Problem Sheet 2

1. This is a warm-up problem. You are asked to verify a few results from the Lecture Notes. This problem is here to encourage you to read the Lecture Notes which cover Lectures 5–8. You do not need to write long derivations (a few lines for each point (a)–(e) will be enough).

(a) Consider the SDE (5.7). Compute $\mathrm{E}[X(t)^k]$ for $k \in \mathbb{N}$.

(b) Consider the SDE (5.21). Show that the variance $V(t)$ of $X(t)$ is given by $V(t) = t$.

(c) Verify that (5.36) is a solution of (5.35).

(d) Show that the Fokker-Planck equation corresponding to (7.11) is given by (7.7).

(e) Verify that (8.9) is a solution of (8.8) and that (5.33) is a solution of (5.32).

2. The Lotka-Volterra (predator-prey) system was studied in your Part A Differential Equations 1 course (see pages 38-39 of your lecture notes from last year). We write it as a chemical system

$$A \xrightarrow{k_1} 2A, \qquad B \xrightarrow{k_2} \emptyset, \qquad A + B \xrightarrow{k_3} 2B, \tag{$*$}$$

for two chemical species A ("prey") and B ("predator"). Its deterministic ODE model is

$$\frac{\mathrm{d}a}{\mathrm{d}t} = k_1 a - k_3\, a\, b, \qquad \frac{\mathrm{d}b}{\mathrm{d}t} = -k_2\, b + k_3\, a\, b, \tag{$\diamondsuit$}$$

where $a(t)$ and $b(t)$ are concentrations of A and B, respectively. Consider the (dimensionless) parameters $k_1 = k_2 = 10$ and $k_3 = 0.1$ and initial condition $a(0) = 50$ and $b(0) = 50$. For the stochastic case, consider (dimensionless) volume $\nu = 1$.

(a) Find critical points of ODEs ($\diamondsuit$). Investigate their stability, sketch the phase diagram and prove that the ODE system ($\diamondsuit$) has periodic solutions.

(b) Implement the Gillespie SSA (a4)–(d4) for the chemical system ($*$). Plot the number of molecules of A and B as a function of time and compare your results with the solutions of ODEs ($\diamondsuit$). Plot both stochastic and deterministic trajectories $(A(t), B(t))$ and $(a(t), b(t))$ in the phase diagram as well. You should observe that, for sufficiently long time, the deterministic and stochastic models give significantly different results. What types of the long-time behaviour can the stochastic model have ?

(c) Give an example of a chemical system which has the same deterministic description given by the ODEs ($\diamondsuit$), but its stochastic description (given by the Gillespie SSA) differs from the stochastic model corresponding to the chemical system ($*$).

(d) Consider the chemical system ($*$) together with two additional reactions

$$2A \xrightarrow{k_4} \emptyset, \qquad \emptyset \xrightarrow{k_5} A + B. \tag{$**$}$$

Then its deterministic ODE model is

$$\frac{\mathrm{d}a}{\mathrm{d}t} = k_1 a - k_3\, a\, b - 2k_4\, a^2 + k_5, \qquad \frac{\mathrm{d}b}{\mathrm{d}t} = -k_2\, b + k_3\, a\, b + k_5. \tag{$\heartsuit$}$$

Use dimensionless parameters $k_4 = 0.01$ and $k_5 = 1$. Show that the deterministic ODE model ($\heartsuit$) for the combined system ($*$)–($**$) does not have periodic solutions. What about its stochastic model? Does it oscillate? If yes, what is its period of oscillations?

3. Consider the compartment-based model (8.13) of diffusion, studied in Section 8.2.

(a) Derive the system of equations (8.24)–(8.25).

(b) Let $K = 2$. Write the system of equations for V_1, V_2 and $V_{1,2}$ and find their values at the steady state.

(c) Consider the stationary diffusion master equation, i.e. the equation for the steady state solution of (8.22). Show that the solution of this equation can be written in the form

$$\frac{C}{n_1!\, n_2! \ldots n_K!}, \tag{$\dagger$}$$

for $n_1 + n_2 + \cdots + n_K = N$, where N is the total number of diffusing molecules and C is the normalization constant. Find the value of C and use (†) to calculate the stationary values of the mean and variance vectors, $\mathbf{M}$ and $\mathbf{V}$, and covariance matrix $\{V_{i,j}\}$ defined by (8.23), (8.26) and (8.27), respectively.

(d) Consider that the number of compartments K is large (i.e. study the formal limit $K \to \infty$) and assume that $N = 10K$. Then equations (8.24)–(8.25) imply that there will be on average 10 molecules in each compartment at the steady state. What is the probability that a given compartment will contain at least 20 molecules?

