Solutions to the Midterm Exam

Martin Z. Bazant

November 16, 2006

1 Discrete versus continuous steps in a random walk

1.1 Finding a generating function and $D_2(a)$

For $p_n = Ca^{|n|}$, the probability generating function is

$$\begin{aligned} P(z) &= \sum_{n=-\infty}^{\infty} p_n z^n \\ &= C\left[\sum_{n=0}^{\infty}(az)^n + \sum_{n=1}^{\infty}\left(\frac{a}{z}\right)^n\right] \\ &= C\left[\frac{1}{1-az} + \frac{a}{z-a}\right] \quad (a < |z| < a^{-1}) \\ &= C\left[\frac{(1-a^2)z}{(1-az)(z-a)}\right]. \end{aligned}$$

For normalization, $P(1) = \sum p_n = 1$, we need

$$C(a) = \frac{1-a}{1+a}$$

and thus

$$P(z) = \frac{(1-a)^2 z}{(1-az)(z-a)}.$$

The second moment is easily calculated as

$$\sigma^2 = \sum_{n=-\infty}^{\infty} n^2 p_n = \sum_{n=-\infty}^{\infty} n(n-1)p_n = P''(1)$$

where we use $\sum np_n = 0$ since $p_n = p_{-n}$. Since

$$P''(z) = 2aC[a(1-az)^{-3} + (z-a)^{-3}], \qquad P''(1) = \frac{2(a+1)aC}{(1-a)^3}$$

we finally obtain the diffusivity,

$$D_2(a) = \frac{\sigma^2}{2\tau} = \frac{C(1+a)a}{(1-a)^3} = \frac{a}{(1-a)^2}$$

since the time step in the continuum approximation is $\tau = 1$.

1.2 Continuum approximation

Now we consider the continuum approximation,

$$p(x) = \frac{1}{2b}e^{-|x|/b}, \quad (b = -1/\log a)$$

which has the same exponential decay as p_n for $|n| \gg 1$. The Fourier transform should look familiar (from problem set 2), but it's easy enough to work out again:

$$\begin{aligned}
\hat{p}(k) &= \int_{-\infty}^{\infty} e^{-ikx} p(x)dx \\
&= \frac{1}{2b}\left(\int_0^{\infty} e^{-x(ik+1/b)}dx + \int_{-\infty}^{0} e^{x(-ik+1/b)}dx\right) \\
&= \frac{1}{2}\left(\frac{1}{1+ibk} + \frac{1}{1-ibk}\right) \\
&= \frac{1}{1+(bk)^2}.
\end{aligned}$$

The cumulant generating function is

$$\psi(k) = \log \hat{p}(k) = -\log(1+(bk)^2) = \sum_{m=1}^{\infty} \frac{(-1)^m (bk)^{2m}}{m} \equiv \sum_{n=1}^{\infty} \frac{(-i)^n c_n k^n}{n!}$$

which implies $c_{2m+1} = 0$ and

$$c_{2m} = \frac{(2m)! b^{2m}}{m}.$$

The coefficients in the modified Kramers-Moyall expansion are then $\bar{D}_{2m+1} = 0$ and

$$\bar{D}_{2m} = \frac{b^{2m}}{m} = \frac{1}{m(\log a)^{2m}}.$$

1.3 Log-linear plot

The two diffusivities are

$$D_2(a) = \frac{a}{(1-a)^2} \qquad \text{and} \qquad \bar{D}_2(b(a)) = \frac{1}{(\log a)^2}.$$

In the limit $a \to 1$ the width of the distribution $b = -1/\log a$ becomes much larger than the lattice spacing, and thus the continuum approximation should become exact, $D_2 \sim \bar{D}_2$, which is easily verified. In the opposite limit, $a \to 0$, the decay length for the distribution is much less than the lattice spacing, and the two models should be very different. In fact,

$$\frac{\bar{D}_2}{D_2} \sim \frac{1}{a(\log a)^2} \to \infty \qquad \text{as } a \to 0.$$

These limits are also clear in figure 1.

