Lecture 18: First Passage in Higher Dimensions

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SUMMARY

This lecture reviews key results on first passage times from Lecture 17 to examine the probability of that a random walker on a lattice returns to his starting point (Polya's theorem). The Lecture also examines a simpler way of obtaining low order moments of the first passage time for continous stochastic processes by solving a time-independent PDEs, building on the time-dependent formalism of Lecture 16. This method is particularly powerful in complicated geometries in higher dimensions, where discrete random walks would be very difficult to analyze. It also easily produces the location of the eventual first passage, via an elegant analogy with electrostatics.

1 First passage on a periodic lattice

1.1 First passage time

This section is mainly a review of the last lecture. In class this section was presented as "1-D Random Walks," but the formulas are identical for higher dimensions.

Consider a random walk with identically distrubuted, independent steps on a periodic lattice in d dimensions. The key fact about the lattice is that it is periodic, while its structure is not essential. The lattice is not necessarily hypercubic; it may be simple cubic, face-centered cubic, body-centered cubic, or any other periodic arrangement of points in d dimensions.

Our goal is to analyze the random time it takes the walker to return to its starting point.

Define the following PDFs for a walker that starts at x_0 and makes n steps.

- $p(\Delta x)$ – a walker makes a step Δx (independent of x and n).

- $P_n(x \mid x_0)$ – walker is at x (in general, a vector with d components).

- $F_n(x \mid x_0)$ – the walker is at x for the *first* time. (Note: this is a PDF for n not x or x_0, despite the notation.)

Figure 1 motivates the following formula for F_n:

$$P_n(x \mid x_0) = \sum_{j=1}^{n} F_j(x \mid x_0) P_{n-j}(x \mid x) + \delta_{n,0}\delta_{x,x_0}$$
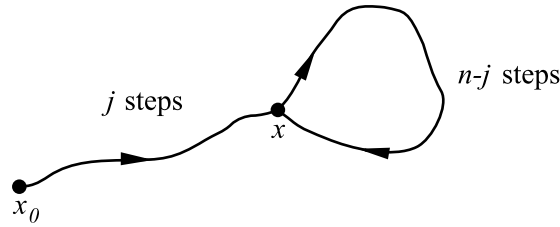
Figure 1: The topology of a general path from x_0 to x in n steps, which arrives for the first time after $j < n$ steps.

To solve for F_n, we introduce generating functions[1], and apply the discrete convolution theorem:

$$P(x \mid x_0; z) = F(x \mid x_0; z)P(x \mid x; z) + \delta_{x,x_0} \quad \Rightarrow$$

$$F(x \mid x_0; z) = \frac{P(x \mid x_0; z) - \delta_{x,x_0}}{P(x \mid x; z)}$$

Inverting the transform (using the formula for Taylor coefficients), we obtain

$$F_n(x \mid x_0) = \frac{1}{n!} \frac{\mathrm{d}^n F(x \mid z_0; z)}{\mathrm{d}z^n} \bigg|_{z=0}$$

1.2   Return probability on a lattice

Without obtaining the complete distribution of the first passage time, we can study the probability that the walker will eventually return to the origin (regardless of how long it takes):

$$R(x \mid x_0) = \sum_{n=1}^{\infty} F_n(x \mid x_0) = F(x \mid x_0; 1)$$

From our general expression above, we obtain a simple formula for the return probability:

$$R(x_0 \mid x_0) = 1 - \frac{1}{P(x_0 \mid x_0; 1)} \tag{1}$$

Let us now consider the case of an unbiased random walk on a lattice in d dimensions, where the steps have finite variance: $\langle \Delta x \rangle = 0$, $\langle x^2 \rangle < \infty$. (In this case, the Central Limit Theorem holds for the position of the random walk after many steps.) The return probability has a fascinating dependence on *dimension*, which was pointed out by George Pólya (1919, 1921):

$$\boxed{R(0 \mid 0) = \begin{cases} 1 & \text{for } d = 1, 2 \\ R < 1 & \text{for } d \geq 3 \end{cases}}$$

