An introduction to python programming

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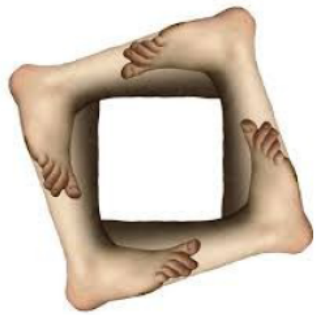

About my Sci-Programming Working group

Pablo Alcain, Rodrigo Lugones, Graciela Molina, and I

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What is python?

Multi-paradigm language:
Structured, object oriented & functional styles are all supported.

- Paradigms is not enforced by language
- Clean syntax
- Highly extensible: small core, large standard lib

`https://www.python.org`

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Why shoud I learn python if I know ***?

- Easy to learn
- Big community of developers
- Huge library
- Excellent science support!!
- Quick development turnaround
- Plot with python libraries is nice and easy
- Open source license

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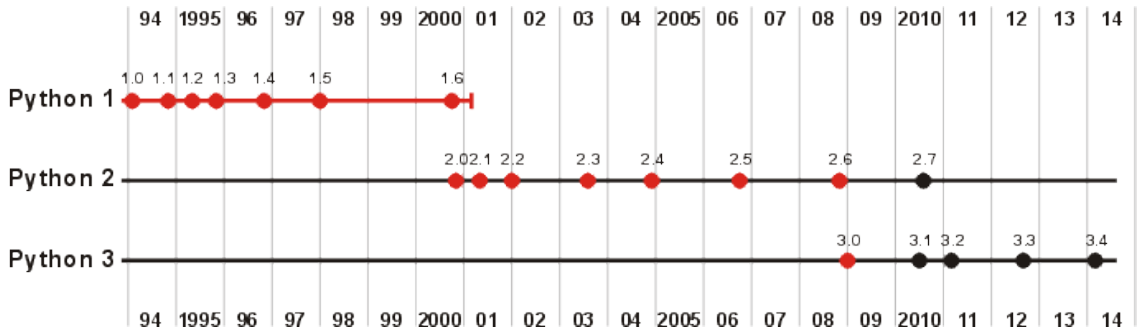
A little of History

- Main development started 1989
- Author Guido van Rossum (if you want to follow him @gvanrossum)



On the design decisions

Zen of Python, by Tim Peters

- Beautiful is better than ugly.
- Explicit is better than implicit.
- Simple is better than complex.
- Complex is better than complicated.
- Readability counts.
- If the implementation is hard to explain, it's a bad idea.

Use of the Interpreter

To start:

- Install the Python interpreter on your computer.
  (Linux distributions also frequently include Python and it is readily upgraded.)
- Call interpreter:

```
python
```

- It has an interative mode to introduce instructions one by one and see the result.

```
>>> 1 + 1
2
>>> a = range(10)
>>> print a
[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
```

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Basic ideas

- In a statically typed language, every variable name is bound both
  - to a type (at compile time, by means of a data declaration) to an object.
  - to an object.
- In a dynamically typed language, every variable name is (unless it is null) bound only to an object.

```
1 x = 1
2 x = "text" # dynamic typing :)
```

Data types

A list of the most common data types:

Class	Description	Immutable?
bool	Boolean value	✓
int	integer (arbitrary magnitude)	✓
float	floating-point number	✓
list	mutable sequence of objects	
tuple	immutable sequence of objects	✓
str	character string	✓
set	unordered set of distinct objects	
frozenset	immutable form of set class	✓
dict	associative mapping (aka dictionary)	

`https://docs.python.org/2/library/types.html`

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Python Syntax

In C or C++: use of ; at the end of statements

```
if(a>b)
    foo();
    bar();
baz();
```

In python: indentation level of your statements is significant! Last statement is executed out of the conditional

```
if(a>b):
    foo()
    bar()
baz()
```

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Python Syntax

Control flow

```
for i in list:
    baz(i)
```

```
if a>b:
    foo()
elif b!=c:
    bar()
else:
    baz()
```

```
while a>b:
    foo()
    bar()
```

```
pass
```

```
break
continue
```

