Introduction to Python for Data Analysis

How to manipulate and represent data with python

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Preamble

These notes contain the material for lecture of a data scientist university degree proposed at Université Clermont-Auvergne (UCA), which is mostly based on a NumPy tutorial that I gave at the Laboratoire de Physique de Clermont in April 2019. No prerequisite knowledge is assumed but being familiar with one progamming language might be useful. It is better to know about some basic mathemtatics like simple vectorial operation or statistics. All the material of this lecture can be found in this github repository.

Python offers a rapidly evolving ecosystem to perform data analysis and it is both out of scope and hopeless to be extensive in this lecture. The main goal is therefore to make people familiar with teh basic of python and data analysis tools in order to *make them able to extend their knowledge on themself*. Object oriented programming is not presented in this lecture. Pratical exercises are also available to provide few working examples as a starting point.

This lecture is only a support to help you doing things *yourself*. As any other language, you must practice it if you want to progress. If you don't write and test code on your own, this lecture is close to be useless. I am available for any questions or general feedback on this lecture, so feel free to use my e-mail: romain.madar@clermont.in2p3.fr.

Chapter 1

Brief introduction to Python

1.1 General information

Python and jupyter-notebook can be installed using anaconda, this is probably the easiest way to follow this lecture and make your own notes. The goal of this first chapter is to give a *very quick introduction basis*, but practice is mandatory to get confortable with python objects and synthax. Practicing is possible with a web browser only using the www3school python tutorials. I recommand to follow these tutorials up to *Arrays*.

In python, there is one instruction per line. Variable assignment is done with with =, indentation is used to group instructions together under a loop or a condition block: there is no backet (like in C++) or equivalent. Comments (*i.e.* uninterpreted text) start with #. Importation of external modules or fonction can be done with three different ways: `import module`, `import module as m` or `from module import this_function`.

In the following example, the result of the command will be printed so that people can check that the computer is doing what is expected. The instruction `print(x)` will print the content of `x`. If several variables are printed, is it convenient to use `print('x={} and y={}'.format(x, y))` synthax that will print `x` and `y` in bracket fields with one command - even if they have different types.

1.2 Object types

1.2.1 Numbers

There are three type of numbers: int, float and complex. The usual operations (+, -, *, /) are available. In addition, there is also `a**b` (which means a^b), `a // b` and `a % b` (which are the result of integer divisions - see example below).

```
# Basic numbers and operations
a = 2
b = 3.14
print(a+b)
print(a**b)
```

```
5.140000000000001
8.815240927012887
```

```
# Complex numbers and power
a = 1j
a**2
```

```
(-1+0j)
```

```
# Integer division example (// and % operators)
a , b = 10, 4
divisor, rest = a//b, a%b
print('{} = {}x{} + {}'.format(a, divisor, b, rest))
```

```
10 = 2x4 + 2
```

1.2.2 Strings

String allows to manipulate words, sentence or even text with specific methods. String are also python lists and list methods work as well (see below). The common and useful string manipulations can be counting the number of letters with `len(word)` or even manipulate a collection of words using `sentence.split(' ')`. Many methods exist, which can be looked at by typing `help(str)` in a python terminal or a jupyter nootebook.

```
w1 = 'hello'
print(w1, len(w1), w1[3])
```

```
hello 5 l
```

```
# Summing two strings is possible (all other operators dont work)
blank, w2 = ' ', 'world'
sentence = w1 + blank + w2
print(sentence)
```

```
hello world
```

```
# Multiplying a string by an integer is also possible
repetition = sentence*3
print(repetition)
```

```
hello worldhello worldhello world
```

```
# Get a list of words from a sentence (cf. below for list objects)
s = 'It is rainy today'
list_words = s.split(' ')
print(list_words)
```

```
['It', 'is', 'rainy', 'today']
```

```
# Looping over the words and get the number of letters
for w in s.split(' '):
    print(w, len(w))
```

```
It 2
is 2
rainy 5
today 5
```

1.3 Object collections

There are four types of collection, which share several methods but differ from various aspects:

- list
- dictionnary
- tuple
- set

The most commonly used are the lists and dictionnary. The specificy of the set is that it is unordered, while the specificyt of the tuple is that it cannot be modified. The common methods are

- number of items: `len(x)`
- loop over items with `for element in x:`
- check if a item is in the list: `element in x`

1.3.1 Lists

This one of the most used collection object in python because it is the next-to-simplest level, after individual variables. A python list is a *list of objects* with possibly different types. One can search, loop, count with list. One can also add two lists or multiply a list by an integer, which makes a *concatenation* or a *duplication* (these points will be important for numpy arrays). The indexing of elements is also a nice way to access the information of interest: one can access the i^{th} element with `my_list[i]` or get a sub-list with `my_list[i:j]`. One can also take only one element every `n` with `my_list[i:j:n]` (more precisely this takes elements of index $i + p \times n$ until j, with $p = 0, 1, 2, ...$). With this synthax, reverting the order of the list is easy: `reverted_list = my_list[::-1]`, where empty variable are default values (namely `0` and `len(my_list)`).

```
# Defining a list and access basic information
my_list1 = [1, 3, 4, 'banana']
print('Second element is {}'.format(my_list1[1]))
print('Number of elements: {}'.format(len(my_list1)))
print('Is \'banana\' in the list? {}'.format('banana' in my_list1))
```

```
Second element is 3
Number of elements: 4
Is 'banana' in the list? True
```

```
# Sum of two lists
my_list2 = ['string', 1+3j, [100, 1000]]
my_list = my_list1 + my_list2
print(my_list)
```

```
[1, 3, 4, 'banana', 'string', (1+3j), [100, 1000]]
```

```
# List multiplied by an integer
my_list = my_list*2
print(my_list)
```

```
[1, 3, 4, 'banana', 'string', (1+3j), [100, 1000], 1, 3, 4, 'banana', 'string', (1+3j), [100,
1000]]
```

```
# Looping over list element and print the type of seven first elements in the reversed order.
for element in my_list[6:0:-1]:
    print('{} is {}'.format(element, type(element)))
```

```
[100, 1000] is <class 'list'>
(1+3j) is <class 'complex'>
string is <class 'str'>
banana is <class 'str'>
4 is <class 'int'>
3 is <class 'int'>
```

1.3.2 sets and tuples

Tuples and set are modified version of python list. Tuples are ordered but cannot be modified (no assignment, no addition, while sets are not ordered but can be mofided. In this context, order means indexing (so `x[i:j:n]` synthax, among others). Search or loop over elements work in the same way as for list.

```
# Tuple
t = (1, 3, 7)
print(t)

# Access the third element
print(t[2])

# Try to modify the second element - using the 'try - except' synthax
try:
    t[1] = 'hello'
except TypeError:
    print('Impossible to change the value of a tuple')
```

```
(1, 3, 7)
7
Impossible to change the value of a tuple
```

Sets can modified with methods like `s.add(x)` or `s.update([x, y])`.

```
# Set
s = {'apple', 'banana', 'orange'}
print(s)

# Add one element
s.add('pineapple')
print(s)

# Add a list
s.update(['pear', 'prune'])
print(s)
```

```
{'apple', 'banana', 'orange'}
{'apple', 'pineapple', 'banana', 'orange'}
{'apple', 'pineapple', 'pear', 'prune', 'banana', 'orange'}
```

```
# Try to access the second element - using the 'try - except' synthax
try:
    print(s[1])
except TypeError:
    print('Impossible to access element via indexing')
```

```
Impossible to access element via indexing
```

1.3.3 Dictionnaries

Other types are important to manipulate and organize data. The most common one is the dictionnary which work with a pair of (`key`, `value`). The `key` must be a non-modifiable object, in practice string or integer, but cannot be a list. This is a very powerful concept to store different types of information into the same object. One can easily loop, search, modify a given key value, or even add a new key quite easily.

```
# dictionnary
person = {'name': 'Charles', 'age': 78, 'size': 173, 'gender': 'M'}
print(person)
```

```
{'name': 'Charles', 'age': 78, 'size': 173, 'gender': 'M'}
```

```
# Accessing value using the key
template = '{} ({}) is {} years old and is {} cm'
print(template.format(person['name'], person['gender'], person['age'], person['size']))
```

```
Charles (M) is 78 years old and is 173 cm
```

```
# Adding a key and its value
person['eyes'] = 'blue'
print(person)
```

```
{'name': 'Charles', 'age': 78, 'size': 173, 'gender': 'M', 'eyes': 'blue'}
```

```
# Test if a key is present
print('name' in person)
print('brand' in person)
```

```
True
False
```

1.4 Loops

Loops are at the core of programming and especially for data analysis oriented tasks. There are two way of repeating a instruction several times: the `for` loop and the `while` loop. Several instructions are common to both loops, such as `continue` (skip instruction after and switch to the next element) or `break` (stop the loop), but the use case of these two ways are different.

