

Random Walks on a Lattice

1D Walk

A particle on the origin, $x = 0$, of a one dimensional lattice makes a step to the right (or left) with probability $0 \leq r \leq 1$ ($q = 1 - r$). The jump lengths are $\Delta x = \pm 1$ and their PDF and characteristic function are:

$$f_{1D}(\Delta x) = r\delta(\Delta x - 1) + q\delta(\Delta x + 1) \quad ; \quad \tilde{f}_{1D}(k) = re^{ik} + qe^{-ik}. \quad (1)$$

The probability of finding the particle on $x = 0, \pm 1, \pm 2, \dots$ after N steps is denoted as ${}^1D p_N(x)$.

(note that $\tilde{f}(k) = \int_{-\infty}^{\infty} f(x) e^{ikx} dx$ and therefore, $|\tilde{f}(k)| = \left| \int_{-\infty}^{\infty} f(x) e^{ikx} dx \right| \leq \int_{-\infty}^{\infty} |f(x)| |e^{ikx}| dx = \int_{-\infty}^{\infty} |f(x)| dx = 1$).

The following rules are easy to understand:

After a single step, ${}^1D p_1(1) = r$ (coefficient of e^{ik} in $[\tilde{f}_{1D}(k)]^1$) and ${}^1D p_1(-1) = q$ (coefficient of e^{-ik} in $[\tilde{f}_{1D}(k)]^1$).

After two steps, ${}^1D p_2(2) = r^2$ (coefficient of e^{i2k} in $[\tilde{f}_{1D}(k)]^2$), ${}^1D p_2(-2) = q^2$ (coefficient of e^{-i2k} in $[\tilde{f}_{1D}(k)]^2$) and ${}^1D p_2(0) = 2rq$ (coefficient of e^{-ik0} in $[\tilde{f}_{1D}(k)]^2$).

Generally, ${}^1D p_N(x) =$ coefficient of e^{ikx} in $[\tilde{f}_{1D}(k)]^N$. To filter the coefficients of e^{ikx} we use the following relation,

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-ikx+imk} dk = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{i(m-x)k} dk = \delta_{m,x}. \quad (2)$$

Hence,

$${}^1D p_N(x) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-ikx} \tilde{f}_{1D}^N(k) dk = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-ikx} (re^{ik} + qe^{-ik})^N dk \quad (3)$$

$$= \sum_{m=0}^N \frac{N! r^m q^{N-m}}{m!(N-m)!} \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-ikx} e^{ikm} e^{-ik(N-m)} dk = \sum_{m=0}^N \frac{N! r^m q^{N-m}}{m!(N-m)!} \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-ik(N-2m+x)} dk \quad (4)$$

$$= \sum_{m=0}^N \frac{N! r^m q^{N-m} \delta_{x,2m-N}}{m!(N-m)!} = \sum_{m=0}^N \frac{N! r^m q^{N-m} \delta_{m,(x+N)/2}}{m!(N-m)!} = \frac{N! r^{\frac{N+x}{2}} q^{\frac{N-x}{2}}}{\left(\frac{N-x}{2}\right)! \left(\frac{N+x}{2}\right)!}, \quad (5)$$

under the condition that x has the same parity as N and $|x| \leq N$.

In the case of an unbiased, symmetric, random walk, $r = 1/2 = q$, the expression simplifies a bit and may be written as:

$${}^1D,^s p_N(x) = \frac{2^{-N} N!}{\left(\frac{N-x}{2}\right)! \left(\frac{N+x}{2}\right)!}. \quad (6)$$

