Return probability on a lattice

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To begin, we consider a basic example of a discrete first passage process. Consider an unbiased Bernoulli walk on the integers starting at the origin. We wish to determine the probability, R, that the walker eventually returns to 0, regardless of the number of steps it takes.

Without loss of generality, say the walker's first step is to 1. From here, the walker can either step left to 0 or can return to 1 n times before stepping back to 0. To avoid double counting, we must also assert that if the walker comes back to 1 n times, it cannot step left to 0 any of those times except the last. Since half of the possible paths from 1 back to 1 stay to the right of 1, the probability of returning to 1 exactly once before hitting 0 is $R/2$. Likewise, the probability of returning to 1 n times before stepping back to 0 is $(R/2)^n$. Thus

$$R = \frac{1}{2} + \left[\sum_{n=1}^{\infty}(R/2)^n\right] \times \frac{1}{2} = \left[\sum_{n=0}^{\infty}(R/2)^n\right] \times \frac{1}{2} = \frac{1}{2(1-R/2)} = \frac{1}{2-R}.$$

This means

$$R^2 - 2R + 1 = 0 \implies (R-1)^2 = 0$$

and since probabilities cannot be negative, this means $R = 1$. In essence, we've just deduced that a drunk man who wanders away from a pub will eventually return, as long as he is confined to a long narrow street. Based on the continuum analysis of the previous lecture, however, he will probably not make it back the same day (or the same week), since the expected return time is infinite!

The preceding simple analysis is not easily generalized to higher dimensions, where the situation can be quite different, e.g. if the drunk man wanders about in a two-dimensional field. As the dimension increases, it makes sense that the walker is less likely to ever find by chance the special point where he started. In the next lecture, we will address the effect of dimension in the return problem (Polyá's theorem), but first we will develop a "transform" formalism for discrete random walks on a lattice, analogous to the Fourier and Laplace transform methods used earlier for continuous displacements. Of course, we could use the same continuum formulation with generalized functions (like $\delta(x)$) to enforce lattice constraints, but it is simpler to work with discrete "generating functions" right from the start.

1 Generating Functions on the Integers

Rather than keeping track of a sequence of discrete probabilities, $P(X = n)$, it is convenient to encode the same information in the expansion coefficients, $P_n = P(X + n)$, of the "probability

*Based on notes by Ken Kamrin and Kirill Titievsky (2005).

generating function" (PGF), defined as

$$f(\xi) = \sum_{n=n_0}^{\infty} P_n \xi^n.$$

There are two common cases:

1. For probabilities defined on all integers, $n_0 = -\infty$, the PGF is the analytic continuation of a Laurent series
$$f(z) = \sum_{n=-\infty}^{\infty} P_n z^n$$
which converges in some annulus in the complex plane, $R_1 < |z| < R_2$. The probabilities are recovered from the PDF by a contour integral around this annulus once counter clockwise,
$$P_n = \frac{1}{2\pi i} \oint \frac{f(z)dz}{z^{n+1}}.$$
When evaluated on the unit circle, $z = e^{i\theta}$, the Laurent series reduces to a complex Fourier series
$$f(e^{i\theta}) = \sum_{n=-\infty}^{\infty} P_n e^{in\theta}$$
which is the discrete analog of our previous Fourier transform in "space".

2. For probabilities defined on the non-negative integers, $n_0 = 0$, the PGF is the analytic continuation of a Taylor series
$$f(z) = \sum_{n=0}^{\infty} P_n z^n$$
which converges in a disk in the complex plane, $|z| < R$. When evaluated on the real axis inside the unit disk with $z = e^s (s > 0)$, the Taylor series resembles a discrete Laplace transform,
$$f(e^{-s}) = \sum_{n=0}^{\infty} P_n e^{-sn},$$
which is the discrete analog of our previous Laplace transform in "time".

For an intuitive discussion of generating function and their relation to Fourier and Laplace transforms in the present context see *A Guide to First Passage Processes* by Sidney Redner (recommended reading).

For the remainder of this lecture, we will focus on case 2, which has relevance for the return problem in one dimension. In this case, similar to the continuous transforms, the PGF has some very useful properties:

- $f(1) = \sum_{n=0}^{\infty} P(X = n) = 1$ (by normalization), which implies that the PGF converges inside the unit disk, $|\xi| < 1$.

- All of the moments of the distribution are encoded in the Taylor expansion of the PGF as $\xi \to 1^-$ (analogous to the Taylor coefficients of the Fourier transform at the origin). For example, $f'(\xi) = \sum_{n=0}^{\infty} P(X = n) n \xi^{n-1} \implies f'(1) = \sum_{n=0}^{\infty} nP(X = n) = \langle X \rangle$. Similarly, $f''(\xi) = \sum_{n=0}^{\infty} n(n-1)\xi^{n-2} P(X = n) = \langle X^2 \rangle - \langle X \rangle$ implying that $\langle X^2 \rangle = f''(1) + f'(1)$.

