CHEM-LV03 Analysis and Simulation of Stochastic Reaction-diffusion Systems
Department of Chemical and Metallurgical Engineering
Aalto University
Summer 2022 Exercise 4

Classroom problems

Problem 1. *(Riemann integrals) Assume that we have some function $f(t)$ which we want to integrate over the range of $t \in [0, T]$. First, partition the interval into $0 = t_0, t_1, \ldots, t_n, \ldots, t_{N-1}, t_N = T$. Let $S(T)$ denote the result of such integration over the interval $[0, T]$.*

$$
\begin{aligned}
S(T) &= \int_0^T f(t)dt \\
&= \lim_{N\to\infty} \sum_{n=0}^{N} f(\tau_n)\Delta t_n, \quad \Delta t_n = t_{n+1} - t_n, \quad \tau_n \in [t_n, t_{n+1}].
\end{aligned}
$$

Show that the integral $S(T)$ converges to the same value no matter where you fix τ_n in the interval $[t_n, t_{n+1}]$. Choose $T = 1$ and $\Delta t_n = \Delta t = 0.2$. ***Hint:*** *you can start by computing the integral with the left boundary $\tau_n = t_n$, and then compare it with the integral using the midpoint $\tau_n = \frac{1}{2}(t_n + t_{n+1})$. If the results diverge, try increasing N, that is, choose a smaller Δt.*

Problem 2. *(Stochastic integrals, Itô vs Stratonovich) We now consider the following class of stochastic differential equations (SDEs):*

$$
dX(t) = f(X(t), t)dt + g(X(t), t)dW(t), \quad X : [0, \infty) \to \mathbb{R}^{D_x}.
$$

Here, W stands for Brownian motion. First consider the integration of the SDE for the Brownian motion itself, that is:

$$
W(t) = W(0) + \int_0^t dW(s), \quad t \in [0, T],
$$

and, with the solution W at hand, approximate the following stochastic integral

$$
S(T) = \int_0^T W(t)dW(t).
$$

More specifically, check the difference between the Itô and Stratonovich interpretations of $S(T)$. ***Hint 1:*** *compute an estimator for $\mathbb{E}[S(T)]$ for $T = 50$ with each type of integral. Check whether the two values match. You are free to choose the number of realisations needed for your estimation of the expectation, as well as the value of Δt.* ***Hint 2:*** *should you plot the process $\{S(t)_{t\in[0,T]}\}$, 25 is a reasonable number of realisations.*

Problem 3. *Partition the interval $t \in [0, 20]$ in N equidistant subintervals and find solutions $X = (X_t, t \in [0, 20])$ to each of the following stochastic differential equations:*

3.1) $dX(t) = dW(t), \quad X : [0, \infty) \to \mathbb{R}, \quad X(0) = 0.$

3.2) $dX(t) = dt + dW(t), \quad X : [0, \infty) \to \mathbb{R}, \quad X(0) = 0.$

3.3) $dX(t) = \begin{bmatrix} \sqrt{2D} & 0 \\ 0 & \sqrt{2D} \end{bmatrix} dW(t), \quad X : [0, \infty) \to \mathbb{R}^2, \quad X(0) = [0, 0]^\top, D > 0.$

Consider Itô integrals and plot few realisations of the solution X, say 5. You are free to choose the intensity D of the noise.

Problem 4. *(System with multiple favourable states, revisited) Consider a chemical species $\mathcal{A}$ being subjected to four chemical reactions in a container of volume V:*

R1) $3\mathcal{A} \xrightarrow{\kappa_1} 2\mathcal{A}$

R2) $2\mathcal{A} \xrightarrow{\kappa_2} 3\mathcal{A}$

R3) $\mathcal{A} \xrightarrow{\kappa_3} \emptyset$

R4) $\emptyset \xrightarrow{\kappa_4} \mathcal{A}$.

The following ODE approximates the evolution of the average number $\overline{n_{\mathcal{A}}}$ of molecules of $\mathcal{A}$:

$$d\overline{n_{\mathcal{A}}}(t) = -\frac{\kappa_1}{6V^2}\overline{n_{\mathcal{A}}}^3(t) + \frac{\kappa_2}{2V}\overline{n_{\mathcal{A}}}^2(t) - \kappa_3\overline{n_{\mathcal{A}}}(t) + \kappa_4 V, \quad \overline{n_{\mathcal{A}}}(0) = 0,$$

where the equation rates are in the time scale of minutes. Consider the first 40 minutes of the reaction and the following rate constants:

$$\kappa_1 = 1.5 \times 10^{-3}, \quad \kappa_2 = 0.36, \quad \kappa_3 = 37.5, \quad \kappa_4 = 2200.$$

(a) plot the time evolution of the copy number by solving the SDE corresponding to the scenario above. Compare it with the deterministic solution. Are there any significant differences between the stochastic and deterministic solutions?

(b) change V to $20V$ and solve the corresponding ODE and SDE. What is the effect of changing the volume V?

Homework

Problem 5. *Consider again the chemical system of Problem 3.1, consisting of two chemical species $\mathcal{A}$ and $\mathcal{B}$ in the volume V subject to the following chemical reactions:*

$$\emptyset \xrightarrow{\kappa_1} \mathcal{A}, \qquad \mathcal{A} \xrightarrow{\kappa_2} \emptyset$$
$$\mathcal{A} \xrightarrow{\kappa_3} \mathcal{B}, \qquad \mathcal{B} \xrightarrow{\kappa_4} \emptyset.$$

Suppose that there are initially 100 molecules of $\mathcal{A}$ and 25 molecules of $\mathcal{B}$ in a vessel of volume $V = 10$, and consider the following rate constants:

$$\kappa_1 = 2, \quad \kappa_2 = 0.2, \quad \kappa_3 = 0.2, \quad \kappa_4 = 0.1.$$

(a) obtain the empirical distribution for the number of molecules of $\mathcal{A}$ and $\mathcal{B}$ at time $T = 20$ with 10^4 realisations of the Gillespie algorithm.

(b) obtain again the empirical distribution, now with 10^4 realisations of the corresponding SDE. Compare it with the result in (a).