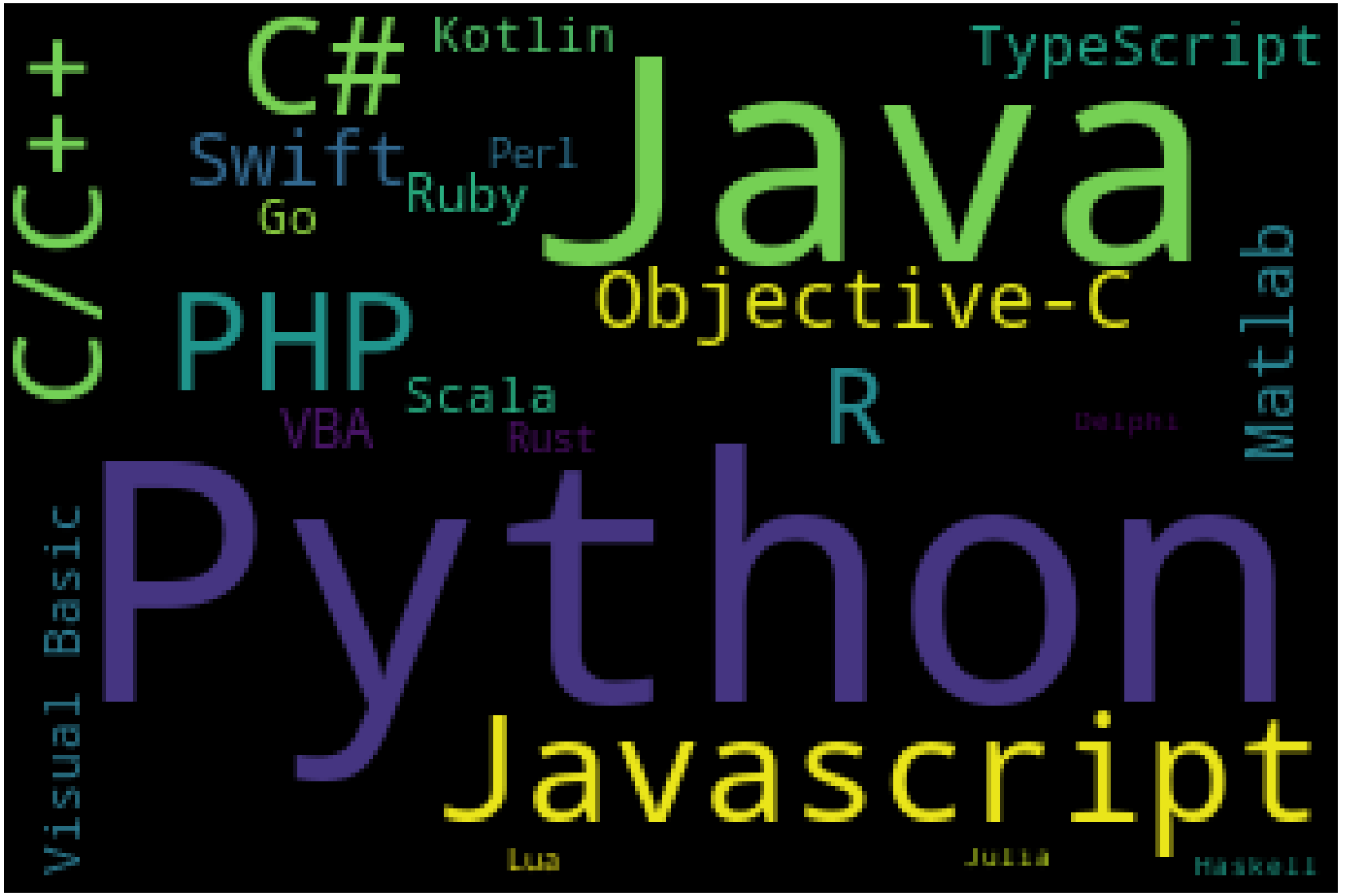
- Expectations



Overview

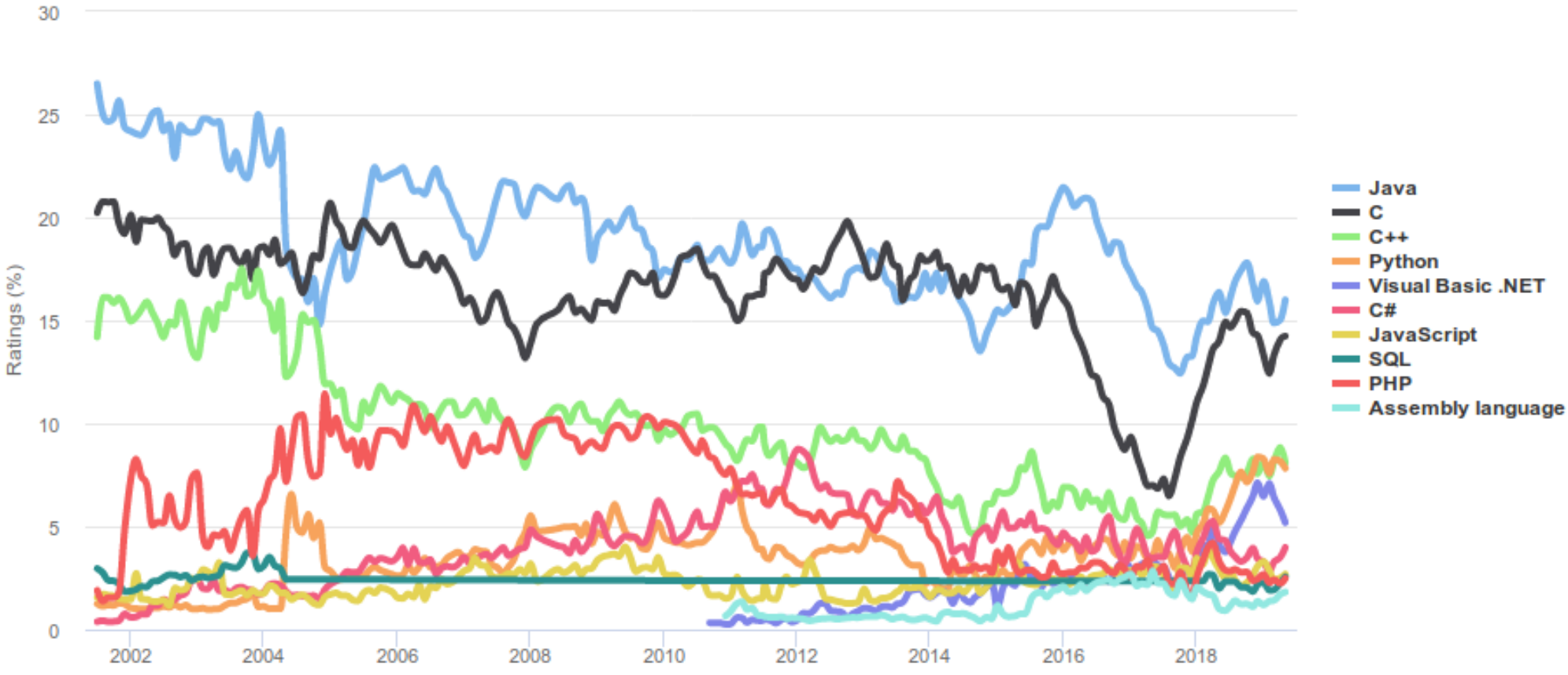
- Why Python
- Language basics
- Working with files
- Working with arrays: Numpy
- Data visualization: matplotlib
- Structured data: Pandas
- Functions and modules
- Scientific modules. Scipy
- Classes and objects (bare minimum!)
- Other scientific modules: sckikit-learn, biopython…
- Profiling and optimization and beyond Python

