Python for Scientists

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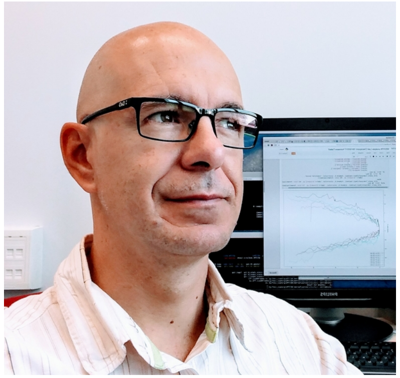


Us

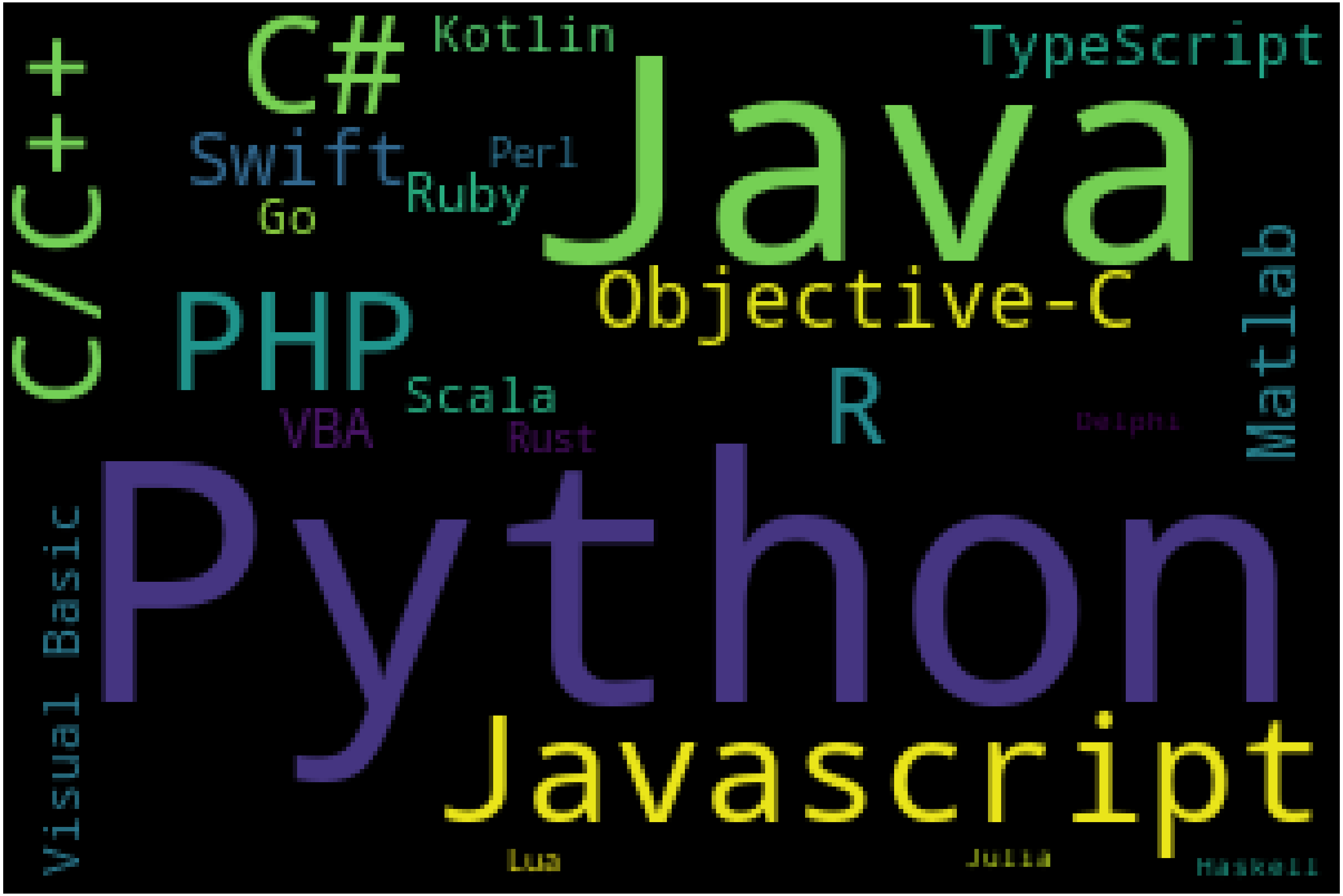
- Researcher at the CSIC
- Computational biochemistry &biophysics
- Started with Fortran. Learnt some Perl, R, Mathematica
- But now mainly use Python
- Analysis of simulations
- Implementing new methods