1.4.1 For loops

For data analysis, I think these are the most used ones. But as we will see in the introduction to numpy, for loops must not be used for heavy computations in python. For loops are relevant for small (~1000) data samples (and computations). We'll come back to this point in the lecture. Below, few example are given.

```
# Compute sum(i^2) for i from 0 to 9
x = 0
for i in range(0, 10):
    x += i**2
print(x)
```

```
285
```

```
# Loop over fruit via a set and print only ones with a 'p'
for fruit in s:
    if 'p' in fruit:
        print(fruit)
```

```
apple
pineapple
pear
prune
```

There are several ways to loop over dictionnary depending on how we want to access the information. Indeed, you can access information by keys, values, or both. An example of each are given below.

```
# Loop over keys for a dictionnary and access the value of each
for properties in person:
    value = person[properties]
    print('{}: {}'.format(properties, value))
```

```
name: Charles
age: 78
size: 173
gender: M
eyes: blue
```

```
# Loop over dictionnary values only
for v in person.values():
    print(v)
```

```
Charles
78
173
M
blue
```

```
# Loop over both keys and values directly
for key, value in person.items():
    print('{}: {}'.format(key, value))
```

```
name: Charles
age: 78
size: 173
gender: M
eyes: blue
```

Tip: how to sort a dictionnary? It an can be noted that dictionnary are natively *not ordered*. This means that you cannot access a item with its index, since there is no index. However, it can be convenient to sort dictionnary keys according ot their values, using the general python function `sorted(collection, key=function)` and a type of object called `OrderDict` from `collections` module, as explained below.

```
# Define a dictionnary
students_marks = {
    'Jean': 12,
    'Chloe': 17,
    'Olivier': 8,
    'Helene': 10
    }
```

```
# Print the key, values items
for name, mark in students_marks.items():
    print(name, mark)
```

```
Jean 12
Chloe 17
Olivier 8
Helene 10
```

The `sorted()` function works on any type of collection than can be looped over (called *iterable*). It needs the collection and the function which return a key on which to sort for each object of the collection. This can be for *e.g.* a letter or a number. Let's try both by defining a function getting either the mark or the first letter of the name, from a dictionnary item `(name, mark)`.

```
# Order it by increasing marks
def get_mark(item):
    return item[1]

# Or by the first letter of the name
def get_name(item):
    return item[0][0]

# Testing with an item
item_test = ('Jacques', 12)
print('{} has a mark of {} and {} as 1st letter'.format(item_test, get_mark(item_test),
↪  get_name(item_test)))
```

```
('Jacques', 12) has a mark of 12 and J as 1st letter
```

We can now apply the `sorted()` function to the collection of items of the initial directory. This will return a collection of sorted items that can be later converted into a dictionnary. This last step depends on python version (in version 2.5, one has to use `OrderDict` from `collections` module while it's not needed in python 3 - the version of python can be dynamically checked with `sys.version_info` from `sys` module).

```
# Get all items and sort them by increasing mark
all_items = students_marks.items()
items_sorted_by_marks = sorted(all_items, key=get_mark)
items_sorted_by_names = sorted(all_items, key=get_name)
```

```
# Check the version of python
import sys
version = sys.version_info[0]
isPython2 = version == 2
```

```
# Final conversion of collection of items into a dictionnary
if isPython2:
    from collections import OrderedDict
    marks_sorted_dict = OrderedDict(items_sorted_by_marks)
    names_sorted_dict = OrderedDict(items_sorted_by_names)

else:
    marks_sorted_dict = {k: v for k, v in items_sorted_by_marks}
    names_sorted_dict = {k: v for k, v in items_sorted_by_names}
```

```
# Check the mark sorted results:
for k, v in marks_sorted_dict.items():
    print(k, v)
```

```
Olivier 8
Helene 10
Jean 12
Chloe 17
```

```
# Check the name sorted results:
for k, v in names_sorted_dict.items():
    print(k, v)
```

```
Chloe 17
Helene 10
Jean 12
Olivier 8
```

1.4.2 While loops

While loops are bit less used in practive but they are quickly discribed for completness. The idea is to repeat a given instruction until a condition is reached.

```
# Cast (ie change type) the set s into a list
my_list = list(s)

# Remove item one by one until there are no items left.
while len(my_list)>0:
    my_list.pop()
    print(my_list)
```

```
['apple', 'pineapple', 'pear', 'prune', 'banana']
['apple', 'pineapple', 'pear', 'prune']
['apple', 'pineapple', 'pear']
['apple', 'pineapple']
['apple']
[]
```

1.5 Few python synthax tips

1.5.1 Comprehension

```
# List
list_squares = [i**2 for i in range(1, 10)]
print(list_squares)

# Dictionnary
dict_squares = {i:i**2 for i in list_squares[0:5]}
print(dict_squares)
```

```
[1, 4, 9, 16, 25, 36, 49, 64, 81]
{1: 1, 4: 16, 9: 81, 16: 256, 25: 625}
```

```
# Comprehension list with a condition (e.g. keep only even numbers)
list_even = [i for i in range(0, 10) if i%2==0]
print(list_even)
```

```
[0, 2, 4, 6, 8]
```

```
# Comprehension with nested loops
sum_integers = [i*10+j for i in range(0,5) for j in range(0, 5)]
print(sum_integers)
```

```
[0, 1, 2, 3, 4, 10, 11, 12, 13, 14, 20, 21, 22, 23, 24, 30, 31, 32, 33, 34, 40, 41, 42, 43,
44]
```

1.5.2 Looping with `enumerate` and `zip`

The keywork `enumerate` return directly a counter together with the element arising in the loop. This is useful if you need to count the number of iterations of the loop. This can be done without `enumerate` but you need to add two lines (initialisation of the counter, and incrementation).

```
# Position of each word in a sentence
sentence = 'I would like to analyse this sentence in term of word position'
words = sentence.split(' ')
for i, w in enumerate(words):
    print(w.ljust(10) + ':  ' + str(i))
```

```
I         :  0
would     :  1
like      :  2
to        :  3
```

```
analyse   :  4
this      :  5
sentence  :  6
in        :  7
term      :  8
of        :  9
word      :  10
position  :  11
```

The `zip(list1, list2)` synthax allows to form pairs using elements of each list at *the same position*. This is quite convenient to associate some objects which are stored in different collections in a very quick and readable way. If `list1` and `list2` don't have the same size, the mimimum of the two lenght is taken. Finally, the `zip()` command can take more than two collections and return then a group of element which has the size of the number of collection.

```
# Associate fruits and colors
fruits = ['banana', 'orange', 'pineapple', 'pear', 'prune']
colors = ['yellow', 'orange', 'brown', 'green', 'purple']
for f, c in zip(fruits, colors):
    print('{} is {}'.format(f, c))
```

```
banana is yellow
orange is orange
pineapple is brown
pear is green
prune is purple
```

```
# Using zip() with three lists
l1, l2, l3 = range(0, 10), range(0, 100, 10), range(0, 1000, 100)
for i, j, k in zip(l1, l2, l3):
    print(i, j, k, i+j+k)
```

```
0 0 0 0
1 10 100 111
2 20 200 222
3 30 300 333
4 40 400 444
5 50 500 555
6 60 600 666
7 70 700 777
8 80 800 888
9 90 900 999
```

1.6 Functions

Functions are defined as a set of instruction encapsulated into one object. This is particulary convenient when one has to the same list of instructions several times. A good guideline to know when to write a function could be

> If you copy-paste the same pieace of code more than two times, then make a function

1.6.1 Definition

A function takes some arguments, perform some instruction an return a result. The syntax to define and call a function is showed below. In python, function must be defined *before* being used (as opposed to C++ where it can be different, as soon as the function is declared). This makes the concept of *package* quite relevant to wrapp-up several function into a python file which can be imported in the main code.

```
# Definition syntax
def function(argument):
    result = argument * 3
    return result

# Call syntax
function(2)
```

```
6
```

The type of the arguement is not fixed (since it is a general feature of python) so the same instruction will be interpreted differently depending on the type. The following example shows the different result of the function above for two argument types.

```
# Print the result for two types of arguements
print('function(10) = {}'.format(function(10)))
print('function(\'ouh\') = {}'.format(function('ouh')))
```

```
function(10) = 30
function('ouh') = ouhouhouh
```

```
def person_printer(p):
    template = '{} ({}) is {} years old and is {} cm'
    print(template.format(p['name'], p['gender'], p['age'], p['size']))
    return


def grow_old(p, n_years):

    # 1. copy the dictionnary person (otherwise p *will* be modified)
    res = p.copy()

    # 2. Compute the new age and size
    new_age = res['age'] + n_years
    new_size = res['size'] - n_years*0.13

    # 3. Assign the new age/size to the result
```

```
    res['age'] = new_age
    res['size'] = new_size

    # 4. Return the result
    return res
```

```
# Print before growing old
person_printer(person)

# Growing old
old_guy = grow_old(person, 10)

# Print after growing old
person_printer(old_guy)
```

```
Charles (M) is 78 years old and is 173 cm
Charles (M) is 88 years old and is 171.7 cm
```

1.6.2 Docstring

This offers the possibility to document your code in a proper way, which is quite useful for others (and for you, when you will re-use a code after several years). This is then a good practice to do, even if it takes time. This can be accessed using the command `help(function)` or by using the keyboard shortcut `Shift+Tab` in jupyter notebook (when the cursor is after the opening parenthesis of the function). The syntax to add docstring is `'''My documentation'''` at the very begining of the function.

```
def grow_old(p, n_years):
    '''
    Take a person dictionnary and update the age and the size to make the person older.

    Parameters
    ----------
    p: dictionnary
        Person object as defined earlier in the code, with at least 'age' (year)
        and 'size' (cm) keys, to get old.
    n_years: integer
        Number of years to be added to the age of the person.

    Return
    ------
    person: dictionnary
       Person object as defined earlier in the code with age and size updated as
         age  -> age+n_years
         size -> size-n_years*0.13
    '''

    # 1. copy the dictionnary person (otherwise p will be modified, which might problematic)
```

```
    res = p.copy()

    # 2. Compute the new age and size
    new_age = res['age'] + n_years
    new_size = res['size'] - n_years*0.13

    # 3. Assign the new age/size to the result
    res['age'] = new_age
    res['size'] = new_size

    # 4. Return the result
    return res
```

```
help(grow_old)
```

```
Help on function grow_old in module __main__:

grow_old(p, n_years)
    Take a person dictionnary and update the age and the size to make the person older.

    Parameters
    -----
    p: dictionnary
        Person object as defined earlier in the code, with at least 'age' (year)
        and 'size' (cm) keys, to get old.
    n_years: integer
        Number of years to be added to the age of the person.

    Return
    ---
    person: dictionnary
       Person object as defined earlier in the code with age and size updated as
         age  -> age+n_years
         size -> size-n_years*0.13
```

There are several ways to organise the docstring and the example above is based on numpy docstring style. Note that docstring can be also added to a module (in practice, a python file) to document the content, goal and usage of this module.

