HW 2

Homework Assignment 2
for the course FFR120/FIM750 in HT24

Instructions
HW2 consists of four exercises. For each exercise, the corresponding chapter is indicated.
Each exercise has a score of 2.5 points.
The maximum number of points for HW2 is 10.
The assessment of your solution of HW2 happens during the HW2 correction session on Wednesday, 20 November.

Remember to:
1. Register to the HW2 correction by Monday 18 November 23:59 *at the latest*. After that time, it won't be possible to get a slot for the HW2 correction.
2. Submit your solution for the HW2 to Canvas by Tuesday 19 November 23:59 *at the latest*. The solution must be in pdf format and should contain figures and code.

On correction day:
1. Arrive to the correction room about 10-20 minutes before your registered time slot.
2. Prepare the solution report ready on your computer, so the assessment can start without further delays.
3. Bring along a valid ID.

Chapter 05: Brownian Dynamics

Exercise 1. [Score: 2.5 pt] **Brownian particle in a harmonic trap.**

A Brownian particle (radius R, neglect the mass) immerse in water (temperature T, viscosity η) is held in an optical trap with stiffness k_x, k_y. Consider a pure 2d motion. The finite difference equations describing its trajectory are:

$$\begin{cases} x_i &= x_{i-1} - \dfrac{k_x}{\gamma} x_{i-1}\Delta t + \sqrt{2D\Delta t}\, w_{x,i} \\ y_i &= y_{i-1} - \dfrac{k_y}{\gamma} y_{i-1}\Delta t + \sqrt{2D\Delta t}\, w_{y,i} \end{cases}$$

Use the following values:

k_B	T	η	R	k_x	k_y
$1.380 \times 10^{-23}\,\mathrm{J/K}$	$300\,\mathrm{K}$	$1 \times 10^{-3}\,\mathrm{N\,s/m^2}$	$1 \times 10^{-6}\,\mathrm{m}$	$1 \times 10^{-6}\,\mathrm{N/m}$	$9 \times 10^{-6}\,\mathrm{N/m}$

and set

$$\gamma = 6\pi\eta R, \qquad D = \frac{k_B T}{\gamma}$$

The noise terms $w_{x,i}$ and $w_{y,i}$ are to be independently generated from Gaussian random distribution with mean 0 and standard deviation 1.
The motion in the trap has a characteristic relaxation time τ_{trap}

$$\tau_{\text{trap}} = \frac{\gamma}{k}$$

To simulate the system, choose the time step Δt such that:

$$\Delta t \ll \tau_{\text{trap}}$$

Generate the trajectory starting from the initial conditions $x_0 = 0$, $y_0 = 0$ and for a duration $t_{\text{tot}} = 30\,\mathrm{s}$
Address the following points:

Q1 - Calculate $\tau_{\text{trap}} = \gamma/k$. *[Remember you have two different stiffnesses here (k_x and k_y)...]*. Choose a value for Δt for the simulation. Write it down. Motivate your choice.

P1 - Plot the trajectory of the disk in the Cartesian plane.

P2 - Plot the *probability distribution* of the positions in x and in y (two separate histograms: one for x and one for y). Compare each case with the expected Boltzmann distribution:

$$\text{Probability Distribution} \propto \exp\left(-\frac{U}{k_B T}\right),$$

where you set $U(x) = \dfrac{1}{2} k_x\, x^2$ for the x positions and $U(y) = \dfrac{1}{2} k_y\, y^2$ for the y positions.

Q2 - Calculate the *variance* of the x and y position: $\sigma_x^2 = \langle x^2 \rangle$ and $\sigma_y^2 = \langle y^2 \rangle$. Which one has the larger variance? x or y? Check and compare the theoretical value for the variance in a harmonic trap: $\sigma^2 = \frac{k_B T}{k}$

P3 - Calculate and plot the *position autocorrelation function* $C_x(t) = \langle x(t+t')x(t') \rangle$ and $C_y(t) = \langle y(t+t')y(t') \rangle$. In the finite difference formalism, you can calculate $C_x(t)$ and $C_y(t)$ as follows:

$$C_x(n\Delta t) = \frac{1}{N-n} \sum_{i=1}^{N-n} x_{i+n}\, x_i \qquad \text{and} \qquad C_y(n\Delta t) = \frac{1}{N-n} \sum_{i=1}^{N-n} y_{i+n}\, y_i$$

The position autocorrelation function indicates how long it takes for the particle to forget its current location. Compare with the theoretical value for a harmonic trapping potential:

$$C(t) = \frac{k_B T}{k} \exp\left(-\frac{k\,t}{\gamma}\right).$$

Chapter 06: Anomalous Diffusion

Exercise 2. [Score: **2.5** pt] **Simulating a Lévy walk**

A Lévy walk (LW) trajectory with anomalous diffusion exponent α can be simulated with the following steps:

1. Choose a constant velocity v.
2. Generate the walking times $\delta t_i = r_i^{-1/(3-\alpha)}$ where r_i is a uniform random number between 0 and 1.
3. Calculate the positions:

case 1-d: Describe your system with the only variable x. Set:

$$x_{i+1} = x_i + w_i\, v\, \delta t_i$$

where w_i is a random number that represents the direction of the random movement ($w_i \in \{-1, 1\}$).

case 2-d: Describe your system with the variables x, y, ϕ, with ϕ the instantaneous orientation (direction of the velocity). Set:

$$\begin{cases} \phi_{i+1} &=& \phi_i + w_i \\ x_{i+1} &=& x_i + v\, \cos\phi_i\, \delta t_i \\ y_{i+1} &=& y_i + v\, \sin\phi_i\, \delta t_i \end{cases} \tag{1}$$

where w_i is a random number that represents the direction of the random movement ($w_i \in \{-1, 1\}$).