Python Syntax

Function definition:

```
1 def function(x,y,z):
2     x=3*y
3     return x+y-z
```

Also functions can be pass as values

```
1 def func(x, p1,p2):
2     return p1*(x)+p2
```

Python Syntax example

In C indentation is optional:

```c
int factorial(int x)
{
if (x == 0)
return 1;
else
return x * factorial(x - 1);
}
```

In python is mandatory:

```python
def factorial(x):
    if x == 0:
        return 1
    else:
        return x * factorial(x - 1)
```

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Python Boolean and operators

Math operators:

Name	Function	symbol
+ Addition	Adds values on either side of the operator.	a + b = 30
- Subtraction	Subtracts right hand operand from left hand operand.	a – b = -10
* Multiplication	Multiplies values on either side of the operator	a * b = 200
/ Division	Divides left hand operand by right hand operand	b / a = 2
% Modulus	Divides left hand operand by right hand operand and returns remainder	b % a = 0
** Exponent	Performs exponential (power) calculation on operators	a**b =10 to the power 20

Boolean:

Operation	Result
x or y	if x is false, then y, else x
x and y	if x is false, then x, else y
not x	if x is false, then True, else False

Strings

It is possible to use ' or " on string definition

```
1  a= "I am Cecilia"
2  b= 'I am from Argentina'
```

To print on screen we use the print function:

```
print ('---All rigth!!!----')
```

Strings examples

An example:

```
'I ate %d %s today' %(12,'apples')
```

other example: I ate today.format(12,'apples')

structures

- List

```
1 a=[1,'apple',1.2]
```

- Tuple

```
1 a=(1,'apple',1.2)
```

- Dict

```
1 a={'name':'Giovanni', 'age':42}
```

- Set

```
1 a={1,'apple',1.2}
```

Lists

- Very useful structure on python
- Index and slice access

```
a[0] a[1] a[2:5] a[2:10:2]
```

- Comprehension list

```
[x**2 for x in range(1,11)]
```

List Methods

```
list.append(obj)
```

Appends object obj to list

```
list.count(obj)
```

Returns count of how many times obj occurs in list

```
list.extend(seq)
```

Appends the contents of seq to list

```
list.index(obj)
```

Returns the lowest index in list that obj appears

```
list.insert(index, obj)
```

Inserts object obj into list at offset index

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List Methods

```
list.pop(obj=list[-1])
```

Removes and returns last object or obj from list

```
list.remove(obj)
```

Removes object obj from list

```
list.reverse()
```

Reverses objects of list in place

Main reason to use python in scientific programing

Three libraries to work with:

- NumPy:
  `http://www.numpy.org/`
- SciPy:
  `http://www.scipy.org/`
- MatPlotLib:
  `http://matplotlib.org/`

All are open source!

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Main reason to use python in scientific programing

- NumPy provides functionality to create, delete, manage and operate on large arrays of type "raw" data (like Fortran and C/C++ arrays)
- SciPy extends NumPy with a collection of useful algorithms like minimization, Fourier transforms, regression and many other applied mathematical techniques
- Both packages are add-on packages (not part of the Python standard library) containing Python code and compiled with (fftpack, BLAS)
- MatPlotLib is a nice library to plot

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Numpy

NumPy is the fundamental package for scientific computing in Python.

- A powerful N-dimensional array object
- Sophisticated (broadcasting) functions
- Tools for integrating C/C++ and Fortran code
- Useful linear algebra, Fourier transform, and random number capabilities
- Operations on matrices and vectors in NumPy are very efficient because they are linked to compiled in BLAS/LAPACK code

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Scipy

One of the core packages that make up the SciPy stack. SciPy is built on top of NumPy and implements many specialized scientific computation tools:

- Manly user-friendly
- Efficient numerical routines such as routines for numerical integration and optimization.

  - Clustering,
  - Fourier transforms
  - numerical integration, interpolations
  - data I/O, LAPACK
  - sparse matrices, linear solvers, optimization
  - signal processing
  - statistical functions

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Matplotlib

Is a Python 2D plotting library which produces publication quality figures in a variety of hardcopy formats and interactive environments across platforms. Can be used in:

- Python scripts
- The Python and IPython shell
- The jupyter notebook
- Web application servers
- Graphical user interface toolkits

How to start?

