Biological Physics II - Tutorial

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Week 9 - Master equations and Random Walk

A. The two-state Promoter

Recall the two state gene regulatory system of previous tutorials. In our simplified model, we consider one gene which is either active (in state A) if it transcribes, or inactive (in state I) if it does not. In the former, mRNA is produced, which decays at a certain rate. The reactions of this system may be written as:

$$I \xrightarrow[k_{-}]{k_{-}} A \xrightarrow{k} \mathrm{mRNA} \xrightarrow{\gamma} \emptyset$$

1) Explain the different terms, and ideally draw a small sketch of the system with all its constituents.

2) Write one Master equation for the time evolution of the probability $p_I(m,t)$ (probability to find m mRNA molecules at time t in the state I), and one for the time evolution of the probability $p_A(m,t)$ (probability to find m mRNA molecules at time t in the state A). Hint: there are 4 terms in the first equation, and six terms in the second equation.

Next week, we will try to find the first and second moment, as well as the Fano factor of the amount m of mRNA molecules.

B. Random Walk

All molecules inside a cell are subject to random collision with other molecules or molecules of the surrounding medium (water). These random collisions impair momentum and produce a movement which is known as Brownian motion described by the Langevin equation:

$$\gamma \mathbf{v} = g\xi$$

Here, γ is the friction coefficient, **v** is the velocity of the molecule, ξ is a stochastic collision term, and g is the strength of the collisions.

1) Numerically solve this equation as following:

- Choose an initial position of the molecule (in 1D or 2D or 3D) and $\mathbf{v}_0 = 0$ (in any dimension).
- Choose appropriate (constant) parameter values for γ , g, and Δt (for example, $\gamma = g = 1$, and $\Delta t = 0.1$, with 1000 total steps). To implement the collisions, draw one, two, or three (depending on the number of dimensions you are working on) normally distributed random numbers ξ (mean: 0, standard deviation: 1, for example with the function normrnd(0,1) in MATLAB).
- Update the position according to: $\mathbf{x}_{t+1} = \mathbf{x}_t + \frac{g}{\gamma} \xi \sqrt{\Delta t}$ (if you work in more than 1 dimension, do this for every dimension).

2) For each realization $\mathbf{x}(t)$, calculate the mean-square displacement $MSD(t) = (\mathbf{x}(t) - \mathbf{x}(0))^2$. Average the MSD over 1000 realizations, and plot the result as a function of time. You should observe a linear behaviour.

3) BONUS: What is the slope of this line? Why are the random collisions modelled by a normally distributed numbers? What would the true (biological) value of γ be, for example for spherical molecules? Is Brownian motion an effective means of transport inside the cell? What other means of transport are there in a cell?

Good luck!