Random Walk

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Introduction

- Statistical Mechanics
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- Announcement and other communication will be through:
- `http://statphys.chungbuk.ac.kr/doku.php?id=2018asm`
- on Tuesday 2 pm - 5 pm (S1-1-205).
- (OR) on Tuesday 1 pm - 4 pm (S1-1-205).

What is Probability?

The asymptotic frequency of success in the limit of an infinite number of trials

$$p = \lim_{N \to \infty} \frac{N_s}{N}. \tag{1}$$

The probabilities must satisfy the conditions that

$$0 \leq P(i) \leq 1, \tag{2}$$

for all i. An impossible event has probability zero and a certain event has probability 1. The normalization condition of the probability distribution is

$$\sum_i P(i) = 1. \tag{3}$$

Mean, Variance, and Standard Deviation

The n-th moment of x can be defined as

$$\langle x^n \rangle = \sum_i x^n P(i). \tag{4}$$

Mean, variance, and standard deviation can be expressed as the moments of the probability distribution

$$\langle x \rangle = \sum_i x P(i),$$
$$\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2,$$
$$\sigma = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}.$$

Binomial Distribution

The binomial distribution is given by

$$P(n|N) = \binom{N}{n} p^n (1-p)^{N-n} \tag{5}$$
$$= \frac{N!}{n!(N-n)!} p^n (1-p)^{N-n}.$$

It represents the probability distribution of the number of successes (yes-no question) with the probability p, out of total N trials.

Coin Tossing

- Prob(Head)=1/2 and Prob(Tail)=1/2
- Let us flip a coin N times.
- What is the probability of getting h heads?

Counting

After N trials, we examine the probability of the number of head n out of total N steps $P(n)$.

$$
\begin{aligned}
N=1: \quad & P(1) = p. \\
& P(0) = q. \\
N=2: \quad & P(2) = p^2. \\
& P(1) = pq. \\
& P(1) = qp. \\
& P(0) = q^2. \\
N=3: \quad & P(3) = p^3. \\
& P(2) = 3p^2 q. \\
& P(1) = 3pq^2. \\
& P(0) = q^3.
\end{aligned}
$$

Coin Tossing

- Prob(Head)=1/2 and Prob(Tail)=1/2
- Let us flip a coin N times.
- What is the probability of getting h heads?

$$P(h|N) = \binom{N}{h} p^h q^{N-h} \tag{6}$$
$$= \frac{N!}{h!(N-h)!} p^h (1-p)^{N-h}.$$

Stirling's Approximation for $N!$

For large N,

$$N! \approx \sqrt{2\pi N}\left(\frac{N}{e}\right)^N, \tag{7}$$

$$\log N! \approx N \log N - N.$$

$$\begin{aligned}\log N! \approx \int_1^N \log x dx &= [x \log x - x]_1^N \\ &= N \log N - N + 1.\end{aligned}$$

Continuous probability theory

Given the probability density $P(x)$, the probability of finding x in an interval $[a, b]$ is

$$P([a,b]) = \int_a^b P(x)dx. \tag{8}$$

The n-th moment of the distribution is

$$\langle x^n \rangle = \int_{-\infty}^{\infty} x^n P(x)dx. \tag{9}$$

Dirac Delta Functions

$$\delta(x - x_0) = \begin{cases} +\infty, & x = x_0 \\ 0, & x \neq x_0 \end{cases}$$

$$\int_{-\infty}^{\infty} \delta(x) dx = 1.$$

$$\int_{-\infty}^{\infty} f(x)\delta(x - \alpha) dx = f(\alpha).$$

$$\delta(x - \alpha) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ip(x-\alpha)} dp.$$

Gaussian (Normal) Distribution

The Gaussian distribution with the mean x_0 and the standard deviation σ is given by

$$g(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x-x_0)^2}{2\sigma^2}\right]. \tag{10}$$

- Gaussian Integral

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}. \tag{11}$$

Gaussian (Normal) Distribution

- Gaussian approximation to the Binomial Distribution

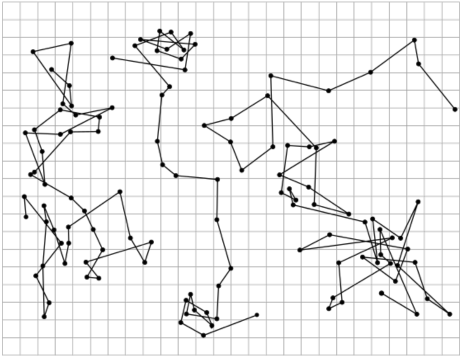
- Central limit theorem:

  Sum of independent and identically distributed random variables with finite variance σ^2 is converging to the normal distribution with variance σ^2 in the limit $N \to \infty$.

  We will prove it later.

