Math 6780 Homework Exercises, Spring 2018

1 Homework Set 1, Due Feb. 20, 2018.

1. Consider the following three state model for sodium channels:

$$I \xleftarrow{\delta} C \underset{\beta}{\overset{\alpha}{\rightleftarrows}} O \xrightarrow{\gamma} I \tag{1}$$

Here C represents the closed state, O represents the open state, and I represents an inhibited state.

(a) Calculate the splitting probability (i.e., the probability that the state I is entered from state O or state C), the expected time to enter state I, and the expected number of times state O is entered before going into state I, assuming in all cases that the process is initially in state C.

(b) Simulate this process using the Gillespie algorithm using parameters $\alpha = 1/\text{ms}$, $\beta = 0.4/\text{ms}$, $\gamma = 1.6/\text{ms}$ and $\delta = 1/\text{ms}$. Collect data from a large number of simulations and use this to verify the calculations from the first part of this problem.

2. Consider a birth-death process in which the death rate β is constant ($k_n^- = n\beta$) and the birth rate is population size dependent, decreasing as a function of population size, $k_n^+ = \alpha(N-n)$.

(a) Write the master equation for this process. Find the steady state solution (a binomial distribution).

(b) Find the equation for the generating function for this process.

(c) Find the steady solution of the generating function equation.

(d) Simulate this process using the Gillespie algorithm. Compare the results of the simulation with the steady distribution you found using the master equation. (Without loss of generality, take $\beta = 1$.)

2 Homework Set 2, Due March 15, 2018

1. Consider the birth-death process in which the death rate β is constant ($k_n^- = n\beta$) and the birth rate is population size dependent, decreasing as a function of population size, $k_n^+ = \alpha(N-n)$.

   (a) Write the master equation for this process. (This was done in the previous Homework Set.)

   (b) Use the large N approximation to find an approximate Fokker-Planck equation for this process.

   (c) Find an approximate steady state distribution for this process. (You will need to approximate the diffusion coefficient using the steady state of the deterministic flux.)

   (d) Compare this approximate solution with the result of a Gillespie simulation.

2. Consider the chemical reaction

$$X + A \underset{\beta}{\overset{\alpha}{\rightleftarrows}} 2X, \tag{2}$$

   with $[A] + [X]$ fixed.

   (a) Write the master equation for this reaction.

   (b) Use a large N approximation to find an approximate Fokker-Planck equation for this process.

   (c) Find an approximation to the steady state distribution for this process. (You will need to use a linear approximation to the deterministic drift term and a constant approximation of the diffusion coefficient.)

   (d) Compare this distribution to the result of a Gillespie simulation.

3. A small particle that is permanently tethered to position $x = 0$ moves diffusively (drag coefficient ξ, spring constant k, diffusion coefficient $\frac{k_B T}{\xi}$) can bind or unbind with another large particle with binding rate α and unbinding rate β. When it is bound to the large particle it moves with drag coefficient η and no diffusion. Suppose both α and β are large. Use adiabatic reduction to find an approximate equation for the motion of this system.

4. Suppose that there are three states underlying the random variable X (with values $x = 0, 1, 2$) with transitions

$$S_0 \underset{\beta}{\overset{2\alpha}{\rightleftarrows}} S_1 \underset{2\beta}{\overset{\alpha}{\rightleftarrows}} S_2. \tag{3}$$

   (a) Use the Gillespie algorithm to find sample paths for the solution of

$$\frac{dy}{dt} = x. \tag{4}$$

   Use this to estimate the mean and the variance as a function of time for this process.

   (b) What is the master equation for this stochastic differential equation?

   (c) Suppose that α and β are much greater than 1. Use the rapid equilibrium approximation to find an approximate Fokker Planck equation and the equivalent Langevin equation for this process. Compare the result of this calculation with the numerical estimates found numerically in part a.

3 Homework Set 3, Due April 17, 2018

1. Find the mean first exit time for a particle starting at position $x = 0$ from the piecewise linear potential
$$U(x) = \begin{cases} -\frac{\Delta G x}{L} & -L < x < 0 \\ \frac{\Delta G x}{L} & 0 < x < L \end{cases}, \tag{5}$$
with a reflecting boundary at $x = -L$ and absorbing boundary at $x = L$, and with a force F. Assume the particle has drag coefficient ξ.

2. Suppose a diffusing particle is pulled with force F along a line of length L, but there is a binding site to which it can bind at position $x = a$, $0 < a < L$.

   (a) Find the splitting probability for binding, i.e., the probability that binding will occur at site a for a particle that starts at $x = 0$. Assume that the particle cannot escape through $x = 0$ but it can escape through $x = L$.

   (b) Suppose that the particle can both bind and unbind from the binding site. Find the mean exit time at $x = L$, as a function of force F.