Language popularity



http://pypl.github.io/PYPL.html

Language popularity



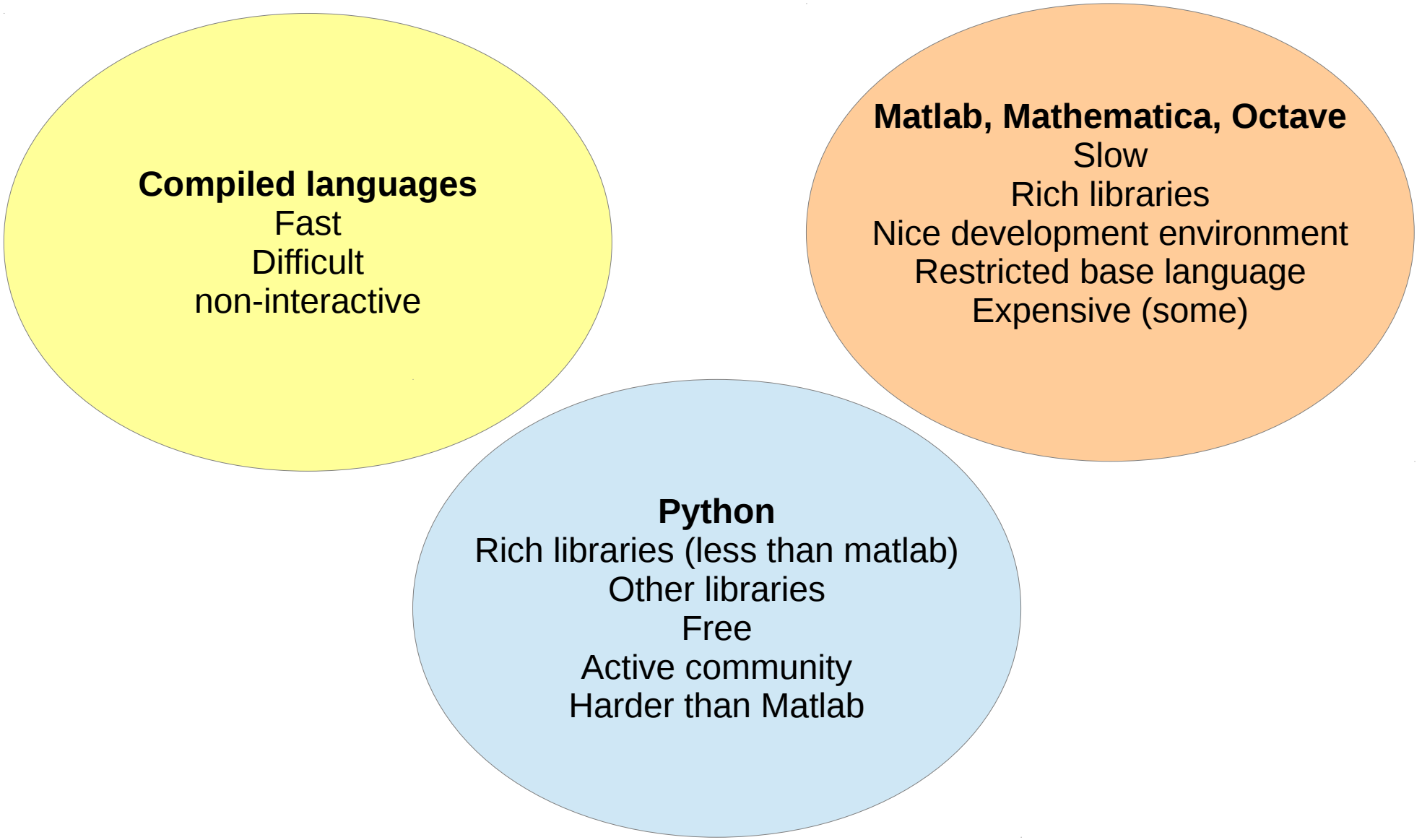
http://www.tiobe.com/index.php/content/paperinfo/tpci/index.html

Python for science

- A high level language gives more time to more complex problems
  - At the expense of hiding important details
- Example:
  - A reaction mechanism
  - Optimisation of an energy function
    - Steepest descent, conjugate gradients, quasi-Newton
  - Implementation of BFGS quasi-Newton
    - Memory issues, diagonalization, matrix inversion…
  - Calculation of numerical gradients or hessians:
    - machine precision, central differences, etc.

http://fperez.org/py4science/why_python.html

Python for science

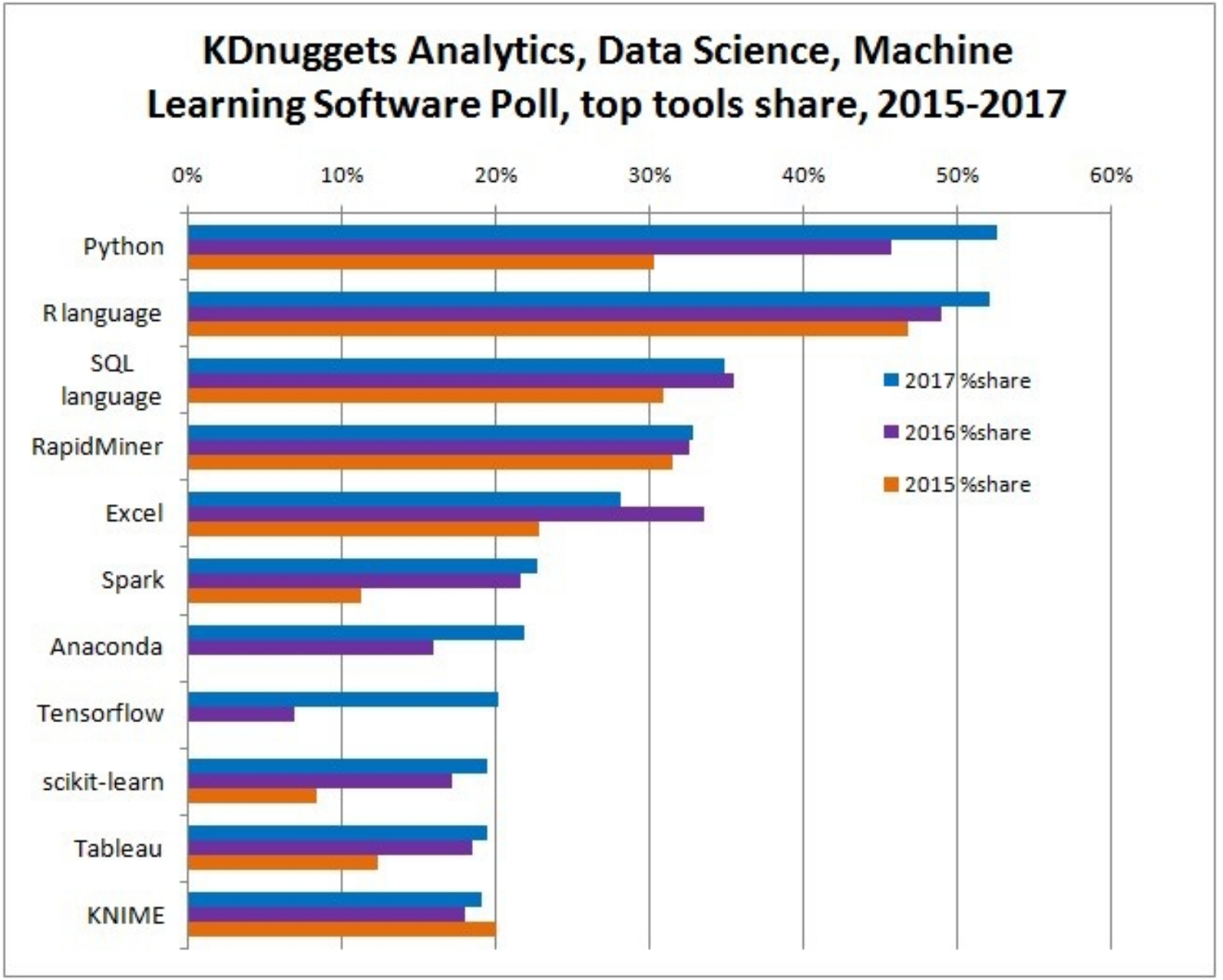


Matlab, Mathematica?

- Scientific computing:
  - ipython + scipy + matplotlib
- Free
- Open source
- Extensible

- Bioinformatics
  - Biopython
- Molecular Dynamics
  - MMTK
- Efficiency
  - Numba, Cython, Fortran, C
- Server control
- XML parser

Python for data science



Python for data science

- Which is better for data analysis: R or Python?
  http://www.quora.com/Which-is-better-for-data-analysis-R-or-Python
- SAS vs. R (vs. Python) – which tool should I learn?
  http://www.analyticsvidhya.com/blog/2014/03/sas-vs-vs-python-tool-learn/
- Python Vs R Machine learning
  http://datascience.stackexchange.com/questions/326/python-vs-r-machine-learning
- How to Choose Between Learning Python or R First
  http://blog.udacity.com/2015/01/python-vs-r-learn-first.html
- Python, Machine Learning, and Language Wars
  http://sebastianraschka.com/blog/2015/why-python.html

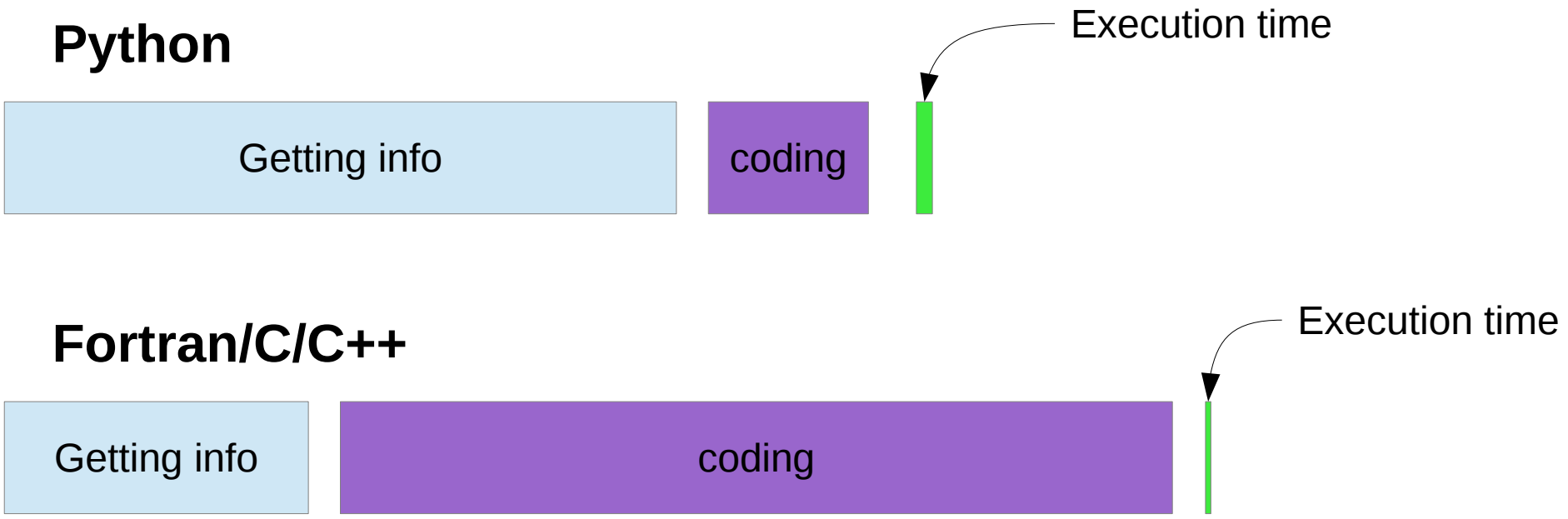
Low level vs. high level

- Python is a high level language
- You can focus on:
  - Low level issues
  - Higher complexity of problems