- 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

Overview

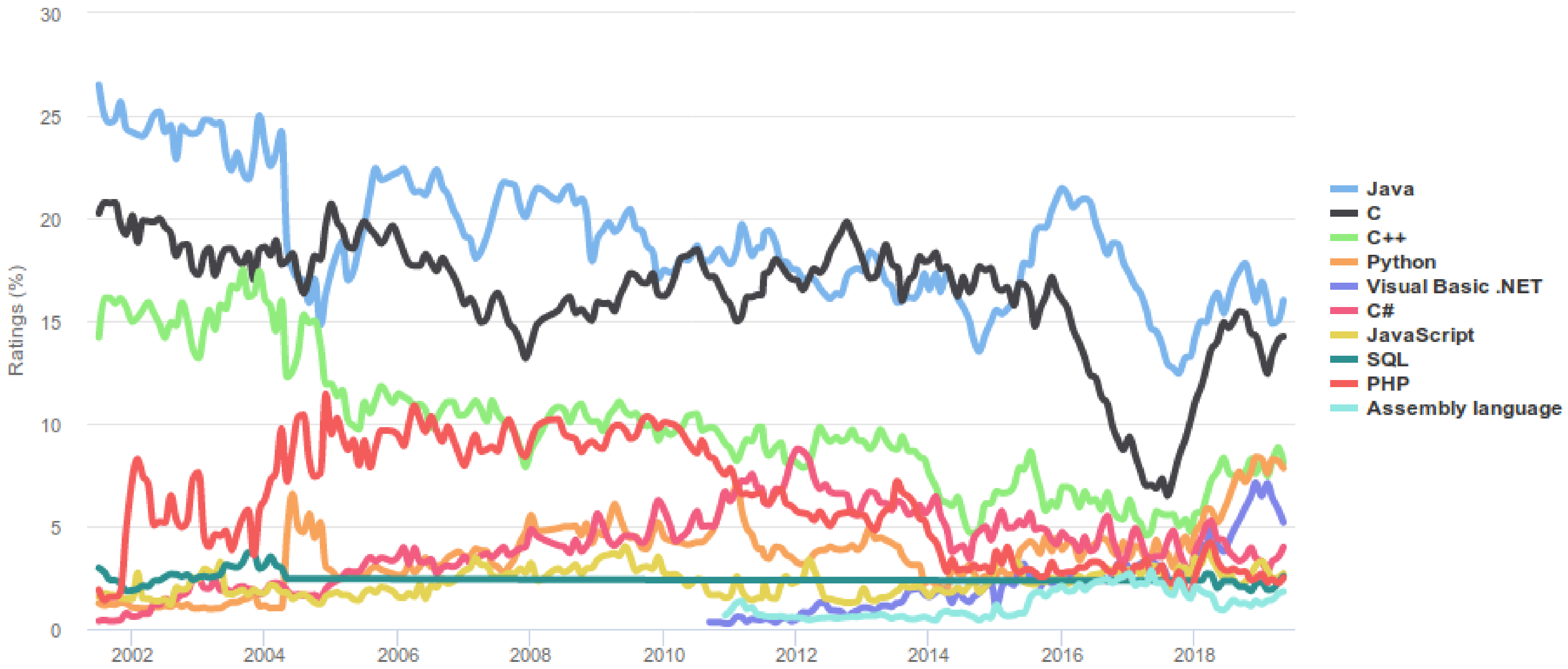
- Why Python
- Language basics
- Working with files
- Working with arrays: Numpy
- Data visualization: matplotlib
- Structured data: Pandas
- Functions and modules
- Scientific modules. Scipy
- Classes and objects (bare minimum!)
- Other scientific modules: sckikit-learn, biopython…
- Profiling and optimization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

Compiled languages
Fast
Difficult
non-interactive

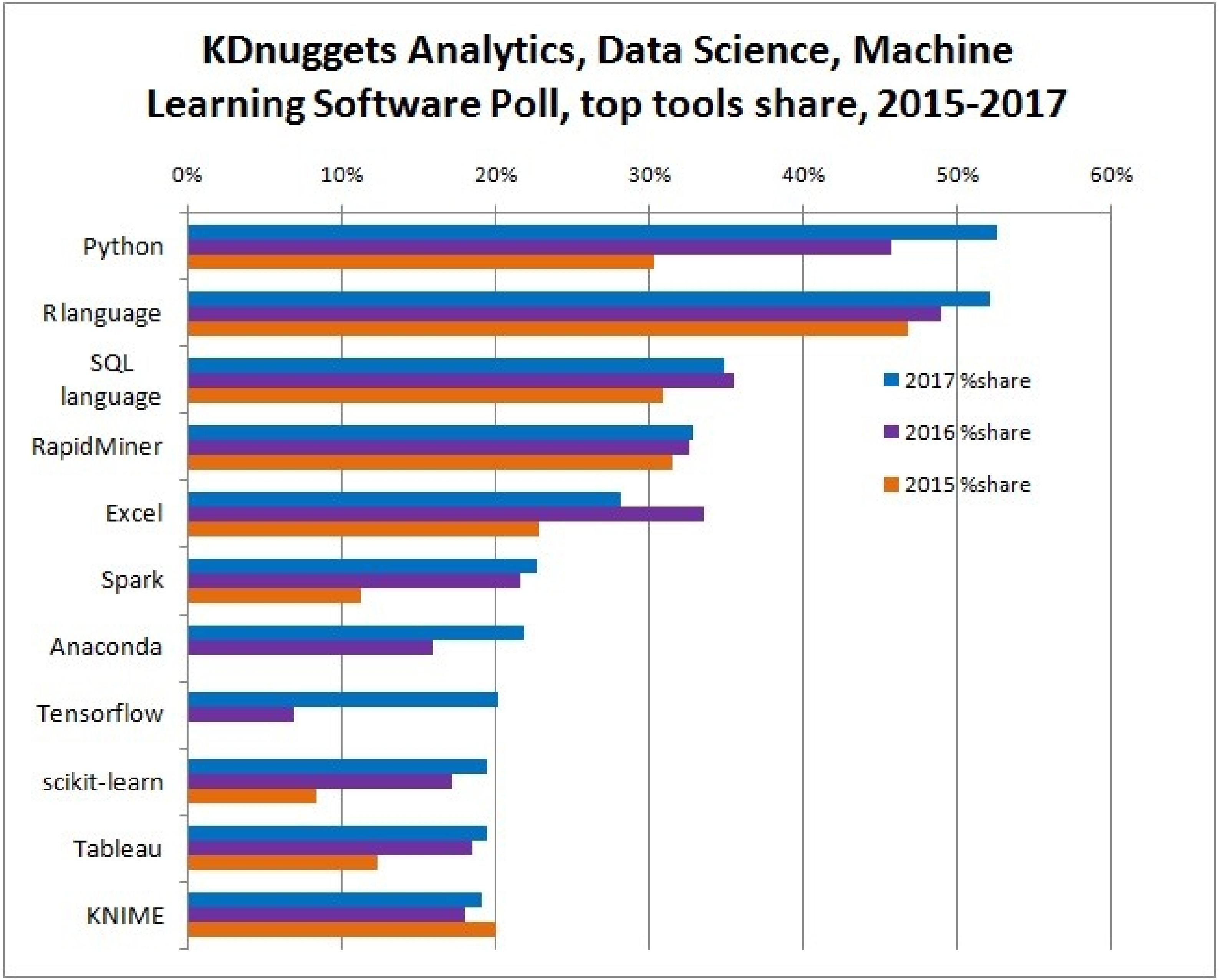
Matlab, Mathematica, Octave
Slow
Rich libraries
Nice development environment
Restricted base language
Expensive (some)

