6.055J / 2.038J The Art of Approximation in Science and Engineering
Spring 2008

Chapter 9
Discretization

9.1 Diaper usage

9.2 Pendulum period

9.3 Random walks

Random walks are everywhere. Do you remember the card game War? How long does it last, on average? A molecule of neurotransmitter is released from a vesicle. Eventually it binds to the synapse, and your leg twitches. How long does it take to get there? On a winter day, you stand outside wearing only a thin layer of clothing. Why do you feel cold?

These physical situations are examples of random walks. In a physical random walk, for example a gas molecule moving and colliding, the walker moves a variable distance and can move in any direction. This general situation is complicated. Fortunately, the essential features of the random walk do not depend on these complicated details.

Simplify by discarding the generality. The generality arises from the continuous degrees of freedom: the direction is continuous and the distance between collisions is continuous. So, discretize the direction and the distance: Assume that the particle travels a fixed distance between collisions and that it can move only along the coordinate axes. Furthermore, analyze the special case of one-dimensional motion before going to the more general cases of two- and three-dimensional motion.

In this discretized, one-dimensional model, a particle starts at the origin and moves along a line. At each tick it moves left or right with probability 1/2 in each direction. Let the position after n steps be x_n, and the expected position after n steps be $\langle x_n \rangle$. Because the random walk is unbiased – because moving in each direction is equally likely – the expected position remains constant:

$$\langle x_n \rangle = \langle x_{n-1} \rangle.$$

So $\langle x \rangle$, the so-called first moment of the position, is an invariant. However, it is not a fascinating invariant because it does not tell us much that we do not already understand intuitively.

Given that the first moment is not interesting, try the next-most-complicated moment: the second moment $\langle x^2 \rangle$. This analysis is easiest in special cases. Suppose that after a while wandering, the particle has arrived at 7, i.e. $x = 7$. At the next tick it will be at either $x = 6$ or $x = 8$. Its expected squared position – not its squared expected position! – has become

$$\langle x^2 \rangle = \frac{1}{2}\left(6^2 + 8^2\right) = 50.$$

The expected squared position increased by 1.

Let's check this pattern in a second example. Suppose that the particle is at $x = 10$, so $\langle x^2 \rangle = 100$. After one tick, the new expected squared position is

$$\langle x^2 \rangle = \frac{1}{2}\left(9^2 + 11^2\right) = 101.$$

Yet again $\langle x^2 \rangle$ has increased by 1! Based on those two examples, the conclusion is that

$$\langle x_{n+1}^2 \rangle = \langle x_n^2 \rangle + 1.$$

In other words,

$$\langle x_n^2 \rangle = n.$$

Since each step takes a constant time, in this discretized analysis, the conclusion is that

$$\langle x_n^2 \rangle \propto t.$$

The result that $\langle x^2 \rangle$ is proportional to time applied to the one-dimensional random walk. And it works for any dimension. Here's an example in two dimensions. Suppose that the particle's position is $(5, 2)$, so $\langle x^2 \rangle = 29$. After one step, it has four equally likely positions:
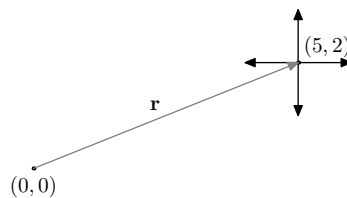
Rather than compute the new expected squared distance using all four positions, be lazy and just look at the two horizontal motions. The two possibilities are $(6, 2)$ and $(4, 2)$. The expected squared distance is

$$\langle x^2 \rangle = \frac{1}{2}(40 + 20) = 30,$$

which is one more than the previous value of $\langle x^2 \rangle$. Since nothing is special about horizontal motion compared to vertical motion – symmetry! – the same result holds for vertical motion. So, averaging over the four possible locations produces an expected squared distance of 30.

For two dimensions, the pattern is:

$$\langle x_{n+1}^2 \rangle = \langle x_n^2 \rangle + 1.$$

No step in the analysis depended on being in only two dimensions. In fancy words, the derivation and the result are invariant to change of dimensionality. In plain English, this result also works in three dimensions.

