

Short introduction to Python for Matlab users

Claus Führer, Numerical Analysis, Matematikcentrum

Najmeh Abiri, Computational Biology, Fysikum

Python Compact - Part 1

What do we cover in this introduction lecture?

1. [Preparation](#)
2. [Elementary Datatypes](#)
3. [Program Flow](#)
4. [Container Types](#)
5. [Functions](#)
6. [Arrays](#)
7. [Plotting](#)
8. [Exceptions](#)
9. [Training Tasks](#)

What is also interesting to know?

- Testing, Profiling
- Iterators

Preparation

Everywhere in this course: in files, in shells we start with

```
In [1]: from scipy import *  
        from matplotlib.pyplot import *
```

Tools you will need in this course:

- Ipython
- Spyder
- jupyter-notebook

Elementary datatypes

Numeric Types

```
In [2]: i = 1          # an integer
        x = 2.         # a float
        z = y = 3.e-8
        c = 1.-3       # automatic type conversion
        d = 1.+3.j     # a complex number
```

Elementary datatypes

Strings

```
In [3]: text = 'We learn Python'
        speed = 'fast'
        how = 'fast. ' if speed else 'slow. ' # note the conditioned assignment
        now = text + ' ' + how               # concatenation by "+"
        2 * now
```

```
Out[3]: 'We learn Python fast. We learn Python fast. '
```

Summary: Elementary Datatypes

- we saw integers, floats, complex numbers, Booleans and strings
- we saw different ways to assign values to a variable
- we saw concatenation of strings
- we saw `print()` and `type()`

Program Flow: Block commands

The flow is controlled by loops, conditional statements and functions

```
In [4]: for i in range(3):
        print(i)
        j = i**2
        print(j)
```

```
0
0
1
1
2
4
```

Mind the indentation!

Nested Loop:

```
In [5]: for i in range(5):  
        for j in range(i + 1):  
            print( (i,j), end = ' ' )  
        print('\n')      # Makes a new line
```

```
(0, 0)  
  
(1, 0) (1, 1)  
  
(2, 0) (2, 1) (2, 2)  
  
(3, 0) (3, 1) (3, 2) (3, 3)  
  
(4, 0) (4, 1) (4, 2) (4, 3) (4, 4)
```

Conditional statement

```
In [6]: b = False  
        if b :  
            j = 2 * j  
        else:  
            j = None  
        print(j)
```

```
None
```

Loop constructions: break, else

```
In [7]: j = 30  
        for i in range(100):  
            if i == j:  
                break  
        else:  
            raise Exception('j not found')  
        print('j found')
```

```
j found
```

Container types

Lists

```
In [8]: a = [1,2,'aha']  
        print(a)  
        b = [1,a]  
        a[0]  
        print(a[0])  
        print(b[1][2])
```

```
[1, 2, 'aha']  
1  
aha
```

```
In [9]: a+b
```

```
Out[9]: [1, 2, 'aha', 1, [1, 2, 'aha']]
```

```
In [10]: c = list(range(0,8))
          print(c[-1])
          print(c[-4:])
          print(c[0:2]) # Note the "hotel booking" rule.

7
[4, 5, 6, 7]
[0, 1]
```

List comprehension

```
In [11]: base_list = [5,9,22,38]

          new_list = [l**2+1 for l in base_list]

          other_list=[l+1 for l in base_list if l%2 == 0 ]

          print(new_list,end=3 * '\n')

          print(other_list)

[26, 82, 485, 1445]

[23, 39]
```

List Operations

note the *inplace* operations

```
In [12]: L=[1,2,3,29,-10]
          L.sort()
          print('sorted list L=', L)
          L.reverse()
          print('reversed list L=',L)
          L.append(70)
          print('extended list L=', L)
          L.pop()
          print('last element removed L=',L)

sorted list L= [-10, 1, 2, 3, 29]
reversed list L= [29, 3, 2, 1, -10]
extended list L= [29, 3, 2, 1, -10, 70]
last element removed L= [29, 3, 2, 1, -10]
```

Summary

- Lists and lists of lists
- indexing and slices
- negative indexing
- 'Hotel'booking rule
- List comprehension
- list(range(...))

Dictionaries

```
In [13]: truck={'bodies':['frWheel','reWheel','Chassis','Cabine','Load'],
              'total length':15,'total weight':30000}
```

```
In [14]: truck.keys()
```

```
Out[14]: dict_keys(['total length', 'bodies', 'total weight'])
```

Tuples

```
In [15]: a=2,3
         print(a)
         b=('anna',23)
         print(b)
         print(a+b)
         print(b[1])

(2, 3)
('anna', 23)
(2, 3, 'anna', 23)
23
```

A tuple is an immutable list. What means immutable?

```
In [16]: b[1]=-2
```

```
-----
TypeError                                 Traceback (most recent call last)
<ipython-input-16-74c169ca2cd8> in <module>()
----> 1 b[1]=-2

TypeError: 'tuple' object does not support item assignment
```