- Low level issues
  - Variable types
  - Machine precision
- But also
  - Extend
  - Mantain
  - Document code

Python vs. Fortran/C

Different time distribution to get a task done

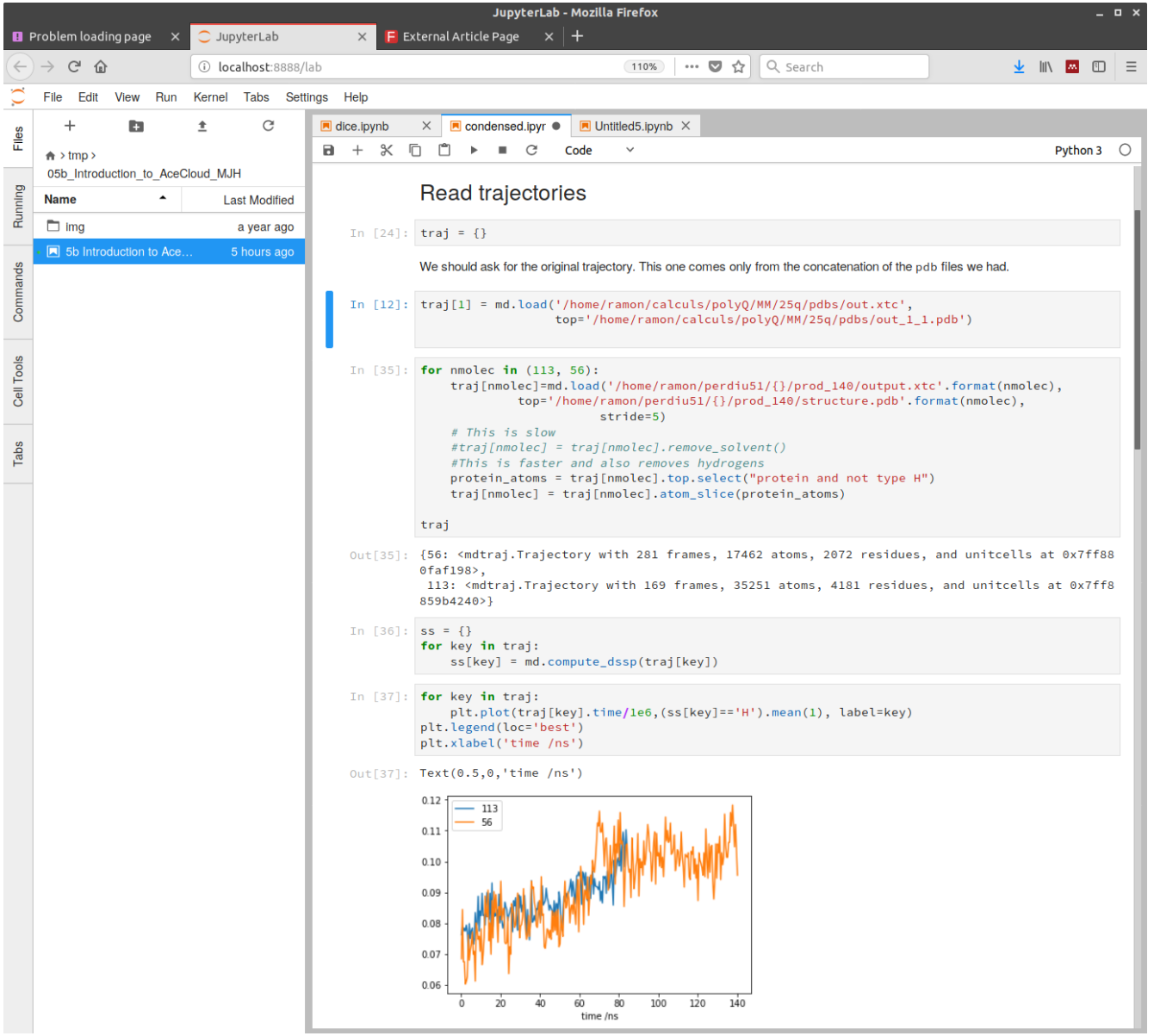


Python for science

- The homogenization of scientific computing, or why Python is steadily eating other languages' lunch
  http://www.talyarkoni.org/blog/2013/11/18/the-homogenization-of-scientific-computing-or-why-python-is-steadily-eating-other-languages-lunch/
- 10 Reasons Python Rocks for Research (And a Few Reasons it Doesn't)
  http://www.stat.washington.edu/~hoytak/blog/whypython.html

Interactive shells

- python
- IDLE
- JupyterLab (previously called ipython)
  - console
  - notebook
- spyder
- eric
- PIDA
- Sage



Python distributions

- Anaconda
  - https://www.continuum.io/downloads
- Enthought Canopy
  - https://www.enthought.com/products/canopy/

Which python version?

- Language is fast evolving
- 2 versions now coexist: 3.x and 2.x
- These versions are not completely compatible
- 3.x is better and continued
- 2.x has some software still not ported
- Both can safely coexisit
  - Packages and shells are for a specific version
- `2to3 -w hello.py`

Short jupyter-lab tutorial

beyond python

TAB autocomplete:

- functions
- methods
- files
- …

`reload` command

cursor keys get history (for console only):

- even previous sessions!
- text + keys: previous match

?: intro to ipython

`%quickref`

Without ipython:

`python3 -u script.py` enters interactive mode

Magic functions

```
%timeit x=10     : time the 'x=10' statement with high precision.
%%timeit x=2**100
x*100            : time 'x*100' with a setup of 'x=2**100'; setup code is not
                   counted.  This is an example of a cell magic.

%history
%load_ext
%run
%pdb: Control the automatic calling of the pdb interactive debugger.
%timeit
%pwd
%cd
%%bash
```

http://ipython.org/ipython-doc/dev/interactive/tutorial.html

Running scripts

`%run script.py`

`import script.py`

are not the same!

`%run script.py` is like `python3 script.py`

Imports are only “imported” once in a session (see later `%autoreload` magic function)

ipython notebook

- Nice presentation
- Allows parallel execution
- Combines text and code
- Executable or exportable to:
  - html
  - LaTeX
  - python
- Start with: `jupyter lab`
- Examples:
  https://github.com/jrjohansson/scientific-python-lectures

Files

Files

- Files can be *text* or *binary*
- Files can be opened for read, write or append
  - `'r', 'w', 'a+'`
- **`with open('name') as filein:`**
  - Allows automatic file closure
  - Explanation of the **`with`** statement: http://effbot.org/zone/python-with-statement.htm

Reading / Writing Files

```
file_in=open('indata.txt','r')
file_out=open('outdata.txt','w')
for line in file_in:
    # Take some information (split() method is very useful!)
    x = float(line.split()[0])
    # Apply a given function (fact)
    fx = fact(x)
    # Write the result in an output file with a defined format
    file_out.write('{:010.3f}\n'.format(fx))
```

But for loading numerical data **Numpy** is more efficient. And **pandas** even more.

File parsing

- The basic:

```
for line in filein:
    do something
```

- Common things:

```
if 'optimized' in line:
    do something
line = line.split()
if line.upper().startswith('GEOM'): …
energy = float(line[2])
```

skipping lines

- Lines can be skipped by calling **`next()`** to a file:

```
for line in filein:
    if 'Optimized' in line:
        next(filein); next(filein) #skip two lines
        do something...
```

Formatting

- There are several function:

```
'12'.rjust(5), '12'.zfill(5)
```

- But `format` is more general:

```
print('{0:2d} {1:3d}'.format(x, x*x))
print("{:10.3f} {:10.3f} {:10.3f}".format(x,y,z))
```

- List of unkown length (use argument unpacking):

```
vals = np.linspace(0,1,11)
print((len(vals)*"{:10.2e} ").format(*vals))
```

http://docs.python.org/3/library/string.html#formatspec

Useful modules

- Similar to `ls`:

```
import glob
files = glob.glob(pattern)
```

- Working with shell-like commands:

```
import os
os.rename(src, dst)
os.mkdir(path)
os.chown(path, uid, gid)
os.getenv(key)
os.walk(directory)
```

http://docs.python.org/3/library/os.html

Useful modules

- Reading Excel files http://www.python-excel.org/:

```
import xlrd
```

  - Pandas uses this library
- Working with image files
  - http://scikit-image.org/
  - http://pillow.readthedocs.io/en/latest/

Numpy

Why Numpy / Scipy?

