An Introduction to Random Walks from Pólya to Self-Avoidance

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Outline

1. Brief introduction to probability
2. Random walk
3. Pólya's theorem
4. Self-avoiding random walk

1. Brief Introduction to Probability

- Perform an experiment
- Set of all possible outcomes of an experiment is called <u>sample space</u>, denoted Ω

Ex: Toss coin. $\exists$ 2 outcomes: Heads or Tails

$$\therefore \Omega = \{H, T\}$$

Definition: A <u>probability</u>, P, is a function $P : S \to [0, 1]$, $S \subset \Omega$, st:

1. $P(\phi) = 0$
2. $P(\Omega) = 1$
3. $P(A \cup B) = P(A) + P(B) \quad \forall A, B \subset \Omega$ with A, B disjoint

Ex:
$P(H) = \frac{1}{2}$,
$P(T) = \frac{1}{2}$,
$P(H \text{ or } T) = 1$,
$P(H \text{ and } T) = 0$.

Definition: A <u>random variable</u>, X, is a real number representing values of possible outcomes of an experiment.

Ex: Let $H = 1$, $T = 0$. Flip a coin twice and count the number of heads. Then there can be either 0,1 or 2 heads.

$X = 0$ No Heads
$X = 1$ One Head
$X = 2$ Two Heads

Thus,

$$P(X = 0) = \frac{1}{4} \text{ TT is only way to get no heads}$$
$$P(X = 1) = \frac{2}{4} \text{ HT or TH}$$
$$P(X = 2) = \frac{1}{4} \text{ HH only}$$

Definition: The expected value (or average value or mean) of a (discrete) random variable is defined as:

$$\mathbb{E}(X) = \sum_{x \in \Omega} x P(X = x)$$

(i.e. sum over all possible outcomes)

Ex: Roll a die. Observe face. What is expected outcome?

$X = 1$	$P(X = 1) = \frac{1}{6}$
$X = 2$	$P(X = 2) = \frac{1}{6}$
$X = 3$	$P(X = 3) = \frac{1}{6}$
$X = 4$	$P(X = 4) = \frac{1}{6}$
$X = 5$	$P(X = 5) = \frac{1}{6}$
$X = 6$	$P(X = 6) = \frac{1}{6}$

$$\begin{aligned}\therefore \mathbb{E}(X) &= \sum_{x} x P(X = x) \\ &= 1 \cdot P(X = 1) + \ldots + 6 \cdot P(X = 6) \\ &= \frac{1}{6}(1 + 2 + 3 + 4 + 5 + 6) \\ &= 3.5\end{aligned}$$

Note: Expectation is additive:

$$\mathbb{E}(X + Y) = \mathbb{E}(X) + \mathbb{E}(Y)$$

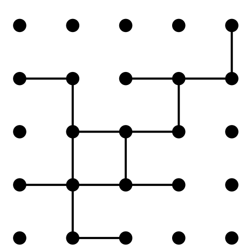
2. Random Walk

$\mathbb{R}^d$: d-dimensional Euclidean space

$\mathbb{Z}^d$ = set of all d-tuples with integer coefficients
$= \{(z_1, \ldots, z_d) : z_i \in \mathbb{Z}\}$
"$d-$dimensional lattice"

A particle starts at the origin of $\mathbb{Z}^d$. At each unit of time the particle randomly selects one of its $2d$ nearest neighbours and moves there. This is called a <u>random walk</u>.

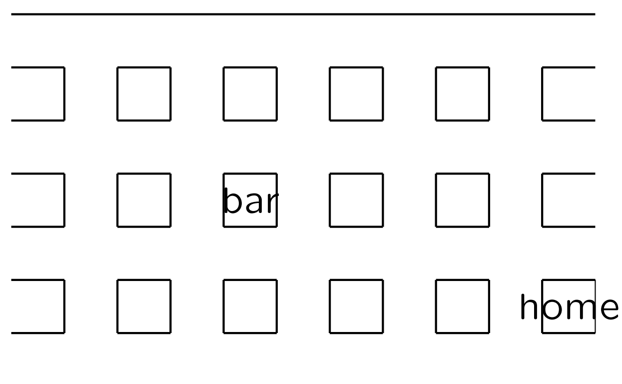
For Example, on $\mathbb{Z}^2$:



At each step the particle can move either up, down, left or right. This is sometimes called a <u>drunkard's walk</u>.

