

7. Assignment

Complex Systems for Bioinformaticians

SS 2025

Deadline: June 10, 12:00 (**before** the lecture)

The homework should be worked out individually, or in groups of 2 students. Pen & paper exercises should be handed at the designated deadline. Each solution sheet must contain the names and 'Matrikulationsnummer' of all group members and the name of the group. The name of the group must include the last names of the group members, in alphabetic order, e.g. "AlbertRamakrishnanRastapopoulos", for group members Mandy Albert, Mike Ramakrishnan, and Marcus Rastapopoulos. Please staple all sheets.

Programming exercises must be submitted via Whiteboard.

Homework 1 (Drift equations (pen & paper), 2 points)

For the quad-well potential

$$V(\mathbf{z}) = (|z_1| - 1)^2 + (|z_2| - 1)^2, \quad (1)$$

derive the ODEs describing the drift in z_1 , z_2 direction.

Homework 2 (Programming, 2 + 1points)

Perform a random walk on a two-dimensional (z_1, z_2) plane using the Euler-Maryama algorithm.

a) (**to be uploaded via Whiteboard**) Write a program implementing this model with plane size $[-2, 2]$ in each dimension, noise level $\sigma = 0.3$, clipped boundaries and time step $\tau = 1$. Consider a single particle, which is initially placed at random (uniform) on the plane. Set the random 'seed' to the value given in the Input.txt file, i.e.:

```
seed = int(np.loadtxt('Input.txt'))
```

```
np.random.seed(seed)
```

Simulate until $T_{end} = 100$ and save the location of your particle at each time step into file 'Task2Traj.txt' in comma-separated format using two digits after the comma. Name your code 'Ex2a.py' and upload via whiteboard.

b) (**to be uploaded via Whiteboard**) Change your program, such that it generates an mp4 movie and writes it into the file Task2bTraj.mp4. Name your code 'Ex2b.py' and upload via whiteboard.

Homework 3 (Programming, 1 + 2points)

Extend your program from Task 2, by adding a drift term that corresponds to your quad-well potential from Task 1, with weights $\sigma_{drift} = 0.1$ and $\sigma_{random} = 0.3$.

a) (**to be uploaded via Whiteboard**) Consider a single particle, which is initially placed at random (uniform) on the plane. Set the random 'seed' to the value given in the Input.txt file. Simulate until $T_{end} = 100$ and save the location of your particle at each time step into file 'Task3Traj.txt' in comma-separated format using two digits after the comma. Name your code 'Ex3a.py' and upload via whiteboard.

b) (**to be uploaded via Whiteboard, and plotted**) Simulate 100 particles simultaneously, assign them four different types (e.g. 'colors': black, green, blue, red), whereby the types are assigned depending in which quadrant the particles are initially positioned, with $(0, \cdot)$, $(\cdot, 0)$ separating the plane into four quadrants.

- Let your program generate an mp4 movie and write it into the file Task3bTraj.mp4. Name your code 'Ex3b.py' and upload via whiteboard.

- Plot the shannon entropy in each quadrant as a function of time. Print and discuss what happens when you decrease σ_{random} .

Homework 4 (Programming – Schelling model, 2points)

Write a program implementing the Schelling segregation model on a plane of size $[0, 1]$ in each dimension. Initialize 300 agents with random locations (uniform) on the plane. Assign each agent one of two possible types (for example 'rich' vs. 'poor'; or 'AFD' vs. 'no thanks'; [whatever you like]) at random. Use a neighbourhood radius $r^2 = 0.1$ and randomly (uniform) draw a new location for an agent if $\leq 50\%$ of the agent's neighbours are not his/hers type. Update 10 random agents at a time (that is check their neighbourhood and eventually move them) and perform 300 time steps in total.

Let your program generate an mp4 movie and write it into the file Task4Traj.mp4. Name your code 'Ex4.py' and upload via whiteboard.

Good luck!