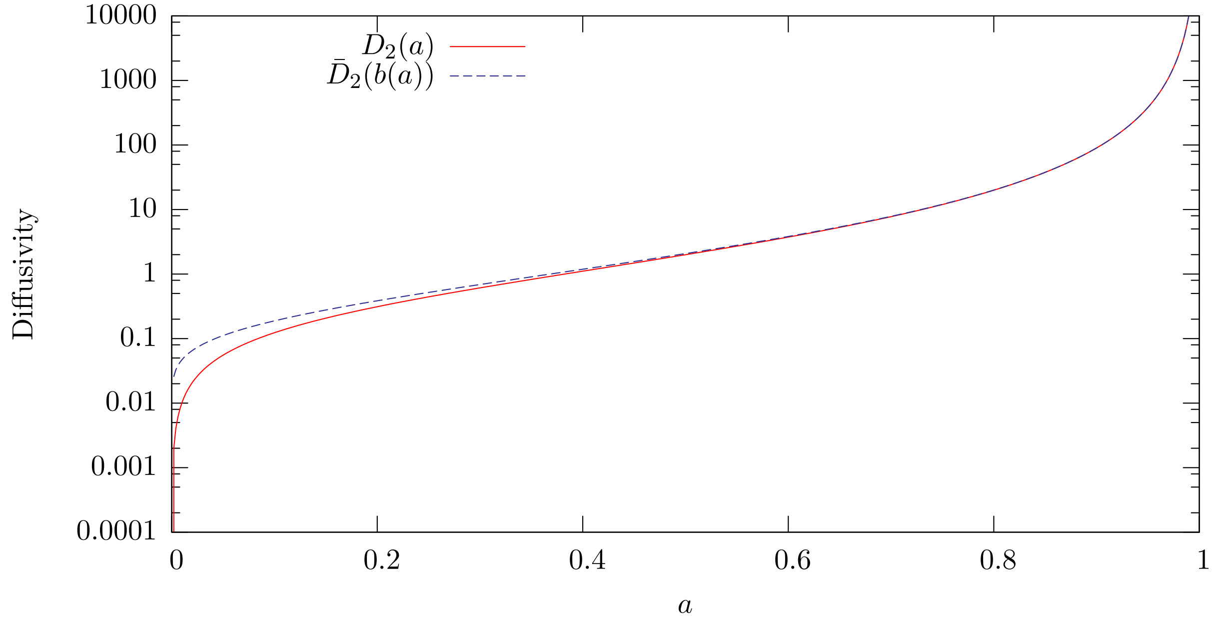

Figure 1: A log-linear plot of $D_2(a)$ and $\bar{D}_2(b(a))$.

2 First passage of N random walks in two dimensions

2.1 First passage position of a single walker

Since the diffusivity is a scalar (isotropic process), the Green function for the x-component (marginal probability density, after integrating out the y-component) will describe a one-dimensional x diffusion process with the same D,

$$G(x,t|0) = \frac{e^{-x^2/4Dt}}{\sqrt{4\pi Dt}}.$$

By symmetry, the x process plays no role in determining the first passage time, whose (Smirnov[1]) probability density will be same as for a one-dimensional y diffusion process with the same D,

$$f(t|a) = -S'(t|a) = \frac{ae^{-a^2/4Dt}}{\sqrt{4\pi Dt^3}}$$

where the survival probability is

$$S(t|a) = \text{erf}\left(\frac{a}{\sqrt{4Dt}}\right).$$

The hitting probability density can be calculated as

$$\varepsilon(x|a) = \int_0^\infty f(t|a)G(x,t|0)dt$$

since this is an integral over all times t of the probability that the x-component is x given that first passage occurs at time t. As noted above, these events are independent, so the integrand is just a

[1]There is a typo in the Exam 2, problem 2 solution from 2005: t should be t^3 under the square root. However, it is correct in Lecture 16 2005 notes and was correct in lecture this year.

