CHAPTER 10

Diffusion and Random Walks

10.1 Random walk against odds

We consider a gambling game in which your objective is to win N dollars, starting with $n < N$. We assume that if you run out of money, you can always borrow 1 dollar to continue the game. Therefore, to achieve your objective is certain. The question is how long; and a more challenging question how much you have to borrow.

Of couse, playing with a casino means the odd of doubling a dollar, p is always a little less than that lossing the dollar $q > p$, $p + q = 1$. Let T_n be the mean time to reach your objective. Then

$$T_n = qT_{n-1} + pT_{n+1} + 1. \tag{10.1}$$

This is a linear, constant coefficient, 2nd order, inhomogeneous difference equation. So to solve it, we first consider the corresponding time homogeneous equation

$$\widetilde{T}_n = q\widetilde{T}_{n-1} + p\widetilde{T}_{n+1}. \tag{10.2}$$

Let $\widetilde{T} = \alpha\beta^n$, then we have the characteristic equation

$$\alpha\beta^n = q\alpha\beta^{n-1} + p\alpha\beta^{n+1}. \tag{10.3}$$

This yields for $\alpha \neq 0$,

$$\beta = q + p\beta^2 \ \Rightarrow \beta_{1,2} = \frac{1 \pm \sqrt{1 - 4pq}}{2p} = 1 \text{ and } \frac{q}{p}. \tag{10.4}$$

The general solution to the homogeneous equation (10.2) is

$$\widetilde{T}_n = \alpha_1\beta_1^n + \alpha_2\beta_2^n. \tag{10.5}$$

We need to also fine a particular solution to the inhomogeneous equation (10.1). It can be the form

$$T_n^* = \frac{an}{q - p}, \text{ in which } a = 1. \tag{10.6}$$

Therefore, the general solution to the inhomogeneous equation (10.1) is

$$T_n = \alpha_1 + \alpha_2 \left(\frac{q}{p}\right)^n + \frac{n}{q - p}. \tag{10.7}$$

To determine the two αs, we have

$$T_0 = T_1, \quad T_N = 0. \tag{10.8}$$

This gives two simultaneous equations for α_1 and α_2

$$\left(1-\frac{q}{p}\right)\alpha_2=\frac{1}{q-p},\;\;\alpha_1+\left(\frac{q}{p}\right)^N\alpha_2=-\frac{N}{q-p}, \tag{10.9}$$

which yield

$$\alpha_1=\frac{q\big(q/p\big)^{N-1}+N(p-q)}{(q-p)^2},\;\;\alpha_2=-\frac{p}{(q-p)^2}. \tag{10.10}$$

That is,

$$T_n \;=\; \frac{p}{(q-p)^2}\left[\left(\frac{q}{p}\right)^N-\left(\frac{q}{p}\right)^n+(N-n)\left(1-\frac{q}{p}\right)\right]. \tag{10.11}$$

We see that if $q<p$, then with large N and n, $T_n\approx\frac{N-n}{p-q}$. If $q=p$, then $T_n=(N-n)(N+n-1)$. Finally, the most interesting and important case, when $q>p$, then for $N,n\gg 1$:

$$T_n\approx\frac{p}{(q-p)^2}\left(\frac{q}{p}\right)^N. \tag{10.12}$$

We see even though the random "walker" started at n, it is as if it were started at $n=0$. The time to arrive at N is exponentially long. On the other hand, if $p>q$, then the time is directly proportional to $N-n$ and inversely proportional to $p-q$. $(p-q)$ is actually the expected gain, in dollar amout, *per* one dollar bet.

10.2 Barrier crossing in bistable systems

$$D\frac{dT^2(x)}{dx^2}+F(x)\frac{dT}{dx}=-1, \tag{10.13}$$

with boundary condition $T_x(0)=0$ and $T(L)=0$.

10.3 Heat equation and immigration

Heat is often considered as "things" that can move, from high temperature region to low temperature region. A similar argument also applies to movement of dye molecules in water.

The movement of "heat" in space is usually described by the *heat equation*, first developed by Jean Baptiste Joseph Fourier (1768-1830):

$$\frac{\partial u(x,t)}{\partial t}=D\frac{\partial^2u(x,t)}{\partial x^2}, \tag{10.14}$$

where D is called heat diffusion constant.