- A "drunk" steps out of the bar and is so intoxicated that he stumbles at random.

- Imagine the bar situated at the centre of a large grid of streets.



- With each step the drunk is equally likely to go north, south, east or west.

- Imagine that the drunk also has a home.

Now, suppose that we release the drunk and let him walk (randomly) and that

- At the bar, he has a drink and leaves at the next time step.

- At home, he has a nap and leaves at the next time step.

CLAIM

The drunkard returns to the bar infinitely often; but also returns home infinitely often.

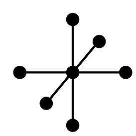
IN FACT

- In one dimension, the drunk <u>will</u> return to the bar infinitely often.
- In two dimensions, the drunk <u>will</u> return to the bar infinitely often.
- In three dimensions, the drunk <u>will not</u> return to the bar infinitely often. That is, he will go to the bar one final time, have his final drink, and wander off ... never to return again.

More formally,

a simple random walk on $\mathbb{Z}^d$ is a random walk in which the probability of moving from a point to any one of its $2d$ nearest neighbours is $\frac{1}{2d}$.

e.g.



Simple random walk on $\mathbb{Z}^3$
Choose any neighbour with probability $\frac{1}{6}$

Now, let's begin a simple random walk on $\mathbb{Z}^d$ starting at the origin.

Let $p_{esc} = Pr\{\text{walk never returns to } 0\}$

Definition: A random walk is recurrent iff $p_{esc} = 0$.
A random walk is transient iff $p_{esc} > 0$.

We can now formulate the theorem of Pólya.

3. Theorem: Pólya, 1928

A simple random walk on the d-dimensional lattice $\mathbb{Z}^d$ is recurrent for $d = 1$ and $d = 2$, but is transient for $d \geq 3$.

That is, for $d = 1, 2$ it is "certain" to return to the origin, but for $d \geq 3$ it is not.

Proof: I will prove this theorem for the $d = 1, 2$ recurrent cases and the $d = 3$ transient case. The $d > 3$ cases are very similar to the $d = 3$ case except for some messier algebra.

But first ...

Recurrence $\equiv$ infinite expected number of returns

- $u = Pr\{\text{random walk started at 0 returns to 0}\}$
- $Pr\{\text{walker is there }\underline{\text{exactly}}\ k \text{ times}\} = u^{k-1}(1-u)$
- $m =$ expected number of times at 0

$$
\begin{aligned}
\therefore m &= \sum_{k=1}^{\infty} k \cdot u^{k-1}(1-u) \\
&= (1-u) \sum_{k=1}^{\infty} k \cdot u^{k-1} \\
&= (1-u) \sum_{k=1}^{\infty} \frac{d}{du} u^{k} \\
&= (1-u) \frac{d}{du} \sum_{k=1}^{\infty} u^{k} \\
&= (1-u) \frac{d}{du} \frac{1}{1-u} \\
&= \frac{1}{1-u}
\end{aligned}
$$

$\therefore$ if $m = \infty$, then $u = 1$ and so the walk is recurrent
if $m < \infty$, then $u < 1$ and so the walk is transient

Alternatively,

let $u_n = Pr\{$walk starting at 0 is at 0 on n^{th} step$\}$
$u_0 = 1$

Define a random variable as follows:

$$e_n = \begin{cases} 1, & \text{if walker is at 0 at time n} \\ 0, & \text{otherwise} \end{cases}$$

Thus, $T = \sum_{n=0}^{\infty} e_n$ is the total number of times at 0.

So, $m = \mathbb{E}(T) = \sum_{n=0}^{\infty} \mathbb{E}(e_n)$

But, $\mathbb{E}(e_n) = 1 \cdot u_n + 0 \cdot (1 - u_n)$

So,

$$\boxed{m = \sum_{n=0}^{\infty} u_n}$$

recurrence $\Leftrightarrow \sum u_n$ diverges transience $\Leftrightarrow \sum u_n$ converges

$\boxed{\mathbf{D=1}}$

To return to origin walker must take same number of steps left as right.