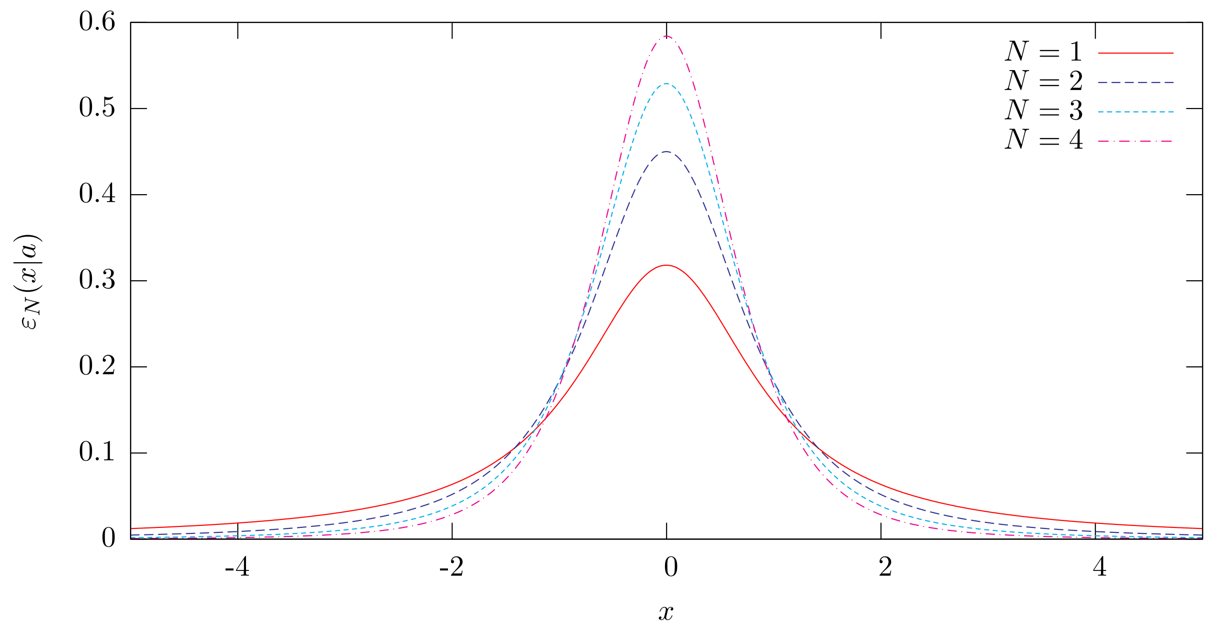

Figure 2: Plots of $\varepsilon_N(x|a)$ for several different values of N, for the case when $a = D = 1$. The case of $N = 1$ is the Cauchy distribution, while the cases $N > 1$ are from numerical integration of equation 1. The substitution $1/t = -\log\alpha$ was employed to change the integral into one over a finite range $0 < \alpha < 1$, and the resulting expression was evaluated using Simpson's rule.

product of the two probabilities. The integral is easily evaluated:

$$\begin{aligned}\varepsilon(x|a) &= \frac{a}{4\pi D}\int_0^\infty e^{-(x^2+a^2)/4Dt}\frac{dt}{t^2} \\ &= \frac{1}{\pi}\frac{a}{a^2+x^2}\end{aligned}$$

which is the same Cauchy distribution we obtained in lecture by conformal mapping. Note that $\langle x^2\rangle = \int_{-\infty}^{\infty} x^2\varepsilon(x|a)dx = \infty$.

2.2 First passage position of the first of N independent walkers

The probability that N independent walkers survive is just the product of the individual survival probabilities, $S_N(t) = S(t)^N$. Therefore, the PDF of the minimum first passage time is

$$f_N(t|a) = -\frac{d}{dt}S(t)^N = Nf(t|a)S(t)^{N-1}.$$

The hitting probability of the first walker is given by the x diffusion process sampled at this time,

$$\varepsilon_N(x|a) = \int_0^\infty f_N(t|0)G(x,t|0). \tag{1}$$

It does not seem that this integral can be performed analytically, so some numerical integrations are shown in figure 2.