9.3.1 Difference between a random walk and a regular walk

In a standard walk in a straight line, $\langle x \rangle \propto$ time. Note the single power of x. The interesting quantity in a regular walk is not x itself, since it can grow without limit and is not invariant, but the ratio x/t, which is invariant to changes in t. This invariant is also known as the speed.

In a random walk, where $\langle x^2 \rangle \propto t$, the interesting quantity is $\langle x^2 \rangle/t$. The expected squared position is not invariant to changes in t, but the ratio $\langle x^2 \rangle/t$ is an invariant. This invariant is, except for a dimensionless constant, the *diffusion constant* often denoted D. It has dimensions of $L^2 T^{-1}$.

The difference between a random and a regular walk makes intuitive sense. A random walker, for example a gas molecule or a very drunk person, moves back and forth, sometimes making progress in one direction, and other times undoing that progress. So a random walker should take longer than a regular walker would take to travel the same distance. The relation $\langle x^2 \rangle/t \sim D$ confirms and sharpens this intuition. The time for a random walker to travel a distance l is $t \sim l^2/D$, which grows quadratically rather than linearly with distance.

9.3.2 Diffusion equation

The discretized model of a random explains where the diffusion equation comes from. Imagine a gas of particles with each particle doing a random walk in one dimension. How does the concentration, or number, change with time?

Slice the one-dimensional world into slices of width Δx, and look at the slices at $x - \Delta x$, x, and $x + \Delta x$. In every time step, one-half the molecules in each slice move left, and one-half move right. So the number at x changes from $N(x)$ to

$$\frac{1}{2}(N(x - \Delta x) + N(x + \Delta x)),$$

for a change of

$$\begin{aligned} \Delta N &= \frac{1}{2}(N(x - \Delta x) + N(x + \Delta x)) - N(x) \\ &= \frac{1}{2}(N(x - \Delta x) - 2N(x) + N(x + \Delta x)). \end{aligned}$$

This last relation can be rewritten as

$$\Delta N \sim (N(x + \Delta x) - N(x)) - (N(x) - N(x + \Delta x)),$$

which in terms of derivatives is

$$\Delta N \sim (\Delta x)^2 \frac{\partial^2 N}{\partial x^2}.$$

The slices are separated by a distance such that most of the molecules travel from one piece to the neighboring piece in the time step τ. If τ is the time between collisions – the mean free time – then the distance is the mean free path λ. Thus

$$\frac{\Delta N}{\tau} \sim \frac{\lambda^2}{\tau} \frac{\partial^2 N}{\partial x^2},$$

or

$$\dot{N} \sim D\frac{\partial^2 N}{\partial x^2}$$

where $D \sim \lambda^2/\tau$ is a diffusion constant.

This partial-differential equation has interesting properties. The second spatial derivative means that a linear spatial concentration gradient remains unchanged: Its second derivative is zero so its time derivative must be zero. Diffusion smashes only curvature – roughly speaking, the second derivative – and does not try to change just the gradient. Heat often diffuses by a random walk, either via phonons (in a liquid or solid) or via molecular random walks (in a gas), so if you maintain one end of a bar at T_1 and the other end at T_2, then the bar will eventually linearly interpolate between the two temperatures, as long as heat is fed into the hot end and drawn out of the cold end.

9.3.3 Keeping warm

One consequence of random walks is how to keep warm on a cold day. We need to calculate the flux of heat: the energy flowing per unit area per unit time. We start from the definition of flux and reason physically.

Flux of stuff is defined as

$$\text{flux of stuff} = \frac{\text{stuff}}{\text{area} \times \text{time}}.$$

The flux depends on the density of stuff and on how fast the stuff travels:

$$\text{flux of stuff} = \frac{\text{stuff}}{\text{volume}} \times \text{speed}.$$

You can check that the dimensions are the same on both sides.