Warning: Changing in sub list has side effects!

```
In [17]: a=[1,2,3]
         b=[4,5,a]
         print(b)
         a[2]=-300
         print(b)

[4, 5, [1, 2, 3]]
[4, 5, [1, 2, -300]]
```

```
In [18]: b=tuple(b)
         print(b)
         a[2]=70
         print(b)

(4, 5, [1, 2, -300])
(4, 5, [1, 2, 70])
```

```
In [19]: b=[1,2]
         a=b
         b[1]=-234
         print(a[1])

-234
```

Copy removes these side effects

```
In [20]: a=b.copy()
         b[1]=1
         a[1]
```

```
Out[20]: -234
```

Unpacking , Packing

```
In [21]: a=1
         b=b
         c,d=a,b
```

or even

```
In [22]: b,a = a,b # the swapping trick
```

Summary:

- lists, list indexing, slices
- dictionaries, keys, values, items
- tuples, immutable
- copy
- packing, unpacking

Functions

```
In [23]: def my_func(p1, p2, p3 = None):
         a = p1*p2 + p3 if p3 != None else p1*p2
         b = p1**2
         return a, b
```

```
In [24]: r1, r2 = my_func(1, 2, 5)
```

Lambda Functions: Defining functions on the fly

```
In [25]: f = lambda x: sin(x) * cos(x)
         f(pi)
```

```
Out[25]: -1.2246467991473532e-16
```

Passing arguments

- by position
- by key
- when mixing: **always** first those by position

```
In [26]: def my_func(p1, p2 ,p3):  
         pass                                # a statement which does nothing, just to pleas  
         e the syntax
```

```
In [27]: my_func(2, 3, 25)  
         my_func(p3 = 25, p1 = 2, p2 = 3)    # note, how default values are defined  
         my_func(2, 3, p3 = 25)
```

Starred Arguments

You can expand a list to form positional arguments and a dictionary to form keyword arguments of a function

```
In [28]: li = [2, 3, 25]  
         di={'p1':2, 'p2':3, 'p3':25}  
         my_func(*li)  
         my_func(**di)
```

Scope of a variable

```
In [29]: a = 3; l=[1, 2, 3]  
         def func1(b):  
             return a * b    # a is a global variable  
  
         def func2(b):  
             a = 17          # a is a local variable  
             return a * b
```

```
In [30]: print(func1(3))  
         a = -10            # Be aware of side effects  
         print(func2(3))  
         print(a)  
  
9  
51  
-10
```

Arrays and Linear Algebra

```
In [31]: from scipy import *  
         from scipy.linalg import *
```

a vector ...

```
In [32]: v = array([1.,2.,3.])  
         w = array([1.,0.,1])  
         v.reshape((3,))
```

```
Out[32]: array([1., 2., 3.])
```

Dot product, cross product, outer product

```
In [33]: a = v @ w # or a=dot(v,w)
A = outer(v,w)
u = cross(v,w)
```

Filling vectors

```
In [34]: v = linspace(0,3,10) # filling with equidistant floats
i = arange(0,3) # filling with integers
o = ones((3,))
z = zeros((3,))
```

Matrices are two dimensional arrays

```
In [35]: A = array([[1.,2.,7],[7,9,13],[-1,2,6.]])
A.shape
```

```
Out[35]: (3, 3)
```

a particular element is addressed by a **dubble index**

```
In [36]: trace = A[0,0] + A[1,1] + A[2,2]
print(trace)
```

```
16.0
```

the same but with list comprehension:

```
In [37]: trace = sum( [A[i,i] for i in range(A.shape[0])] )
print(trace)
```

```
16.0
```

Filling 2D arrays

```
In [38]: I = eye(3)
Z = zeros((3,3)) # the argument is a tuple
Z = zeros_like(I)
F = 5. * ones((3,3)) # the argument is a tuple
R = rand(3,3) # the argument is *not* a tuple
a = pi/3
Rot = array([[cos(a), sin(a)],
             [-sin(a), cos(a)]])
```

Operations on arrays


```
In [39]: F @ Z
v = array([3,4])
vr = Rot @ v

from scipy.linalg import solve

abs(solve(Rot,vr) - v) < 1.e-8 # mind round-off

Out[39]: array([ True,  True])
```

Views

```
In [40]: f = arange(0, 10)
F = f.reshape(2, 5)
FT = F.T # the transpose
F[-1,-1] = 17
print(FT[-1, -1], f[-1]) # everything affected

17 17
```

Universal functions

Many functions operate directly on arrays -- componentwise

```
In [41]: sin(F)
abs(F)

Out[41]: array([[ 0,  1,  2,  3,  4],
               [ 5,  6,  7,  8, 17]])
```

Addition, multiplication, division are **elementwise** operations on arrays

```
In [42]: print(F)
print(F + F)
print(F * F)

[[ 0  1  2  3  4]
 [ 5  6  7  8 17]]
[[ 0  2  4  6  8]
 [10 12 14 16 34]]
[[ 0  1  4  9 16]
 [ 25 36 49 64 289]]
```