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[1]Generating functions are discrete transforms, introduced in Lecture 17. Here, the sequence of probabilities, P_0, P_1, $P_2, \ldots$ is encoded in the power-series coefficients of the generating function, $P(z) = \sum_{n=0}^{\infty} P_n z^n$

Pólya proved this result for the simplest case of nearest-neighbor steps of equal probability on a hypercubic lattice (generalizing the Bernoulli walk on the integers), but the result carries over to the general case of "normal diffusion" on the lattice, where the CLT applies to the position of the walk. (For a detailed discussion of Pólya's theorem and a review of recent results, see Hughes, Ch. 3.3.)

Before providing a derivation, we consider an intuitive justification of the theorem. When the CLT holds, the random walker visits a sequence of N lattice sites, effectively confined to the "central region" of volume, $O(N^{d/2})$, or linear dimension, $O(\sqrt{N})$. (As $N \to \infty$, it is exponentially unlikely to find the walker far outside the central region.) For $d = 1$, the number of visited sites, N grows faster than the number of accessible sites, $\sqrt{N}$, so the walker must loop back and forth frequently, returning the origin (and any other visited site) infinitely many times as $N \to \infty$. On the other hand, for $d \geq 3$, the number of accessible sites in the central region grows faster than the number of visited sites, so the walker will generally explore fresh sites, without necessarily returning to any previously visited site[2] This argument also predicts that two dimensions is a borderline case, which requires a more careful treatment.

1.3 Proof of Pólya's theorem

Note that the walker returns with probability one, if and only if $P(0 \mid 0; 1) = \infty$. Recall that the Bachelier's equation provides us the PDF for finding the walker at $P_n(x \mid x_0)$

$$P_{n+1}(x) = \sum_{\Delta x} p(\Delta x) P_n(x - \Delta x)$$

where $x_0 = 0$. The convolution is reduced to a product by Fourier transform, as usual:

$$\hat{P}_n(x) = \hat{p}(k)^n$$

The only difference to keep in mind here is that x is restricted to a discrete, periodic lattice, which implies that k is restricted to a finite, continuous region called the "first Brillouin zone". This is elementary cell of periodicity in d-dimensional k-space, associated with the periodicity of the lattice in d-dimensional x-space[3]. (See the Appendix for a brief discussion of the connection between discrete and continuous Fourier transforms.)

The probability generating function for the position is then given by

$$
\begin{aligned}
P(x \mid 0; z) &= \sum_{n=0}^{\infty} P_n(x) z^n & (2) \\
&= \int e^{ik \cdot x} \sum_{n=0}^{\infty} \hat{P}_n(x) z^n \frac{\mathrm{d}x}{(2\pi)^d} & (3) \\
&= \int e^{ik \cdot x} \sum_{n=0}^{\infty} (\hat{p}(k) z)^n \frac{\mathrm{d}x}{(2\pi)^d} & (4)
\end{aligned}
$$

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[2]This argument also explains why the random walk is a *fractal* of fractal dimension, $D_f = 2$, when embedded in any dimension $d \geq 3$.

[3]Brillouin zones play a central role in solid state physics, which focuses on electronic wave functions and lattice vibrations in periodic crystal lattices in three dimensions. To better understand the first Brillouin zone, think of the reverse situation for $d = 1$, which is the familiar case of Fourier series: A continuous periodic function in x, defined on one period, has a Fourier modes k restricted to a discrete integer lattice, corresponding to sines and cosines of the same period in x.