4. We revisit the problem studied in Question 5 on Problem Sheet 1. We consider the chemical system (3.25), i.e.

$$3A \underset{k_2}{\overset{k_1}{\rightleftarrows}} 2A, \qquad\qquad A \underset{k_4}{\overset{k_3}{\rightleftarrows}} \emptyset \tag{3.25}$$

and choose the values of (dimensionless) rate constants k_1, k_2 and k_3 as

$$k_1/\nu^2 = 2.5 \times 10^{-4}, \qquad k_2/\nu = 0.18, \qquad k_3 = 37.5.$$

We will vary the value of $k_4\nu$ in the interval $(1700, 2500)$ and study the dependence of the behaviour of the chemical system (3.25) on this parameter.

(a) Write the chemical Fokker-Planck equation corresponding to the system (3.25). Plot the stationary distribution p_s given by the chemical Fokker-Planck equation for (i) $k_4\nu = 1750$; (ii) $k_4\nu = 2100$; (iii) $k_4\nu = 2200$; and (iv) $k_4\nu = 2450$. Compare with the results computed in Question 5 on Problem Sheet 1 (using the Gillespie SSA and the chemical master equation). If there are any differences, explain them.

(b) Plot the graph of local maxima and minima of p_s as a function of $k_4\nu$ for $k_4\nu \in (1700, 2500)$. Compare with the graph of steady states of the deterministic ODE model obtained in Question 5 on Problem Sheet 1. If there are any differences, explain them.

(c) Plot the average switching time between two favourable states of the system as a function of $k_4\nu \in (1700, 2500)$. To obtain this plot, use formula (7.20). Compare the results with the Gillespie SSA for (i) $k_4\nu = 2100$; and (ii) $k_4\nu = 2200$.

(d) Use $k_4\nu = 2100$. Plot the stationary distribution. Now, change ν to 10ν. That means that we will use the following parameters:

$$k_1/\nu^2 = 2.5 \times 10^{-4}/100 = 2.5 \times 10^{-6}, \qquad k_2/\nu = 0.18/10 = 0.018,$$

$$k_3 = 37.5, \qquad k_4\nu = 2100 \cdot 10 = 21000.$$

Plot the stationary distribution. What is the effect of changing the volume ν on the shape of the stationary distribution?

A couple of additional questions (OPTIONAL)

5. This problem is about generating random numbers. Let us assume that you are able to sample random numbers which are uniformly distributed in $(0,1)$.

(a) How would you sample random numbers which are uniformly distributed on a sphere with radius R ?

(b) Suppose that r_1 and r_2 are two random numbers uniformly distributed in $(0,1)$. Define

$$\xi_1 = \sqrt{2|\log r_1|}\,\cos(2\pi r_2), \qquad \xi_2 = \sqrt{2|\log r_1|}\,\sin(2\pi r_2).$$

Show that ξ_1 and ξ_2 are random numbers sampled from normal distribution with zero mean and unit variance.

Note: This method for sampling normally distributed random numbers is called the Box-Muller transform or the Box-Muller algorithm.

6. A particle moves in a one-dimensional interval $[0,L]$, where $L>0$, according to the discretized stochastic differential equation:

$$X(t+\Delta t) = X(t) + f(X(t))\,\Delta t + \sqrt{2\Delta t}\,\xi,$$

where $X(t)\in[0,L]$ is the particle position at time $t\geq 0$, $f:[0,L]\to\mathbb{R}$, $f(0)=0$, $\Delta t>0$ is the time step and ξ is a random number which is sampled from the normal distribution with zero mean and unit variance. The initial condition is $X(0)=0$. The boundary $x=0$ is reflective, i.e. whenever the particle crosses this boundary, it is reflected back to the domain. In parts (a) and (b), we will consider $L=\infty$ which means that $X(t)\in[0,\infty)$.

(a) Let $L=\infty$. Let $p(x,t)$ be the distribution of the probability that $X(t)=x$. Write the Fokker-Planck equation satisfied by $p(x,t)$ in the limit $\Delta t\to 0$. Write the boundary condition for the Fokker-Planck equation at $x=0$.

(b) Let $L=\infty$ and $f(x)=-x$. Find the stationary distribution.

(c) Let $L=10$ and $f(x)\equiv 0$ for $x\in[0,L]$. Let $X(0)=0$. What is the average time to reach the right boundary, i.e. the point $x=L$?

(d) Let $L=1$ and $f(x)=x(1-x)$, with a reflective boundary condition at $x=L$. Find the stationary distribution. Express it in the form $p_s(x)=Ch(x)$ where C is the normalization constant. You need not calculate the normalization constant C explicitly.