It is necesary to import libraries:

```
1 import numpy
2 import scipy
3 import matplotlib.pyplot
```

There are different way to import libraries:

```
1 import numpy
2 import numpy as np
3 from numpy import *
```

I use:

```
1 import numpy as np
2 import scipy
3 import matplotlib.pyplot as pp
```

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Things from Numpy

NumPy functionality:

- Polynomial mathematics
- Statistical computations
- Pseudo random number generators
- Discrete Fourier transforms
- Size / shape / type testing of arrays

Fundamental things from Numpy: np.array

There are 5 general mechanisms for creating arrays:

- Conversion from other Python structures (e.g., lists, tuples)
- Intrinsic numpy array array creation objects (e.g., arange, ones, zeros, etc.)
- Reading arrays from disk, either from standard or custom formats
- Creating arrays from raw bytes through the use of strings or buffers
- Use of special library functions (e.g., random)

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Numpy array examples

(>>> means input)

```
mport numpy as np
>>> x = np.array([2, 3, 1, 0])
>>> print x
[2 3 1 0]

>>> np.arange(10)
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])

>>> np.arange(2, 10, dtype=np.float)
array([ 2., 3., 4., 5., 6., 7., 8., 9.])

>>> np.arange(2, 3, 0.1)
array([ 2. , 2.1, 2.2, 2.3, 2.4, 2.5, 2.6, 2.7, 2.8, 2.9])

>>> np.linspace(1., 4., 6)
array([ 1. ,  1.6,  2.2,  2.8,  3.4,  4. ])
```

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Changing array shape

```
>>> a = np.zeros((5, 2))
>>> print a
[[ 0.  0.]
 [ 0.  0.]
 [ 0.  0.]
 [ 0.  0.]
 [ 0.  0.]]
```

reshape:

```
>>> b = a.reshape((2, 5))
>>> print b
[[ 0.  0.  0.  0.  0.]
 [ 0.  0.  0.  0.  0.]]
```

Array transpose and Fill:

Some routine examples:

```
>>> x = np.array([1.,2.,3.,4.])
>>> x
array([ 1.,  2.,  3.,  4.])
>>> x.T
array([ 1.,  2.,  3.,  4.])
```

```
>>> a = np.array([1, 2])
>>> a.fill(0)
>>> a
array([0, 0])
>>> a = np.empty(2)
>>> a.fill(1)
>>> a
array([ 1.,  1.])
```

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Some elemental operations with Numpy:

```
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

>>>print(x + y)
>>>print(np.add(x, y))
 [[ 6.0  8.0]
 [10.0 12.0]]

# Elementwise difference; both produce the array

>>>print(x - y)
>>>print(np.subtract(x, y))
 [[-4.0 -4.0]
 [-4.0 -4.0]]
```

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Some elemental operations with Numpy:

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

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

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

More operations with arrays

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

v = np.array([9,10])
w = np.array([11, 12])

# Inner product of vectors; both produce 219
print(v.dot(w))
print(np.dot(v, w))

# Matrix / vector product; both produce the rank 1 array [29 67]
print(x.dot(v))
print(np.dot(x, v))

# Matrix / matrix product; both produce the rank 2 array

print(x.dot(y))
print(np.dot(x, y))
```

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On array creation

```
a = np.zeros((2,2))   # Create an array of all zeros
print(a)              # Prints "[[ 0.  0.]
                      #          [ 0.  0.]]"
b = np.ones((1,2))    # Create an array of all ones
print(b)              # Prints "[[ 1.  1.]]"
c = np.full((2,2), 7) # Create a constant array
print(c)              # Prints "[[ 7.  7.]
                      #          [ 7.  7.]]"
d = np.eye(2)         # Create a 2x2 identity matrix
print(d)              # Prints "[[ 1.  0.]
                      #          [ 0.  1.]]"
e = np.random.random((2,2))  # Create an array filled with random values
print(e)                     # Might print "[[ 0.91940167  0.08143941]
                             #              [ 0.68744134  0.87236687]]"
```

How to create a data set, plot and save in txt

