Diffusive and Stochastic Processes Programming assignment 2024

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- The programming assignment will count for 20% of the final grade.
- You need to do the assignment by yourself alone.
- Deadline for this assignment is 14 June (Fri) 2024 noon. Submission of your result should be done through the absalon assignment page.
- You can upload one main file in PDF, plus as many appendixes files as you like in any format. For the main file, make plots asked for in the assignment with clear labels so that I can understand what is plotted. When it is asked to calculate a certain quantity, state the value you have obtained clearly. You should also submit the codes as separate files so that I can run them. Make sure that the uploaded files are readable and executable as it is. If you use Jupyter notebook, you can submit the PDF version of it as the main file, and the ipynb file as the code.
- If you add more than what is asked in the assignment in your answer, it does not affect the grade.
- If you have a question about formulation of the problem (e.g., you think there is a mistake in the formulation that prevents you from solving it), write to Namiko an e-mail (mitarai@nbi.ku.dk). TA will not answer any questions regarding this assignment.
- When X is a stochastic variable and $f(X)$ is a function of X, $\langle f(X)\rangle$ means the ensemble average of $f(X)$.
- When taking ensemble averages to compute the quantities asked, average over at least 100 samples.

1. We consider a Brownian particle in the over-damped limit and under the effect of force from potential $U(X)$.

   The potential has the functional form

$$U(X) = \frac{1}{4}X^4 - \frac{1}{2}X^2 + X. \tag{1}$$

   The potential is plotted in Fig. 1. Hence, the force is given by

$$-U'(X) = -\left(X^3 - X + 1\right), \tag{2}$$

   where the prime denotes the derivative by its argument.

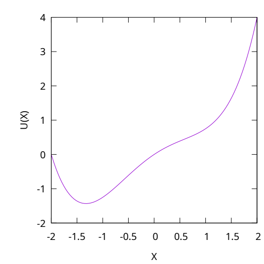

Figure 1: $U(X)$ defined in eq. (1).

   The position of the particle at time t, $X(t)$, obeys the following Langevin equation:

$$\frac{dX}{dt} = -\frac{1}{\eta}\left(X^3 - X + 1\right) + \xi(t). \tag{3}$$

   Here, η is the drag coefficient and a positive constant. $\xi(t)$ is a Gaussian white noise, and it satisfies

$$\langle \xi(t)\rangle = 0, \quad \langle \xi(t_1)\xi(t_2)\rangle = 2D\delta(t_1 - t_2). \tag{4}$$

   Here, D is the diffusion coefficient and a positive constant. Set $D = 0.2$, $\eta = 2$. **Set the initial position to be** $X(0) = 1$. Numerically simulate the trajectory $X(t)$ by using the Euler method. Set the time step for integration to $\Delta t = 0.01$. Plot the following quantities.

(i) (4 points) Plot one example trajectory $X(t)$ as a function of time from $t = 0$ to $t = 50$.

(ii) (2 point) Plot the mean trajectory $\langle X(t) \rangle$ as a function of time from $t = 0$ to $t = 50$.

(iii) (2 points) Plot the variance $\left\langle (X(t) - \langle X(t) \rangle)^2 \right\rangle$ as a function of time from $t = 0$ to $t = 50$.

2. Suppose there are Ω people in total in a community (Ω is an integer and a constant). N people in the community have flu. If a person with the flu meets a healthy person who does not have the flu, there is a chance for a healthy person to catch the flu. The person who has the flu recovers at a constant rate per person. The recovered healthy person can catch the flu again. Also, a healthy person can catch the flu spontaneously at a small constant rate per person, representing the rare event of catching a cold from people outside of the community. Assuming that the population is well-mixed inside the community, we express this process as

   - $N \to N + 1$ at a rate $\alpha \frac{N}{\Omega}(\Omega - N) + \epsilon(\Omega - N)$.
   - $N \to N - 1$ at a rate γN.

   Here, α, ϵ, and γ are positive constants. $(\Omega - N)$ is the number of healthy people in the community and $\frac{N}{\Omega}$ is proportional to the density of people who have a cold. Set $\Omega = 100$, $\alpha = 2.5$, $\epsilon = 0.01$, and $\gamma = 1$. Set the initial number of people with the flu at time zero to 1, i.e., $N(0) = 1$. Simulate the process by using the Gillespie method. Do the following.

   (i) (4 points) Plot one simulated trajectory of $N(t)$ as a function of time t from $t = 0$ to $t = 100$.

   (ii) (4 points) After some time, the system reaches a steady state. Numerically calculate the mean $\langle N \rangle$ and the variance $\langle (N - \langle N \rangle)^2 \rangle$ in the steady-state from the simulation. When you are taking averages, pay attention that inter-event intervals in Gillespie simulation is uneven.

3. Let's modify the previous model to take into account immunity. Suppose a community has Ω people in total (Ω is an integer and a constant). N people in the community have the flu. We assume that a recovered person becomes immune to the flu and, hence, does not catch the flu. The immunity is lost at a constant rate per person. Denoting the number of immune people as M, the number of healthy but non-immune people becomes $(\Omega - N - M)$. We express this process as

   - $N \to N + 1$ at a rate $\alpha \frac{N}{\Omega}(\Omega - N - M) + \epsilon(\Omega - N - M)$.
   - $N \to N - 1$ and $M \to M + 1$ at a rate γN.
   - $M \to M - 1$ at a rate βM.

   Here, α, ϵ, γ, and β are positive constants. Set $\Omega = 100$, $\alpha = 2.5$, $\epsilon = 0.01$, $\gamma = 1$, and $\beta = 0.3$. Set the initial number of people who have the flu at time zero to be 1, i.e., $N(0) = 1$, and no one is immune at the start, i.e., $M(0) = 0$. Simulate the process by using the Gillespie method.

   (i) (4 points) Plot one simulated trajectory of $N(t)$ and $M(t)$ as a function of time t from $t = 0$ to $t = 100$.