Exercise 05

Please hand in your solution before **Thursday, 01 Dec, 8.00 a.m.**

1 Phython exercise 10 points

1.1

Import the file "data_matrix.txt" and save its content in a numpy matrix A.

1.2

Create a function calculating the average of a given array of floats.

1.3

Use this function to calculate the average of each column of the matrix A.
Create a new matrix B, by subtracting the elements of each column by the respective average.

1.4

Save the matrix B to a file called `"data_b.txt"` (save floats with 14 decimal places).

1.5

Save the averages of each column to a file called `"data_averages.txt"`. The file should have one line (not one column) containing the averages of the respective columns.

1.6

Reduce the original data matrix by calculating the average of 10 consecutive rows for each column, resulting in a 10x10 matrix (since the original matrix has 100 rows and 10 columns).
Save this matrix to a file called `"data_reduced.txt"`.

2 Commutators 10 points

Evaluate the following commutators by applying them to a function $f(x)$

- $\left[\left(\frac{d}{dx}\right) - x, \left(\frac{d}{dx}\right) + x, \right]$
- $\left[\frac{d}{dx}, x^2\right]$
- $\left[\frac{d^2}{dx^2}, x\right]$
- $\left[x\frac{\partial}{\partial y}, y\right]$ (apply to $f(x, y)$)

3 Expectation value 10 points

Consider a wave function, written as superposition of eigenfunctions of a particle in a 1D box:

$$\psi(x,t) = \sum_{n=1}^{\infty} c_n \phi_n(x) \tag{1}$$

with eigenfuctions:

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) \tag{2}$$

and energy eigenvalues:

$$E_n = \frac{\hbar^2}{2m}k^2 = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{L^2} \tag{3}$$

For this kind of system the coefficents c_n are defined as:

$$c_n = \begin{cases} \frac{1}{\sqrt{2}} & n = 2 \\ 0 & n = 4, 6, 8, ... \\ \frac{4\sqrt{2}(-1)^{\frac{n+1}{2}}}{(n-2)(n+2)\pi} & n = 1, 3, 5 \end{cases} \tag{4}$$

- Calculate analytically the energy expectation value $\langle E \rangle$.
- Write a program which models the outcome of an energy measurement, drawing random numbers from the distribution which is given by:

$$|\psi(x,t)|^2 = |c_n|^2$$

- Calculate the average of the energy measurements in python. Compare the average of your measurements to the exact expectation value.
- Construct a histogram of your measurement series and compare the histogram to the expansion coefficients of $\psi(x,t)$.

Use the following parameters:

$$x_0 = 0; \qquad \Delta x = 0.01; \qquad L = 10; \qquad \hbar = 1; \qquad m = 1$$

Extract a random number from a given distribution The following PYTHON code implements the *probability integral transform*. Such method gives us a simple way to transform a random number extracted from a given distribution (e.g. the uniform distribution) into a number extracted from any other distribution P:

```
import numpy as np

ncoefs = 10                # Number of coefficients
nexps = 1000               # Number of experiments
cn = np.zeros((ncoefs))    # Create Coefficent vector

for n in range(1,ncoefs+1):
   #Define here the coefficients cn

#Prob. density function:
P = cn**2

#The first element has to be 0
P = np.append([0], P)

#Cumulative sum to get the cumulative density distribution
cP = np.cumsum(P)

#Generate nexps experiments
a = np.random.uniform(0,1,(nexps))

#Array where to store the new distribution
b = np.zeros(nexps)

for n in range(nexps):
   b[n] = np.sum(a[n]>cP) - 1

b = b.astype(int)
```

The vector `a` contains 1000 float numbers between 0 and 1, drawn from the uniform distribution. The vector `b` contains 1000 integer numbers between 0 and 9, drawn from the distribution P. Each element of `b`, basically represents the outcome of an experiment. For example if `b[0]=5`, it means that during the first experiment, the contribution to the wave function $\psi(x,t)$ came only from the eigenfunction $\phi_6(x)$ (be careful to indexing!). Thus, the energy of the first experiment would be the eigenvalue E_6. You can now construct a vector containing the energy of each experiment. The arithmetic average of this vector is approximately equal to the analytical value $\langle E \rangle$.