```
from math import *
import numpy as np
import matplotlib.pyplot as pp
#File creation
f_out_max = open('tabla.txt', 'w')
#data generation
x    = np.arange(441)
Sin1 = 1*np.sin(2*pi*(25/441.0)*x)
Sin2 = 0.25*np.sin(2*pi*((25./2)/441.0)*x)
Sin  = Sin1+Sin2
Vec  = np.c_[x,Sin]
#printing
print ('Vec: ',Vec.shape)
#save in .txt file
np.savetxt(f_out_max,Vec,fmt='%f',delimiter='\t',header="x #f(x)")
f_out_max.close()
#plot figure
pp.figure()
pp.plot(x*1./44100.,Sin, color='r',label='Sin vs x')
pp.xlabel('Time (s)')
pp.savefig("fig_01.jpg",dpi=200)
```

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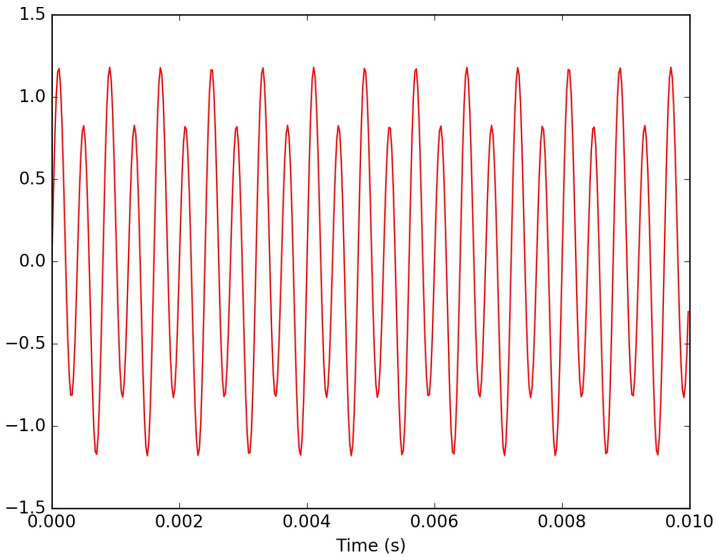
```

We obtain:

A basic figure and table in a txt file:



# x	#f(x)
0.000000	0.000000
1.000000	0.392994
2.000000	0.740813
3.000000	1.003819
4.000000	1.152764
5.000000	1.172342
6.000000	1.062998
7.000000	0.840786
8.000000	0.535279
9.000000	0.185801
10.000000	-0.163538
11.000000	-0.469389
12.000000	-0.694586
13.000000	-0.812779
14.000000	-0.811673
15.000000	-0.694499
16.000000	-0.479506
17.000000	-0.197559
18.000000	0.111860 ...

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How to open a table in .txt or cvs

A very easy way is using numpy:

```
1  import numpy as np
2
3  file_name_you_want        = np.loadtxt(fname,delimiter=" ")
4
5  print "First column element: ",file_name_you_want[0]
6  #to get the full column:
7
8  Transpose_your_file       = file_name_you_want.T
9
10 print "First column: ", Transpose_your_file[0]
```

How to perform a simple Fit and nicely plot it

```
1  import numpy as np
2  import matplotlib.pyplot as pp
3  from scipy.optimize import curve_fit
4
5  def fitFunc(t, a, b, c):
6      return a*np.exp(-b*t) + c
7
8  t                          = np.linspace(0,4,50)
9  temp                       = fitFunc(t, 2.5, 1.3, 0.5)
10 noisy                      = temp + 0.25*np.random.normal(size=len(temp))
11 fitParams, fitCovariances = curve_fit(fitFunc, t, noisy)
12
13 pp.figure(figsize=(12, 6))
14 pp.ylabel('Temperature (C)', fontsize = 16)
15 pp.xlabel('time (s)', fontsize = 16)
16 pp.xlim(0,4.1)
17 pp.errorbar(t, noisy, fmt = 'ro', yerr = 0.2)
18 sigma = [fitCovariances[0,0], fitCovariances[1,1], fitCovariances[2,2] ]
19 pp.plot(t, fitFunc(t, fitParams[0], fitParams[1], fitParams[2]))
20 pp.plot(t, fitFunc(t, fitParams[0] + sigma[0], fitParams[1] - sigma[1], fitParams[2] + sigma[2]))
21 pp.plot(t, fitFunc(t, fitParams[0] - sigma[0], fitParams[1] + sigma[1], fitParams[2] - sigma[2]))
22 pp.savefig('dataFitted.pdf', bbox_inches=0, dpi=600)
23 pp.show()
```