- Python (alone) is not efficient for numerical calculations
- Python (alone) is not practical for array manipulation
- Numpy provides the data types and methods for arrays
- Scipy provides more elaborate numerical methods
  - Optimization
  - Fast Fourier Transform
  - Linear algebra, etc

```
import numpy as np
import scipy.optimization
import scipy.stats as stats
```

numpy arrays

- without numpy:

```
> a=[[1,2],[3,4]]
> b=[[10,20], [30,40]]
> a+b
[[1, 2], [3, 4], [10, 20], [30, 40]]
```

- with numpy:

```
> a=np.array(a)
> b=np.array(b)
> a+b
array([[11, 22],[33, 44]])
```

- Array creation

```
a=np.array([1,2,3,4]).reshape([2,2])
a=np.array([[1,2], [3,4]])
a=np.zeros([2,2], dtype=int)
a[0,0]=1.
a=np.ones((4,4))
a=np.arange(10)
a=np.diag([1,2,3,4])
a=np.tile(a, (10,2))
a=np.identity(3)
a=np.linspace(-5,5, 20)
```

Ufuncs

- Unary:

```
a.min()
a.sum()
a.cumsum()
a.mean()
np.argmin(a)
np.exp(-a)
np.cov(a)
a.tolist()
```

- Binary:

```
a + b
np.dot(a, b)
```

- Applying to parts of an array:

```
> a=np.array([[1,2], [3,4]])
> a.min(axis=0)
array([1, 2])
a.sum(axis=1)
array([3, 7])
```

- `Python functions are less efficient than numpy functions:`

  `a.sum()` better than `sum(a)`

  `np.min(a)` better than `min(a)`

many implemented as methods and functions

Accessing array elements

- Slicing:

```
> a[2:5]

> b[:, ::5]

> a[1:4, ...]
```

- Fancy indexing:
  - Boolean arrays (masks):

```
> a = np.arange(10,15)
> indices = (a**2 > 115) & (a < 14)
> a[indices]
array([11, 12, 13])
```

  - With lists:

```
> a = np.arange(10,15)
> y=a[[4,4,1]]
> y
array([14, 14, 11])
> a[[4,4,1]] = [-2, -4, 5]
> a
array([10,  5, 12, 13, -4])
```

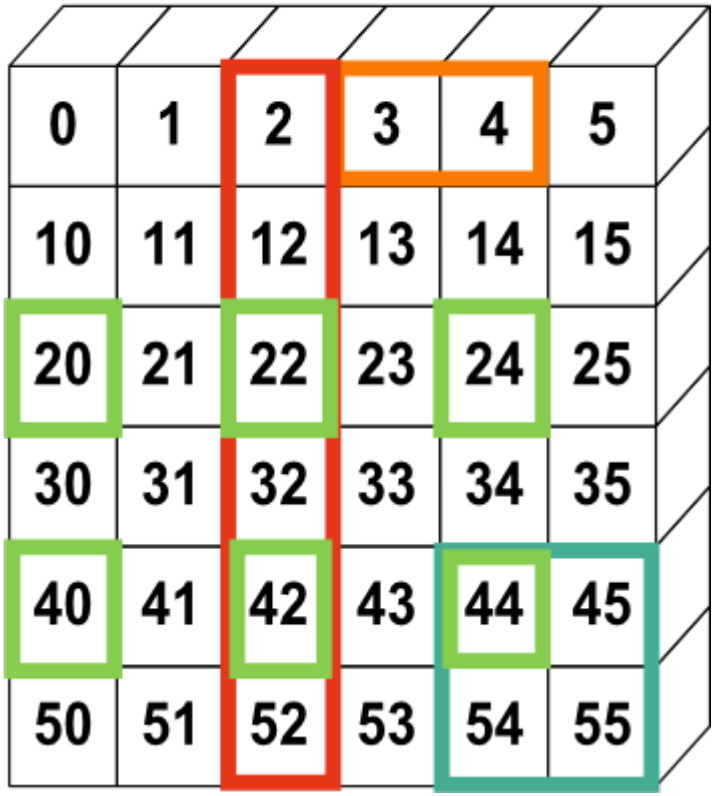
Accessing array elements

```
>>> a[0,3:5]
array([3,4])

>>> a[4:,4:]
array([[44, 45],
       [54, 55]])

>>> a[:,2]
array([2,12,22,32,42,52])

>>> a[2::2,::2]
array([[20,22,24]
       [40,42,44]])
```



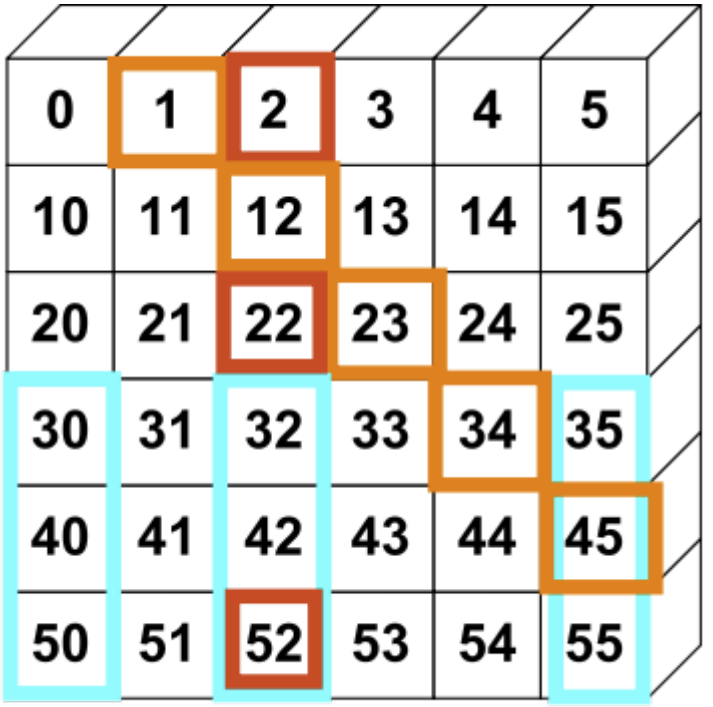
From: https://scipy-lectures.github.io/intro/numpy/array_object.html

Accessing array elements

```
>>> a[(0,1,2,3,4),(1,2,3,4,5)]
array([ 1, 12, 23, 34, 45])

>>> a[3:,[0, 2, 5]]
array([[30, 32, 35],
       [40, 42, 45]])
       [50, 52, 55]])

>>> mask = array([1,0,1,0,0,1],
                 dtype=bool)
>>> a[mask,2]
array([2,22,52])
```



From: https://scipy-lectures.github.io/intro/numpy/array_object.html

Accessing array elements

- Slices return views

```
> a = np.arange(5)
> y=a[2:5]
> y *= -1
> a
array([ 0,  1, -2, -3, -4])
> y.flags.owndata
False
```

- np.where

```
> np.where((a>=2)&(a<4), a**2, -1)

Array([-1, -1,  4,  9, -1])
```

- np.choose
  - Powerful, but complex!
- np.nonzero

- Boolean arrays return copies

```
> a = np.arange(5)
> y = a[a>1]
> y *= -1
> a
array([0, 1, 2, 3, 4])
> y.flags.owndata
True
```

- Fancy indexing returns copies:

```
> a = np.arange(5)
> y=a[[2,3,4]]
> y *= -1
> a
array([0, 1, 2, 3, 4])
> y.flags.owndata
True
```

Broadcasting

```
> a = 4.
> b = np.array([1,2,3])
> c = np.array([[1,2,3], [4,5,6]])
> b+a, c+a
(array([ 5.,  6.,  7.]), array([[  5.,   6.,   7.],
        [  8.,   9.,  10.]]))
> b+c
array([[2, 4, 6],
       [5, 7, 9]])
> c.dot(b)
> b.dot(c)
ValueError: objects are not aligned
> b[1:]*c
ValueError: operands could not be broadcast together with shapes (2) (2,3)
> b[1:]*c.T
```

- Use `matrix` if you want more algebra-like behaviour

Broadcasting

- Change the shape to allow for broadcasting:

```
> c = np.array([[1,2,3], [4,5,6]])
> b = c.mean(axis=1)
> c+b[:,np.newaxis] #or c+b[:,None]
> c+b.reshape((-1,1))
```

- Or keep the shape:

```
> b = c.mean(axis=1, keepdims=True)
> c+b
```

- See also:
  - `np.atleast_2d`, `np.atleast_1d` and `np.atleast_3d`

Broadcasting

- Broadcasting rules:

  When operating on two arrays, NumPy compares their shapes element-wise. It starts with the trailing dimensions, and works its way forward. Two dimensions are compatible when

  1) they are equal, or
  2) one of them is 1

- More examples and longer explanation here:
  - https://docs.scipy.org/doc/numpy-1.13.0/user/basics.broadcasting.html

np.einsum

- Complex but powerful function to avoid the use of loops
  - Dot product, outer product, and others can be written as **einsum**

```
> c = np.array([[1,2,3], [4,5,6]])
> np.allclose(c.dot(c.T), np.einsum('ij, kj->ik',c,c))
```

True

- See numpy documentation and the following blog entry:
  - http://docs.scipy.org/doc/numpy-1.10.0/reference/generated/numpy.einsum.html
  - http://ajcr.net/Basic-guide-to-einsum/

array functions and methods

- Array reduction and logical operations:

```
> a=np.arange(5)
> np.all(a>3)
False
> np.any(a>3)
True
> a > 3
array([False, False, False, False,
 True], dtype=bool)
> (a > 3) & (a < 5)
array([False, False, False, False,
 True], dtype=bool)
```

- Some details of memory use:
- `> a.flags`

```
 C_CONTIGUOUS : True
 F_CONTIGUOUS : True
 OWNDATA : True
 WRITEABLE : True
 ALIGNED : True
 UPDATEIFCOPY : False
```

Loading and saving data

- Pickle is the usual way to save and restore data in Python
- We often have data file in text format:

```
#Dist Energy
1.0 34.
1.2 38.
2.4 42.
```

- `f=np.loadtxt("energies.dat")`
- `f=np.genfromtxt("energies.dat")`

```
> f
array([[  1. ,  34. ],
       [  1.2,  38. ],
       [  2.4,  42. ]])
```