Using Stirling's formula, $n! \simeq \sqrt{2\pi n} (n/e)^n$ we find for $x \ll N$

$$\begin{aligned} {}^1D,^s p_N(x) &= \frac{2^{-N} N!}{\left(\frac{N-x}{2}\right)! \left(\frac{N+x}{2}\right)!} \simeq \frac{2^{-N} \sqrt{2\pi N} (N/e)^N}{\sqrt{2\pi \frac{N-x}{2}} \left(\frac{N-x}{2}/e\right)^{\frac{N-x}{2}} \sqrt{2\pi \frac{N+x}{2}} \left(\frac{N+x}{2}/e\right)^{\frac{N+x}{2}}} \quad (7) \\ &= \frac{2}{\sqrt{2\pi N} (1-x/N)^{\frac{N-x+1}{2}} (1+x/N)^{\frac{N+x+1}{2}}} \simeq 2 \frac{e^{-\frac{x^2}{2N}}}{\sqrt{2\pi N}}, \end{aligned}$$

under the parity conditions mentioned above (note the factor of 2 due to the parity issue). In the above derivation we used,

$$\begin{aligned}
\ln\left(\left(1 - \frac{x}{N}\right)^{\frac{N-x+1}{2}}\right) &= \frac{N-x+1}{2} \ln\left(1 - \frac{x}{N}\right) \\
&\sim \frac{N-x+1}{2} \left(-\frac{x}{N} - \frac{x^2}{2N^2} + O\left(\left(\frac{x}{N}\right)^3\right)\right) \\
&\rightarrow \left(1 - \frac{x}{N}\right)^{\frac{N-x+1}{2}} \sim e^{\frac{N-x+1}{2} \left(-\frac{x}{N} - \frac{x^2}{2N^2} + O\left(\left(\frac{x}{N}\right)^3\right)\right)} \\
\ln\left(\left(1 + \frac{x}{N}\right)^{\frac{N+x+1}{2}}\right) &= \frac{N+x+1}{2} \ln\left(1 + \frac{x}{N}\right) \\
&\sim \frac{N+x+1}{2} \left(\frac{x}{N} - \frac{x^2}{2N^2} + O\left(\left(\frac{x}{N}\right)^3\right)\right) \\
&\rightarrow \left(1 + \frac{x}{N}\right)^{\frac{N+x+1}{2}} \sim e^{\frac{N+x+1}{2} \left(\frac{x}{N} - \frac{x^2}{2N^2} + O\left(\left(\frac{x}{N}\right)^3\right)\right)}
\end{aligned} \tag{8}$$

(If the lattice space is a , the time between jumps is τ , and $\lim_{a \rightarrow 0, \tau \rightarrow 0} \frac{a^2}{\tau} = 2D$ we find that the limiting continuous PDF corresponding to the random walk we described is ${}^{1D}p_t(x) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}$).

2D

The above arguments can be generalized for a random walk on a 2-dimensional square lattice. The probability of hopping from lattice site $(x, y) \rightarrow (x+1, y)$ is r_x , from $(x, y) \rightarrow (x-1, y)$ is q_x , from $(x, y) \rightarrow (x, y+1)$ is r_y , and from $(x, y) \rightarrow (x, y-1)$ is q_y . Obviously, $q_x + q_y + r_x + r_y = 1$. The characteristic function, $\tilde{f}_{2D}(k_x, k_y)$, is

$$\begin{aligned}
\tilde{f}_{2D}(\vec{k}) &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{i(k_x \Delta_x + k_y \Delta_y)} f_{2D}(\Delta_x, \Delta_y) d\Delta_x d\Delta_y \\
&= r_x e^{ik_x} + q_x e^{-ik_x} + r_y e^{ik_y} + q_y e^{-ik_y}.
\end{aligned} \tag{9}$$

The probability, ${}^{2D}p_N(x, y)$, is

$${}^{2D}p_N(x, y) = \left(\frac{1}{2\pi}\right)^2 \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} [r_x e^{ik_x} + q_x e^{-ik_x} + r_y e^{ik_y} + q_y e^{-ik_y}]^N e^{-ik_x x - ik_y y} dk_x dk_y. \tag{10}$$