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19 pp.plot(t, fitFunc(t, fitParams[0], fitParams[1], fitParams[2]))
20 pp.plot(t, fitFunc(t, fitParams[0] + sigma[0], fitParams[1] - sigma[1], fitParams[2] + sigma[2]))
21 pp.plot(t, fitFunc(t, fitParams[0] - sigma[0], fitParams[1] + sigma[1], fitParams[2] - sigma[2]))
22 pp.savefig('dataFitted.pdf', bbox_inches=0, dpi=600)
23 pp.show()
```

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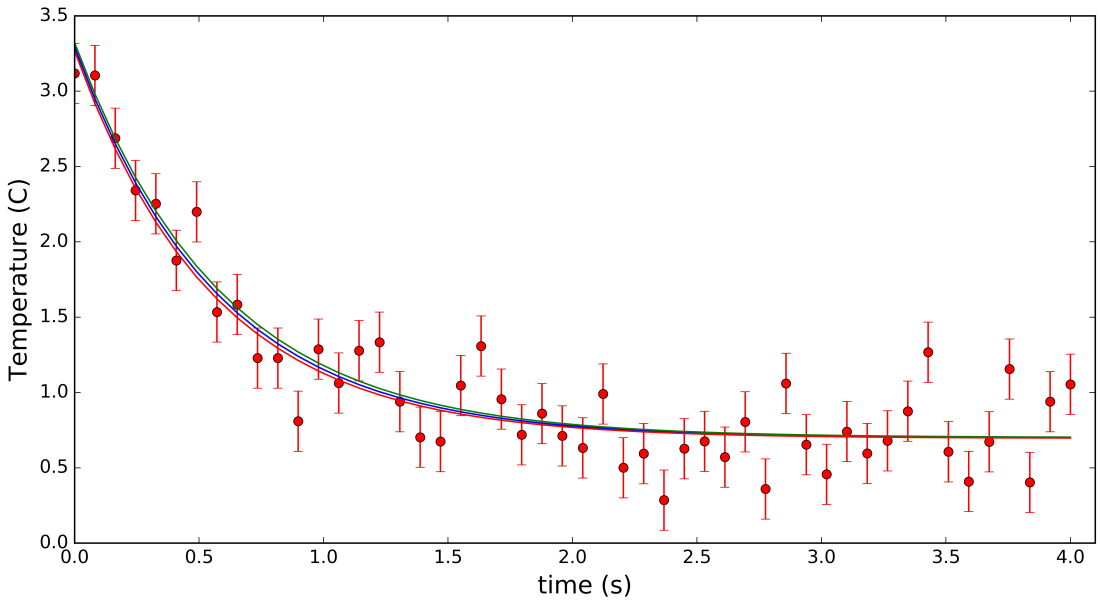
How to perform a simple Fit

We obtain the fit parameters:

```
[ 2.595658    1.74438726  0.69809511]
```

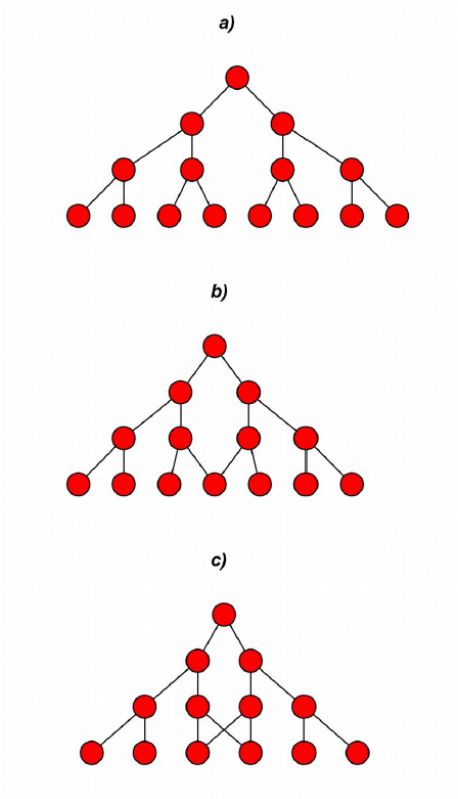
The covariance matrix:

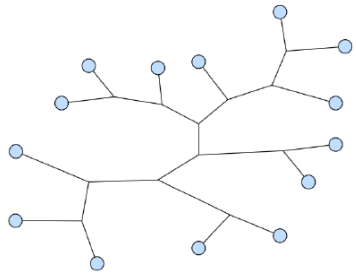
```
[[ 0.02506636  0.01490486 -0.00068609]
 [ 0.01490486  0.04178044  0.00641246]
 [-0.00068609  0.00641246  0.00257799]]
```



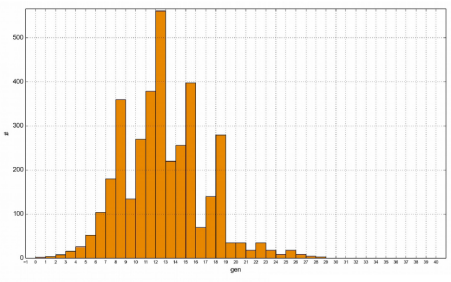
Other more advance kind of plots

```
1 import networkx as nx
2 import pygraphviz
```



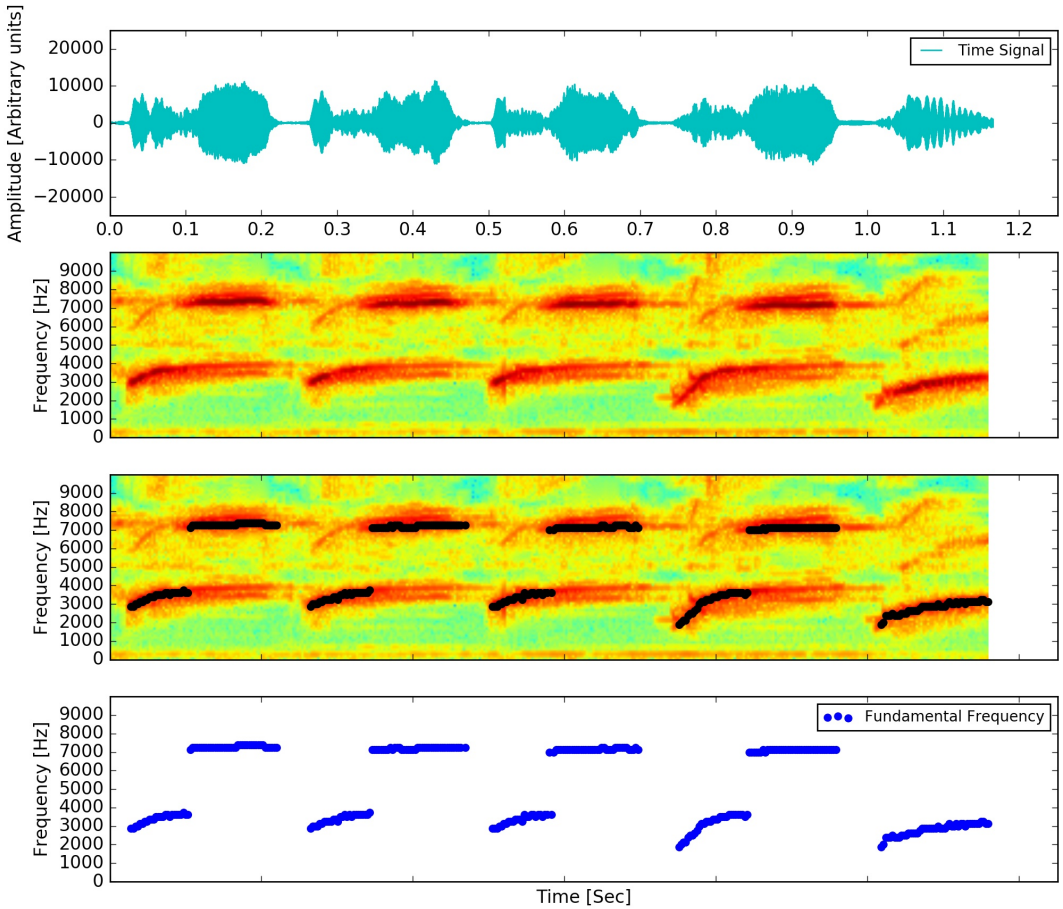


