Random walks

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1 Why study random walks?

Random walks have a huge number of applications in statistical mechanics. You have already seen that they can be used as a model of diffusion. We can include absorbing boundaries to model adsorption or other similar processes. A self-avoiding random walk (defined in the next section) can be used as a model for a polymer. Some types of energy transfer processes can also be modeled as random walks. There are lots of other examples. There are also lots of applications in other areas, including ecology (movement of animals in an environment) and economics (modeling short-term market fluctuations).

2 Types of random walks

The random walk described in the textbook is an **unbiased and unbounded random walk in one dimension**. We can of course look at random walks in higher dimensional spaces. We can also study **biased** random walks in which the probabilities of moving to the right or left are different. Another variation is a bounded random walk, in which the space on which the random walk occurs is finite. There are at least two versions of these: We can have a random walk with a **reflecting boundary**, modeling for instance diffusion in a container of finite size. We can also have a random walk with an **absorbing boundary**, which describes a process that stops when some particular value of a variable is reached. An example of the latter is the famous gambler's ruin problem: A gambler starts with x dollars and stops when he runs out of money. What is the probability that the gambler will run out of money, and what is the expected time to ruin?

In addition to looking at random walks in different numbers of spatial dimensions, we can also study random walks in spaces of different connectivity. For example, we can study random walks on square lattices or on hexagonal lattices. We can also study random walks on lattices where each site is only connected to some of its nearest neighbors. This might be a model of diffusion through a zeolite or other porous material.

Generally, in random walk models, the time is a discrete variable: The time steps are numbered, and at each time step the walker takes a step. In some variations, the walker

can stay in its location instead of taking a step, but time is still discrete. It is also possible to treat the case where the time between steps is a random variable. This kind of model is particularly useful for describing chemical reactions and related processes.

Another important type is the **self-avoiding random walk**. A self-avoiding random walk is one that is not allowed to revisit the same site twice. Special techniques are required to generate self-avoiding random walks since there is a tendency, particularly in two dimensions, for simple methods to get "stuck", i.e. to advance the walker to a position where it is completely surrounded by sites it has already visited. Since self-avoiding walks are often used to simulate polymer conformations, we need to be able to generate walks with a preset number of steps (monomers or segments), so getting stuck after some small number of steps is something we need to avoid.

3 Some questions associated with random walks

Depending on the application, we may be interested in asking different questions about a random walk process. However, there are some questions that come up over and over again:

Root-mean-squared distance: How does the root-mean-squared distance travelled depend on the number of steps taken?

Mean recurrence time: What is the average interval of time (number of steps) between visits to a particular site (e.g. the origin of the walk)? In some cases (e.g. an unbiased random walk in three dimensions), the mean recurrence time is infinite, which means that a random walker will eventually wander away and not return.

Mean time to capture: What is the average time required for a walker to be captured by (e.g.) an absorbing boundary?

Capture/escape probability: What is the probability that a walker will be captured (or not) by an absorbing boundary or site(s)?

Mean first-passage time: What is the average time required to reach a particular target?

Theoretical expressions can be obtained for all of these quantities in some simple cases. In other cases, we need to use simulations.

4 Markov processes

Loosely, a **Markov process** is a random process for which the probabilities of future states depend only on the current state, and not on the prior history. An ordinary random walk is clearly a Markov process: If I know where the random walker is now, I can calculate the probability that it will reach some given site at a later time without knowing how it reached its current position.

Let $P_n(x)$ be the probability that a random walker has reached coordinate x after n steps from some specified initial condition (often $x = 0$). The transition probability $W_k(X|x)$ is

the probability that, if the random walker was at coordinate x at step n, then it will be at $x = X$ k steps later. Markov processes obey the following relationship:

$$P_n(X) = \sum_x W_k(X|x) P_{n-k}(x), \tag{1}$$

where the sum is taken over all values of x_1 at which the walker could have been k steps earlier.

5 The biased random walk in one dimension

We are going to look at a biased random walk in one dimension. If an unbiased random walk is a model of diffusion, a biased walk might be a model of diffusion with an added drift velocity. We will in fact now derive a **diffusion-advection** equation for a random walk, i.e. an equation with both a diffusion term and a directed drift component.