Array Examples

A projection matrix P and its eigenvalues and eigenvectors

$$P = I - \frac{vv^T}{v^T v}$$

```
In [43]: from scipy.linalg import *

v = array([1., 0., 0., 1., 5.])
P = eye(v.shape[0]) - outer(v, v)/(v @ v)

evalue, evector = eig(P)
print('P v =', P @ v, end=2*'\n')
print('Eigenvalues: ', evalue,
      'Eigenvectors: ', evector, sep=2*'\n')

P v = [2.22044605e-16  0.00000000e+00  0.00000000e+00  2.22044605e-16
 0.00000000e+00]

Eigenvalues:

[1.+0.j 0.+0.j 1.+0.j 1.+0.j 1.+0.j]

Eigenvectors:

[[ 0.98130676 -0.19245009  0.22187058  0.          0.          ]
 [ 0.          0.          0.          1.          0.          ]
 [ 0.          0.          0.          0.          1.          ]
 [-0.03774257 -0.19245009 -0.9637218  0.          0.          ]
 [-0.18871284 -0.96225045  0.14837025  0.          0.          ]]

In [44]: for i in range(evalue.shape[0]):
          if allclose(evector[:,i], -v/norm(v,2)) or allclose(evector[:,i], -v/norm
(v,2)):
              print('v is an eigenvector of the projection matrix corresponding to
eigenvalue ', evalue[i].real)

v is an eigenvector of the projection matrix corresponding to eigenvalue 0.0
```

Boolean Arrays

```
In [45]: A = rand(4,4)
small = abs(A) < 0.5

C = A.copy()
C[small] = 0
print(A, C, small, sep=2*'\n')

[[0.79513052 0.2886361  0.09312346 0.39255937]
 [0.36544745 0.09243608 0.46101068 0.18904672]
 [0.03383226 0.39205689 0.04890219 0.57672891]
 [0.42758111 0.02100887 0.20230901 0.3542879 ]]

[[0.79513052 0.          0.          0.          ]
 [0.          0.          0.          0.          ]
 [0.          0.          0.          0.57672891]
 [0.          0.          0.          0.          ]]

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

Continuation from eigenvalue example above

(note the decorator `vectorize` to make a universal function)

```
In [46]: @vectorize
def near(x, y, eps = 1.e-8):
    return (y-eps) < x.real < (y+eps) and -eps < x.imag < eps

if (near(abs(evalue),1) + near(evalue,0)).all():
    print('All eigenvalues of a symmetric projection matrix are either +- 1
or 0')
```

All eigenvalues of a symmetric projection matrix are either +- 1 or 0

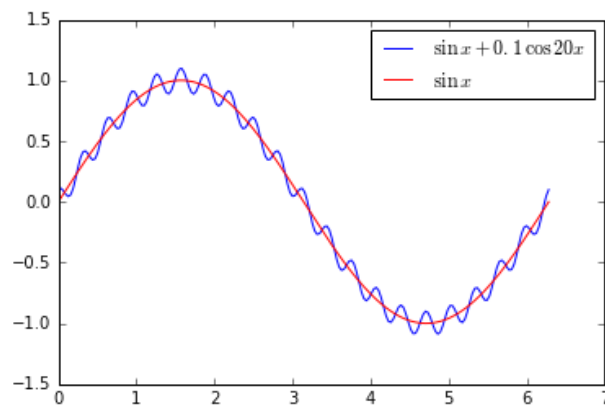
Elementary Plotting

write in IPython as one of the first commands `%matplotlib` when you want to want the plots to be embedded in the current session.

```
In [47]: %matplotlib inline
```

```
In [48]: x = linspace(0, 2 * pi, 200)
plot(x, sin(x) + 0.1*cos(20*x), label='$\sin\,x+0.1\,\cos\,20x$')
plot(x, sin(x), 'r', label='$\sin\,x$')
legend(loc = 'best')
```

```
Out[48]: <matplotlib.legend.Legend at 0x7f7f88d089b0>
```



Exceptions

```
In [49]: x_list = [1, 2, 3, 0, 23, 65]
y = []

for x in x_list:
    try:
        y.append(1./x)
    except ZeroDivisionError:
        y.append('no inverse')

print(x_list, y, sep='\n')

[1, 2, 3, 0, 23, 65]
[1.0, 0.5, 0.3333333333333333, 'no inverse', 0.043478260869565216, 0.01538461
5384615385]
```

Important Exception Types

- IndexError
- ValueError
- NameError
- ZeroDivisionError
- SyntaxError

... or just unspecified.

Task:

1. Generate a vector with random numbers. Check all its elements and count the number of sign changes.
2. write a function which takes an axis-label ('x', 'y', 'z') and an angle as input and returns a rotation matrix, e.g., `rot3D(2*pi, 'x')` should return a 3D rotation matrix about the 'x'-axis.
3. Test if the product of three rotation matrices is orthogonal and has determinant 1
4. Compute the eigenvalues of this composed rotation matrix and plot them as small stars in the complex plane.