```
1 import matplotlib.pyplot as pp
2 pp.hist([vector,bins=bins)
```



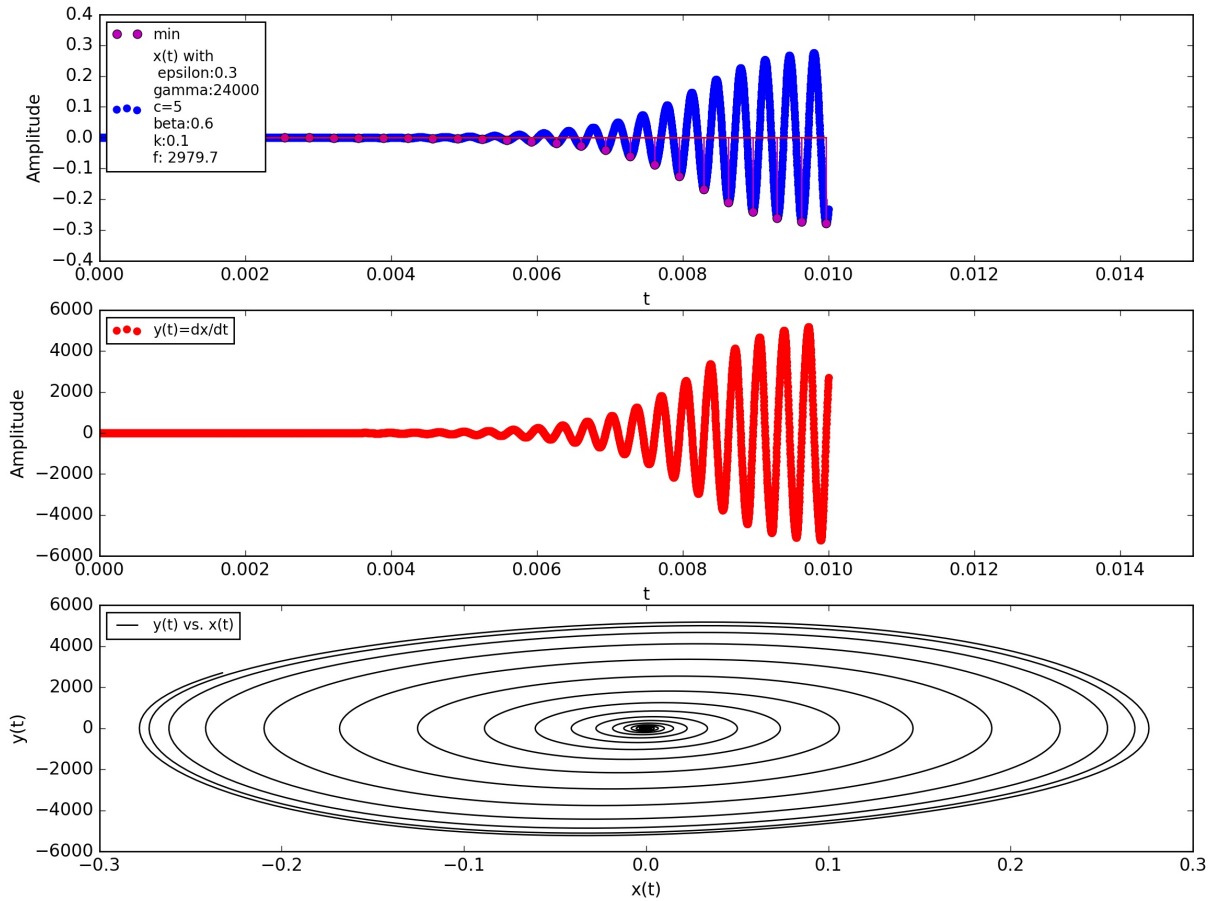
Fourier transform and Spectrograms