Python
Rich libraries (less than matlab)
Other libraries
Free
Active community
Harder than Matlab

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

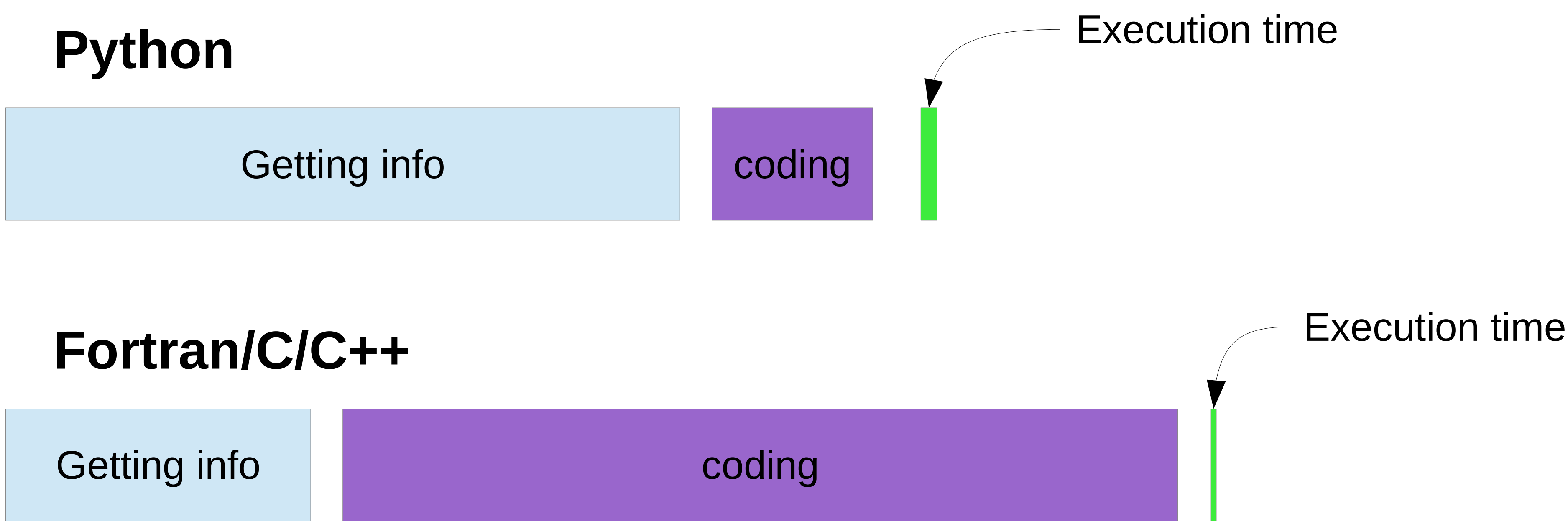


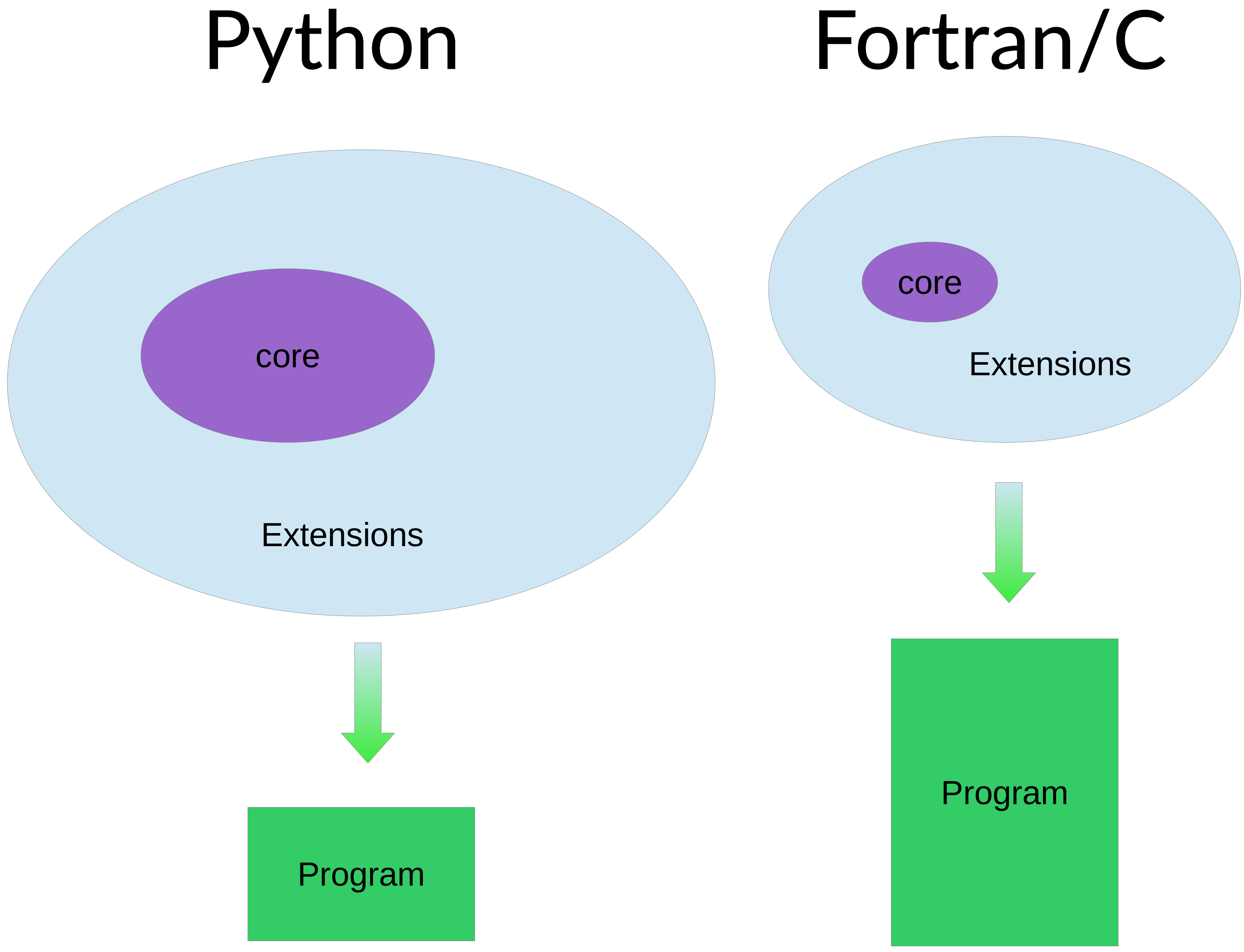
Python for data science

- 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

Python vs. Fortran/C

Different time distribution to get a task done




Python
Fortran/C
core
Extensions
Program
core
Extensions
Program

Hello World program

```
print(“Hello World!”)
```

```
print(“Hello World!”)
```