It turns out, spatical movements of any population, be it animals, biological organisms, or molecules, all can be described by the same *diffusion equation* (10.14). We have talked about *birth* and *death* of individuals in a population. We now address the spatial movement, i.e., *immigration*, of individuals in a population. In 1-dimensional space, we have

$$\frac{\partial u(x,t)}{\partial t} = -\frac{\partial J(x,t)}{\partial x} + b(x,t) - d(x,t), \tag{10.15}$$

in which $J(x,t)$ is the immigration (transport) flux.

10.4 Random walk and diffusion

Let us again consider the drunken walker. In fact, we consider a hugh population of drunken walkers, distributed in space and time $n(x,t)$, where x and t take discrete values $x = 0, \pm\delta x, \pm 2\delta x, \cdots$, and $t = 0, \delta t, 2\delta t, \cdots$.

The result will be like a Pascal's triangle:

$$u(x, t+\delta t) = pu(x-\delta x, t) + qu(x+\delta x, t), \tag{10.16}$$

where $p + q = 1$. They do not have to be the same. When $p = q = \frac{1}{2}$, we say the random walk is unbiased. Otherwise, it is biased.

Eq. (11.2) can be re-written as

$$u(x,t+\delta t) - u(x,t) = -p\left(u(x,t) - u(x-\delta x,t)\right) + q\left(u(x+\delta x,t) - u(x,t)\right), \tag{10.17}$$

Therefore, if we identify

$$\frac{u(x,t+\delta t) - u(x,t)}{\delta t} = \frac{\partial u(x,t)}{\partial t}, \quad \frac{u(x+\delta x,t) - u(x,t)}{\delta x} = \frac{\partial u(x,t)}{\partial x},$$

then we have

$$\frac{\partial u(x,t)}{\partial t} = D\frac{\partial^2 u(x,t)}{\partial x^2} - V\frac{\partial u(x,t)}{\partial x} \tag{10.18}$$

with $D = (\delta x)^2/(2\delta t)$ and $V = (p-q)\delta x/\delta t$. We see that when $p = q = \frac{1}{2}$, we have the well-known heat equation. And more generally, Fourier-Fick's law for the transport flux

$$J(x,t) = -D\frac{\partial u(x,t)}{\partial x} + Vu(x,t). \tag{10.19}$$

Note that the Fourier-Fick's law should be understood as a population behavior. It should *not* be interpreted as an individual knowing anything about what others are doing!

10.5 Advection and moving frame of reference

The D-term and V-term in Eq. (11.6) are known as *diffusion* and *advection*, respctively. The advection can be understood from a very different perspective, as described in the Appendix of Chap. 12 in the text.

Consider a pure diffusion superimposed with a constant drift with velocity V leftward . Now in a moving frame which moves with *the flow*, one has its distribution $\widetilde{u}(x,t) = u(x+Vt,t)$, where $u(x,t)$ is what observed in the stationary frame of reference. Now in the moving frame of reference, the $\widetilde{u}(x,t)$ is a pure diffusion:

$$\frac{\partial \widetilde{u}(x,t)}{\partial t} = D\frac{\partial^2 \widetilde{u}(x,t)}{\partial x^2}.$$

Therefore, applying the chain rule

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

Let us now solve a problem of diffusion with advection $-V$ against a wall at $x = 0$: $x \geq 0$.

$$D\frac{d^2u(x)}{dx^2} + V\frac{du(x)}{dx} = 0,$$

$$D\frac{du(x)}{dx} + Vu(x,t) = \text{ const. },$$

$$\text{const. } = 0 \text{ at } x = 0.$$

$$D\frac{du(x)}{dx} = -Vu,$$

$$u(x) = u(0)e^{-Vx/D}.$$

10.6 Solution to the random walk problem

A single particle starting at $n = 0$ at $t = 0$, the solution $u(x,t)$ to Eq. (11.2) is $u\big(m\delta x, n\delta t\big) = u_{m,n}$,