```
1 import matplotlib.pyplot as pp
2 pp.specgram(signal, NFFT=nfft, Fs= sample_rate, noverlap=par, cmap='jet'
      )
```



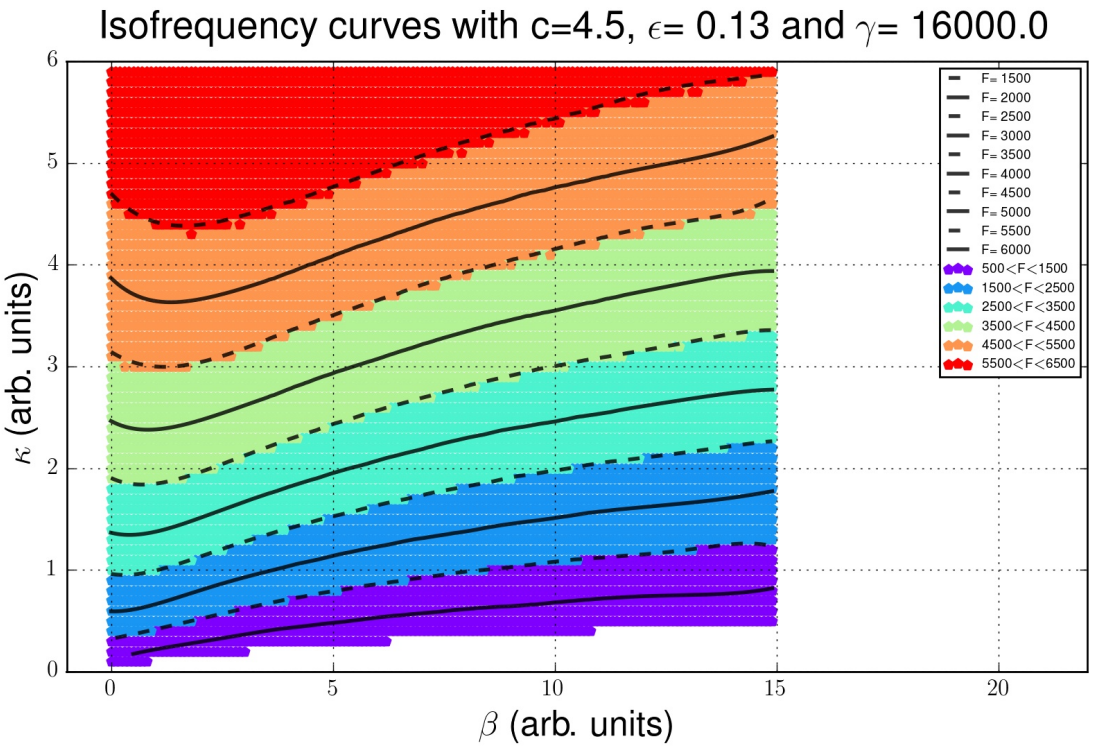
Numerical integration

```
from scipy.integrate import odeint
dy/dt = func(y, t0, ...)
sol   = odeint(func, X0, t)
```



Scatter plot of multiple numerical integrations

- Each point represent the value of the parameters in a numerical integration of the previous equation.
- Colors represent frequency regions



Conclusions

- Python is a very versatile language to write scripts or complex programs combining C, or Fortran
- Scientific libraries with a lot of examples
- Possibility of re-use and improve existing code
- A guide of style in: `https://google.github.io/styleguide/pyguide.html`
- Matplotlib examples: `http://matplotlib.org/gallery.html`

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Additional libraries for data analysis

- Scikit learn:
  `http://scikit-learn.org`
- Pandas
  `http://pandas.pydata.org/`

Additional libraries for data analysis