SSSBB Winter 2017
HW assignment 2
(Master equations and Monte Carlo simulations)

Due: TBA

1. Consider the following chemical reaction (that frequently occurs in biological processes)

$$X \xrightarrow{c} X^*$$

The above reaction can be modeled by the following master equation

$$\frac{\partial P(x,t)}{\partial t} = c[(x+1)P(x+1,t) - xP(x,t)]$$

x is the number of X molecules (c is a kinetic constant). P(x,t) is defined as the probability of having x molecules at time t.

(a) (2 pts) Discuss the significance of each term in the above equation (justify inclusion of the multiplicative factor *x+1* or *x*). Also discuss the biological relevance of the chemical reaction considered in this problem.

(b) (4 pts) Solve the above master equation (initial condition $X = x_0$ at t=0) to obtain

$$P(x,t) = \frac{x_0!}{x!\,(x_0-x)!}(e^{-ct})^x(1-e^{-ct})^{x_0-x}$$

You may use a characteristic function of the form

$$G(s,t) = \sum_{x=0}^{\infty} s^x P(x,t)$$

(c) (2 pts) Show that the average <*X*> satisfies the deterministic equation $dx/dt = -cx$. It might be possible to justify the expression of P(x,t) obtained in part (c) based on the solution of the deterministic equation, discuss it.

(d) (3.5 pts) Obtain a solution of the above master equation using Monte Carlo simulations. Compare your results with the result P(x,t) in part (a). Also compare the average behavior obtained in those two cases (exact solution and MC simulation). You need to provide graphical plots (you need to show 10 MC run results for x(t) on the plot where you show the average behavior).

(e) (3.5 pts) Find an exact expression for the variance in the number of molecules of X. Find the maximal variance and estimate the time corresponding to it. Show an approximate graphical plot of the variance (as a function of time).

Estimate the variance using Monte Carlo simulations. Compare your MC result with the exact expression. You need to do it for at least three different c values (should capture order of magnitude variation in c).

(f) Challenge Problem: Suppose the reverse reaction $X^* \rightarrow X$ also takes place. Write and solve the appropriate master equation for this case to obtain P(x,t). You may consult the book Stochastic Methods by C Gardiner.

2. (Challenge Problem)
The following two-step process can be studied to provide insights into cell-to-cell stochastic variability and all-or-none type behavior in biological systems

$$X \overset{c_1}{\rightarrow} Y \overset{c_2}{\rightarrow} Z$$

(a) Write down the master equation for the above process and obtain solutions for it using Monte Carlo (MC) simulations (c_1 and c_2 are kinetic constants).

(b) Study the following scenario $c_1 << c_2$. Plot Z(t) for individual MC runs to show stochastic variability. Also plot the average Z(t).

(c) Estimate P(Z,t) for various time-points (this is a data analysis tool to assess stochastic variability in the system).

(d) Write down and solve the deterministic equations (in terms of the number of molecules) for the above two-step process. Compare your results with the solutions obtained from Monte Carlo simulations (consider $c_1 << c_2$).