Imperial College London

Department of Bioengineering

4 October 2017

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Training coursework 7

Simulating an overdamped particle

In this exercise, we will consider an overdamped particle moving in the potential $V(x) = 2(x+1)^2(x-1)^2$, in a medium with viscosity $\gamma = 10$ and temperature $k_B T = 1$ (don't worry about the lack of units; it simply means we're defining all dimensional quantities relative to each other). We will generate long sample trajectories by numerically integrating the Langevin equation; if we run these simulations for long enough, the sample trajectories will sample states in a manner consistent with the stationary distribution. We can then use these samples to understand properties of the stationary distribution; this is an extremely common approach!

1. Plot the potential $V(x)$ for the range $-2 \leq x \leq 2$. How do you expect the particle to behave?
2. Use Euler's method to obtain a sample trajectory $x(t)$ by integrating the differential equation
$$\frac{\mathrm{d}x}{\mathrm{d}t} = -\frac{1}{\gamma}\frac{\mathrm{d}V(x)}{\mathrm{d}x} + \eta(t) \tag{1}$$
for a total time of 1000, using a time step of 0.01, starting from a position of $x = 0$. Plot your sample trajectory $x(t)$ as a function of time. You will need to use the fact that
$$\int_{t_0}^{t_0+\Delta t} \eta(t)\mathrm{d}t \tag{2}$$
is a sample drawn from a Gaussian with mean 0 and standard deviation $\sqrt{(2k_B T\Delta t)/\gamma}$.
3. By running long simulations (for a total time of 10000) and measuring the energy at each step, estimate the average energy of the particle in the stationary distribution. What happens if you change your time step to 0.2? The exact answer is 0.545728.
4. Construct a histogram to record the states visited in the stationary distribution as sampled from a simulation of total time 3000. How does this histogram change if you increase the number of time steps to 30000? Which is more trustworthy?
5. What is the Boltzmann distribution $\pi(x)$ for this system? Plot this function. Are your histograms approximately consistent with this prediction?
6. (Optional) Matlab cannot actually generate truly random numbers; instead, it uses a complex formula to generate a sequence of numbers that look random (ie., it is difficult to predict the next number knowing the current one). However, the sequence is actually fully determined by a single integer "seed". If we set this seed to be the same, we'll get the same sequence of random numbers. This seed is automatically set to 0 every time you restart Matlab, so you'll always get the same "random" trajectory if you simply open matlab and press go. Explore what happens as you change the seed using the `rng(seed)` instruction.

> In this coursework you may need to use the following Matlab commands: `normrnd` and `hist` or `histogram` (depending on version). You will also find it useful to define functions analogously to `f= @(x) x^2`; f(x) will then return x^2. You can check the Matlab help by using `help COMMAND`.