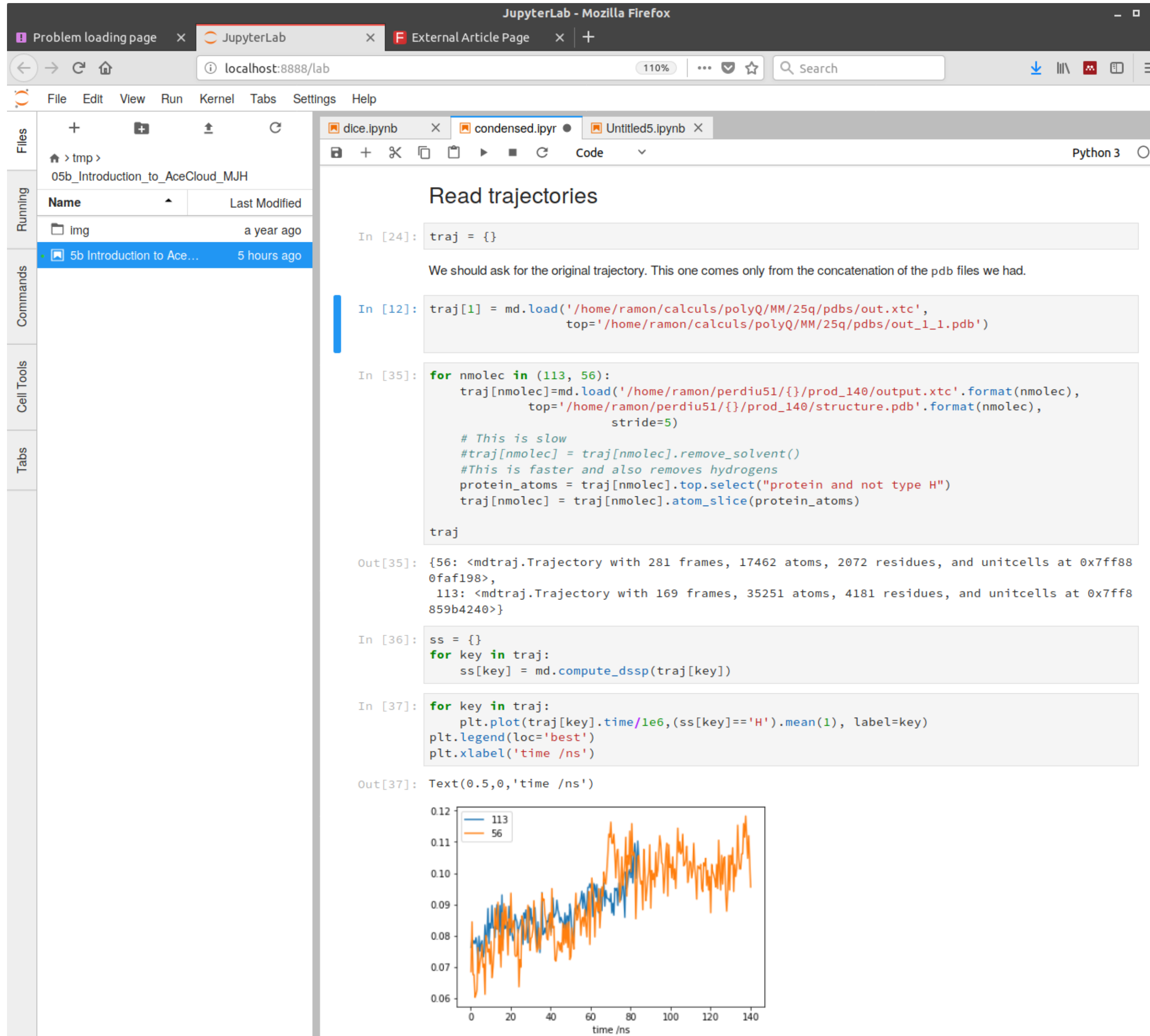
```
$ python3 hello.py
```

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
- See also PDF articles in the repository

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):

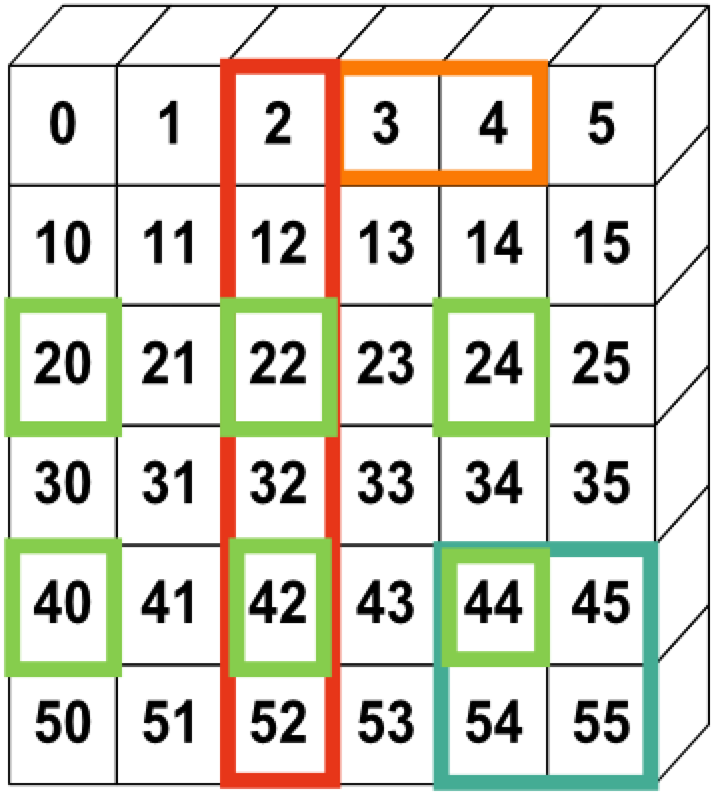
```
> a = np.arange(10,15)
> indices = (a**2 > 115) & (a < 14)
> a[indices]
array([11, 12, 13])
```