- Save single arrays with:

```
> np.save('result_y', y)
```

- Save in text mode with:

```
> np.savetxt('result_y', y)
```

- and multiple arrays with (saves a dictionary):

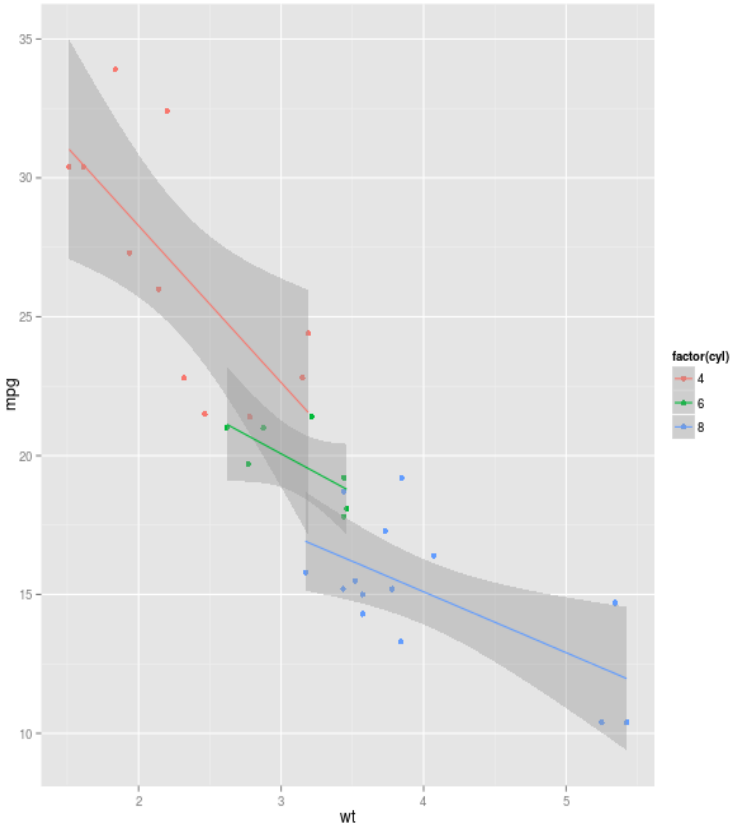
```
> np.savez('results', x, y)
```

- Recover them with load:

```
> y=np.load('results_y.npy')
> npz=np.load('results.npz')
```

Acess R from python

- Use the rpy2 module.
- From the documentation:




```
import math, datetime
import rpy2.robjects.lib.ggplot2 as ggplot2
import rpy2.robjects as ro
from rpy2.robjects.packages import importr
base = importr('base')
datasets = importr('datasets')


mtcars = datasets.data.fetch('mtcars')['mtcars']
pp = ggplot2.ggplot(mtcars) + \
     ggplot2.aes_string(x='wt', y='mpg', col='factor(cyl)') + \
     ggplot2.geom_point() + \
     ggplot2.geom_smooth(ggplot2.aes_string(group = 'cyl'),
                         method = 'lm')
pp.plot()
```

Other tutorials

- Take a look at these tutorials:
  - http://wiki.scipy.org/Tentative_NumPy_Tutorial
  - From: http://jrjohansson.github.io/
    - Lecture-2-Numpy.ipynb
    - Lecture-3-Scipy.ipynb

Extensions

- When your data is too large to fit in memory:
  - PyTables https://www.pytables.org/
- or to compute in a single machine:
  - DASK https://dask.pydata.org/en/latest/
- Multidimensional Pandas dataframes:
  - Xarray https://xarray.pydata.org/en/stable/

matplotlib

Matplotlib

- A module for plotting 2D and 3D data
- Combines well with numpy
- Starts with

```
import matplotlib.pyplot as plt
%matplotlib inline
```

`import pylab` or similar is deprecated.

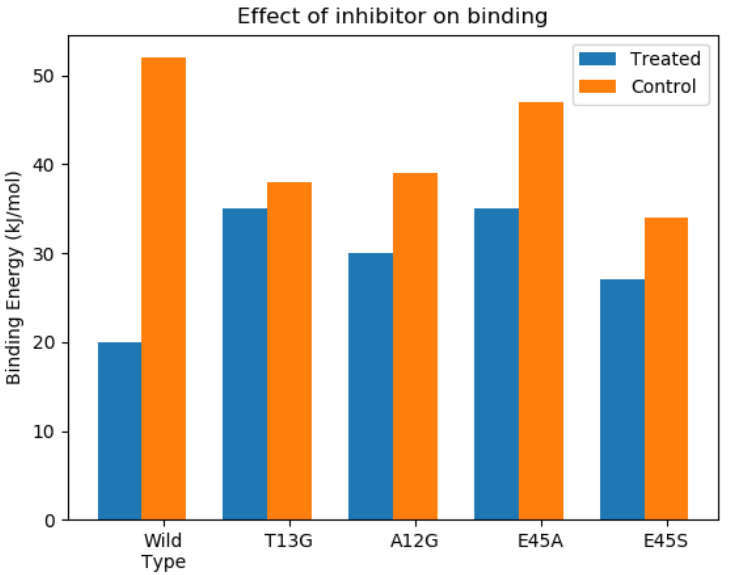
Matplotlib

Simplest plots:

```
> plt.plot([1,2,3], [1,4,9])
> plt.plot(x, sin(x), '--') #where x is a numpy array
> plt.figure() # creates new figure
> plt.clf() # Clears current figure
> plt.matshow(m) # m is a 2D array
> plt.imshow(m) # m is a 2D array. Same as matshow.
> d = np.loadtxt('data.txt')
> plt.plot(d[:,0], d[:,1], 's') #just slightly longer than gnuplot
```

Matplotlib

Totally reproducible figures




```
N = 5
treated = (20, 35, 30, 35, 27)
control = (52, 38, 39, 47, 34)
ind = np.arange(N)  # the x locations for the groups
width = 0.35       # the width of the bars

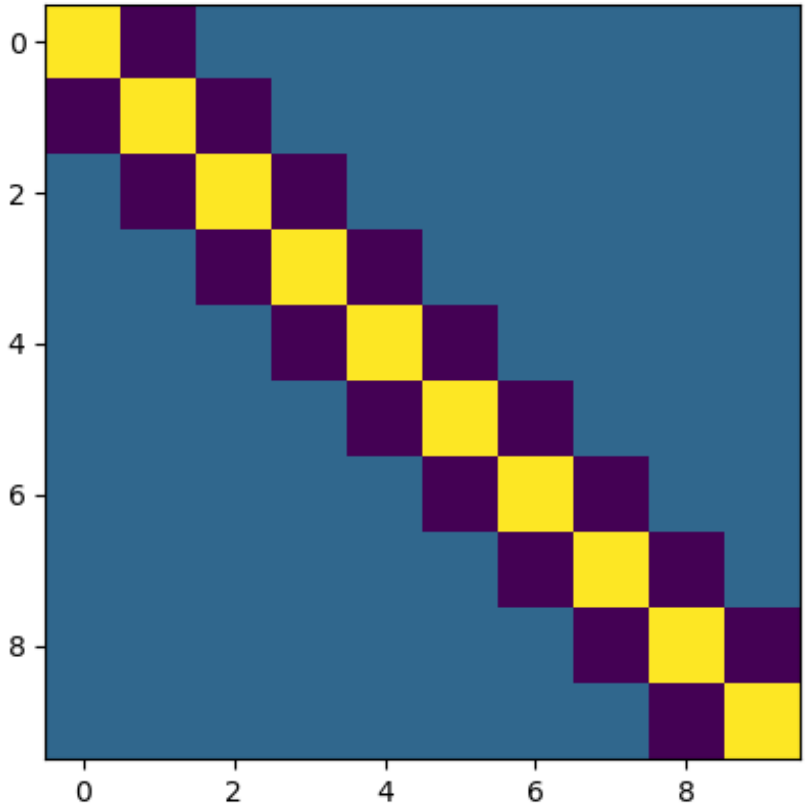
fig, ax = plt.subplots()
rects1 = ax.bar(ind, treated, width, label='Treated')
rects2 = ax.bar(ind+width, control, width, label = 'Control')

# add some
ax.set_ylabel('Binding Energy (kJ/mol)')
ax.set_title('Effect of inhibitor on binding')
ax.set_xticks(ind+width)
ax.set_xticklabels( ('Wild\nType', 'T13G', 'A12G', 'E45A', 'E45S') )
ax.legend()
```

Plotting matrices

```
m=np.diag(2*np.ones(10))+np.diag(-1*np.ones(9),1)+np.diag(-1*np.ones(9), -1)

plt.imshow(m)              # plt.matshow(m) is very similar
```