4. Calculate the corresponding times as the cumulative sum of δt, i.e., $t_i = \sum_{k=1}^{i} \delta t_k$.
5. Regularize the trajectory (see definition in the book, Chapter 6, page 6-4, and jupyter notebook shared on Canvas).

This model can only generate anomalous diffusion trajectories that are superdiffusive ($\alpha > 1$) or diffusive ($\alpha = 1$). For this exercise, we focus on $\alpha = 2$.

P1 - Generate five different LW trajectories in **one** dimension for $\alpha = 2$, $v = 1$. Plot them on the same plot.

P2 - Generate five more in **two** dimensions for $\alpha = 2$, $v = 1$. Plot them on the same plot.

P3 - Calculate and plot the eMSD and tMSD for a 1-dimensional LW with $\alpha = 2$. Follow the same method presented in class (see Lecture_06_AD jupyter notebook uploaded on Canvas > Files).

For a comparison, refer also to Fig. 6.6 in the book.

Chapter 07: Multiplicative Noise

Exercise 3. [Score: **2.5** pt] **Particle in a box with** $\sigma(x) = \sigma_0\ \exp\left(-\frac{x^2}{2\ w_0^2}\right)$

In this exercise, we will simulate a particle in a 1-dimensional box of length L centered in 0 (i.e., the particle position x is in the interval $[-L/2, L/2]$) and with reflective boundary conditions, as we have done at lecture. The initial position of the particle is x_0. See Lecture_07_MN jupyter notebook uploaded on Canvas > Files. Here, we will use the following dependence for the standard deviation of the position-dependent (i.e., multiplicative) noise $\sigma(x)$:

$$\sigma(x) = \sigma_0 \ \exp\left(-\frac{x^2}{2\ w_0^2}\right).$$

As illustrated in class, the trajectory according to the integration convention α is:

$$x_{j+1} = x_j + \underbrace{\alpha\sigma(x_j)\frac{\mathrm{d}\sigma(x_j)}{\mathrm{d}x}\,\Delta t}_{\text{noise-induced drift}} + \sigma(x_j)\sqrt{\Delta t}\,w_i. \tag{2}$$

For this exercise w_i comes from a Gaussian distribution with mean 0 and standard deviation 1.
Use the following values:

Δt	t_0	σ_0	L	w_0	x_0
1	100	1	100	25	0

P1 - Plot the dependence for the term $s(x) = \sigma(x)\frac{\mathrm{d}\sigma(x)}{\mathrm{d}x}$:

$$s(x) = -x\left(\frac{\sigma_0}{w_0}\right)^2 \exp\left(-\frac{x^2}{w_0^2}\right)$$

for $x \in [-L/2, L/2]$

P2 - Simulate the system (use Eq. 2) initially according to the Itô convention ($\alpha = 0$). Plot the distribution of the final point after t_0, $5\,t_0$, $10\,t_0$, $25\,t_0$, $50\,t_0$, $100\,t_0$.

P3 - Simulate the system initially according to the Stratonovich convention ($\alpha = 0.5$). Plot the distribution of the final point after t_0, $5\,t_0$, $10\,t_0$, $25\,t_0$, $50\,t_0$, $100\,t_0$.

P4 - Simulate the system initially according to the anti-Itô convention ($\alpha = 1$). Plot the distribution of the final point after t_0, $5\,t_0$, $10\,t_0$, $25\,t_0$, $50\,t_0$, $100\,t_0$.

Q1 - Comment your plots: are the distribution of the final points symmetrical? Why or why not?

Chapter 08: The Vicsek Model

Exercise 4. [Score: **2.5** pt] **Two subpopulations.**

Simulate the Vicsek model, as shown in class. Set a number of particle equal to $N = 200$. Start from a random configuration (i.e., random position and orientation). Use periodic boundary conditions. The side of the squared arena is L. The speed of each particle is v. The noise parameter affecting the orientation is η. The flocking radius is R_f. Simulate the system according to the following parameters

Δt	L	η	v	R_f
1	100	0.01	1	2

Task 1: Let the system evolve for at least $T = 6000$ time steps.

P1 - Plot the configuration at $t = 0\,\Delta t$, $2000\,\Delta t$, $4000\,\Delta t$, $6000\,\Delta t$. When plotting, include also the particles orientation.

P2 - Calculate and plot global alignment coefficient ψ and global clustering coefficient c as a function of the time step.

Task 2: Simulate a Vicsek model with two subpopulation of particles. Set a number of particle equal to $N = 200$.

- Half of the particles will behave like in task 1.
- The other half of the particles will instead feel more noise on their orientation: instead of $\eta = 0.01$, they will behave accordingly to $\boxed{\eta_\mathrm{mod} = 0.3}$.

Let the system evolve for at least $T = 6000$ time steps.

P3 - Plot the configuration at $t = 0\,\Delta t$, $2000\,\Delta t$, $4000\,\Delta t$, $6000\,\Delta t$. When plotting, include also the particles orientation. Plot the two subpopulations of particles with a different color.

P4 - Calculate and plot global alignment coefficient ψ and global clustering coefficient c as a function of the time step.

Q1 - Inspecting the animation of the simulation and the plot of ψ and c in time: what is the effect of having a population with two distinct traits?