CHEM-LV03 Analysis and Simulation of Stochastic Reaction-diffusion Systems
Department of Chemical and Metallurgical Engineering
Aalto University
Summer 2022 Exercise 2

Chemical master equations of elementary reactions

Classroom problems

Problem 1. *(Stochastic Simulation of Production and Degradation - Continuation) Consider again the chemical reactions*

$$\mathcal{A} \xrightarrow{\kappa_1} \emptyset$$
$$\emptyset \xrightarrow{\kappa_2} \mathcal{A},$$

from Ex.1 (Problem 3c), where $\mathcal{A}$ is the chemical species of interest and κ_1, κ_2 were the rate constants of the reactions. Consider $n_{\mathcal{A}}(0) = 0$ as the initial condition on the number of molecules, $\kappa_1 = 0.1 sec^{-1}$ and $\kappa_2 = 1 \times 10^3 sec^{-1} m^{-3}$ as the reaction rates, and $V = 10^{-3} m^3$ as the volume of the vessel where the reactions take place. Draw 10^6 realizations for the first 100 seconds and plot a normalized histogram of your realizations at the stopping time. Compare the histogram with the solution to the steady-state version of the chemical master equation, $\phi(\cdot)$, given by

$$\begin{aligned}
\phi(0) &= 1, \\
\phi(1) &= \frac{\kappa_2 V}{\kappa_1}\phi(0), \\
\phi(n+1) &= \frac{1}{\kappa_1(n+1)}[\kappa_1 n\phi(n) + \kappa_2 V\phi(n) - \kappa_2 V\phi(n-1)], \quad \text{for } n \geq 1.
\end{aligned}$$

Problem 2. *Consider the chemical reaction*

$$A \xrightarrow{\kappa} \emptyset.$$

Let $p_n(t)$ denote the probability that there are n molecules of A at time t. Derive and solve ordinary differential equations for the mean

$$M(t) = \sum_{n=0}^{\infty} n p_n(t)$$

and variance

$$V(t) = \sum_{n=0}^{\infty} (n - M(t))^2 p_n(t).$$

Problem 3. *For this problem, we will consider the dimerisation kinetics of a protein P, at very low concentrations in a bacterial cell. Consider two chemical reactions*

$$2P \xrightarrow{\kappa_1} P_2, \text{ and } P_2 \xrightarrow{\kappa_2} 2P.$$

(a) suppose there are initially 301 molecules P and no molecules of P_2. Denote by $p(t,n)$ the probability that there are n molecules of P_2 at time t, and by $\phi(n)$ the corresponding stationary probability distribution. Find $\phi(n)$ as a function of the rate constants κ_1 and κ_2.

(b) assume that the values of κ_1 and κ_2 have been determined from an experiment and found to be $\kappa_1 = 1.66 \times 10^{-3}$ and $\kappa_2 = 0.2$. Draw 10^6 realizations during the first 10 seconds of the reaction and plot a normalized histogram of your realizations at the stoppting time $T = 10$ sec. Compare the histogram for molecules of P_2 with $p(10, n)$ and with $\phi(n)$.

Homework

Problem 4. *(Gene transcription and translation - Cont...)*

We allow for the possibility that the protein from Ex.1 (Problem 3) dimerizes via the reaction $2P \xrightarrow{\kappa_3} D$ *. The degradation of the dimer is allowed by the reaction* $D \xrightarrow{d_d} \emptyset$*. The set of species for the model is now* (G, M, P, D)*.*

R5) $2P \xrightarrow{\kappa_3} D$ *(dimerization)*

R6) $D \xrightarrow{d_d} \emptyset$ *(degradation)*

Consider the same choice of rate constants and initial quantities, and consider $\kappa_3 = 0.01$*,* $d_d = 1$ *and* $D(0) = 0$*. Draw a realization of the stochastic model and plot it together with the solution to its associated deterministic model.*