  - 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

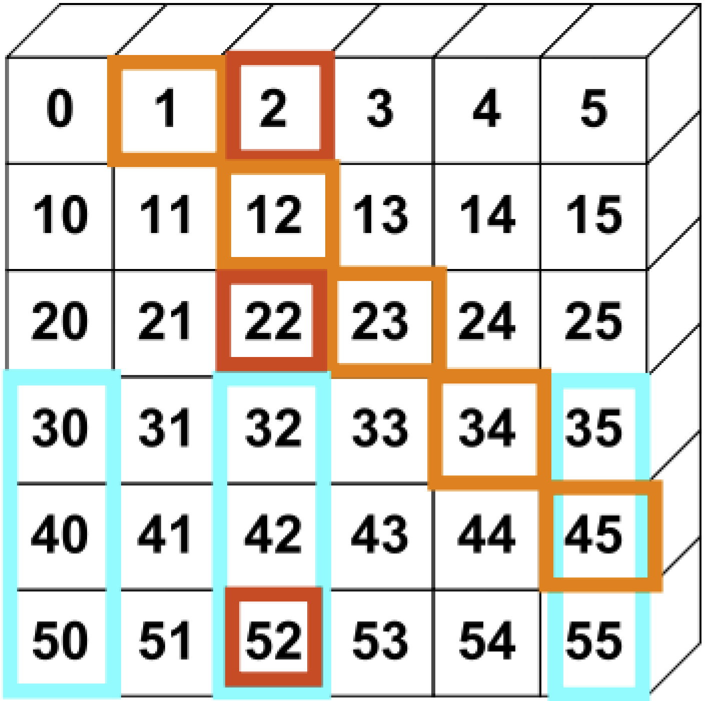
```
>>> a[0,3:5]
array([3,4])

>>> 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):

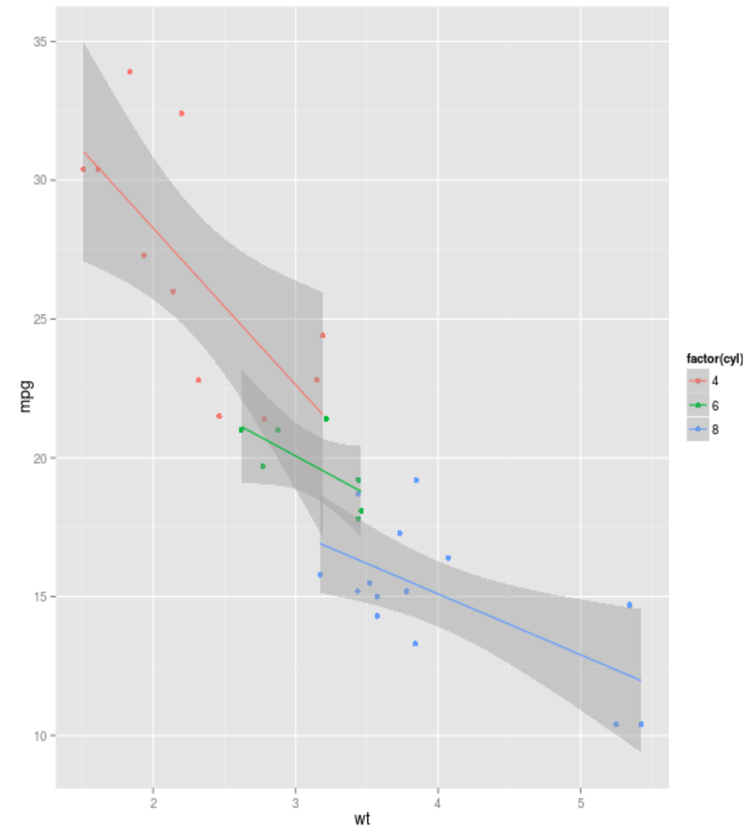
```
> np.savez('results', x, y)
```

- 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.

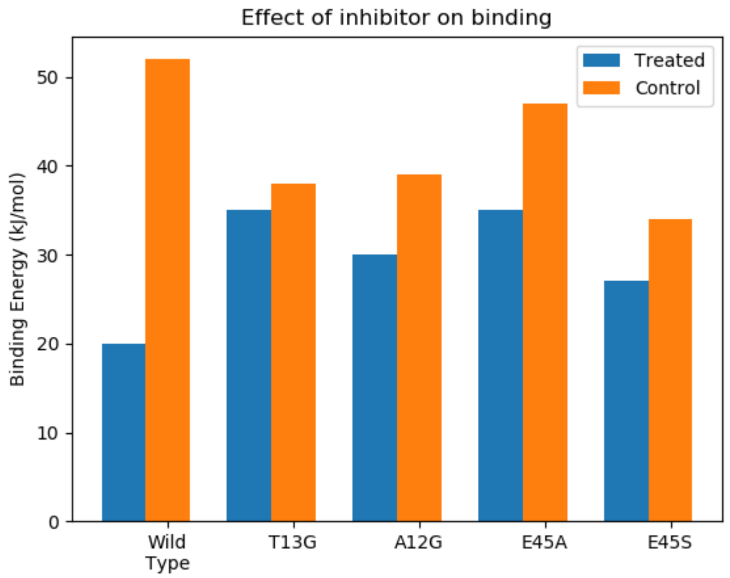
Matplotlib

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

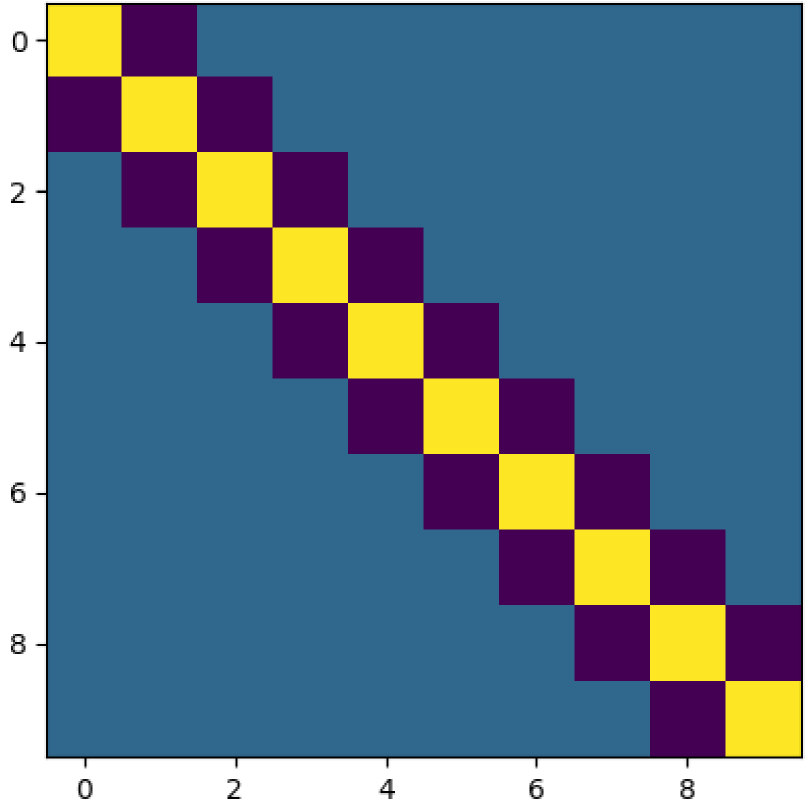
Totally reproducible figures




