

## Exercise 00

### Introduction to Linux and Python

For next week you should do some practice with the Linux commands and solve three exercises with Python (+NumPy). At the end of each line you can find [between square brackets] the reference to the "Linux and Python" manual with the functions necessary.

Send your protocol as a single pdf file to [stevan.aleksic@fu-berlin.de](mailto:stevan.aleksic@fu-berlin.de) by 4<sup>th</sup> May 10 a.m. This first session of exercises will be corrected, but not evaluated.

## 1 Linux I

1. Create a folder called "TCexercises" in your home directory. [1.3]
2. Enter in the folder and create a subdirectory "exercise00". [1.3]
3. Create a Python file for each exercise. [1.4.1]

## 2 Python

1. (a) Create the following matrix  $5 \times 5$  (2 dimensional NumPy array):

$$M = \begin{pmatrix} 17 & 24 & 1 & 8 & 15 \\ 23 & 5 & 7 & 14 & 16 \\ 4 & 6 & 13 & 20 & 22 \\ 10 & 12 & 19 & 21 & 3 \\ 11 & 18 & 25 & 2 & 9 \end{pmatrix}$$

What is the sum of the rows? What is the sum of the columns? [2.4.1, 2.4.5]

- (b) Exchange the first row with the first column. [2.4.3]
  - (c) Create a vector (1d NumPy array)  $\vec{u} = (1, 2, 3, 4, 5)$  and sum each element of the first column with each element of the vector. [2.4.3, 2.4.4]
  - (d) Multiply by 2 the last two elements of the first and of the second column. [2.4.3, 2.4.4]
  - (e) Replace by 3 all the elements of the matrix greater than 15. [2.4.3]
  - (f) Compute the trace (sum of the elements of the diagonal) of the matrix  $M$ . There are many ways to compute the trace of a matrix, try the following:
    - i. Implement a for loop to extract all the elements of the diagonal. [2.6.1]
    - ii. Use the function `diagonal()` to extract all the elements of the diagonal. [2.4.5]
    - iii. Use the function `np.trace()` to check your previous results. [2.4.5]
  - (g) Find the eigenvalues and the eigenvectors of the matrix  $M$  and verify the relation  $M\vec{v} = \lambda\vec{v}$ . [2.4.5, 2.4.4]
  - (h) Create a second  $5 \times 5$  matrix  $A$  of random integer numbers (from a uniform distribution) in the interval  $[0,9]$ . [2.4.2, 2.4.5]
  - (i) Compute the determinant of the matrices and verify the relation  $\det(M \cdot A \cdot M^{-1}) = \det(M) \cdot \det(A) \cdot \det(M^{-1})$ . [2.4.5, 2.4.4]
2. (a) In this second exercise, you will practise with the plot functions, so first of all, import the matplotlib.  
Generate a vector  $x$  of  $N = 10000$  equally spaced points in the interval  $[-50, 50]$  and compute  $y_1 = \frac{\sin(x)}{x}$  and  $y_2 = \left| \frac{\sin(x)}{x} \right|$ . [2.4.2, 2.4.6]
  - (b) plot  $y_1$  and  $y_2$  using two different colors and two different line styles [2.5].
  - (c) Reduce the x-axis to  $[-4\pi, 4\pi]$  and set ticks only for  $-4\pi, -2\pi, 0, 2\pi, 4\pi$ . [2.5]
  - (d) Add title, x-label, y-label and legend to the graph and save it in the EPS format. [2.5]
  - (e) Compute  $y_3 = \exp(x)$  with  $x \in \mathbb{R}$  and  $y_4 = \log(x)$  with  $x \in \mathbb{R}^+$ . [2.4.3, 2.4.6]

- (f) Plot in a new figure  $y_1$  and  $y_2$  using two different colors and two different line styles. [2.5]
- (g) Reduce the y-axis to  $[-3, 2]$ . [2.5]
- (h) Add title, x-label, y-label and legend to the graph and save it in EPS format. [2.5]
3. (a) Generate an array  $P$  of size  $N \times 3$ , with  $N = 1000$  random numbers (from a uniform distribution). Each row of the array represents the position in the 3d space of a particle. [2.4.1]
- (b) Create a Python file where to define a new function (you can also use the file `userfunctions.py` created during the tutorial) that generates a symmetric matrix  $d$  of size  $N \times N$ , where each element  $d_{ij}$  is the euclidean distance between each pair of points  $(i, j)$ :

$$d_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$$

There are many methods to implement this function, you should implement the following three.

- i. The first method should use two for loops. [2.6.1]

```
def distance1(P):    #P is the array $Nx3$
    x = P[:,0]      #we store each column in a vector
    y = ...
    ...
    for i in range(N):
        for j in range(N):
            d[i,j] = np.sqrt((x[i] - x[j])**2 + ... )
    ...
```

- ii. Inside the double for loop, we have computed the difference between each pair of elements of the vectors  $x$ ,  $y$  and  $z$ . This method is quite slow, but we can improve it vectorizing the algorithm.

We can create the same matrices  $x_i - x_j$  doing a difference between the "row vector"  $x$  and the "column vector"  $x$ . To do this, we need the function `np.newaxis` that adds "a new dimension to the array". Basically it just transforms a row vector in a column vector.

If  $X$  is a vector,  $X[:,\text{np.newaxis}]-X$  is a matrix  $M$  where each element  $M_{ij}$  is  $X_i - X_j$ . You should generate these matrices for each dimension and use them to compute the distance with the "elementwise operations". [2.4.4]

```
def distance2(P):    #P is the array $Nx3$
    x = P[:,0]
    y = ...
    ...
    dx = x[:,np.newaxis]-x #dx is a matrix NxN
    ...
    d = np.sqrt(dx**2 + ... )
    ...
```

- iii. Import from SciPy the function `distance` and check your previous results:

```
import scipy.spatial.distance as dist

d = dist.cdist(x,x)
```

To measure the execution time, you have to use the function `time` as follows:

```
import time

t_begin = time.time()
#instructions...
t_end = time.time()

print "Elapsed time: ", t_end - t_begin
```

Plot the results

### 3 Linux II

You can try the following linux commands with the three python files.

1. List the created files and check their dimension. [1.5.1]
2. Create a folder "backup" and copy all the files in it. [1.5.2]
3. Enter in the folder "backup" and delete the files 00-1.m and 00-2.m. [1.3, 1.5.2]
4. Go back in the up directory and delete the full directory "backup". [1.3, 1.5.2]
5. Create a TAR archive of the exercise folder. [1.6]