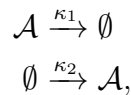


Chemical master equations of elementary reactions

Classroom problems

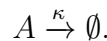
Problem 1. (*Stochastic Simulation of Production and Degradation - Continuation*) Consider again the chemical reactions



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, $\kappa_1 = 0.1 \text{sec}^{-1}$ and $\kappa_2 = 1 \times 10^3 \text{sec}^{-1} \text{m}^{-3}$ as the reaction rates, and $V = 10^{-3} \text{m}^3$ 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



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

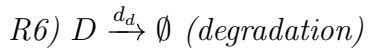
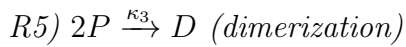


- suppose there are initially 301 molecules P and no molecules of P_2 . Denote by $p(t, n)$ the probability that there are n molecules of P_2 at time t , and by $\phi(n)$ the corresponding stationary probability distribution. Find $\phi(n)$ as a function of the rate constants κ_1 and κ_2 .
- assume that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



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.