The sum is easily evaluated, since it is a geometric series[4]

$$P(x \mid 0; z) = \int \frac{e^{ik \cdot x}}{1 - \hat{p}(k)z} \frac{dk}{(2\pi)^d}$$

The return probability is one, if and only if

$$P(0 \mid 0; z) = 1 - \left[\int \frac{e^{ik \cdot x}}{1 - \hat{p}(k)} \frac{dk}{(2\pi)^d} \right]^{-1} = 1$$

or, equivalently, the integral diverges. Since the integral is carried out over the Brillouin zone – a finite region of k-space around $k = 0$ – the integral can only diverge due to singularities in the integral, which occur where $hatp(k) \to 1$, or $k \to 0$. To explore whether the integral diverges, it suffices to consider integrating only over some ball of radius ϵ centered at the origin:

$$\int_{B(\epsilon)} \frac{1}{1 - \hat{p}(k)} \frac{dk}{(2\pi)^d} \sim \int_{B(\epsilon)} \frac{dk}{k \, m_2 \, k}$$

where we have also substituted the Taylor expansion of $\hat{p}(k)$ for an unbiased random walk with steps of finite variance:

$$\hat{p}(k) \approx 1 - i \, m_1 \, k - \frac{1}{2} k \cdot m_2 \cdot k + \cdots$$

As discussed in Lecture 2, the moments m_k are generally tensors of rank k with d^k elements. We now make a change of variables $u = \sqrt{m_2}k$ (and $u \cdot u = k \cdot m_2 \cdot k$) and switch to spherical coordinates:

$$\int_{B(\epsilon)} \frac{dk}{k \cdot m_2 \cdot k} \sim \int_0^{\epsilon} \frac{u^{d-1}}{u^2} = \int_0^{\epsilon} u^{d-3} dk$$

It is now clear that the integral converges for $d \geq 3$ ($R = 1$) and diverges for $d < 3$ ($0 < R < 1$), which completes the proof of Pólya's theorem.

2   First passage to a complicated boundary

2.1   Continuum formulation

In higher dimensions, it is difficult to analyze discrete random walks in complicated geometries, especially when calculating the first passage time. It is much easier to obtain results from a continuum diffusion formulation in terms of PDEs. In Lecture 16 we derived a formalism to obtain the PDF for the time a continuous stochastic process takes to reach an absorbing boundary. The random process could be viewed as a continuum approximation of a discrete random walk or as a true mathematical stochastic process, as discussed in Lecture 13.

The calculation is considerably simplified if one only requires the low-order moments of the first passage time $\langle T^n \rangle$, and not its complete PDF.

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[4]The series converges for $|z| < 1$ since p is a PDF and therefore $|\hat{p}(k)| < \hat{p}(0) = 1$. The series also converges for $|z| = 1$ for $k \neq 0$. The exchange of sum and integral is also justified due to the uniform convergence of the geoemetric series, within the disk of convergence.

Let $S(t)$ be the survival probability of the walker having not yet reached the absorbing boundary,

$$S(t) = \int P(x, t \mid x_0, 0) \mathrm{d}x$$

so the first passage time PDF is $f(t) = -S'(t)$. Then the moments are given by

$$
\begin{aligned}
\langle T^n \rangle &= \int_0^\infty t^n f(t) \mathrm{d}t \\
&= -\int_0^\infty t^n S'(t) \mathrm{d}t \\
&= t^n S \big|_0^\infty + n \int_0^\infty t^{n-1} S(t) \mathrm{d}t
\end{aligned}
$$

The first term may be set equal to zero since $S(\infty) < 0$ for $S(t)$ to be a PDF. As an aside, note the following simple formula for the mean first passage time:

$$\langle T \rangle = \int_0^\infty S(t) dt \tag{5}$$

We now express the moments as integrals over space, not time:

$$\langle T^n \rangle = n \int_0^\infty t^{n-1} S(t) \mathrm{d}t = n \int_0^\infty t^{n-1} \int P(x, t \mid x_0, 0) \mathrm{d}x \mathrm{d}t = n \int g_{n-1}(x \mid x_0) \mathrm{d}x$$

where

$$g_n(x \mid x_0) = \int_0^\infty t^n P(x, t \mid x_0, 0) \mathrm{d}t \tag{6}$$

is the nth moment in time of the probability of finding the walker at x, after release from x_0.