For simplicity we will focus on the unbiased random walk in which $r_x = r_y = q_x = q_y = 1/4$. In this case,

$$\begin{aligned}
{}^{2D}p_N(x, y) &= 2^{-N} \left(\frac{1}{2\pi}\right)^2 \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} [\cos(k_x) + \cos(k_y)]^N e^{-ik_x x - ik_y y} dk_x dk_y, \\
&= 4^{-N} \sum_{m=0}^N \sum_{s=0}^m \sum_{u=0}^{N-m} \left[\begin{aligned} &\frac{N!}{m!(N-m)!} \frac{m!}{s!(m-s)!} \frac{(N-m)!}{u!(N-m-u)!} \\ &\times \left(\frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-ik_x(m-2s+x)} dk_x \right) \\ &\times \left(\frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-ik_y(N-m-2u+y)} dk_y \right) \end{aligned} \right] \\
&= 4^{-N} \sum_{m=0}^N \sum_{s=0}^m \sum_{u=0}^{N-m} \frac{N!}{m!(N-m)!} \frac{m!}{s!(m-s)!} \frac{(N-m)!}{u!(N-m-u)!} \delta_{x, 2s-m} \delta_{y, 2u+m-N}.
\end{aligned} \tag{11}$$

Note that according to our derivation for the RW on 1D, we found

$$\begin{aligned} {}^1D p_m(x) &= 2^{-m} \sum_{s=0}^m \frac{m! \delta_{x,2s-m}}{s! (m-s)!} = 2^{-m} \frac{m!}{\left(\frac{m-x}{2}\right)! \left(\frac{m+x}{2}\right)!}, \\ {}^1D p_{N-m}(y) &= 2^{m-N} \sum_{u=0}^{N-m} \frac{(N-m)!}{u! (N-m-u)!} \delta_{y,2u+m-N} = 2^{m-N} \frac{(N-m)!}{\left(\frac{N-m-y}{2}\right)! \left(\frac{N-m+y}{2}\right)!}. \end{aligned}$$

Therefore,

$${}^2D p_N(x, y) = 2^{-N} \sum_{m=0}^N \frac{N!}{m! (N-m)!} {}^1D p_m(x) {}^1D p_{N-m}(y). \quad (12)$$

The specific case of ${}^2D p_N(0, 0)$ yields

$${}^2D p_N(0, 0) = \frac{N!}{\left(\frac{N}{2}\right)!^2} 2^{-2N} \sum_{m=0}^N \frac{\left(\frac{N}{2}\right)!^2}{\left[\left(\frac{m}{2}\right)!\right]^2 \left[\left(\frac{N-m}{2}\right)!\right]^2} \quad (13)$$

Realizing that returning to the origin is only possible if there were even numbers of jumps on both x and y directions, leads us to define $N = 2n$; $m = 2k$;

$${}^2D p_N(0, 0) = \frac{N!}{\left(\frac{N}{2}\right)!^2} 2^{-2N} \sum_{k=0}^n \left(\frac{n!}{k! (n-k)!}\right)^2 = \left(\frac{N!}{\frac{N}{2}! \frac{N}{2}!}\right)^2 2^{-2N} \quad (14)$$

In the equation above we used the identity

$$\sum_{k=0}^n \left(\frac{n!}{k! (n-k)!}\right)^2 = \frac{(2n)!}{n! n!}. \quad (15)$$

Using the Stirlings formula we may write

$$\begin{aligned} {}^2D p_N(0, 0) &\sim \left(\frac{\sqrt{2\pi N} (N/e)^N}{\sqrt{2\pi N/2} (N/2e)^{N/2} \sqrt{2\pi N/2} (N/2e)^{N/2}}\right)^2 2^{-2N} \\ &= \left(\frac{\sqrt{2} 2^N}{\sqrt{\pi N}}\right)^2 2^{-2N} = \frac{2}{\pi N}. \end{aligned} \quad (16)$$