$\therefore$ only even return times are possible

$u_{2n} = \left(\frac{1}{2}\right)^{2n} \cdot$ #possible paths

$u_{2n} = \binom{2n}{n} \left(\frac{1}{2}\right)^{2n}$

Using the well-known Stirling Formula, we can get an asymptotically equivalent expression for u_{2n}.

Stirling Formula: $n! \approx \sqrt{2\pi n}\, e^{-n}\, n^n$

$$\begin{aligned}\therefore u_{2n} &= \frac{(2n)!}{n!(2n-n)!}\frac{1}{2^{2n}} \\ &\approx \frac{\sqrt{2\pi 2n}\, e^{-2n}\, (2n)^{2n}}{(\sqrt{2\pi n}\, e^{-n}\, n^n)^2\, 2^{2n}} \\ &= \frac{1}{\sqrt{\pi n}}\end{aligned}$$

Thus,

$$\sum_n u_{2n} \approx \sum_n \frac{1}{\sqrt{\pi n}} \text{ which \underline{diverges}}$$

$\therefore$ Simple rw in one dimension is recurrent. $\square$

$\boxed{\mathbf{D = 2}}$

To return the walker must take ...

- same number of steps left as right, AND
- the same number of steps up as down.

$\therefore$ every path that returns in $2n$ steps has probability $\left(\frac{1}{4}\right)^{2n}$ of occurring

The number of paths with k steps left, k steps right, $n-k$ steps up, $n-k$ steps down is $\binom{2n}{k,k,n-k,n-k} := \frac{(2n)!}{k!k!(n-k)!(n-k)!}$

$$
\begin{aligned}
u_{2n} &= \left(\frac{1}{4}\right)^{2n} \sum_{k=0}^{n} \frac{(2n)!}{k!k!(n-k)!(n-k)!} \\
&= \left(\frac{1}{4}\right)^{2n} \sum_{k=0}^{n} \frac{(2n)!}{n!n!} \frac{n!n!}{k!k!(n-k)!(n-k)!} \\
&= \left(\frac{1}{4}\right)^{2n} \binom{2n}{n} \sum_{k=0}^{n} \binom{n}{k}^2
\end{aligned}
$$

Note: $\displaystyle\sum_{k=0}^{n} \binom{n}{k}^2 = \binom{2n}{n}$.

So, $\boxed{u_{2n} = \left(\frac{1}{2^{2n}}\binom{2n}{n}\right)^2}$

Thus, $m = \sum_n u_{2n} \approx \sum_n \frac{1}{\pi n} = \infty$

(It is just the square of the one dimensional result.)

$\therefore$ Simple rw in two dimensions is also recurrent. $\square$

$\boxed{\mathbf{D=3}}$
Similarly, to return to the origin, the walker must take

- same number of steps left as right, AND
- same number of steps up as down, AND
- same number of steps forward as backward

$\therefore$ every path that returns in $2n$ steps has probability $\left(\frac{1}{6}\right)^{2n}$ of occurring

The number of paths with k steps left, k steps right, j steps up, j steps down, $n-k-j$ steps forward, $n-j-k$ steps backward is

$$\binom{2n}{k,k,j,j,n-k-j,n-k-j} := \frac{(2n)!}{k!k!j!j!(n-k-j)!(n-k-j)!}$$

So,

$$u_{2n} = \frac{1}{6^{2n}} \sum_{\substack{j,k \\ j+k \leq n}} \frac{(2n)!}{k!k!j!j!(n-j-k)!(n-j-k)!}$$

$$= \frac{1}{2^{2n}} \binom{2n}{n} \sum_{\substack{j,k \\ j+k \leq n}} \left(\frac{1}{3^n} \frac{n!}{k!j!(n-k-j)!} \right)^2$$

Now,

$$\frac{1}{3^n} \binom{n}{k, j, n-j-k} = \frac{1}{3^n} \frac{n!}{k!j!(n-j-k)!}$$

$$= \text{probability of placing } n \text{ balls in 3 boxes}$$

This is maximized when k, j, $(n-k-j)$ are as close to $\frac{n}{3}$ as possible.