We first need to define our random walk model. Let p be the probability that the random walker takes a step to the right in the next time step, i.e. the probability that the coordinate (m) will be incremented by 1. Similarly, let q be the probability that the random walker takes a step to the left. We allow for the possibility that the walker stays where it is in a time step, i.e. that $p + q < 1$ such that the probability of staying in place is $1 - p - q$. The constants p, q and $1 - p - q$ are the transition probabilities in this model. If we apply equation 1 with $k = 1$, we get

$$P_n(m) = pP_{n-1}(m-1) + qP_{n-1}(m+1) + (1-p-q)P_{n-1}(m),$$

or

$$P_n(m) - P_{n-1}(m) = pP_{n-1}(m-1) + qP_{n-1}(m+1) - (p+q)P_{n-1}(m),$$

The quantity on the left of the equal sign looks a little like a time derivative. In fact, if one time step takes time Δt,

$$\frac{\partial P(x,t)}{\partial t} \approx \frac{P_n(m) - P_{n-1}(m)}{\Delta t}.$$

The quantity on the right of the equal sign needs more work. It can be rewritten in the form

$$\begin{aligned} pP_{n-1}(m-1) + qP_{n-1}(m+1) + -(p+q)P_{n-1}(m) & \\ = \frac{1}{2}(p+q)\left[P_{n-1}(m-1) - 2P_{n-1}(m) + P_{n-1}(m+1)\right] & \\ - \frac{1}{2}(p-q)\left[P_{n-1}(m+1) - P_{n-1}(m-1)\right]. & \end{aligned} \tag{2}$$

If the steps of our random walk are of length Δx, then the last term in this equation is related to the spatial derivative of P:

$$\frac{\partial P(x, t-\Delta t)}{\partial x} \approx \frac{P_{n-1}(m+1) - P_{n-1}(m-1)}{2\Delta x}. \tag{3}$$

(Note that $x = m\Delta x$.) This may be less obvious, but the quantity after the equal sign in equation 2 is in fact related to the second derivative with respect to position. The second derivative is defined by

$$\begin{aligned}\frac{\partial^2 P(x,t-\Delta t)}{\partial x^2} &\approx \frac{1}{\Delta x}\left[\frac{\partial P(x+\Delta x,t-\Delta t)}{\partial x} - \frac{\partial P(x,t-\Delta t)}{\partial x}\right] \\ &\approx \frac{1}{\Delta x}\left[\frac{P_{n-1}(m+1)-P_{n-1}(m)}{\Delta x} - \frac{P_{n-1}(m)-P_{n-1}(m-1)}{\Delta x}\right] \\ &= \frac{1}{(\Delta x)^2}\left[P_{n-1}(m+1) - 2P_{n-1}(m) + P_{n-1}(m-1)\right].\end{aligned}$$

Putting it all together, we get

$$\Delta t\frac{\partial P(x,t)}{\partial t} = \frac{(\Delta x)^2(p+q)}{2}\frac{\partial^2 P(x,t-\Delta t)}{\partial x^2} - \Delta x(p-q)\frac{\partial P(x,t-\Delta t)}{\partial x}.$$

The above derivation assumes that Δt is small. That being the case, and assuming that P is a continuous function of t, $P(x,t-\Delta t) \approx P(x,t)$. We get

$$\frac{\partial P(x,t)}{\partial t} = \frac{(\Delta x)^2}{2\Delta t}(p+q)\frac{\partial^2 P(x,t)}{\partial x^2} - \frac{\Delta x}{\Delta t}(p-q)\frac{\partial P(x,t)}{\partial x}.$$

If we identify

$$D = \frac{(\Delta x)^2}{2\Delta t}(p+q) \tag{4}$$

$$\text{and} \quad u = \frac{\Delta x}{\Delta t}(p-q), \tag{5}$$

we get

$$\frac{\partial P(x,t)}{\partial t} = D\frac{\partial^2 P(x,t)}{\partial x^2} - u\frac{\partial P(x,t)}{\partial x}. \tag{6}$$

Note that if $p = q = \frac{1}{2}$, equation 4 is the Einstein-Smoluchowski equation for the diffusion coefficient. This equation is therefore a generalization of the Einstein-Smoluchowski result to the biased random walk. Also note that u defined by equation 5 is a velocity. Equation 6 can be transformed to a form which is more clearly a diffusion-advection equation by noting that, for a system that contains N_0 particles undergoing the biased random walk process, the lineal concentration is $c(x,t) = N_0 P(x,t)/\Delta x$ so that c satisfies the equation

$$\frac{\partial c(x,t)}{\partial t} = D\frac{\partial^2 c(x,t)}{\partial x^2} - u\frac{\partial c(x,t)}{\partial x}. \tag{7}$$