1.6.3 Arbitrary number of arguments: `*args` and `**kwargs`

The example above are relatively simple and generally function takes several arguments. Sometime it is even convenient to have an unfixed number of arguments, so that the function is rather evolutive when the code grows. Python offres a nice way to define such a function thanks to the *packing* and *unpacking* notion, which is describe right below.

1.6.3.1 *Apparte* packing and unpacking

In short, this is the possibity to convert a list into a serie of objects (unpacking) or vis-versa (packing). This way of writing collection makes code developments very consise and fast, especially to call function with a several arguments in a nice way. This also allows to define function with an arbitrary number of arguments as already mentioned. The following dummy function is used to illustrate the concept of packing/unpacking with both a list and a dictionnary.

```
# Test function
def mean(a, b, c):
    return (a+b+c)/3.
```

It is possible to use a list of three number to specify the argument values of the `mean(a, b, c)` function, using the unpacking syntax for list: `*list`. This is demonstrated below:

```
# Packing & unpacking with a list (or a tuple): *list
my_numbers = [10, 12, 15]
mean(*my_numbers)
```

```
12.333333333333334
```

This is also sometime convenient to call the argument by their name (mostly to make the code more readable). This type of arguments are called *keyword arguments* and can be packed/unpacked into a dictionnary. Each argument name is a key of this dictionnary and the value is the values passed to the function. The unpacking is done with `**dict`.

```
# Packing & unpacking with a dictionnary: **dict
my_numbers = {'a': 10, 'b': 12, 'c': 15}
mean(**my_numbers)
```

```
12.333333333333334
```

Coming back to the initial motivation, *i.e.* having an arbitrary number of arugments. It is possible to define such a function as follow - which in that case just print number and the list of arguments:

```
# Function definition with *args
def test_function(*args):
    print('There are {} arguments: '.format(len(args)))
    for a in args:
        print('  -> {}'.format(a))
    print('')
    return
```

```
# Test with different numbers/types of arguments
test_function()
```

```
test_function('hoho')
test_function('hoho', 3)
test_function('hoho', 3, [1,'banana'], {'mood': 'happy', 'state': 'holidays'})
```

```
There are 0 arguments:

There are 1 arguments:
  -> hoho

There are 2 arguments:
  -> hoho
  -> 3

There are 4 arguments:
  -> hoho
  -> 3
  -> [1, 'banana']
  -> {'mood': 'happy', 'state': 'holidays'}
```

```
# Function definition with kwargs
def test_function(**kwargs):
    print('There are {} arguments: '.format(len(kwargs)))
    for k, v in kwargs.items():
        print(' {}={}'.format(k, v))
    print('')
    return
```

```
test_function()
test_function(x='hoho')
test_function(word='hoho', multiplicity=3)
test_function(a='hoho', N=3, shopping=[1,'banana'], feeling={'mood': 'happy', 'state':
↪  'holidays'})
```

```
There are 0 arguments:

There are 1 arguments:
 x=hoho

There are 2 arguments:
 word=hoho
 multiplicity=3

There are 4 arguments:
 a=hoho
 N=3
 shopping=[1, 'banana']
 feeling={'mood': 'happy', 'state': 'holidays'}
```

This can be used to declare argument in a very readable and concise way. This might be helpful for some cosmetic argument of plot that can be common to several plots (but not all). We'll see some concrete example later in the lecture. In the meanwhile, here is the equivalent of last call from the code above:

```
# Pack all keyword arguments in a dictionnary first
my_args = {
           'a': 'hoho',
           'N': 3,
           'shopping': [1,'banana'],
           'feeling': {'mood': 'happy', 'state': 'holidays'}
          }

# Then call the function
test_function(**my_args)
```

```
There are 4 arguments:
 a=hoho
 N=3
 shopping=[1, 'banana']
 feeling={'mood': 'happy', 'state': 'holidays'}
```

1.7 File manipulation

File handling is quite important since it enable interaction between your code and input/ouput data (called I/O). There are several features related to file handeling in python and this short section just give few basic practices.

1.7.1 Open/close a file

Python has native methods to open and close file. While closing a file doesn't allow for many variations, the opening can be done in different mode, depending if we want to read, write or append to the openned file. The basic syntax is:

```
# Open
f = open('my_file_name.txt', option)

# Close
f.close()
```

where option is a one letter string which can be: + `r` read (default): to just read the file + `a` append: to add content at the end of an existing file + `w` write: to write content in a file (it creates a new file) + `x` create: to create a new file

1.7.2 Write a file

```
# Text to be written (can be one line string 'my text' or multiple lines string - docstring)
text = '''Gervaise avait attendu Lantier jusqu'à deux heures du matin. Puis,
toute frissonnante d'être restée en camisole à l'air vif de la fenêtre,
elle s'était assoupie, jetée en travers du lit, fiévreuse, les joues
trempées de larmes.
'''

# Open in write mode
f = open('test.txt', 'w')

# Write string
f.write(text)

# Close
f.close()
```

1.7.3 Read a file

The following example load the precedent file and loop over each line to analyse its content. One can note several issues: first one sentence can be on two lines, and second, each end of line containt a `\n` (which is an invisible caracter meaning "go-to-next-line"). There is a method to clean a line, called `line.strip()` and remove all spaces and invisible caracteres, unless specifed otherwise - see `help(str.strip)`.

```
# Open the file in read mode
f = open('test.txt', 'r')

# Loop over the lines
for line in f:

    # Print a header to make the ouput clearer
    print('\n\n{}'.format('='*50))

    # Print the line as it is given
    print('This line: {}'.format(line))

    # Split by '.' to isolate sentence
    sentences = line.split('.')
    print('This line has {} sentences: '.format(len(sentences)))

    # Split each sentence by ' ' to isolate words
    for i,s in enumerate(sentences):
        sclean = s.strip()
        words = sclean.split(' ')
        print(' - sentence {}: {}'.format(i, words))
```

```
f.close()
```

```
==================================================
This line: Gervaise avait attendu Lantier jusqu'à deux heures du matin. Puis,

This line has 2 sentences:
 - sentence 0: ['Gervaise', 'avait', 'attendu', 'Lantier', 'jusqu'à', 'deux', 'heures', 'du',
'matin']
 - sentence 1: ['Puis,']


==================================================
This line: toute frissonnante d'être restée en camisole à l'air vif de la fenêtre,

This line has 1 sentences:
 - sentence 0: ['toute', 'frissonnante', 'd'être', 'restée', 'en', 'camisole', 'à', 'l'air',
'vif', 'de', 'la', 'fenêtre,']


==================================================
This line: elle s'était assoupie, jetée en travers du lit, fiévreuse, les joues

This line has 1 sentences:
 - sentence 0: ['elle', 's'était', 'assoupie,', 'jetée', 'en', 'travers', 'du', 'lit,',
'fiévreuse,', 'les', 'joues']


==================================================
This line: trempées de larmes.

This line has 2 sentences:
 - sentence 0: ['trempées', 'de', 'larmes']
 - sentence 1: ['']
```

1.7.4 Re-write a modifed version of a file into a new file

It can be quite convenient to modify an existing file to correct a systematical mistake automatically, or simply do more complexe operation. The example below shows how to remove all the "e" from the text below and write it in a new file.

```
# Open the in/out files
f_i = open('test.txt', 'r')
f_o = open('test_without_e.txt', 'w')

# Loop over line, remove all "e" for each, and write the result in the output file
for line in f_i:
    line_without_e = line.replace('e', '') # replace "e" by nothing
```

```
    f_o.write(line_without_e)

# Close all files
f_i.close()
f_o.close()
```

```
# Open in read mode and check the result
f = open('test_without_e.txt', 'r')
print(f.read())
```

```
Grvais avait attndu Lantir jusqu'à dux hurs du matin. Puis,
tout frissonnant d'êtr rsté n camisol à l'air vif d la fnêtr,
ll s'était assoupi, jté n travrs du lit, fiévrus, ls jous
trmpés d larms.
```

1.7.5 Read a csv file to get data

This use case is quite important since it allows to convert a file with data into variables accessible in the code (for some computation, plotting, etc …). One the most basic format to store data is called *csv* (for comma-separated values) which can import/export from any spreadsheet software (like excel). This format is not necessarily appropriate for large dataset but is quite useful if a large number of situations. one must be able to manipulate it easily, as shown in the example below.