- A "discrete convolution theorem" also holds. Suppose Y has probability generating function $g(\xi)$. Then the PGF of $Z = X + Y$ is $h(\xi) = \sum_{n=0}^{\infty} P(X + Y = n)\xi^n = \sum_{n=0}^{\infty}\sum_{i=0}^{n} P(X = i)P(Y = n - i)\xi^n$. Letting $k = n - i$ we have $h(\xi) = \sum_{i=0}^{\infty} P(X = i)\sum_{k=0}^{\infty} P(Y = k)\xi^{i+k} = f(\xi)g(\xi)$.

For example, consider a Poisson distribution with parameter λ:

$$P(X = n) = e^{-\lambda}\lambda^n/n!$$

$$\Longrightarrow f(\xi) = \sum_{n=0}^{\infty} e^{-\lambda}(\lambda\xi)^n/n! = e^{-\lambda}e^{\lambda\xi} = e^{\lambda(\xi-1)}.$$

We get $f(1) = e^0 = 1$ as we expect and $f'(1) = \lambda = \langle X\rangle$. If we let Y be Poisson with parameter μ, we may define the variable $Z = X + Y$. By the last property we get that the PGF for Z is $h(\xi) = e^{(\lambda+\mu)(\xi-1)}$ thus telling us that the sum of two Poisson variables also has a Poisson distribution (with parameter $\lambda + \mu$).

2 First Passage on a Lattice

Define $P_n(s|s_0)$ as the probability of being at lattice point s after n steps given that the walk started at s_0. Also, define $F_n(s|s_0)$ as the probability of arriving at site s for the first time on the n^{th} step, given that the walker begins at s_0. One condition we know must hold is

$$\sum_s P_n(s|s_0) = 1$$

since the walker must be somewhere on the lattice. We may also define

$$R(s|s_0) = \sum_{n=1}^{\infty} F_n(s|s_0)$$

as the probability that site s is ever reached by a walker starting from site s_0. Our initial conditions for a walker beginning at s_0 are

$$P_0(s|s_0) = \delta_{ss_0}\text{and}F_0(s|s_0) = 0$$

where δ is the Kronecker delta function. Use the following notation for the generating functions:

$$P(s|s_0;\xi) = \sum_{n=0}^{\infty} P_n(s|s_0)\xi^n$$

$$F(s|s_0;\xi) = \sum_{n=0}^{\infty} F_n(s|s_0)\xi^n.$$

The odds of a walker reaching s from s_0 are the same as the odds of a walker first arriving to s in j steps and then returning to s in $n - j$ steps. Thus we can write:

$$P_n(s|s_0) = \sum_{j=1}^{n} F_j(s|s_0)P_{n-j}(s|s)$$

as long as $n \geq 1$. In the case that $n = 0$, $P_0(s|s_0) = \delta_{ss_0}$ so altogether we have

$$P_n(s|s_0) = \delta_{ss_0}\delta_{n0} + \sum_{j=1}^{n} F_j(s|s_0)P_{n-j}(s|s)$$

By the convolution-like property of PGFs we can now write

$$P(s, s_0; \xi) = \delta_{ss_0} + F(s|s_0; \xi)P(s|s; \xi)$$

$$\Longrightarrow F(s|s_0; \xi) = \frac{P(s|s_0; \xi) - \delta_{ss_0}}{P(s|s; \xi)}.$$

This is comparable to the result in the continuum case using a Laplace Transform. Using this, we can write

$$R(s|s_0) = \sum_{n=1}^{\infty} F_n(s|s_0) = F(s|s_0; 1) = \frac{P(s|s_0; 1) - \delta_{ss_0}}{P(s|s; 1)}$$

and thus the probability of return is

$$\boxed{R(s_0|s_0) = 1 - \frac{1}{P(s|s_0; 1)}}. \tag{1}$$

3 First Passage Example

Let us now consider a biased Bernoulli walk on the integers.

$$P_{2m}(0|0) = \binom{2m}{m} p^m q^m$$

where we use $2m$ because a walk that returns must do so in an even number of steps.

$$\begin{aligned} P(0|0; \xi) &= \sum_{m=0}^{\infty} \binom{2m}{m} p^m q^m \xi^{2m} \\ &= (1 - 4pq\xi^2)^{-1/2} \end{aligned}$$

and hence the probability of return is

$$\begin{aligned} R(0|0) &= 1 - \sqrt{1 - 4pq} \\ &= 1 - \sqrt{1 - 4p(1-p)} \\ &= 1 - \sqrt{(2p-1)^2} \\ &= 1 - |2p - 1| \end{aligned}$$

This result agrees with our first example; just let $p = 1/2$ and we get $R = 1$. As p approaches 0 or 1, the return probability vanishes.