The last term in this equation is an advection (drift) term. If $u > 0$ ($p > q$), then this term will cause the distribution $c(x,t)$ to drift to the right. To see this, consider figure 1 and imagine a case where diffusion is weak so that the advective term dominates. In the tail of the distribution (small x), $\partial c/\partial x > 0$, so $\partial c/\partial t < 0$. The tail therefore dies away. At the leading edge (to the right of the maximum), $\partial c/\partial x < 0$, so $\partial c/\partial t > 0$. The leading

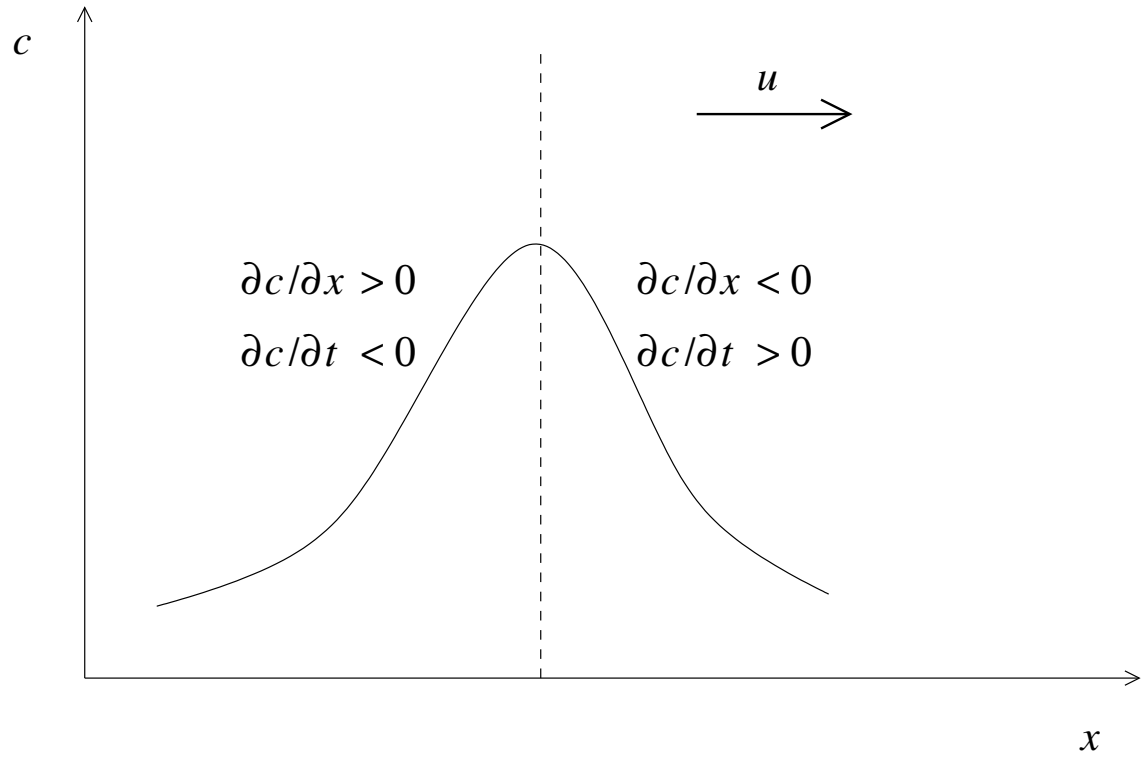

Figure 1: Motion of a concentration distribution for equation 7 in the case of weak diffusion with $u > 0$.

edge therefore grows. Growth ahead of the maximum and decay behind it results in a net movement in the direction of u.

The diffusion-advection equation 7 can be solved. The solution for a delta-function initial condition at $x = 0$ is

$$c(x,t) = \frac{N_0}{\sqrt{4\pi Dt}} \exp\left(\frac{-(x-ut)^2}{4Dt}\right).$$

The expression $x - ut$ is characteristic of traveling wave solutions. In this case, because of diffusion, the wave both travels and dissipates.