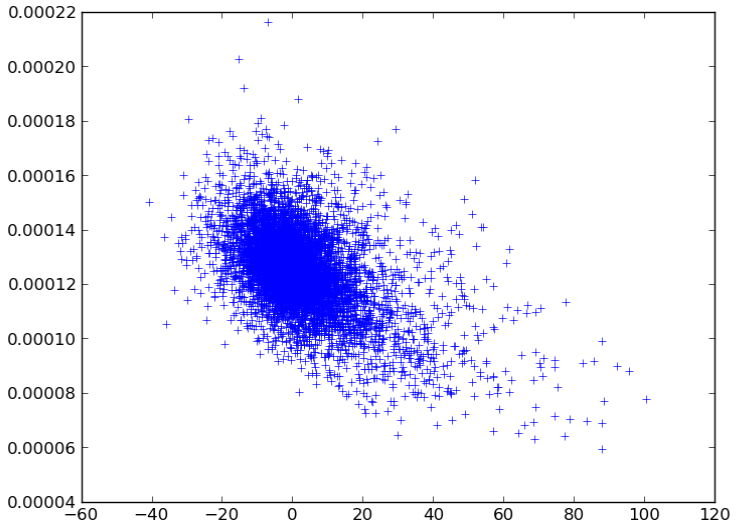


Matplotlib styles

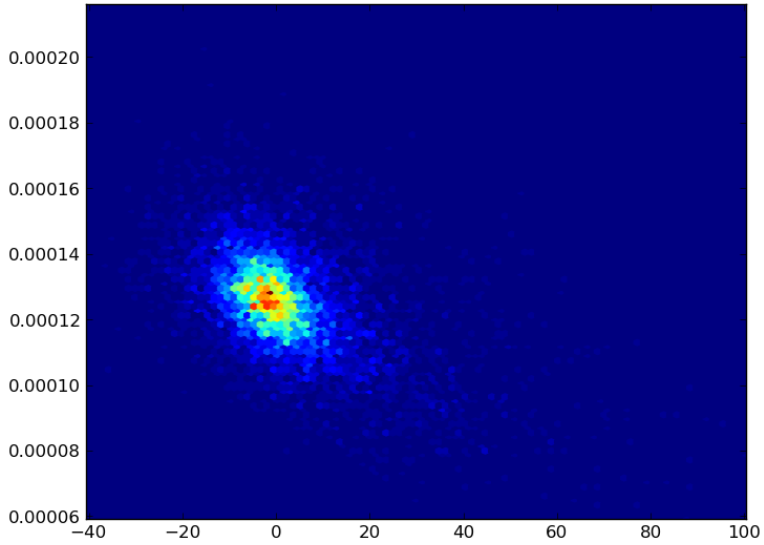
- Since version 1.5 several default styles.
- Try the following code

```
x= np.linspace(0, np.pi, 100)
for s in plt.style.available:
    with plt.style.context(s):
        plt.figure()
        plt.title(s)
        plt.plot(x,np.sin(x)*np.cos(x**2), label='A')
        plt.plot(x,np.sin(x)*np.cos(x**2)*np.cos(x), label='B')
        plt.plot(x,np.sin(x)-np.cos(x)*np.sin(x), label='C')
        plt.legend(loc='best')
```

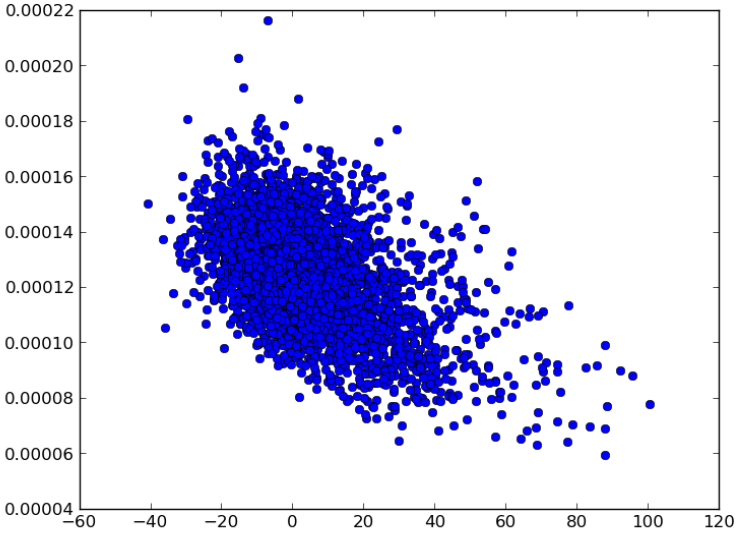
Plotting lots of points:hexbin



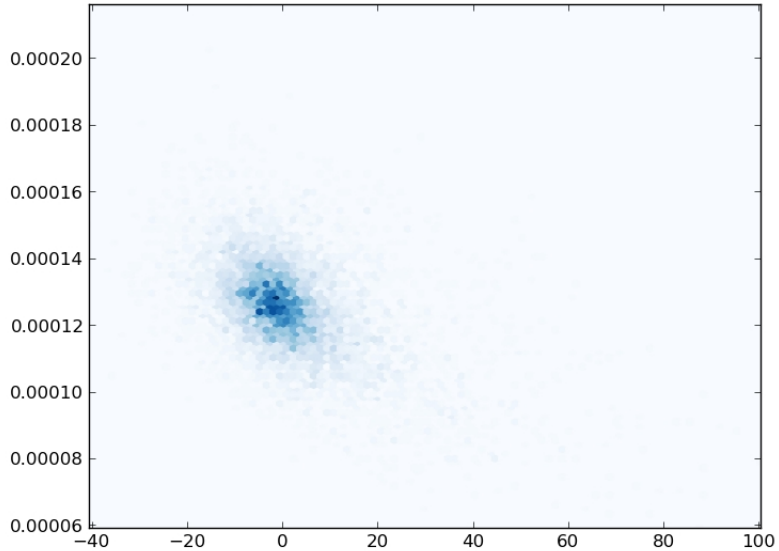

```
plt.plot(x, y, '+')
```




```
plt.hexbin(x, y)
```

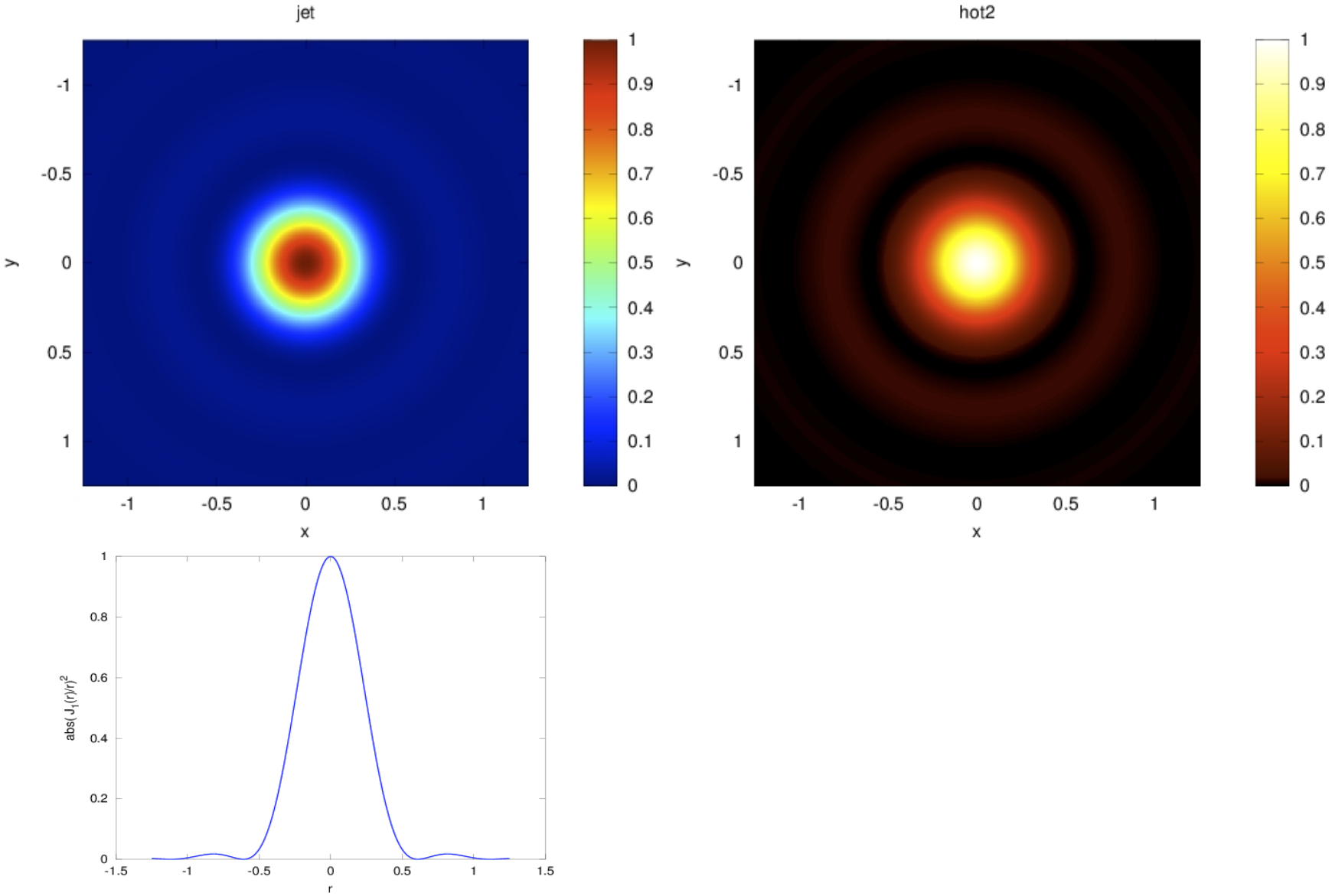



```
plt.plot(x, y, 'o')
```




```
plt.hexbin(x, y, cmap=pylab.cm.Blues)
```

Jet is not a good colormap



http://cresspahl.blogspot.com.es/2012/03/expanded-control-of-octaves-colormap.html
https://jakevdp.github.io/blog/2014/10/16/how-bad-is-your-colormap/

Matplotlib

- Do Lecture-4-Matplotlib.ipynb from http://jrjohansson.github.io/
  - Other interesting material there…
- Check matplotlib gallery
  - http://matplotlib.org/gallery.html
- Quick reference of symbols and colours:
  - http://www.loria.fr/~rougier/teaching/matplotlib/#quick-references

  (part of a larger tutorial)
- Some more tricks and examples:
  - http://wiki.scipy.org/Cookbook/Matplotlib

Extensions

- Altair
  - Declarative Visualization
  - https://altair-viz.github.io/
- Seaborn
  - Data visualization
  - Nice color palettes from http://colorbrewer2.org/
  - https://stanford.edu/~mwaskom/software/seaborn/
- Bokeh:
  - http://bokeh.pydata.org/en/latest/
- Plotly:
  - https://plot.ly/
- http://pbpython.com/visualization-tools-1.html

Functions and modules

Functions

defined by def and a colon:

```
def add(x,y):
    return x+y
```

Remember indentation!