1.7.5.1 Creation of a csv file on the fly using a docstring

```
# Data taken from kaggle: https://www.kaggle.com/jolasa/waves-measuring-buoys-data-mooloolaba
data_csv_format = '''index,date,height,heightMax,period,energy,direction,temperature
1,01/01/2017 00:00,-99.9,-99.9,-99.9,-99.9,-99.9,-99.9
2,01/01/2017 00:30,0.875,1.39,4.421,4.506,-99.9,-99.9
3,01/01/2017 01:00,0.763,1.15,4.52,5.513,49,25.65
4,01/01/2017 01:30,0.77,1.41,4.582,5.647,75,25.5
5,01/01/2017 02:00,0.747,1.16,4.515,5.083,91,25.45
6,01/01/2017 02:30,0.718,1.61,4.614,6.181,68,25.45
7,01/01/2017 03:00,0.707,1.34,4.568,4.705,73,25.5
8,01/01/2017 03:30,0.729,1.21,4.786,4.484,63,25.5
9,01/01/2017 04:00,0.733,1.2,4.897,5.042,68,25.5
10,01/01/2017 04:30,0.711,1.29,5.019,8.439,66,25.5
11,01/01/2017 05:00,0.698,1.11,4.867,4.584,64,25.55
12,01/01/2017 05:30,0.686,1.14,4.755,5.211,56,25.55
13,01/01/2017 06:00,0.721,1.12,4.843,5.813,67,25.5
14,01/01/2017 06:30,0.679,1.22,4.948,4.71,81,25.45
15,01/01/2017 07:00,0.66,1.08,5.068,5.353,90,25.45
16,01/01/2017 07:30,0.662,1.18,5.263,7.436,67,25.4
17,01/01/2017 08:00,0.653,1.21,5.007,6.001,90,25.45
18,01/01/2017 08:30,0.665,1.17,4.952,6.414,90,25.55
```

```
19,01/01/2017 09:00,0.684,1.55,5.022,6.691,88,25.6
20,01/01/2017 09:30,0.679,1.09,4.926,6.804,88,25.65
21,01/01/2017 10:00,0.667,1.12,4.928,6.641,122,25.75
22,01/01/2017 10:30,0.688,1.13,4.808,5.958,91,25.7
23,01/01/2017 11:00,0.644,0.99,4.559,6.691,92,25.9
'''

# Create csv file using these data
f = open('wave_data.csv', 'w')
f.write(data_csv_format)
f.close()
```

1.7.5.2 Reading the csv file and storing values in python objects

In this example, we'll see how to store all information about the wave in a list of dictionnaries.

```
# Open the file in read mode
f = open('wave_data.csv', 'r')

# Get the first line (calling the readline() method once) to extract the feature names.
features = f.readline().strip().split(',')
print(features)

# Loop over lines and store the information
data = []
for l in f:
    values = l.strip().split(',')
    data_single_wave = {var: val for var, val in zip(features, values)}
    data.append(data_single_wave)
```

```
['index', 'date', 'height', 'heightMax', 'period', 'energy', 'direction', 'temperature']
```

```
# helper function for a nice printing
def print_wave(w):
    tmp = 'Wave {} ({}) had a heigh of {}m with a temperature of {} degree'
    print(tmp.format(w['index'], w['date'], w['height'], w['temperature']))

# Print the first 5 waves
for wave in data[:5]:
    print_wave(wave)
```

```
Wave 1 (01/01/2017 00:00) had a heigh of -99.9m with a temperature of -99.9 degree
Wave 2 (01/01/2017 00:30) had a heigh of 0.875m with a temperature of -99.9 degree
Wave 3 (01/01/2017 01:00) had a heigh of 0.763m with a temperature of 25.65 degree
Wave 4 (01/01/2017 01:30) had a heigh of 0.77m with a temperature of 25.5 degree
Wave 5 (01/01/2017 02:00) had a heigh of 0.747m with a temperature of 25.45 degree
```

At the stage, the problem is that the type of object which are stored is string and not numbers … so no computation can be made. Typically, the following code will crash because the division between string is not defined:

```
# Compute the average height
heights = [w['height'] for w in data]
average = sum(heights)/len(heights)
```

One has to cast (*i.e.* change type) the object stored into the dictionnaries. They can all casted as float but the date. The index makes more sense as integer as well. So the following can work:

```
# Manage string to time object conversion
def str_to_time(date_str):
    import datetime
    return datetime.datetime.strptime(date_str, '%d/%m/%Y %H:%M')

# Container with properly converted data
DATA = []

# Loop over waves and make the proper conversion depending on the feature name
for w in data:
    wgood = w.copy()
    for k in w:
        if k == 'index':   # Cast string into an integer
            wgood[k] = int(w[k])
        elif k == 'date':  # cast string into a datetime object
            wgood[k] = str_to_time(w[k])
        else:              # cast string into a float
            wgood[k] = float(w[k])
    DATA.append(wgood)
```

Computing the averaged heigh of wave now works but give a quite strange result:

```
# Compute the average height
heights = [w['height'] for w in DATA]
average = sum(heights)/len(heights)
print('Averaged waveheight is {:.1f} m'.format(average))
```

```
Averaged waveheight is -3.7 m
```

This is due to the first row which has all values at -99. Removing it (using indexing technics) gives a more sensible result:

```
heights = [w['height'] for w in DATA[1:]]
average = sum(heights)/len(heights)
print('Averaged waveheight is {:.1f} m'.format(average))
```

```
Averaged waveheight is 0.7 m
```

Chapter 2

Short introduction to numpy

Why numpy? Numpy stands for *numerical python* and is highly optimized (and then fast) for computations in python. Numpy is one of the core package on which many others are based on, such as scipy (for *scientific python*), matplotlib or pandas (described at the end of this chapter). A lot of other scientific tools are also based on numpy and that justifies to have - at least - a basic understanding of how it works. Very well, but one could also ask why using python?

Why python? Depending on your preferences and your purposes, python can be a very good option or not (of course this is largely a matter of taste and not everyone agrees with this statement). In any case, many tools are available in python, scanning a very broad spectrum of applications, from machine learning to web design or string processing.

2.1 The core object: arrays

The core of numpy is the called numpy array. These objects allow to efficiently perform computations over large dataset in a very consise way from the language point of view, and very fast from the processing time point of view. The price to pay is to give up explicit *for* loops. This lead to somehow a counter intuitive logic - at first.

2.1.1 Main differences with usual python lists

The first point is to differenciate numpy array from python list, since they don't behave in the same way. Let's define two python lists and the two equivalent numpy arrays.

```
import numpy as np
l1, l2 = [1, 2, 3], [3, 4, 5]
a1, a2 = np.array([1, 2, 3]), np.array([3, 4, 5])
print(l1, l2)
```

```
[1, 2, 3] [3, 4, 5]
```

First of all, all mathematical operations act element by element in a numpy array. For python list, the addition acts as a concatenation of the lists, and a multiplication by a scalar acts as a replication of the lists:

```
# obj1+obj2
print('python lists: {}'.format(l1+l2))
print('numpy arrays: {}'.format(a1+a2))
```

```
python lists: [1, 2, 3, 3, 4, 5]
numpy arrays: [4 6 8]
```

```
# obj*3
print('python list: {}'.format(l1*3))
print('numpy array: {}'.format(a1*3))
```

```
python list: [1, 2, 3, 1, 2, 3, 1, 2, 3]
numpy array: [3 6 9]
```

One other important difference is about the way to access element of an array, the so called slicing and indexing. Here the behaviour of python list and numpy arrays are closer expect that numpy array supports few more features, such as indexing by an array of integer (which doesn't work for python lists). Use cases of such indexing will be heavily illustrated in the next chapters.

```
# Indexing with an integer: obj[1]
print('python list: {}'.format(l1[1]))
print('numpy array: {}'.format(a1[1]))
```

```
python list: 2
numpy array: 2
```

```
# Indexing with a slicing: obj[slice(1,3)]
print('python list: {}'.format(l1[slice(1,3)]))
print('numpy array: {}'.format(l1[slice(1,3)]))
```

```
python list: [2, 3]
numpy array: [2, 3]
```

```
# Indexing with a list of integers: obj[[0,2]]
print('python list: IMPOSSIBLE')
print('numpy array: {}'.format(a1[[0,2]]))
```

```
python list: IMPOSSIBLE
numpy array: [1 3]
```

2.1.2 Main caracteristics of an array

The strenght of numpy array is to be multidimensional. This enables a description of a whole complex dataset into a single numpy array, on which one can do operations. In numpy, dimension are also called *axis*. For example, a set of 2 position in space $\vec{r}_i$ can be seen as 2D numpy array, with the first axis being the point $i = 1$ or $i = 2$, and the second axis being the coordinates (x, y, z). There are few attributes which describe multidimentional arrays:

- `a.dtype`: type of data contained in the array
- `a.shape`: number of elements along each dimension (or axis)
- `a.size`: total number of elements (product of `a.shape` elements)
- `a.ndim`: number of dimensions (or axis)

```
points = np.array([[ 0,  1, 2],
                   [ 3,  4, 5]])

print('a.dtype = {}'.format(points.dtype))
print('a.shape = {}'.format(points.shape))
print('a.size  = {}'.format(points.size))
print('a.ndim  = {}'.format(points.ndim))
```

```
a.dtype = int64
a.shape = (2, 3)
a.size  = 6
a.ndim  = 2
```

2.2 The three key features of numpy

2.2.1 Vectorization

The *vectorization* is a way to make computations on numpy array **without explicit loops**, which are very slow in python. The idea of vectorization is to compute a given operation *element-wise* while the operation is called on the array itself. An example is given below to compute the inverse of 100000 numbers, both with explicit loop and vectorization.

```
a = np.random.randint(low=1, high=100, size=100000)

def explicit_loop_for_inverse(array):
    res = []
    for a in array:
        res.append(1./a)
    return np.array(res)
```

```
# Using explicit loop
%timeit explicit_loop_for_inverse(a)
```

```
204 ms ± 27.1 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

```
# Using list comprehension
%timeit [1./x for x in a]
```

```
188 ms ± 42.4 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
```

```
# Using vectorization
%timeit 1./a
```

```
116 µs ± 13.7 µs per loop (mean ± std. dev. of 7 runs, 10000 loops each)
```

The suppression of explicit *for* loops is probably the most unfamiliar aspect of numpy - according to me - and deserves a bit a of practice. At the end, lines of codes becomes relatively short but ones need to properly think how to implement a given computation in a *pythonic way*.

Many standard functions are implemented in a vectorized way, they are call the *universal functions*, or `ufunc`. Few examples are given below but the full description can be found in numpy documentation.

