# Diffusive and Stochastic Processes Programming assignment 2023

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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 (Wed) 2023 at 11:59am. Submission of your result should be made 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 the plots asked for in the assignment with clear labels so that I can understand what is plotted. When asked to calculate a certain quantity, state your obtained value 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 the formulation of the problem (e.g., you think there is a mistake that prevents you from solving it), write Namiko an e-mail (mitarai@nbi.ku.dk).
- When $X$ is a stochastic variable and $f(X)$ is a function of $X$, $\langle f(X)\rangle$ means the ensemble average of $f(X)$.

1. Consider bacteria growing exponentially but also producing toxic material for themselves that they start to die when the density of bacteria is too high. Suppose the toxic material is short-lived, so its density is proportional to the density of the bacteria in the system. We also assume that there is a small influx of bacteria into the system all the time. Let's model this with the following simple birth-death process.

   - $N \to N+1$ at a rate $\mu N + \epsilon$.
   - $N \to N-1$ at a rate $\gamma \frac{N}{\Omega} \cdot N$.

   Here, $\mu$ is the bacteria's rate of division, $\epsilon$ is the influx rate of the bacteria from outside, $\Omega$ is the volume of the system, and $\gamma N/\Omega$ denotes the death rate per bacteria, which is proportional to the bacteria's density, where $\gamma$ is a constant.

   (a) Set $\Omega = 10$, $\mu = 1$, $\epsilon = 0.1$, and $\gamma = 0.2$. Set the initial number of bacteria to be 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 are uneven.

   (b) What if the bacteria is somewhat immune to the toxin that it makes, but there are two kinds of bacteria that produce different toxin, and they are sensitive to the toxin coming from another bacteria? To consider this problem, I devised the following model for the number of A-bacteria $N$ and the number of B-bacteria $M$.

   - $N \to N+1$ at a rate $\mu N + \epsilon$.
   - $N \to N-1$ at a rate $\gamma \frac{M+N/2}{\Omega} \cdot N$.

- $M \to M + 1$ at a rate $\mu M + \epsilon$.
- $M \to M - 1$ at a rate $\gamma \frac{N+M/2}{\Omega} \cdot M$.

Set $\Omega = 10$, $\mu = 1$, $\epsilon = 0.1$, and $\gamma = 0.2$. Set the initial condition to be $N(0) = 50$ and $M(0) = 50$. Simulate this process using the Gillespie algorithm.

(i) (4 points) Plot FIVE simulated trajectories of $N(t)$ and $M(t)$ as a function of time $t$ from $t = 0$ to $t = 100$ with the initial condition $N(0) = 50$ and $M(0) = 50$.

2. Consider a Brownian particle in the over-damped limit under external force. The particle is charged, and we apply a constant electronic field, and in addition, we apply a harmonic potential. We model the particle's position $X(t)$ by using the following Langevin equation:

$$\frac{dX(t)}{dt} = -\frac{1}{\eta}(kX(t) - c) + \xi(t). \tag{1}$$

Here, $\eta$ is the drag coefficient and a positive constant. The constant $c$ represents the force due to the electronic field, and $k$ is the spring constant that parametrizes the harmonic potential. $\xi(t)$ is a Gaussian white noise, and it satisfies

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

Here, $D$ is the diffusion coefficient and a positive constant. Set $c = 1$, $k = 1$, $D = 0.1$, $\eta = 2$. **Set the initial position to be** $X(0) = 0$. 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 $t = 10$.

(ii) (2 point) Plot the mean trajectory $\langle X(t) \rangle$ as a function of time from $t = 0$ to $t = 10$. Take the average over at least 1 00 samples.

(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 $t = 10$. Take the average over at least 100 samples.