Randomness in Biology [2014 Aug Term]

Homework 4: Assigned Sep 24. Due Oct 1.

1. Simulating the velocity of a Brownian particle

We saw in class that the velocity of a Brownian particle is an exmple of an Ornstein-Uhlenbeck process described by the following Fokker-Planck equation:

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial v}\left(\frac{\Gamma v}{m} p\right) + \frac{\partial^2}{\partial v^2}\left(\frac{\Gamma kT}{m^2} p\right)$$

This is equivalent to the Langevin equation:

$$\frac{dx}{dt} = v$$

$$m\frac{dv}{dt} = -\Gamma v + \xi(t), \qquad < \xi(t)\xi(t+t') > = 2\Gamma kT\ \delta(t')$$

Or, more explicitly,

$$\Delta x = \frac{dx}{dt}\Delta t, \qquad \Delta v = (-\Gamma v/m)\Delta t + \alpha\sqrt{2\Gamma kT/m^2}\sqrt{\Delta t}$$

where α is normally distributed with mean 0 and variance 1. Let measure time in units where the relaxation time is unity ($m/\Gamma = 1$), and measure distance in units such that the RMS velocity is unity ($kT/m = 1$).

1. Focus just on the velocity equation for now. Find a numerical solution to the Langevin equation as follows.

1. Start with $v(t = 0) = 0$ and choose a timestep $\Delta t = 0.1$.
2. Compute Δv as above.
3. Update: $v = v + \Delta v$, and $t = t + \Delta t$.
4. Continue up to a maximum time $t = 100$.
5. Repeat for e.g. 100 realizations, storing just the final velocity in each case.
6. Run again for all combinations of $v(t = 0) = 0, 10$; and $\Delta t = 0.1, 0.01, 0.001$.

For your solution, submit 5 sample trajectories each for all 6 cases above.

(a) Do velocities converge to a reproducible distribution independent of Δt and $v(t = 0)$?
(b) What is the RMS value of the final velocity for the six cases?

2. Bonus. For $v(t = 0) = 0$ and $\Delta t = 0.001$, numerically solve the full equation for x, v. What is the apparent value of the diffusion coefficient? (Plot *x* vs *t* for many realizations, and check how the value of $< \delta x^2 >$ changes with *t*. The slope of this curve will be 2*D*.)