$$u_{m,n} = \binom{n}{\frac{n+m}{2}} p^{\frac{n+m}{2}} q^{\frac{n-m}{2}}, \tag{10.20}$$

in which for odd n, only terms with odd m are non-zero; and for even n, only terms with evne m are non-zero. For example when $p = q = \frac{1}{2}$, we have

$$\begin{array}{cc} 0 & 1 \\ 1 & 1\ 0\ 1 \\ 2 & 1\ 0\ 2\ 0\ 1 \\ 3 & 1\ 0\ 3\ 0\ 3\ 0\ 1 \\ 4 & 1\ 0\ 4\ 0\ 6\ 0\ 4\ 0\ 1 \\ \vdots & \ldots \end{array} \tag{10.21}$$

The variance of the distributions given in (10.21) is 1 per time step. Hence, ℓ for $n = \ell$:

Now substituting $m = \frac{x}{2\delta x}$ and $n = \frac{t}{2\delta t}$, we have

$$u(x,t) = \binom{t/(2\delta t)}{\frac{t/(\delta t)+x/(\delta x)}{4}} \left(\frac{1}{2}\right)^{t/(2\delta t)}. \tag{10.22}$$

Taking the limit of $\delta x, \delta t \to 0$ and $\frac{(\delta x)^2}{2(\delta t)} = D$ we have, according to Stirling's formula:

$$\begin{aligned}
\ln u(x,t) &\approx -\left(\frac{t}{4(\delta t)} + \frac{x}{4(\delta x)}\right)\ln\left(\frac{1}{2} + \frac{x(\delta t)}{2t(\delta x)}\right) - \left(\frac{t}{4(\delta t)} - \frac{x}{4(\delta x)}\right)\ln\left(\frac{1}{2} - \frac{x(\delta t)}{2t(\delta x)}\right) \\
&\quad + \left(\frac{t}{(2\delta t)}\right)\ln\frac{1}{2} \\
&\approx -\left(\frac{t}{4(\delta t)} + \frac{x}{4(\delta x)}\right)\ln\left(1 + \frac{x(\delta x)}{2Dt}\right) - \left(\frac{t}{4(\delta t)} - \frac{x}{4(\delta x)}\right)\ln\left(1 - \frac{x(\delta x)}{2Dt}\right) \\
&= -\left(\frac{t}{4(\delta t)} + \frac{x}{4(\delta x)}\right)\frac{x(\delta x)}{2Dt} + \left(\frac{t}{4(\delta t)} - \frac{x}{4(\delta x)}\right)\frac{x(\delta x)}{2Dt} + O(\delta x) \\
&= -\frac{x^2}{4Dt}.
\end{aligned}$$

Therefore,

$$u(x,t) \propto \exp\left(-\frac{x^2}{4Dt}\right). \tag{10.23}$$

That is,

$$u(x,t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right). \tag{10.24}$$

Solution to the diffusion equation with advection V is

$$u(x,t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{(x-Vt)^2}{4Dt}\right). \tag{10.25}$$

10.7 The meaning and significance of Fourier-Fick's law

10.8 Exit time

$$\frac{\partial u(x,t)}{\partial t} = -\frac{\partial}{\partial x}J(x,t). \tag{10.26}$$

$$\frac{\mathrm{d}}{\mathrm{dt}}\int_a^b u(x,t)\mathrm{d}x = J(a,t) - J(b,t). \tag{10.27}$$

To the interval $[a,b]$, noting that $J(a,t)$ is the flux going into the interval while $J(b,t)$ is the flux going out of the interval, we have

$$\frac{\mathrm{d}}{\mathrm{dt}}\int_a^b u(x,t)\mathrm{d}x = -J_{\text{going out at the boundary}}(t).$$

In terms of probability,

$$\int_a^b u(x,t)\mathrm{d}x = \Pr\left\{T > t\right\}, \tag{10.28}$$

where T is the random time that the diffusor is still inside. Then, the probability density function of T:

$$f_T(t) = -\frac{\mathrm{d}}{\mathrm{d}t}\int_a^b u(x,t)\mathrm{d}x, \tag{10.29}$$

from which, the mean time can be computed.

10.9 How to statistically determine the D and V from a large amount of single diffusor data?