For heat flux, the stuff is thermal energy. The specific heat c_p is the thermal energy per mass, and $\rho c_p T$ is the thermal energy per volume. The speed is the 'speed' of diffusion. To diffuse a distance l takes time $t \sim l^2/D$, making the speed l/t or D/l. The l in the denominator indicates that, as expected, diffusion is slow over long distances. For heat diffusion, the diffusion constant is denoted κ and called the thermal diffusivity. So the speed is l/κ.

Combine the thermal energy per volume with the diffusion speed:

$$\text{thermal flux} = \rho c_{\mathrm{p}} T \times \frac{\kappa}{l}.$$

The product $\rho c_{\mathrm{p}} \kappa$ occurs so frequently that it is given a name: the thermal conductivity K. And the ratio T/l is a discretized version of the temperature gradient $\Delta T/\Delta x$. With those substitutions, the thermal flux is

$$F = K \frac{\Delta T}{\Delta x}.$$

To estimate how much heat one loses on a cold day, we need to estimate $K = \rho c_{\mathrm{p}} \kappa$. Time to put all the pieces together for air:

$$\rho \sim 1 \, \mathrm{kg \, m^{-3}},$$
$$c_{\mathrm{p}} \sim 10^3 \, \mathrm{J \, kg^{-1} \, K^{-1}},$$
$$\kappa \sim 1.5 \cdot 10^{-5} \, \mathrm{m^2 \, s^{-1}},$$

where we are guessing that $\kappa = \nu$, since both are diffusion constants. Then

$$K = \rho c_{\mathrm{p}} \kappa \sim 0.02 \, \mathrm{W \, m^{-1} \, K^{-1}}.$$

Now we can estimate the heat loss outside on a cold day. Let's say that your skin is at $30\,^{\circ}\mathrm{C}$ and the air outside is $0\,^{\circ}\mathrm{C}$, so $\Delta T = 30 \, \mathrm{K}$. A thin T-shirt may have thickness $2\,\mathrm{mm}$, so

$$F = K \frac{\Delta T}{\Delta x} \sim 0.02 \, \mathrm{W \, m^{-1} \, K^{-1}} \times \frac{30 \, \mathrm{K}}{2 \cdot 10^{-3} \, \mathrm{m}} \sim 300 \, \mathrm{W \, m^{-2}}.$$

Damn, I wanted a power not a power per area. Oh, flux is power per area, so all is well. I just need to multiply by my surface area. I'm roughly $2\,\mathrm{m}$ tall (approximately!) and $0.5\,\mathrm{m}$ wide, so my front and back each have area $1 \, \mathrm{m}^2$. Then

$$P \sim FA = 300 \, \mathrm{W \, m^{-2}} \times 2 \, \mathrm{m}^2 = 600 \, \mathrm{W}.$$

No wonder it feels so cold! Just sitting around, your body generates $100\,\mathrm{W}$ (the basal metabolic rate). So, with $600\,\mathrm{W}$ escaping, you lose far more heat more than you generate. After long enough, your core body temperature drops. Chemical reactions in your body slow down, because all reactions go slower at lower temperature, and because enzymes lose their optimized shape. Eventually you die.

One solution is jogging to generate extra heat. That solution indicates that the estimate of $600\,\mathrm{W}$ is plausible. Cycling hard, which generates hundreds of watts of waste heat, is vigorous enough exercise to keep you warm, even on a winter day in thin clothing.

Another simple solution, as parents repeat to their children: Dress warmly by putting on thick layers. Let's recalculate the power loss if you put on a fleece that is $2\,\mathrm{cm}$ thick. You could redo the whole calculation from scratch, but it is simpler is to notice that the thickness has gone up by a factor of 10. Since $F \propto 1/\Delta x$, the flux and the power drop by a factor of 10. So, when wearing the fleece,

$$P \sim 60 \, \mathrm{W}.$$

That heat loss is smaller than the basal metabolic rate, which indicates that you do not feel too cold. Indeed, when wearing a thick fleece, you feel most cold in your hands and face. Those regions are exposed to the air, and are protected by only a thin layer of still air. Because a small Δx means a large heat flux, the moral is: Listen to your parents, bundle up!

9.4 Boundary layers