4 Pólya's Theorem

We will now make use of the above formalism to study Pólya's theorem. Consider the case of an unbiased random walk on a lattice in d dimensions, where the steps have finite variance: $|\Delta x| = 0, |x^2| < \infty$. (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):

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

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 P/'olya's theorem and a review of recent results, see Chapter 3.3 of *Random Walks and Random Environments* by Barry Hughes.)

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 a 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 to 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[1]. This argument also predicts that two dimensions is a borderline case, which requires more careful treatment.

5 Proof of Pólya's Theorem

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

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

where $x_0 = 0$. By using a Fourier transform, the convolution is reduced to a product

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

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 an elementary cell of periodicity in d-dimensional k-space, associated with the periodicity of the lattice in d-dimensional x-space[2]. (See the Appendix for a brief discussion of the connection between discrete and continuous Fourier transforms.)

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

[2] 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 Fourier modes k restricted to a discrete integer lattice, corresponding to sines and cosines of the same period in x.

The probability generating function for the position is then given by

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

Since the sum is a geometric series[3], we obtain

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

and thus the return probability is one if and only if

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

This is equivalent to asking whether or not the integral diverges. Since the integration is carried out over the Brillouin zone (a finite region of k-space around $k = 0$) the integral can only diverge due to singularities, which occur where $\hat{p}(k) \to 1$, or $k \to 0$. Near $k = 0$ we have a Taylor expansion of the form

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

and since we are considering an unbiased walk, $m_1 = 0$. m_2 is a symmetric matrix, and as such there exists an orthogonal matrix O such that $O^{\mathrm{T}} m_2 O = D$ where D is diagonal, and for a non-degenerate case, the diagonal elements of D, labeled as d_i, will all be strictly positive. Let E be the square root of D, which is has diagonal elements e_i. By making use of the coordinate transformations $k = Ov$, $v = E^{-1} l$, we can write the integral as

$$
\begin{aligned}
\int \frac{e^{ik\cdot x}}{1-\hat{p}(k)} \frac{dk}{(2\pi)^d} &= \int \frac{2e^{ik\cdot x}}{k \cdot m_2 \cdot k + \dots} \frac{dl}{(2\pi)^d} \\
&= \int \frac{2e^{iOv\cdot x}}{v \cdot D \cdot v + \dots} \frac{dv}{(2\pi)^d} \\
&= \int \frac{2e^{iOE^{-1}l\cdot x}}{E^{-1}l \cdot D \cdot E^{-1}l + \dots} \frac{|E|^{-1}\, dl}{(2\pi)^d} \\
&= \frac{2}{|E|\,(2\pi)^d} \int \frac{e^{iOE^{-1}l\cdot x}}{|l|^2 + \dots}\, dl
\end{aligned}
$$

To explore whether the integral diverges, it suffices to consider integrating only over some ball of

[3] 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 geometric series, within the disk of convergence.

radius ϵ centered at the origin. Near the origin, the exponential is slowly-varying, and hence

$$\begin{aligned}
\int_{B(\epsilon)} \frac{e^{iOE^{-1}l\cdot x}}{|l|^2 + \dots}\, dl &\sim \int \frac{1}{|l|^2}\, dl \\
&\sim \int_0^{\epsilon} \frac{S(d) w^{d-1}\, dw}{w^2} \\
&\sim \int_0^{\epsilon} S(d) w^{d-3}\, dw
\end{aligned}$$

where we have made the switch to spherical coordinates, $S(d)$ is the surface area of a d-dimensional sphere. It is now clear that the integral converges for $d \geq 3$ $(0 < R < 1)$ and diverges for $d < 3$ $(0 < R < 1)$ which completes the proof of Pólya's theorem.

A Fourier transform on a lattice

Here, we set out to understand the idea of Brillouin zones and the relationship between discrete and continuous Fourier transforms. 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 related to the lattice defined just by the d-dimensional set of integers by a linear transformation. The lattice is periodic, with the shape and size of the repeating cell defined by M.

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:

$$\begin{aligned}
f(x) &= \sum_\alpha w_\alpha \delta(x - x_\alpha) \\
\hat{f}(k) &= \sum_\alpha w_\alpha e^{ikx} \\
f(x_\beta) &= \sum_\alpha w_\alpha \int e^{ikMm} \frac{dk}{(2\pi)^d} \\
&= \sum_\alpha w_\alpha \int e^{ikm} \frac{dk}{(2\pi)^d\, |M|}
\end{aligned}$$

Notice, this since m is an integer vector, carrying the integral out over a shifted part of the lattice cell – that is, the cube $[-\pi, \pi]^d$ – makes the integral equal to unit for $|m| =$ and zero otherwise. This region in k-space, with the linear transformation of M applied, 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 delta functions back.

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