

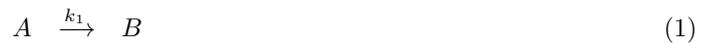
# Stochastic simulation and chemical inference modules

## 1. The Gillespie algorithm for stochastic simulation.

Download a copy of the original paper by Gillespie (*Exact Stochastic Simulation of Coupled Chemical Reactions*, D. T. Gillespie, J. Phys. Chem. **81** 2340 (1977)). Locate the file `GillespieMatlab.m`. Write down a description of the function of each variable in the M-file, and the line numbers corresponding to the steps in boxes 1-3 in Fig. 2 of the original paper.

## 2. A simple stochastic chemical system.

We will first consider the following simple chemical system:



where  $k_i$  are the rates of each reaction.

(a) Write down the stoichiometry matrix for this system.

(b) Use `GillespieMatlab.m` to simulate this system for  $k_1 = k_2$ ,  $k_1 > k_2$  and  $k_1 < k_2$ . Plot the resulting stochastic trajectories to verify that the system behaves as expected.

## 3. Gillespie simulation of the Monod model.

We will now look at a more complicated chemical system, used to model co-operative binding, which we shall see is useful in biological inference. Here, we have a protein which can exist in binding ( $B$ ) or non-binding ( $N$ ) states. The protein has  $n$  sites, to which sugar molecules ( $S$ ) may bind. However, the protein may only swap between  $B$  and  $N$  states when no sugars are bound to it. Sugar binding hence acts to “lock in” a particular state of the protein. This system is described by:



(a) Write down the stoichiometry matrix for this system. Don't forget that sugar molecules are reactants too! Why are some rates a function of  $n$ ?

(b) Use `GillespieSwain.m` to simulate this system for  $K_R = 100$ ,  $K_T = 10$ ,  $L = 2$ ,  $n = 1$ . Explore the occupancy of the  $B$  state as  $S$  varies over orders of magnitude.

(c) Simulate the system for  $n = 2$ . What do you notice about the behaviour at different sugar concentrations as  $n$  changes?