2.2   Hierarchy of PDEs for the moments

Following Lecture 13, we assume that $P(x, t \mid x_0, 0)$ satisfies a PDE expressing conservation of probability:

$$\frac{\partial P}{\partial t} = LP = -\nabla \cdot J = -\nabla \cdot MP, \tag{7}$$

where L and M are operators, related to the probability current J. The PDE for $P(x, t \mid x_0, 0)$ is to be solved with boundary conditions, $P = 0$ on the *absorbing boundary* (the "target" for first passage) and $\hat{n} \cdot J = 0$ on any *reflecting boundary*, and initial condition, $P(x, 0 \mid x_0, 0) = \delta(x - x_0)$, since the walker is released from x_0.

To be specific, in the case of the Fokker-Planck equation, we have

$$J = M P = D_1(x, t) P(x, t) - \nabla(D_2(x, t) P(x, t))$$

where D_1 and D_2 are the drift and diffusion coefficients. Recall that the Fokker-Planck equation either holds exactly (by definition, for a mathematical "Brownian motion", or continuous stochastic

prcess) or approximately (as a continuum approximation of a discrete random walk, often valid after many steps). In the latter case, there are generally corrections, which can be expressed as higher-order spatial derivatives in J ("modified Kramers-Moyall expansion" from Lectures 9 and 13).

In the common case of a constant diffusion coefficient and drift in a time-independent external potential, $\phi(x)$, the Fokker-Planck operator is indepedent of time:

$$J = M\,P = -\mu P \nabla \phi - D \nabla P$$

More generally when the modified Kramers-Moyall coefficients are independent of time, the operators L and M depend only on space, which we will assume hereafter.

Starting from a time integral of t^n times the PDE and applying integration by parts, we have

$$
\begin{aligned}
\int t^n \frac{\partial P}{\partial t} dt &= t^n P|_0^\infty - n \int_0^\infty t^{n-1} P(x, t \mid x_0, 0) dt \\
&= t^n P|_0^\infty - L \int_0^\infty t^n P_t(x \mid x_0) dt
\end{aligned}
$$

The first term vanishes if the nth moment exists, except in the case $n = 0$, where it yields $-\delta(x - x_0)$ from the initial condition. In this way, we arrive at a hierarchy of time-independent PDEs for the functions $g_n(x \mid x_0)$:

$$\boxed{L\,g_0(x \mid x_0) = -\delta(x - x_0)} \tag{8}$$

$$\boxed{L\,g_n(x \mid x_0) = -g_{n-1}(x \mid x_0)} \tag{9}$$

with the boundary conditions, $g_n = 0$ on the absorbing boundary, and $\hat{n} \cdot J_n = 0$ on any reflecting boundary, where $J_n = M\,g_n$. As these PDEs are solved recursively for $n \geq 0$, one obtains the first passage time moments by integrals:

$$
\begin{aligned}
\langle T \rangle &= \int g_0(x \mid x_0) dx \\
\langle T^2 \rangle &= 2 \int g_1(x \mid x_0) dx \\
&\vdots
\end{aligned}
$$

$$\boxed{\langle T^n \rangle = n \int g_{n-1}(x \mid x_0) dx} \tag{10}$$

2.3 Electrostatic analogy

As discussed by Redner (2002), this hierarchy of PDEs has a convenient electrostatic analogy in the case of simple diffusion, $J = -D\nabla P$. In that case, $g_0(x \mid x_0)$ is equivalent to the electrostatic potential of a point charge of magnitude $-D^{-1}$ at x_0, which satisfies Poisson's equation,

$$\nabla^2 g_0 = -D^{-1}\delta(x - x_0) \tag{11}$$

with boundary conditions representing a conductor ($g_0 = 0$) on the absorbing boundary and an insulator ($\hat{n} \cdot \nabla g_0 = 0$) on the reflecting boundary. The next step is to view $-D^{-1}g_0(x \mid x_0)$ as the

charge density in another Poisson equation, where $g_1(x \mid x_0)$ now plays the role of the electrostatic potential, etc.

The advantage of this connection is that the well-developed mathematical theory of electrostatics can be brought to bear on first passage problems. See Redner's book for an example involve the method images to solve for the first passage time from a point to a sphere, which has applications in simulations of diffusion-limited aggregation. The analogous problem of first passage to a plane, which has relevance for polymer surface adsorption, appears on the homework.