```
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
```

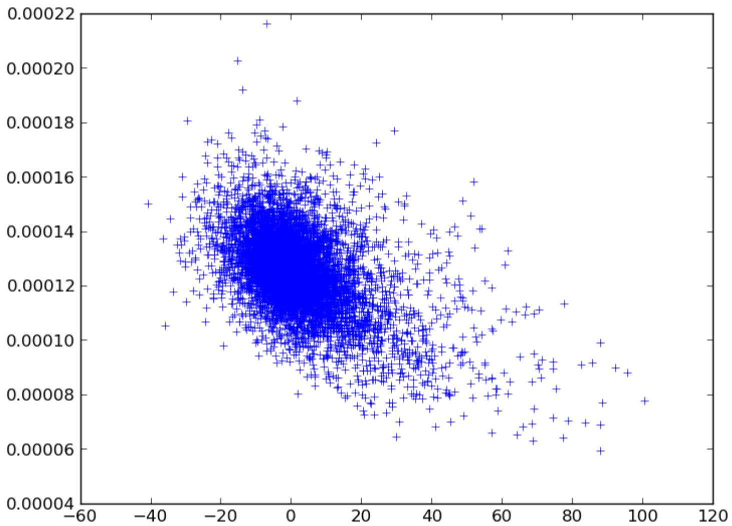


Matplotlib styles

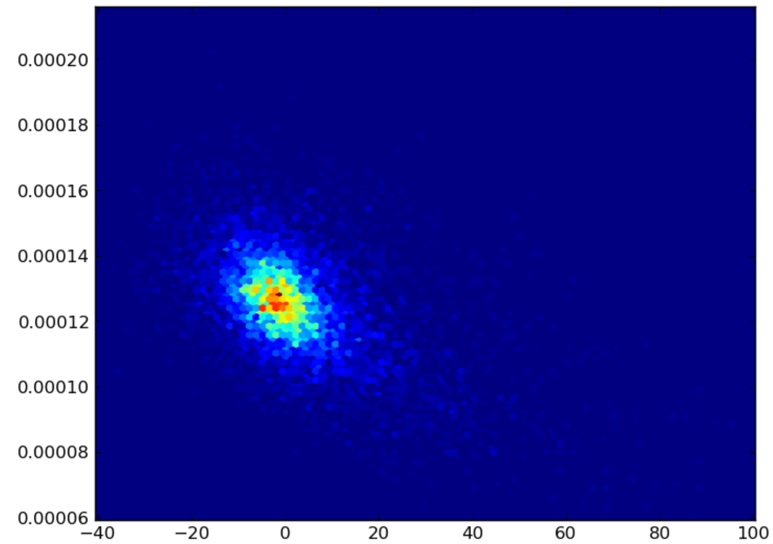
- Since version 1.5 several default styles.
- Try the following code