Automatic (and recommended) documentation:

```
def add(x,y):
    """ Returns the
      sum of 2 numbers"""
    return x+y
```

Functions can be seen as both Fortran procedures and functions but...

Arguments are passed by reference

there is access to global variables:

```
> def x_val(): print(x)
> x=60
> x_val()
60
```

Functions II

Function variables are local :

```
> def x_val():
...   x=40
...   print(x)
> x=60
> x_val()
40
> x
60
```

to assign variables, use `return`

```
def x_val():
...   x=40
...   print(x)
...   return x
> x = xval()
40
> x
40
```

Functions III

Mutable objects are passed by reference:

```
> def square_0(lst):
...  lst[0]*=lst[0]
> a=[3,2,1]
> square_0(a)
> a
[9,2,1]
```

Copy variables that need to be preserved:

```
> a_copy=a[:]
> square_0(a)
> import copy
> a_copy=copy.deepcopy(a)
```

Functions IV

Functions can have default arguments :

```
> def submit(job, priority=10,
   nprocs=1):
...  pass
> submit('job1.sh')
```

Function arguments do not have explicit types.

```
> add('Python ', 'summerschool')
Python summerschool
```

Functions can be recursive

```
def fact(n):
  if n == 1:
      return 1
  else:
      return n * fact(n-1)
```

Argument unpacking

Starred arguments are tuples that collect positional arguments :

```
> def prod(*args): ...

> prod(2,3,4)

> x = (4, 5, 6)

> prod(*x)
```

In `prod, args=(2,3,4)`

Keword arguments can be passed as a dictionary:

```
> options = dict(paper='A4', color = True)

print_setup(options)
```

Unpacking can be a convenient way to print a list:

```
> vals = [1,2,3,4,5]

> print((4*'{:03d} ').format(*vals))

001 002 003 004
```

https://docs.python.org/3/tutorial/controlflow.html#unpacking-argument-lists

Lists or iterators?

- Lists are iterable objects
- Iterators generate objects on-the-fly
- Iterators can be created with a generator function
  - Uses **`yield`** satement
- Relevant for efficiency

```
def rang_llista(n):
    result = []
    i = 0
    while i<n:
        result.append(i)
         i += 1
    return result


def rang_gen(n):
    i = 0
    while i<n:
        yield i
        i += 1
```

Modules

- Modules allow packing libraries or extensions
- There are built-in and external modules
- When imported modules are executed
- Modules can be written in C or Fortran!

```
> import math
> m = math
> import math as m
> from math import cos, sin
> from math import * #dangerous. All into the same namespace
```

Modules

- Python checks if a module is already loaded.
  - The interpreter does not reload a module already imported
  - This can cause unexpected behaviour interactively
- Ipython has a more versatile module loading

```
%load_ext autoreload

autoreload 2 #Will reload a module if it changes
```

Some useful modules

- sys — System-specific parameters and functions
- os — Miscellaneous operating system interfaces
- os.path — Common pathname manipulations
- glob — Unix style pathname pattern expansion
- re — regular expressions
- copy — Shallow and deep copy operations
- argparse — Parser for command-line options, arguments and sub-commands
- subprocess — Subprocess management
- inspect — Inspect live objects

Some useful modules

```
if len(sys.argv!=3):
    print('Error: Use two arguments.')
    sys.exit()

method = sys.argv[1]
filelist = glob.glob('/home/ramon/*')
for fileName in filelist:
    if os.path.isfile(fileName): print(fileName)
```

Modules: too many...

```
>>> import math
>>> import cmath
>>> import numpy.lib.scimath as scimath
>>> math.sqrt(4)
2.0
>>> math.sqrt(-4)
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
ValueError: math domain error
>>> cmath.sqrt(4)
(2+0j)
>>> cmath.sqrt(-4)
2j
>>> scimath.sqrt(4)
2.0
>>> scimath.sqrt(-4)
2j
```

Working with your modules

- Import reads from local directory and from the directories in `sys.path` (`import sys` first)
- Put your modules in a directory and add it to the environtment variable `$PYTHONPATH`.
- Python will add the directories in `$PYTHONPATH` to `sys.path`
- Document your modules and the functions therein.
- Use `if __name__=='__main__':` to execute code only if Python is running the module, and not if it is imported.
  - http://stackoverflow.com/questions/419163/what-does-if-name-main-do

Installing external Modules

- Use conda distribution. Then `$ conda install module`
- Many come as part of the linux distributions (usually older versions that those in conda or PyPI)
  - ipython, numpy, biopython...
- For modules in the PyPI repository(most of them) https://pypi.python.org/pypi
  - `(sudo) pip3 install module`
- Manual installation (dependencies have to be also manually installed):

```
$ python setup.py build
$ (sudo) python setup.py install
```

Updating external Modules

- With conda `$ conda update module`
- For modules in the PyPI repository(most of them) https://pypi.python.org/pypi
  - `pip3 install -U module`
- `pip` can also be used in the conda installation.
- Remeber that modules are installed for a given version of python. If you have python 2.x and 3.x you need to check for which version you are installing. For example using `pip3` or

```
$ which pip
```

Scipy

Linear algebra

- Support for LAPACK, BLAS and ATLAS
  - Can make Scipy compilation more involved

```
> A=matrix(random.rand(5,5))
> A.I
> linalg.det(A)
> linalg.eigvals(A)
> linalg.eig(A)
> linalg.svd(A)
> linalg.cholesky(A)
```

- Solving linear systems:
  - **A.x=b**

```
> b=matrix(random.rand(5)).reshape((5,1))
> linalg.solve(A,b)
```

- LAPACK, BLAS wrappers

```
> from scipy.lib import lapack
> from scipy.lib import blas
blas.fblas.sdot?
```

Optimization

- There are different optimization methods:

```
> import scipy.optimize as so
```

- Some only need the function value:

```
> fmin, fmin_powell
```

- Some need the gradient or the hessian:

```
> fmin_cg, fmin_bfgs, fmin_ncg
```

- Some look for global minima:

```
> anneal
```

- Remember:

```
> scipy.info('optimize')
```

- Pedagogical documentation:
- http://docs.scipy.org/doc/scipy/reference/tutorial/optimize.html
- http://docs.scipy.org/doc/scipy/reference/optimize.html

f2py

- Many things are fast with Numpy
- Iterative algorithms over **array values** are slow
- You can import Fortran functions and subroutines with f2py
- You could also call external fortran programs with

```
> subprocess.call(<program>, shell=True)
```

  - but data exchange has to be through files (slower)

- f2py finds your fortran compiler. Works with gfortran, ifort,...
- f2py creates a module you can import in python
- As simple as:
- `$ f2py -c <file> -m <module>`
  - Tip: first compile it to check it works

f2py II

```
module funcs
implicit none
contains
function f1(x,y)
  real,intent(in):: x,y
  real:: f1
  f1=x+y**2
end function f1

function f2(x,y)
  real,intent(in):: x,y
  real, dimension(3):: f2
  f2(1)=x+y**2
  f2(2)=sin(x*y)
  f2(3)=2*x-y
end function f2
end module
```

```
$ f2py -c test.f90 -m test
```

- go to ipython:

```
> import test
> test.funcs.f1(1,2)
5.0
> test.funcs.f2(1,2)
array([ 5., 0.90929741, 0.],
dtype=float32)
```

f2py III

Using ipython magicfunctions:

```
sudo pip3 install -U fortran-magic
```

Useful for performing long array operations

```
In [5]: %load_ext fortranmagic

In [6]: %%fortran
        subroutine f1(x, y, z)
            real, intent(in) :: x,y
            real, intent(out) :: z

            z = sin(x+y)

        end subroutine f1


In [7]: f1(1.0, 2.1415)

Out[7]: 9.26574066397734e-05
```

Big data, big memory

- Numpy arrays are meant to live in memory
- If that is not possible:
  - Use op= operations (they use half the memory):
    - `p *=alpha` is better than `p = p*alpha`
  - Use `scipy.sparse` matrices
    - http://docs.scipy.org/doc/scipy/reference/sparse.html
  - Use `PyTable` to store (compressed) matrices on disk
    - http://www.pytables.org/
  - Modify your algorithm to work with submatrices

Sympy: Symbolic math

- Symbolic algebra
- Analytic solution of equations
- Integration, derivation
- Polynomials
- Limits

Alternate forms:

```
(cos(x + y)).expand(trig=True)
```

$$-\sin(x)\sin(y) + \cos(x)\cos(y)$$

```
trigsimp(cos(x + y))
```

$$\cos(x+y)$$

```
(cos(x + y)).rewrite(csc, sin, sec, cos, cot, tan)
```

$$\frac{-\tan^2\left(\frac{x}{2}+\frac{y}{2}\right)+1}{\tan^2\left(\frac{x}{2}+\frac{y}{2}\right)+1}$$

```
(cos(x + y)).rewrite(sin, exp, cos, exp, tan, exp)
```

$$\frac{1}{2}e^{i(-x-y)} + \frac{1}{2}e^{i(x+y)}$$

```
>>> integ = Integral(sin(x**2), x)
>>> integ
⌠
⎮  ⎛ 2⎞
⎮ sin⎝x ⎠ dx
⌡
>>> integ.doit()
                    ⎛√2⋅x⎞
3⋅√2⋅√π⋅fresnels⎜────⎟⋅Γ(3/4)
                    ⎝ √π ⎠
──────────────────────────
          8⋅Γ(7/4)
```

http://sympy.org/en/index.htm
l

Add-ons

Add ons: Biopython

Biopython

```
from Bio.PDB import *

p=PDBParser(PERMISSIVE=1)

s=p.get_structure('1OJR', filename)
```