In two dimensions, one can also apply conformal mapping to solve for first passage in more complicated geometries. In fact, this method applies much more generally than just simple diffusion: The probability current can be any "gradient-driven flux density" in the class described by Bazant, Proc. Roy. Soc. A 460, 1433 (2004). For first passage problems, this trick was introduced in the case of advection-diffusion in a potential flow by Koplik, Redner, and Hinch (1994).

2.4   Location of the first passage

The continuum formalism of this section also naturally answers the question of *where* the first passage occurs on the absorbing boundary (regardless of the time it takes). The probability density for eventual first passage at an absorbing boundary point x_a, which Redner calls the *eventual hitting probability*, can be calculated as follows:

$$
\begin{aligned}
\mathcal{E}(x_a) &= \int_0^\infty \hat{n} \cdot J(x_a, t) dt \\
&= \hat{n} \cdot M \int_0^\infty P(x_a, t \mid x_0, 0) dt \\
&= \hat{n} \cdot M \, g_0(x_a \mid x_0) \\
&= \hat{n} \cdot J_0(x_a \mid x_0)
\end{aligned}
$$

where $\hat{n}(x_a)$ is the outward normal at x_a. The first line follows from the definition of the probability current, by integrating the "leakage" of probability at x_a over all time, and the last line shows that the eventual hitting probability is given by the "normal current" of g_0, defined by $J_0 = M \, g_0$ (with g_0 replacing P).

For simple diffusion, this quantity also has an elegant electrostatic analogy. In that case, we have $J_0 = M g_0 = -D \nabla g_0$, which is proportional to the (normal) "electric field" on the conductor.

APPENDIX

(by Kirill Titievsky)

Fourier transform on a lattice

Here, we set out to understand the idea of Brillouin zones and the relationship between discrete and continuous Fourier transform enough for the proof of Polya's theorem to make sense. This is another way in which continuous and discrete ways of thinking about probability distributions differ significantly, but once again, are found to be profoundly related.

For a $d \times d$ matrix M and a d element vector of integers m, products Mm define all points on a lattice. Thus, any lattice we consider is the hypercubic one (just the d-dimensional set of integers) that has been transformed linearly. The lattice is periodic, with the shape and size of the repeating

cell defined by M. By periodic we mean that if there is a lattice point at x, there is also a lattice point at $M(1,0,0)$ and other values of m that involve only ones. Such definition of lattices should cover a broad range of possibilities, but I am not sure it covers all periodic structures.

Suppose we define a discrete probability function, w_α for each point x_α of the lattice. We can define a continuous PDF to represent this function and note its properties:

$$f(x) = \sum_\alpha w_\alpha \delta(x - x_\alpha) \quad \text{``continuous'' field} \tag{12}$$

$$\tilde{f}(k) = \sum_\alpha w_\alpha e^{ikx_\alpha} \quad \text{continuous FT} \tag{13}$$

$$f(x_\beta) = \sum_\alpha w_\alpha \int e^{ikMm} \frac{\mathrm{d}k}{(2\pi)^d} \quad \text{where } Mm = x_\alpha + x_\beta \tag{14}$$

$$= \sum_\alpha w_\alpha \int e^{ikm} \frac{\mathrm{d}k}{(2\pi|M|)^d} \tag{15}$$

Notice, that since m is an integer vector, carrying the integral out over shifted part of the lattice cell – that is, the cube $[-\pi, \pi]^d$ – makes the integral equal to unity for $|m| = 0$ and zero otherwise. This region, with the linear transformation of M applied, in k-space is called the Brillouin zone. Thus, to recover the discrete probability function from the Fourier transform of its continuous representation, we need only to restrict the domain of integration to the repeat unit of the cell! If we carry out the usual inverse Fourier transform, we would get the δ functions back.

So if we are interested in the PDF on a lattice point, as we were in the derivation of Polya's theorem, the domain of integration is limited to a finite region of k space around $k = 0$.