

NATIONAL TAIWAN UNIVERSITY,
GRADUATE INSTITUTE OF BIOMEDICAL ENGINEERING AND BIOINFORMATICS

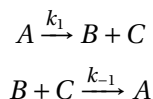
BEBI5009:
Mathematical Modeling of System Biology
Homework 4

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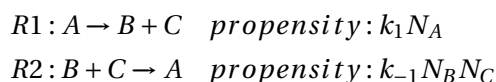
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Consider the reaction network



- Suppose that the system starts with two molecules of A, one molecule of B, and no molecules of C, that is $(N_A, N_B, N_C) = (2, 1, 0)$. Determine the set of possible states the system can adopt and write the chemical master equation that describes the corresponding probability distribution.
- Take $k_1 = 1 \text{ (time}^{-1}\text{)}$ and $k_{-1} = 1 \text{ (time}^{-1}\text{)}$, and solve for the steady-state probability distribution.
- Simulate sample paths of N_A , N_B , and N_C using stochastic simulation algorithm (SSA). Set the initial condition of N_A , N_B , and $N_C = (2, 1, 0)$ or $(10, 5, 0)$ or $(100, 50, 0)$



Note1: To calculate the waiting time, you will need to generate values of a random variable distributed according to an exponential distribution. You could simply generate a random variable U drawn from the uniform distribution on the unit interval $(0, 1)$, and $T = -\ln(U)/\lambda$ will be an exponential random variable, where λ is the rate parameter of the exponential distribution. In this example, λ would be the sum of the reaction propensities.

Another way to generate exponential random number is to use Matlab function `expnrnd(μ)`, where μ is the mean of the exponential distribution $\mu = 1/\lambda$.

Note2: You might need to change the value of k_1 and k_{-1} for different initial conditions due to the volume changes. Use $(k_1, k_{-1}) = (1, 1)$, $(1, 1/5)$ and $(1, 1/50) \text{ (time}^{-1}\text{)}$ for I.C. = $(2, 1, 0)$, $(10, 5, 0)$, and $(100, 50, 0)$.

- Set the initial condition of N_A , N_B , and $N_C = (2, 1, 0)$. Analyzed the statistics of your ensemble, and compare to the steady state probability distribution in (b)
- Write down a deterministic model for the chemical reaction following the mass action law. Simulate the concentration changes of A, B, C with the parameter $k_1 = 1 \text{ (s}^{-1}\text{)}$ and $k_{-1} = 1 \text{ (mM}^{-1} \text{s}^{-1}\text{)}$. Set initial concentrations $[A], [B], [C]$ as 2, 1, and 0 mM. Compare simulation results in (c)