```
a = np.random.randint(low=1, high=100, size=3)
print('a        : {}'.format(a))
print('a^2      : {}'.format(a**2))
print('a/(1-a^a): {}'.format(a/(1-a**a)))
print('cos(a)   : {}'.format(np.cos(a)))
print('exp(a)   : {}'.format(np.exp(a)))
```

```
a        : [22 84 90]
a^2      : [ 484 7056 8100]
a/(1-a^a): [-4.41611606e-18  8.40000000e+01  9.00000000e+01]
cos(a)   : [-0.99996083 -0.6800235  -0.44807362]
exp(a)   : [3.58491285e+09 3.02507732e+36 1.22040329e+39]
```

All these ufunct can work for n-dimension arrays and can be used in a very flexible way depeding on the axis you are refering too. Indeed the mathematical operation can be performed over a different axis of the array, having a totally different meaning. Let's give a simple concrete example with a 2D array of shape (5,2), *i.e.* 5 vectors of three coordinates (x, y, z) Much more examples will be discussed in the section 2.

```
# Generate 5 vectors (x,y,z)
positions = np.random.randint(low=1, high=100, size=(5, 3))

# Average of the coordinate over the 5 observations
pos_mean = np.mean(positions, axis=0)
```

```
print('mean = {}'.format(pos_mean))

# Distance to the origin sqrt(x^2 + y^2 + z^2) for the 5 observations
distances = np.sqrt(np.sum(positions**2, axis=1))
print('distances = {}'.format(distances))
```

```
mean = [47.6 53.6 61. ]
distances = [ 76.4852927   45.14421336 142.91955779 128.23805987  97.49871794]
```

2.2.2 Broadcasting

The *broadcasting* is a way to compute operation between arrays of having different sizes in a implicit (and consice) manner. One concrete example could be to translate three positions $\vec{r}_i = (x, y)_i$ by a vector $\vec{d}_0$ simply by adding `points+d0` where `points.shape=(3,2)` and `d0.shape=(2,)`. Few examples are given below but more details are give in this documentation.

```
# operation between shape (3) and (1)
a = np.array([1, 2, 3])
b = np.array([5])
print('a+b = \n{}'.format(a+b))
```

```
a+b =
[6 7 8]
```

```
# operation between shape (3) and (1,2)
a = np.array([1, 2, 3])
b = np.array([
              [4],
              [5],
             ])
print('a+b = \n{}'.format(a+b))
```

```
a+b =
[[5 6 7]
 [6 7 8]]
```

```
# Translating 3 2D vectors by d0=(1,4)
points = np.random.normal(size=(3, 2))
d0 = np.array([1, 4])
print('points:\n {}\n'.format(points))
print('points+d0:\n {}'.format(points+d0))
```

```
points:
 [[-1.21022003 -1.11118338]
 [-0.85932207  1.10591019]
```

```
 [-0.74296716  1.82954158]]

points+d0:
 [[-0.21022003  2.88881662]
 [ 0.14067793  5.10591019]
 [ 0.25703284  5.82954158]]
```

Not all shapes can be combined together and there are *broadcasting rules*, which are (quoting the numpy documentation):

> 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

In a failing case, one can then add a new *empty axis* `np.newaxis` to an array to make their dimension equal and then the broadcasting possible. Here is a very simle example:

```
a = np.arange(10).reshape(2,5)
b = np.array([10,20])
```

```
try:
    res = a+b
    print('Possible for {} and {}:'.format(a.shape, b.shape))
    print('a+b = \n {}'.format(res))
except ValueError:
    print('Impossible for {} and {}'.format(a.shape, b.shape))
```

```
Impossible for (2, 5) and (2,)
```

```
c = b[:, np.newaxis]
try:
    res = a+c
    print('Possible for {} and {}:'.format(a.shape, c.shape))
    print('a+c = \n {}'.format(res))
except ValueError:
    print('Broadcasting for {} and {}'.format(a.shape, c.shape))
```

```
Possible for (2, 5) and (2, 1):
a+c =
 [[10 11 12 13 14]
 [25 26 27 28 29]]
```

2.2.3 Working with sub-arrays: slicing, indexing and mask (or selection)

As mentioned eariler, *slicing and indexing* are ways to access elements or sub-arrays in a smart way. Python allows slicing with `Slice()` object but `numpy` allows to push the logic much further with what is called *fancy indexing*. Few examples are given below and for more details, please have a look to this documentation page.

Rule 1: the syntax is `a[i]` to access the ith element. It is also possible to go from the last element using negative indices: `a[-1]` is the last element.

```
a = np.random.randint(low=1, high=100, size=10)
print('a = {}'.format(a))
print('a[2] = {}'.format(a[2]))
print('a[-1] = {}'.format(a[-1]))
print('a[[1, 2, 5]] = {}'.format(a[[1, 2, 5]]))
```

```
a = [27 74  9 99 49 21 79 54 97 71]
a[2] = 9
a[-1] = 71
a[[1, 2, 5]] = [74  9 21]
```

Rule 2: numpy also support array of indices. If the index array is multi-dimensional, the returned array will have the same dimension as the indices array.

```
# Small n-dimensional indices array: 3 arrays of 2 elements
indices = np.arange(6).reshape(3,2)
print('indices =\n {}'.format(indices))
print('a[indices] =\n {}'.format(a[indices]))
```

```
indices =
 [[0 1]
 [2 3]
 [4 5]]
a[indices] =
 [[27 74]
 [ 9 99]
 [49 21]]
```

```
# Playing with n-dimensional indices array: 2 arrays of (10, 10) arrays
indices_big = np.random.randint(low=0, high=10, size=(2, 3, 2))
print('indices_big =\n {}'.format(indices_big))
print('a[indices_big] =\n {}'.format(a[indices_big]))
```

```
indices_big =
 [[[8 6]
  [5 8]
  [4 1]]

 [[7 2]
  [7 0]
  [9 2]]]
a[indices_big] =
 [[[97 79]
  [21 97]
```

```
  [49 74]]

 [[54  9]
  [54 27]
  [71  9]]]
```

Rule 3: There is a smart way to access sub-arrays with the syntax `a[min:max:step]`. In that way, it's for example very easy to take one element over two (`step=2`), or reverse the order of an array (`step=-1`). This syntax works also for n-dimensional array, where each dimension is sperated by a comma. An example is given for a 1D array and for a 3D array of shape (5, 2, 3) - that can considered as 5 observations of 2 positions in space.

```
# 1D array
a = np.random.randint(low=1, high=100, size=10)
print('full array a              = {}'.format(a))
print('from 0 to 1: a[:2]        = {}'.format(a[:2]))
print('from 4 to end: a[4:]      = {}'.format(a[4:]))
print('reverse order: a[::-1]    = {}'.format(a[::-1]))
print('all even elements: a[::2] = {}'.format(a[::2]))
```

```
full array a              = [85 57 89 81 79 14 50 79  5  1]
from 0 to 1: a[:2]        = [85 57]
from 4 to end: a[4:]      = [79 14 50 79  5  1]
reverse order: a[::-1]    = [ 1  5 79 50 14 79 81 89 57 85]
all even elements: a[::2] = [85 89 79 50  5]
```

```
# 3D array
a = np.random.randint(low=0, high=100, size=(5, 2, 3))
print('a = \n{}'.format(a))
```

```
a =
[[[90 81 16]
  [87  2 33]]

 [[97 57 17]
  [21 39 87]]

 [[99 12 69]
  [18 23 30]]

 [[95 90 73]
  [76 99 50]]

 [[71 86 20]
  [67 50 63]]]
```

Let's say, one wants to take only the (x, y) coordinates for the first vector for all 5 observations. This is how each axis will be sliced: - first axis (=5 observations): `:`, *i.e.* takes all - second axis (=2 vectors): `1` *i.e.* only the 2nd element - third axis (=3 coordinates): `0:2` *i.e.* from 0 to $2 - 1 = 1$, so only (x, y)

```
# Taking only the x,y values of the first vector for all observation:
print('a[:, 0, 0:2] =\n {}'.format(a[:, 0, 0:2]))
```

```
a[:, 0, 0:2] =
 [[90 81]
 [97 57]
 [99 12]
 [95 90]
 [71 86]]
```

```
# Reverse the order of the 2 vector for each observation:
print('a[:, ::-1, :] = \n{}'.format(a[:, ::-1, :]))
```

```
a[:, ::-1, :] =
[[[87  2 33]
  [90 81 16]]

 [[21 39 87]
  [97 57 17]]

 [[18 23 30]
  [99 12 69]]

 [[76 99 50]
  [95 90 73]]

 [[67 50 63]
  [71 86 20]]]
```

Rule 4: The last part of of indexing is about *masking* array or in a more common language, *selecting* sub-arrays/elements. This allows to get only elements satisfying a given criteria, exploiting the indexing rules described above. Indeed, a boolean operation applied to an array such as `a>0` will directly return an array of boolean values `True` or `False` depending if the corresponding element satisfies the condition or not.