So,

$$u_{2n} \leq \frac{1}{2^{2n}}\binom{2n}{n}\left(\frac{1}{3^n}\frac{n!}{\left[\frac{n}{3}\right]!\left[\frac{n}{3}\right]!\left[\frac{n}{3}\right]!}\right)\underbrace{\left(\sum_{j,k}\frac{1}{3^n}\frac{n!}{k!j!(n-j-k)!}\right)}_{=1 \text{ since it is a distribution}}$$

$$\therefore u_{2n} \leq \frac{1}{2^{2n}}\binom{2n}{n}\left(\frac{1}{3^n}\frac{n!}{\left(\left[\frac{n}{3}\right]!\right)^3}\right)$$

However, Stirling $\Rightarrow u_{2n} \leq \frac{K}{n^{3/2}}$ for some constant $K \in \mathbb{R}^+$

So,

$$m = \sum_n u_{2n} \leq K \sum_n \frac{1}{n^{3/2}} < \infty$$

$\therefore$ Simple rw in three dimensions is transient. $\square$

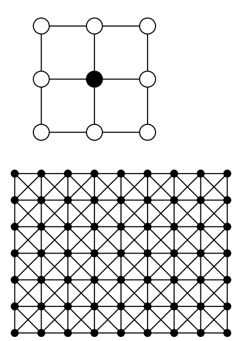
4. Self-Avoiding Random Walk

A <u>self-avoiding random walk</u> is simply a random walk with the additional constraint that you cannot revisit a previously visited site.

One application of self-avoiding random walks is as a model for polymers.

- A polymer is a chain of molecules known as monomers.
- Monomers attach "at random angles" to the end of the chain.
- A monomer cannot attach at an already occupied spot.

For example, suppose that we have a polymer in which monomers are allowed to attach to the chain only at angles which are multiples of 45°. In this case, we are working on an "honeycomb lattice".



Definition: A <u>self-avoiding random walk (SARW)</u> of length n in $\mathbb{Z}^d$ is a sequence ω of points such that

1. $\omega = (\omega_0, \omega_1, \dots, \omega_n)$ where $\omega_i \in \mathbb{Z}^d$

2. $\omega_0 = 0$

3. $\|\omega_j - \omega_{j-1}\| = 1$ for $j = 1, \dots, n$ and distance is measured "on the lattice"

4. $\boxed{\omega_i \neq \omega_j \text{ for } i \neq j}$

1, 2, 3 = RW
1, 2, 3 + 4 = SARW

Although SARWs are similar to RWs, they are tough to analyze. There are still many aspects of them that are unknown.

Ω_n : set of SARWs of length n

$C_n = |\Omega_n| = \#(\Omega_n) = \text{card}(\Omega_n)$

Open Question

"What is C_n?"
"How many elements does Ω_n have?"
"How many n-step self-avoiding random walks are there?"

Some Partial Answers

- There exist $(2d)^n$ simple random walks of length n. So,

$$\boxed{C_n \leq (2d)^n}$$

- Don't let it visit it's last site. (i.e. no immediate returns) $\therefore \exists$ at most $2d-1$ nearest unvistited neighbours. So,

$$\boxed{C_n \leq 2d(2d-1)^{n-1}}$$

- Let the random walk move only in the postive x direction. (Or in *any* one direction for that matter.) This is clearly self-avoiding, so

$$\boxed{d^n \leq C_n}$$

Bounds on Number of n-step SARWs

$$d^n \leq C_n \leq 2d(2d-1)^{n-1}$$

<u>CONJECTURE</u>

There is some number β with

$$C_n \approx \beta^n$$

<u>WELL KNOWN:</u> $\lim_{n\to\infty} C_n^{1/n}$ exists

$$\therefore \lim_{n\to\infty} C_n^{1/n} = \beta$$

<u>FROM ABOVE:</u> $d \leq \beta \leq 2d-1$.

$\boxed{\underline{\text{UNKNOWN:}}\ \beta}$

References

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P. Doyle and J. L. Snell: Random Walks and Electric Networks