Equation (3) may be easily generalized to d dimensions and written as

$${}^d p_N(\vec{0}) = \left(\frac{1}{2\pi}\right)^d \int_{-\pi}^{\pi} \dots \int_{-\pi}^{\pi} \tilde{f}_d^N(\vec{k}) d^d k = \left(\frac{1}{2\pi}\right)^d \int_{-\pi}^{\pi} \dots \int_{-\pi}^{\pi} e^{N(-\frac{1}{2}(k_1^2 \sigma_1^2 + k_2^2 \sigma_2^2 + \dots + k_d^2 \sigma_d^2) + O(k^3))} d^d k, \quad (17)$$

where we used,

$$\begin{aligned} \tilde{f}_d(\vec{k}) &= 1 - \frac{1}{2} (k_1^2 \sigma_1^2 + k_2^2 \sigma_2^2 + \dots + k_d^2 \sigma_d^2) + O(k^3) \\ &\rightarrow \ln(\tilde{f}_d(\vec{k})) = \ln\left(1 - \frac{1}{2} (k_1^2 \sigma_1^2 + k_2^2 \sigma_2^2 + \dots + k_d^2 \sigma_d^2) + O(k^3)\right) \\ &= -\frac{1}{2} (k_1^2 \sigma_1^2 + k_2^2 \sigma_2^2 + \dots + k_d^2 \sigma_d^2) + O(k^3), \end{aligned}$$

and therefore,

$$e^{N \ln(\tilde{f}_d(\vec{k}))} \sim e^{N \ln(1 - \frac{1}{2}(k_1^2 \sigma_1^2 + k_2^2 \sigma_2^2 + \dots + k_d^2 \sigma_d^2) + O(k^3))} = e^{N(-\frac{1}{2}(k_1^2 \sigma_1^2 + k_2^2 \sigma_2^2 + \dots + k_d^2 \sigma_d^2) + O(k^3))}.$$

Changing variables according to $k_i = q_i/\sqrt{N}$ we find that $k_i^2 = q_i^2/N$ and

$${}^d p_N(\vec{0}) = \frac{1}{N^{d/2}} \left(\frac{1}{2\pi}\right)^d \int_{-\pi\sqrt{N}}^{\pi\sqrt{N}} \dots \int_{-\pi\sqrt{N}}^{\pi\sqrt{N}} e^{-\frac{1}{2}(q_1^2\sigma_1^2 + q_2^2\sigma_2^2 + \dots + q_d^2\sigma_d^2) + O\left(\frac{1}{\sqrt{N}}\right)} d^d q. \quad (18)$$

Thus, in the limit $N \rightarrow \infty$

$${}^d p_N(\vec{0}) \sim \frac{c_d}{N^{d/2}}, \quad (19)$$

where c_d is a coefficient independent of N .

Polya's Problem

Let $p_N(x, x_0)$ be the probability of a random walking particle being on x after N steps, starting on x_0 . $F_N(x, x_0)$ is the probability that the particle is on x for the first time after N steps, starting on x_0 . The following generating functions are useful tools

$$\hat{p}_u(x, x_0) = \delta_{x, x_0} + \sum_{N=1}^{\infty} u^N p_N(x, x_0), \quad (20)$$

$$\hat{F}_u(x, x_0) = \sum_{N=1}^{\infty} u^N F_N(x, x_0). \quad (21)$$

$\hat{F}_{u=1}(x, x_0)$ = Probability of reaching x for the first time after 1 step + Probability of reaching x for the first time after 2 steps + ... = Probability of reaching x . If $\hat{F}_{u=1}(x, x_0) = 1$ the particle surely reaches x , though it may take a long time. Often, an important quantity is $\hat{F}_{u=1}(x_0, x_0)$, the probability that a particle starting on x_0 to hop into another lattice point and then return to the point x_0 at some later time. If $\hat{F}_{u=1}(x_0, x_0) = 1$, i.e., the particle returns to its starting point with probability 1, the random walk is called recurrent. If we consider a cubic lattice in d dimensions the translation invariance implies that the return probability does not depend on the starting point (and one can set it to be the origin for simplicity). Polya's problem is to determine the return probability. We will see that for unbiased random walks and lattices with equivalent lattice points, the result critically depends on the dimensionality of the problem.