```
a = np.random.randint(low=-100, high=100, size=(5, 3))
mask = a>0
print('a = \n{}'.format(a))
print('\nmask = \n {}'.format(mask))
```

```
a =
[[-97 -59  35]
 [-92  72  74]
 [-60 -42 -35]
 [-93 -37 -60]
 [ 20  33  59]]

mask =
```

```
 [[False False  True]
 [False  True  True]
 [False False False]
 [False False False]
 [ True  True  True]]
```

```
print('\na[mask] = \n {}'.format(a[mask])) # always return 1D array
print('\na*mask = \n {}'.format(a*mask)) # preserves the dimension (False=0)
print('\na[~mask] = \n {}'.format(a[~mask])) # ~mask is the negation of mask
print('\na*~mask  = \n {}'.format(a*~mask)) # working for a product too.
```

```
a[mask] =
 [35 72 74 20 33 59]

a*mask =
 [[ 0  0 35]
 [ 0 72 74]
 [ 0  0  0]
 [ 0  0  0]
 [20 33 59]]

a[~mask] =
 [-97 -59 -92 -60 -42 -35 -93 -37 -60]

a*~mask  =
 [[-97 -59   0]
 [-92   0   0]
 [-60 -42 -35]
 [-93 -37 -60]
 [  0   0   0]]
```

Note the case of boolean arrays as indices has then a special treatment in numpy (since the result is always a 1D array). There is actually a dedicated numpy object called *masked array* (cf. documentation) which allows to keep the whole array but without considering some elements in the computation (*e.g.* CCD camera with dead pixel). Note however that when a boolean array is used in an mathematical operation (such as `a*mask`) then `False` is treated as `0` and `True` as `1`:

```
print('a+mask = \n{}'.format(a+mask))
```

```
a+mask =
[[-97 -59  36]
 [-92  73  75]
 [-60 -42 -35]
 [-93 -37 -60]
 [ 21  34  60]]
```

This boolean arrays are also very useful to *replace a category of elements* with a given value in a very easy, consise and readable way:

```
a = np.random.randint(low=-100, high=100, size=(5, 3))
print('Before: a=\n{}'.format(a))

a[a<0] = a[a<0]**2
print('\nAfter: a=\n{}'.format(a))
```

```
Before: a=
[[ 84  22  42]
 [-78  79 -55]
 [-68 -70  45]
 [-29  -4  91]
 [-72 -38  58]]

After: a=
[[  84   22   42]
 [6084   79 3025]
 [4624 4900   45]
 [ 841   16   91]
 [5184 1444   58]]
```

2.3 Few powerfull tools: matplotlib, pandas and scipy

2.3.1 Plotting with matplotlib

matplolib is an extremely rich librairy for data visualization and there is no way to cover all its features in this note. The goal of this section is just to give short and practical examples to plot data. Much more details can be obtained on the webpage. The following shows how to quickly make *histograms*, *graph*, *2D and 3D scatter plots*.

The main object of matplotlib is `matplotlib.pyplot` imported as `plt` here (and usually). The most common functions are then called on this objects, and often takes numpy arrays in argument (possibly with more than one dimension) and a lot of `kwargs` to define the plotting style.

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

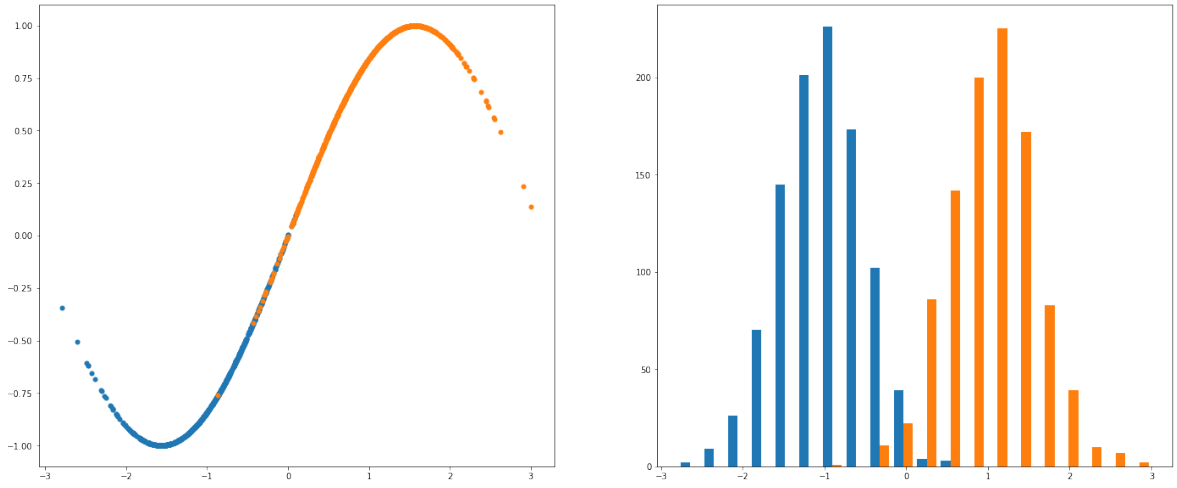
2.3.1.1 Example of 1D plots and histograms

To play with data, we generate 2 samples of 1000 values distributed according to a normal probability density function with $\mu = -1$ and $\mu = 1$ respectively, and $\sigma = 0.5$. These data are stored in a numpy array `x` of shape `x.shape=(1000, 2)`. We then simply compute and store the sinus of all these values into a same shape array `y`:

```
x = np.random.normal(loc=[-1, 1], scale=[0.5, 0.5], size=(1000,2))
y = np.sin(x)
```

The next step is to plot these data in two ways: first we want `y` v.s. `x`, second we want the histogram of the `x` values. We need to first create a figure, then create two *subplots* (specifying the number of line, column, and subplot index). Note that matplotlib take always the first dimension to define the numbers to plot, while higher dimensions are considered as other plots - automatically overlaid.

```
plt.figure(figsize=(24, 10))
plt.subplot(121) # 121 means 1 line, 2 column, 1st plot
plt.plot(x, y, marker='o', markersize=5, linewidth=0.0)
plt.subplot(122) # 122 means 1 line, 2 column, 2nd plot
plt.hist(x, bins=20);
```



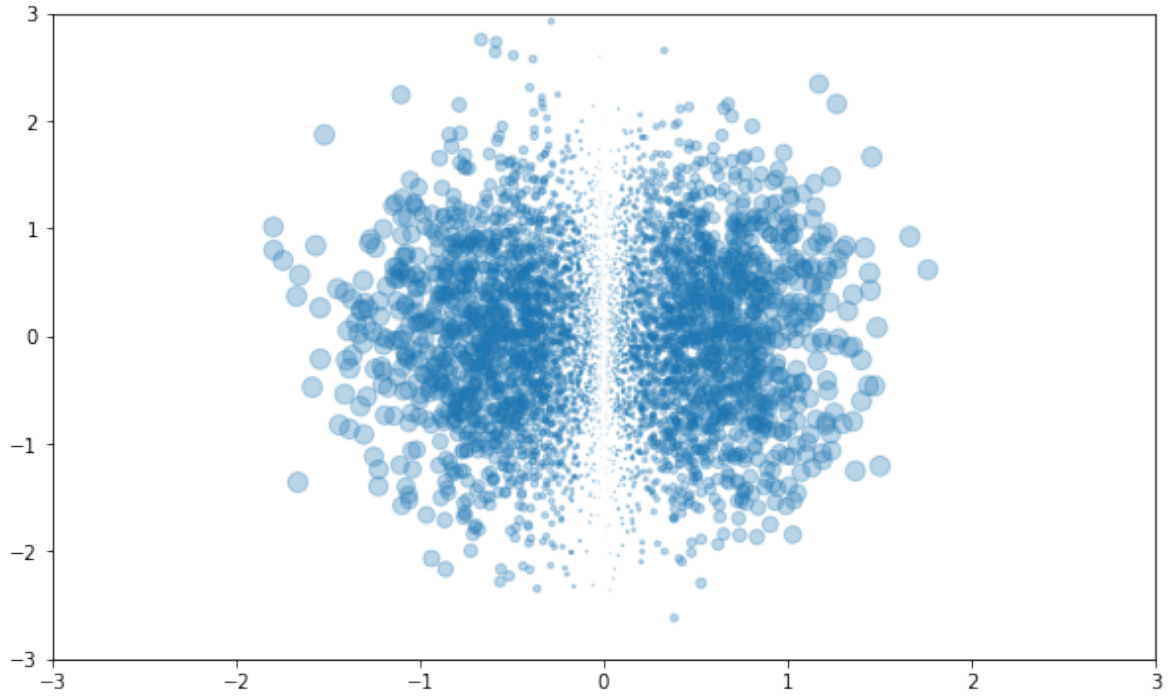
2.3.1.2 Example of 2D scatter plot

A scatter plot allows to draw marker in a 2D space and a thrid information is encoded into the marker size. In order to play, we generated two set of 5000 numbers distributed according to uncorrelated gaussians of ($\mu_0 = \mu_1 = 0$) and (σ_1, σ_2) = (0.5, 0.8) in a numpy array `points` of shape `points.shape=(5000,2)`. These two sets of numbers are then interepreted as (x, y) positions being loaded in two `(5000, 1)` arrays `x` and `y`:

```
points = np.random.normal(loc=[0, 0], scale=[0.5, 0.8], size=(5000,2))
x, y = points[:, 0], points[:, 1]
```

We can then plot the 5000 points in the 2D plan, and here we specify the marker size at $100 \times \sin^2(x)$ using the argument `s` of the `plt.scatter()` function (note that the array `x`, `y` and `s` must have the same shape):

```
plt.figure(figsize=(10,6))
plt.scatter(x, y, s=100*(np.sin(x))**2, marker='o', alpha=0.3)
plt.xlim(-3, 3)
plt.ylim(-3, 3);
```



2.3.1.3 Example of 3D plots

For 3D plots, one can generate 1000 positions in space, and operate a translation by a vector $\vec{r}_0$ using broadcasting:

```
data = np.random.normal(size=(1000, 3))
r0 = np.array([1, 4, 2])
data_trans = data + r0
```

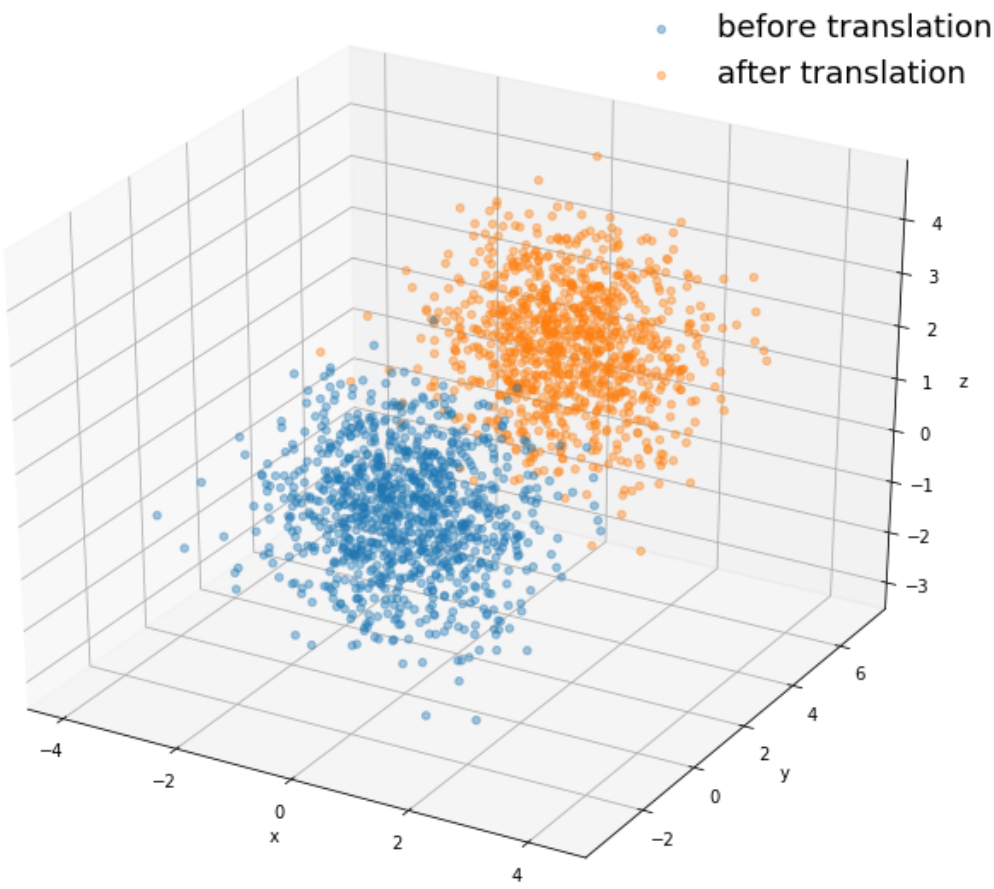
It is then easy to get back the spatial initial (*i.e.* before translation) and final (*i.e.* after translation) coordinates:

```
xi, yi, zi = data[:,0], data[:,1], data[:,2]
xf, yf, zf = data_trans[:,0], data_trans[:,1], data_trans[:,2]
```

An additional module must be imported in order to plot data in three dimensions, and the projection has to be stated. Once it's done, a simple call to `ax.scatter3D(x,y,z)` does the plot. Note that we call a function of `ax` and not `plt` as before. This is due to the `ax = plt.axes(projection='3d')` command which is needed for 3D plotting. More details are available on the matplotlib 3D tutorial.

```
from mpl_toolkits import mplot3d
plt.figure(figsize=(12,10))
ax = plt.axes(projection='3d')
ax.scatter3D(xi, yi, zi, alpha=0.4, label='before translation')
ax.scatter3D(xf, yf, zf, alpha=0.4, label='after translation')
ax.set_xlabel('x')
ax.set_ylabel('y')
```

```
ax.set_zlabel('z')
ax.legend(frameon=False, fontsize=18);
```



2.3.2 Import and manipulate data as numpy array via pandas

The package `pandas` is an very rich interface to read data from different format and produce a `pandas.dataframe` that can be based on `numpy` (but contanining a lot more features). There is no way to fully desribe this package here, the goal is simply to give functional and concrete example easily usable. More more details, please check the pandas webpage.

Many build-in functions are available to import data as pandas dataframe. One, which is particularly convenient, directly reads csv files (one can specify the columns to loads, the row to skip, and many other options ...):

```
import pandas as pd
cols_to_keep = ['HT', 'nlep', 'njet', 'pt_1st_bjet']
df = pd.read_csv('ttW.csv', usecols=cols_to_keep)
print(df.head())
```

```
            HT  njet  nlep  pt_1st_bjet
0   262.100311     2     2    48.112684
1   447.937225     4     4   118.460391
2  1287.348022     6     6    89.715039
3   453.677887     6     6    88.535555
4   268.445099     2     2   116.625023
```

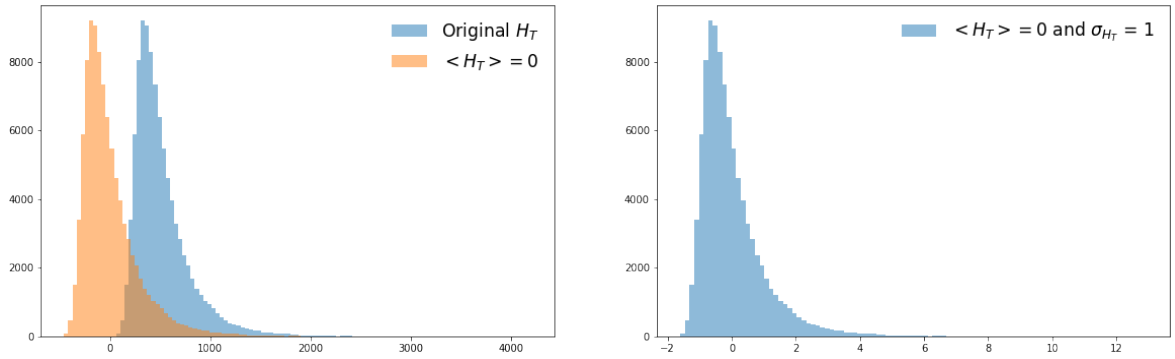
On of the nice feature of pandas is to be able to easily get numpy array, compute and store the result as a new column. For instance, it's a common practice in machine learning to *normalize* the input variables, *i.e.* transform them to have a mean of 0 and a variance of 1.0. The following example shows how to add new H_T distributions (the meaning of this variable doesn't matter for now) as new columns:

```
# Get a numpy arrays
ht = df['HT'].values

# Compute quantities
ht_mean = np.mean(ht)
ht_rms = np.sqrt(np.mean((ht-ht_mean)**2))

# Add them into the pandas dataframe
df['HT_centered'] = ht-ht_mean
df['HT_normalized'] = (ht-ht_mean)/ht_rms

# Print the result
cols_to_print = ['HT', 'HT_centered', 'HT_normalized']
print(df[cols_to_print].head())
```

```
            HT  HT_centered  HT_normalized
0   262.100311  -254.826585      -0.895919
1   447.937225   -68.989671      -0.242554
2  1287.348022   770.421127       2.708646
3   453.677887   -63.249009      -0.222371
4   268.445099  -248.481797      -0.873612
```

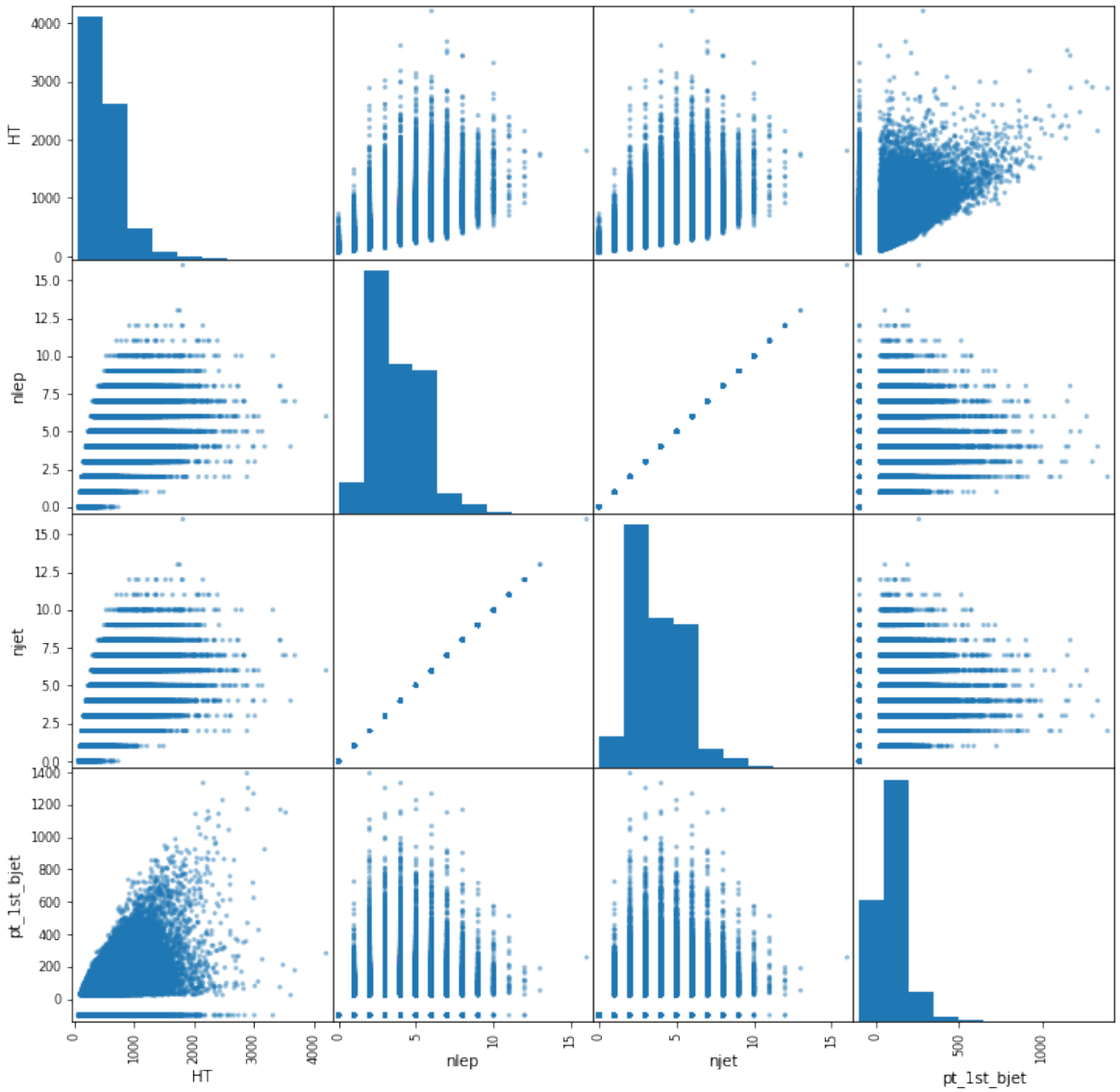
One can simply plot the content of a pandas dataframe using the name of the column. For instance, one can compare the evolution of H_T after each transformation (which is trivial in this illustrative case):