```
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')
```

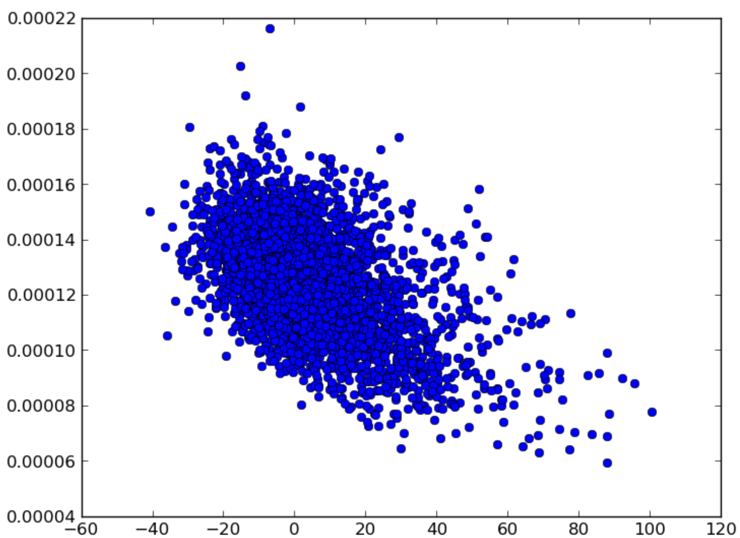
Plotting lots of points:hexbin



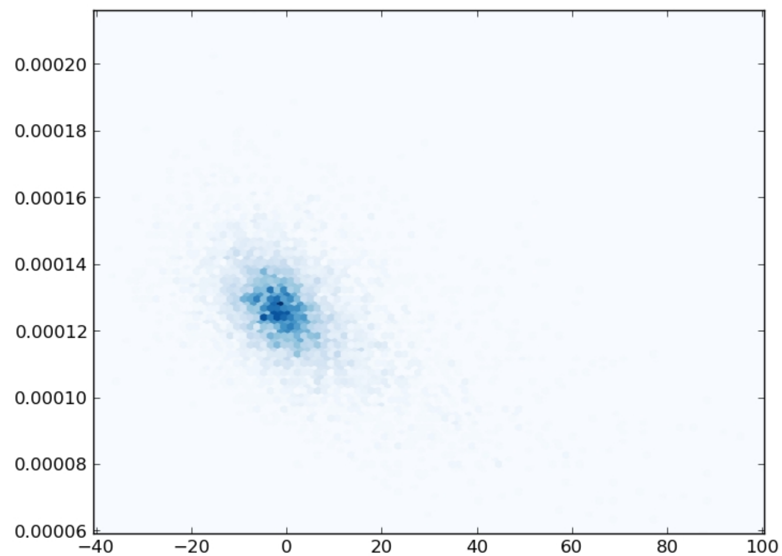
`plt.plot(x, y, '+')`



`plt.hexbin(x, y)`

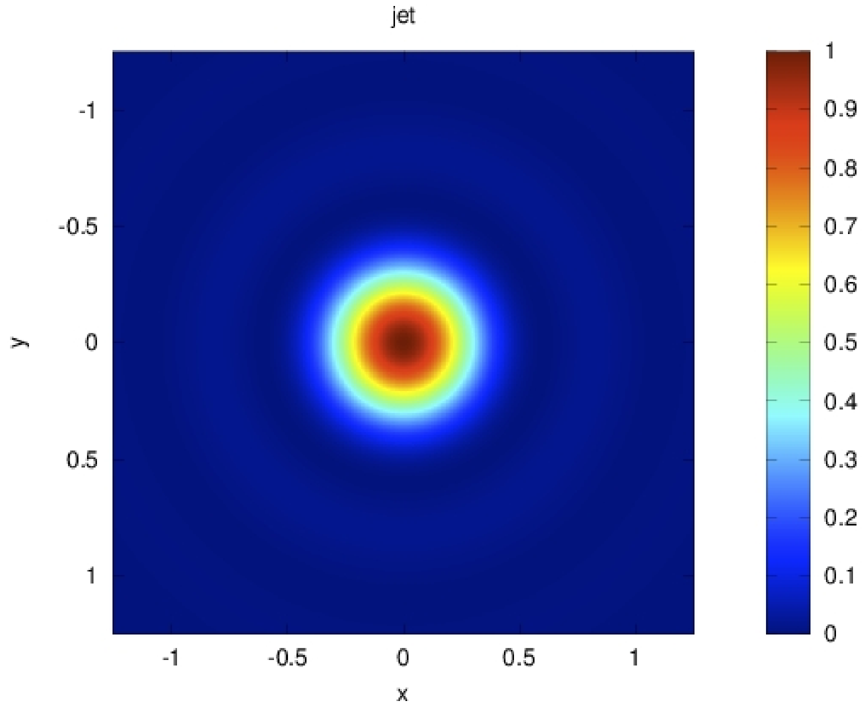


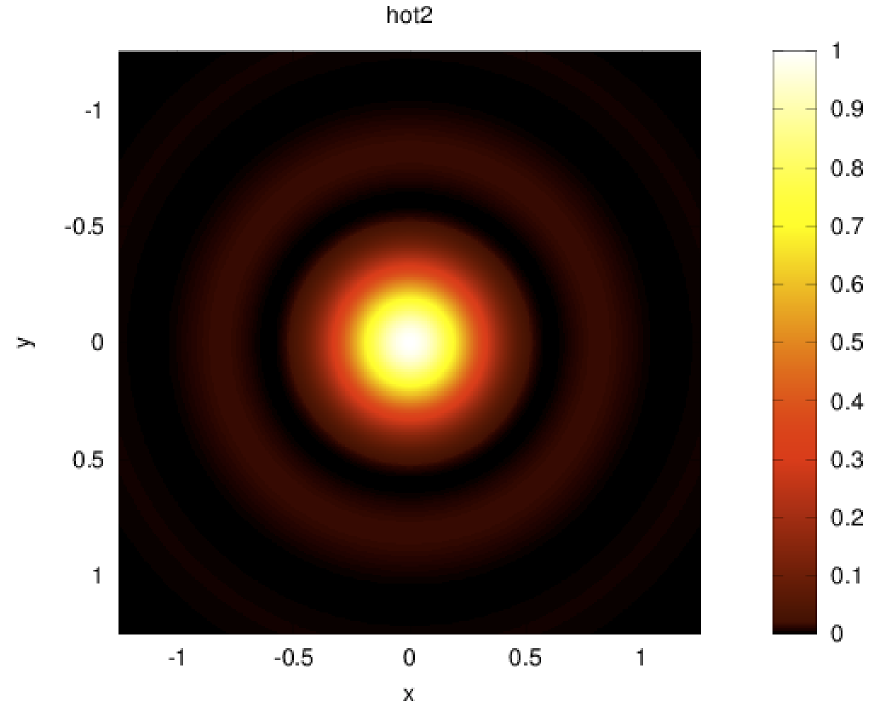
`plt.plot(x, y, 'o')`

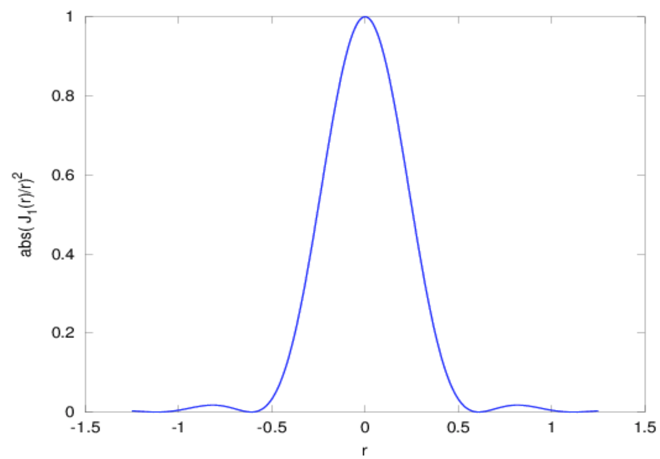


`plt.hexbin(x, y, cmap='Blues')`

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)`

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

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
```

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()
```

$$\frac{3\cdot\sqrt{2}\cdot\sqrt{\pi}\cdot\mathrm{fresnels}\left(\frac{\sqrt{2}\cdot x}{\sqrt{\pi}}\right)\cdot\Gamma(3/4)}{8\cdot\Gamma(7/4)}$$

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