The relation between $p_N(x, x_0)$ and $F_N(x, x_0)$ may be written as:

$$\begin{aligned} p_0(x, x_0) &= \delta_{x, x_0}, \\ p_N(x, x_0) &= \sum_{j=1}^N p_{N-j}(x, x) F_j(x, x_0) \quad N > 0. \end{aligned} \quad (22)$$

In words the relation above means that to reach the point x at the N 'th (time N) step, this point was visited for the first time at some previous time j (with probability $F_j(x, x_0)$) and then the particle is on x after $N - j$ transitions (with probability $p_{N-j}(x, x)$). The sum over j gives all the possible ways of reaching x for the first time. Equations (20,21) are analogous of a discrete Laplace transform and equation (22) is a discrete type of convolution. Substituting equation (22) in equation (20) we may rewrite it as:

$$\begin{aligned} \hat{p}_u(x, x_0) &= \delta_{x, x_0} + \sum_{N=1}^{\infty} u^{N-j} p_{N-j}(x, x) \left[\sum_{j=1}^{\infty} u^j F_j(x, x_0) - \sum_{j=N+1}^{\infty} u^j F_j(x, x_0) \right] \\ &= \delta_{x, x_0} + \left[\sum_{j=1}^{\infty} u^j F_j(x, x_0) \right] \left[\sum_{\tilde{N}=1}^{\infty} u^{\tilde{N}} p_{\tilde{N}}(x, x) \right] \\ &\quad - \left(\sum_{N=1}^{\infty} u^{N-j} p_{N-j}(x, x) \sum_{j=N+1}^{\infty} u^j F_j(x, x_0) \right). \end{aligned} \quad (23)$$

The last term vanishes (because $p_{n<0}(x, x) = 0$), and we write

$$\widehat{p}_u(x, x_0) = \delta_{x, x_0} + \widehat{F}_u(x, x_0) \widehat{p}_u(x, x). \quad (24)$$

We may also write it as

$$\begin{aligned} \widehat{F}_u(x_0, x_0) &= \frac{\widehat{p}_u(x_0, x_0) - 1}{\widehat{p}_u(x_0, x_0)} = 1 - \frac{1}{\widehat{p}_u(x_0, x_0)}, \\ \widehat{F}_u(x, x_0) &= \frac{\widehat{p}_u(x, x_0)}{\widehat{p}_u(x, x)}. \end{aligned} \quad (25)$$

These relations are general in the sense that they are independent of the dimensionality and the bias properties of the random walk (note that we haven't used the translation invariance property either). We did assume, in writing equation (22), that the transition probabilities are time independent. Since all lattice points are identical we may set $x_0 = 0$. The return probability (to the origin) is given by

$$\widehat{F}_{u=1}(x_0, x_0) = 1 - \frac{1}{\widehat{p}_{u=1}(x_0, x_0)} = 1 - \frac{1}{\widehat{p}_{u=1}(0, 0)}. \quad (26)$$

By definition,

$$\widehat{p}_{u=1}(0, 0) = 1 + \sum_{N=1}^{\infty} p_N(0, 0).$$

We showed earlier that ${}^d p_N(\vec{0}) \sim \frac{c_d}{N^{d/2}}$. Thus, for $d = 1, 2$ $\widehat{p}_{u=1}(0, 0) = \infty$ and $\widehat{F}_{u=1}(x_0, x_0) = 1$. For $d \geq 3$, $\widehat{p}_{u=1}(0, 0)$ is finite and hence, $\widehat{F}_{u=1}(x_0, x_0) < 1$.