```
plt.figure(figsize=(20, 6))
plt.subplot(121)
plt.hist(df['HT'], bins=100, alpha=0.5, label='Original $H_T$')
plt.hist(df['HT_centered'], bins=100, alpha=0.5, label='$<H_T> = 0$')
plt.legend(frameon=False, fontsize='xx-large')
plt.subplot(122)
plt.hist(df['HT_normalized'], bins=100, alpha=0.5,
         label='$<H_T> = 0$ and $\sigma_{H_T}$ = 1')
plt.legend(frameon=False, fontsize='xx-large');
```



There are also many plotting function already included into the pandas library. To show only one example (all functions are decribed in the pandas visualization tutorial), here is the *scatter matrix* between variables (defined as a subset of the ones stored the dataframe) obtained in a single line of code:

```
from pandas.plotting import scatter_matrix
var_to_plot = ['HT', 'nlep', 'njet', 'pt_1st_bjet']
scatter_matrix(df[var_to_plot], figsize=(12, 12), alpha=0.5);
```



2.3.3 Mathematics, physics and engineering with scipy

The scipy project is python-based ecosystem of open-source software for mathematics, science, and engineering. In particular, the following core package are part of it: NumPy, matplotlib, pandas, scipy library (very quickly introduced here) and SymPy (symbolic calculations with mathematical expressions *a la* mathematica).

Obviously, there is no way to extensively present the scipy library in this short introduction, but one can quickly summarize few features and illustrate one with a concrete and useful example: fitting data points with a function. Among the main features, the SciPy library contains:

- Integration (`scipy.integrate`): integrals, differential equations, etc ...
- Optimization (`scipy.optimize`): minimization, fits, etc ...
- Interpolation (`scipy.interpolate`): smoothing methods, etc ...
- Fourier Transforms (`scipy.fftpack`): spectral analysis, etc ...
- Signal Processing (`scipy.signal`): transfer functions, filtering, etc ...

- Linear Algebra (`scipy.linalg`): matrix operation, diagonalisation, determinant, etc ...
- Statistics (`scipy.stats`): random number, probability density function, cumulative distribution, etc ...

```
from scipy import optimize
from scipy import stats
```

Let's now show how to perform a fit of data with error bar using one particular function of `scipy.optimize`. First, we need to generate some data where we choose 20 measurements, with some noise of ~30% and an combined uncertainty of an absolute 0.1 uncertainty and 10% relative uncertainy:

```
Npoints, Nsampling = 20, 1000
xcont = np.linspace(-5.0, 3.5, Nsampling)
x = np.linspace(-5, 3.0, Npoints)
y = 2*(np.sin(x/2)**2 + np.random.random(Npoints)*0.3)
dy = np.sqrt(0.10**2 + (0.10*y)**2)
```

Then we need to define functions with which we want to fit our data, for example a degree 1 polynoms. The syntax has to be `func(x, *pars)`:

```
def pol1(x, p0, p1):
    return p0 + x*p1
```

The following lines actually perform the fit and return both the optimal parameters and the covariances for the dgree 1 polynom:

```
p, cov = optimize.curve_fit(pol1, x, y, sigma=dy)
```

One can then generalize the procedure by plotting the result of the fit for polynoms of several degrees, after having plotted the data. This is a good way to compare different models for the same data. First, we define an arbitrary degree polynom `plo_func()` and we *vectorize* it using `np.vectorize` so that it can accept NumPy arrays:

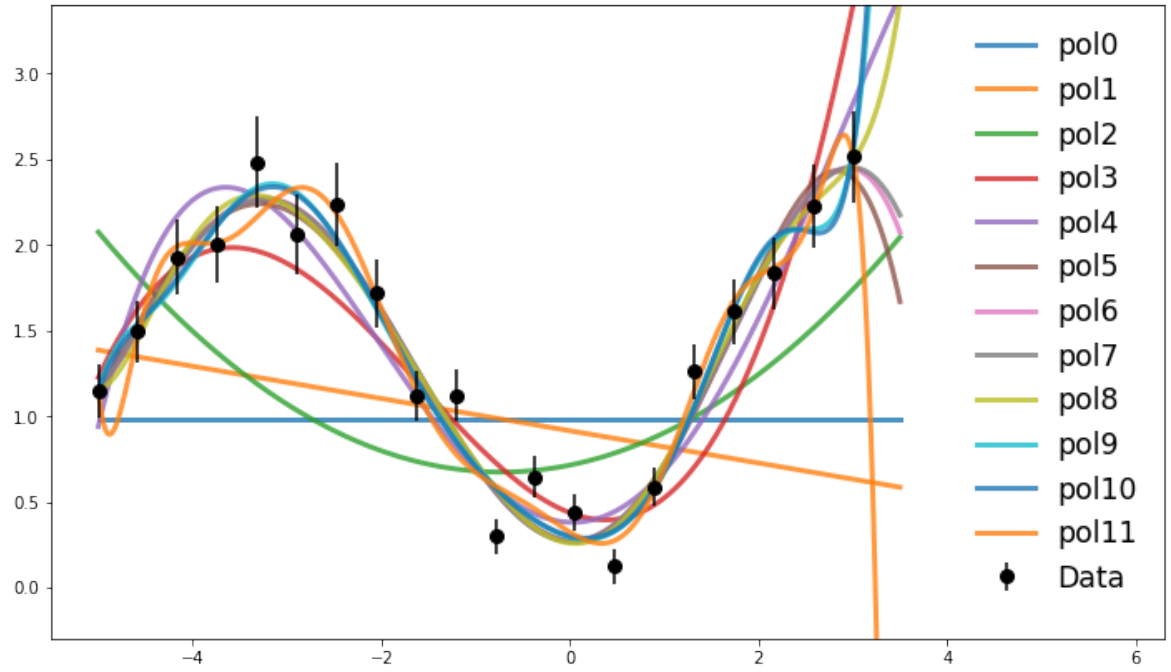
```
def pol_func(x, *coeff):
    a = np.array([coeff[i]*x**i for i in range(len(coeff))])
    return np.sum(a)

pol_func = np.vectorize(pol_func)
```

In the previous call for `optimize.curve_fit()`, we didn't use additional arguement. For this example, we need to specify at least the starting point of the parameters `p0` *because the number of paramter will be assessed using `len(p0)` (it's not known a priori since it is dynamically allocated)*. Other options can be specified, such as the miminum and maximum allowed values of parameters. Here is a wrapp-up function performing the fit for an arbitrary polynom degree:

```
def fit_polynom(degree):
    nPars = degree+1
    p0, pmin, pmax = [1.0]*nPars, [-10]*nPars, [10]*nPars
    fit_options = {'p0': p0, 'bounds': (pmin, pmax), 'check_finite': True}
    par, cov = optimize.curve_fit(pol_func, x, y, sigma=dy, **fit_options)
    return par, cov

degree_max = 12
```

The following code try every polynomial functions up to a degree `degree_max=`, perform the fit and overlay the the result for each together with the experimental data on the same figure:

```
# Figure for the result
fig = plt.figure(figsize=(12,7))

# Fitting & plotting
for d in np.arange(0, degree_max):
    par, cov = fit_polynom(d)
    plt.plot(xcont, pol_func(xcont, *par), label='pol{}'.format(d),
             linewidth=3, alpha=0.8)

# Plotting data
style = {'marker': 'o', 'color': 'black', 'markersize': 8,
         'linestyle': '', 'zorder': 10, 'label': 'Data'}
plt.errorbar(x, y, yerr=dy, **style)

# Plot cosmetics
plt.xlim(-5.5, 6.3)
plt.ylim(-0.3, 3.4)
plt.legend(frameon=False, fontsize='xx-large');
```



It is possible to quantify how well a given model explain the observations, computing what we call the *goodness of fit*. In a frequentist approach, this can be assessed by the fraction of pseudo-data coming from - in principle - repeating the exact same experiment, with to a worst agreement for a given model. The agreement can be quantified using $\chi^2 = \sum_{i=1}^{n} \frac{(y_i - f(x_i))^2}{\sigma_i^2}$ and its probability density function (PDF) directly gives access to the fraction of "worst pseudo-data" (by integrating the PDF from χ^2 to ∞). More precisely, one can use the cumulative distribution function (CDF) of χ^2 computed with n degrees of freedom, for instance `Npoins`, *i.e.* `len(x)`. More details can be found, for examble, in the statistics review of the Particle Data Group. The following two functions allow to compute the goodness of fit:

```
def get_chi2_nDOF(y, dy, yfit):
    r = (y-yfit)/dy
    return  np.sum(r**2), len(y)

def get_pvalue(chi2, nDOF):
    return 1-stats.chi2.cdf(chi2, df=nDOF)
```