Print out the coordinates of all CA atoms with B factor > 50:

```
for model in s.get_list():
  for chain in model.get_list():
    for residue in chain.get_list():
      if residue.has_id("CA"):
        ca=residue["CA"]
        if ca.get_bfactor()>50.0:
          print ca.get_coord()
```

http://biopython.org

Add ons: Machine learning and statistics

- Basic statistics in scipy.stats
  - Tutorial: http://docs.scipy.org/doc/scipy/reference/tutorial/stats.html
  - Reference: http://docs.scipy.org/doc/scipy/reference/stats.html
- Machine learning with sklearn
  - http://scikit-learn.org/stable/
  - Choosing the method: http://scikit-learn.org/stable/tutorial/machine_learning_map/
- More algorithms (and a textbook) with AstroML
  - http://www.astroml.org/

Add ons: itertools

```
> import itertools
> perms = itertools.permutations('ABC', 3)
> list(perms)
[('A', 'B', 'C'),
 ('A', 'C', 'B'),
 ('B', 'A', 'C'),
 ('B', 'C', 'A'),
 ('C', 'A', 'B'),
 ('C', 'B', 'A')]
> list(itertools.combinations('ABC',2))
[('A', 'B'), ('A', 'C'), ('B', 'C')]
```

Add ons: active papers

ActivePapers is a framework for doing and publishing reproducible research. An ActivePaper is a file that contains code (Python modules and scripts) and data (HDF5 datasets), plus the dependency information between all these pieces. You can change a script and re-run all the computations that depend on it, for example. Once your project is finished, you can publish the ActivePaper as supplementary material to your standard paper.

http://khinsen.wordpress.com/2013/09/27/activepapers-for-python/

Optimization and debugging

Optimization

- “Premature optimization is the root of all evil” Knuth
- `%timeit a=np.random.random(100000)`
- ```
  a=np.random.random(100000)
  n_dim=3
  %%timeit
  x=np.zeros(shape=(100000,n_dim),order='F')
  for j in range(0,n_dim):
      x[:,j]=a*j
  ```
- Evaluated in a separate enviroment
  ```

Exceptions and errors

Although the language is interpreted there are some syntax errors that prevent execution:

```
def safe_divide_1(x, y)


File"/home/ramon/python/prova.py",
   line 1
     def safe_divide_1(x, y)
                              ^
SyntaxError: invalid syntax
```

Exceptions leave a trace easy to follow.

Easy debugging with

%pdb

%debug

pdb: python debugger

```
In [1]: pdb
Automatic pdb calling has been turned ON

In [4]: run foo.py
NameError: name 'b' is not defined
> /home/ramon/python/foo.py(2)<module>()
      1 a = 3
----> 2 print(b)

ipdb> ?
```

pdb: python debugger

```
In [9]: run foo.py
---------------------------------------------------------------------------
NameError                                 Traceback (most recent call last)
/home/ramon/python/foo.py in <module>()
      1 a = 3
----> 2 print(b)

NameError: name 'b' is not defined

In [10]: %debug
> /home/ramon/python/foo.py(2)<module>()
      1 a = 3
----> 2 print(b)
ipdb>
```

Numba

- Numba compiles in a virtual machine.
- Developped by Continuum analytics, so easiest install from conda.
- `$ conda install numba`

Cython

- An extension to python that generates C code that can be compiled
- Available in most linux distributions
- Fortran programmers can use f2py, available in scipy.
- See also:
- https://jakevdp.github.io/blog/2013/06/15/numba-vs-cython-take-2/

Other alternatives

- Use Julia
  - A different language
  - Close in syntax to Python
- Theano: “define, optimize, and evaluate mathematical expressions involving multi-dimensional arrays efficiently”
  - https://theano.readthedocs.org/en/latest/
- Parakeet: a runtime compiler for scientific computing in Python
  - http://www.parakeetpython.com/http://www.parakeetpython.com/
- Just-in-time compilers for number crunching in Python
  - http://www.phi-node.com/2013/01/just-in-time-compilers-for-number.html
- See also the notebooks here:
  - http://nbviewer.jupyter.org/github/rasbt/One-Python-benchmark-per-day/tree/master/ipython_nbs/

Resources

Resources

On-line Official documentation (contains Tutorial in PDF or HTML):

http://www.python.org/doc

General introductory books (also in paper):

http://diveintopython.org/ (This one is simpler!)

http://www.greenteapress.com/thinkpython/thinkpython.html

Comparison of codes in different languages:

http://rosetacode.org

http://www.codecodex.com

Python package index: where to find modules

http://pypi.python.org/pypi

Resources

- Interactive tutorial
  - http://pythonmonk.com/
- A Crash Course in Python for Scientists (with applications in Quantum chemistry)
  - http://nbviewer.ipython.org/5920182
  - Written in an ipython notebook
- Python Scientific Lecture notes
  - http://scipy-lectures.github.io/
- Python flow with Pythontutor
  - http://www.pythontutor.com

Python and chemistry

- Parsing Quantum chemistry output files
  - cclib: http://cclib.github.io/
  - ORBKIT: http://orbkit.github.io/
- QM calculation with
- pyQuante: http://pyquante.sourceforge.net/
- NWChem: http://www.nwchem-sw.org/index.php/Python
- Python Library for Automating Molecular Simulation (ADF Suite)
  - https://www.scm.com/doc/plams/index.html
- An open-source "Methodology Discovery" Library
  - http://www.acsu.buffalo.edu/~alexeyak/libra/capabilities.html

Python and chemistry

- Trajectory analysis:
  - MDtraj : http://mdtraj.org
  - MDAnalysis: http://www.mdanalysis.org/
  - Pytraj: https://github.com/Amber-MD/pytraj
- Setup and analyze simulations with HTMD
  - https://www.htmd.org//
- PyEMMA. Markov StateModels. http://emma-project.org/latest/
- PyContact: Rapid, Customizable, and Visual Analysis of Noncovalent Interactions in MD Simulations

Python and chemistry

- Drawing energy diagrams:
  - PyEnergyDiagrams https://github.com/giacomomarchioro/PyEnergyDiagrams
  - CatPlot https://github.com/PytLab/catplot
- https://github.com/lmmentel/awesome-python-chemistry
- Material from UAB “Computational solutions for chemobiotechnology”: https://github.com/insilichem/

Python and chemistry

- QM/MM with pDynamo: http://www.pdynamo.org
- MM with MMTK: http://dirac.cnrs-orleans.fr/MMTK/
- Molecular visualization:
  - VMD: http://www.ks.uiuc.edu/Research/vmd/
  - pymol: http://www.pymol.org/
  - Nglview, chemical structures in juptyer: https://github.com/arose/nglview
- Protein structure with pyRosetta: http://pyrosetta.org/
- Bioinformatics with BioPython: http://biopython.org/

Resources: Books

- Rossant, C, *Learning Ipython for Interactive Computing and Data Visualization*.
  - Basic level. Covers several subjects, includng matplotlib and parallelism. Recipes book.
- Vanderplas, J. *Python Data Science Handbook*.
  - Online: https://jakevdp.github.io/PythonDataScienceHandbook/
- Stewart, J.M., *Python for Scientists*
  - Basic level. Unfortunately in Python 2. Covers a lot on differential equations.
- DeCaria A. J. *Python Programming and Visualization for Scientists*
  - DeCaria teaches Python programming and visualization for meteorology and ocean sciences majors.
- Packt Publishing. Wide variety, lots on GIS and Python.
- https://wiki.python.org/moin/AdvancedBooks

Resources: Video Tutorials

- Check: https://www.youtube.com/user/EnthoughtMedia

- Check: http://www.pyvideo.org/
- Check Scipy Conference and Euroscipy:
  - http://conference.scipy.org/proceedings/scipy2015/
  -

Resources: MOOCs

- General Python programming:
  - https://www.coursera.org/course/programming1
  - https://www.coursera.org/course/programming2
- Advanced scientific programming with Fortran, Python, OMP, OpenMPI…
  - https://www.coursera.org/course/scicomp

Resources: Teaching

- On teaching programming with Python 3

  http://www.comp.leeds.ac.uk/nde/papers/teachpy3.html
- Online Syntax Highlighting

  http://tohtml.com/python/
- Style Guide for Python Code:
- www.python.org/dev/peps/pep-0008/

K. Hinsen views

- “NumPy has introduced incompatible changes with almost every new version over the last years”
- “Given the importance of NumPy in the scientific Python ecosystem, I consider its lack of stability alarming”.
- “What makes me hesitate to recommend not using Python is that there is no better alternative”.
- https://khinsen.wordpress.com/2014/09/12/the-state-of-numpy/

Jake VanderPlas

- Great blog about python with applications in
  - Science
  - Statistics
  - Cycling…
  - All entries are jupyter notebooks.
  - https://jakevdp.github.io/
  - See also his book and library on machine learning:
  - http://www.astroml.org/
  - http://press.princeton.edu/titles/10159.html