The variance of the hitting position is given by

$$\begin{aligned}
\langle x^2 \rangle &= \int_{-\infty}^{\infty} x^2 \varepsilon_N(x|0)\, dx \\
&= \int_0^{\infty} dt\, f_N(t|a) \int_{-\infty}^{\infty} dx\, x^2 G(x,t|0) \\
&= \int_0^{\infty} dt\, f_N(t|a)\, 2Dt.
\end{aligned}$$

For $t \to \infty$ we have $f(t|a) \propto t^{-3/2}$, $S(t) \propto t^{-1/2}$, $f_N(t|a) \propto t^{-1-N/2}$, and thus the integrand decays like $t f_N(t|a) \propto t^{N/2}$. Therefore, the variance is finite only if $N/2 > 1 \Rightarrow N > 2 \Rightarrow N \geq 3$. So, once again $N_c = 3$ is the magic number of walkers such that the first one will hit in a region of finite variance in space. This should come as no surprise, because this is the same critical number needed to have a finite mean first passage time for the first walker, as shown in lecture.

3 First passage to a circle

In the physical z plane, the walker is released at $(x = a, y = 0)$ and hits the unit circle. We would like to map this domain with $w = f(z)$ to the interior of the unit circle with the source at the origin in the mathematical w plane, where we know the complex potential is

$$\Phi = \frac{\log w}{2\pi}.$$

We could choose a Möbius transformation with the constraints, $f(a) = 0$, $f(1) = -1$, $f(-1) = 1$, which yields

$$f(z) = \frac{z-a}{az-1}.$$

The complex potential in the z plane is therefore

$$\Phi = \frac{1}{2\pi} \log\left(\frac{z-a}{az-1}\right) = \frac{1}{2\pi}\Big(\log(z-a) - \log(z-a^{-1}) - \log a\Big)$$

which is clearly the sum of the source term and an image sink at $(a^{-1}, 0)$ (and a constant). The hitting probability density is given by the normal electric field on the circle:

$$\begin{aligned}
\varepsilon(\theta|a) &= \hat{n}\cdot\nabla\phi = -\mathrm{Re}(e^{i\theta}\overline{\Phi'}) \\
&= \mathrm{Re}\left(\frac{1}{1-a^{-1}e^{-i\theta}} - \frac{1}{1-ae^{-i\theta}}\right) \\
&= \frac{1}{2\pi}\left(\frac{1-a^{-1}\cos\theta}{1-2a^{-1}\cos\theta + a^{-2}} - \frac{1-a\cos\theta}{1-2a\cos\theta+a^2}\right).
\end{aligned}$$

Therefore, the

$$\frac{\varepsilon(0)}{\varepsilon(\pi)} = \left(\frac{a+1}{a-1}\right)^2$$

which is nine for source at twice the radius ($a = 2$).

The geometrical interpretation follows from the cumulative distribution function

$$\psi = \mathrm{Im}\Phi = \frac{1}{2\pi}\Big(\arg(z-a) - \arg(z-a^{-1})\Big) = \frac{\gamma}{\pi}$$

where γ is the angle formed at a point on the circle by drawing lines to the "charge" at $z = a$ and its "image" at $z = a^{-1}$. The probability of hitting between angle θ_1 and θ_2 on the circles is just the difference of two such angles, subtended from each of the points to $z = a$ and $z = a^{-1}$:

$$\int_{\theta_1}^{\theta_2} \varepsilon(\theta|a)d\theta = \frac{\gamma_2 - \gamma_1}{2\pi}.$$

For infinitessimal $d\theta = \theta_2 - \theta_1$, we obtain the hitting probability density,

$$\varepsilon(\theta|a) = \frac{1}{2\pi}\frac{d\gamma}{d\theta}.$$