Brownian Motion

In 1827, Robert Brown who was the microscopist found the “Brownian motion” of pollen.



Three tracings of the motion of colloidal particles from “Les Atomes”, Jean Baptiste Perrin.

Albert Einstein (in one of his 1905 papers) and Marian Smoluchowski (1906) brought the solution of the problem.

History

A random work problem which is closely related to the Brownian motion, was in a modern sense introduced by Karl Pearson in 1905. In the letter of Nature:

"A man starts from a point 0 and walks l yards in a straight line; he then turns through any angle whatever and walks another l yards in a straight line. He repeats this process n times. I require the probability that after these n stretches he is at a distance between r and $r + \delta r$ from his starting point 0."

The solution to this random walk problem was provided in the same volume of Nature by Lord Rayleigh ($1842 \sim 1919$). He told that he had solved the problem 25 earlier.

Random Walker

We will consider the simplest example, related to the Brownian motion.

$$P(\rightarrow) = p, \quad P(\leftarrow) = q = 1 - p.$$

Initially, a random walker is located at the origin, $x(t = 0) = 0$. After n steps . . .

Statistical Description

We can trace all the trajectory of a walker, $x(t)$. But it is stochastic (probabilistic) not deterministic. Thus, all we need to know is the statistics of $x(t)$ such as $\langle x(t) \rangle$, $\langle x(t)^2 \rangle$, σ, etc.

Agree? In reality,

- Number of Particles, N is enormous.
- Small errors in the initial conditions leads to drastic a huge difference. We deals with real numbers.
- In many cases, we are not really interested in the trajectories of each particles.

Counting

After n steps, we examine the probability of the number of right steps r out of total n steps $P(r|n)$.

$$
\begin{aligned}
n = 1: \quad & |\rightarrow\rangle, P(1|1) = p. \\
& |\leftarrow\rangle, P(0|1) = q. \\
n = 2: \quad & |\rightarrow, \rightarrow\rangle, P(2|2) = p^2. \\
& |\rightarrow, \leftarrow\rangle, P(1|2) = pq. \\
& |\leftarrow, \rightarrow\rangle, P(1|2) = qp. \\
& |\leftarrow, \leftarrow\rangle, P(0|2) = q^2. \\
n = 3: \quad & P(3|3) = p^3. \\
& P(2|3) = 3p^2 q. \\
& P(1|3) = 3pq^2. \\
& P(0|3) = q^3.
\end{aligned}
$$

Binomial Distribution

The binomial distribution is given by

$$
\begin{aligned}
P(r|n) &= \binom{n}{r} p^r (1-p)^{n-r} \qquad (12) \\
&= \frac{n!}{r!(n-r)!} p^r (1-p)^{n-r}.
\end{aligned}
$$

It represents the probability distribution of the number of right steps with the probability p, out of total n steps.

Binomial Theorem

Binomial Theorem (or expansion) describes the expansion of powers of a binomial.

$$(x+y)^n = \sum_{k=0}^{n} \binom{n}{k} x^k y^{n-k}.$$

The coefficient can be obtained from Pascal's triangle as well.

Sum over All Possible r

Summing over all possible state of r (that is the normalization factor),

$$\begin{aligned} Z &= \sum_r P(r) \\ &= \sum_r \binom{n}{r} p^r q^{n-r} \\ &= (p+q)^n = 1. \end{aligned}$$

Z acts like the Partition function in equilibrium statistical mechanics.

Magic of Partial Derivatives

$$
\begin{aligned}
\langle r \rangle &= \sum_r r P(r) \\
&= \sum_r r \binom{n}{r} p^r q^{n-r} \\
&= p \frac{\partial}{\partial p} \sum_r \binom{n}{r} p^r q^{n-r} \\
&= p \frac{\partial}{\partial p} (p+q)^n \\
&= np(p+q)^{n-1} = np.
\end{aligned}
$$

Magic of Partial Derivatives

$$\begin{aligned}
\langle r^2 \rangle &= \sum_r r^2 P(r) \\
&= p\frac{\partial}{\partial p} p \frac{\partial}{\partial p}(p+q)^n \\
&= p\frac{\partial}{\partial p} np(p+q)^n \\
&= p[n(p+q)^{n-1} + np(n-1)(p+q)^{n-2}] \\
&= np + n(n-1)p^2.
\end{aligned}$$

$$\begin{aligned}
\sigma^2 &= \langle r^2 \rangle - \langle r \rangle^2 \\
&= n(n-1)p^2 + np - n^2p^2 = np - np^2 = np(1-p) = npq.
\end{aligned} \tag{13}$$

Mean and Variance

- $\langle r \rangle = np.$
- $\sigma^2 = npq.$

Diffusion Equation (Continuum limit)

$$g_{n+1}(x) = pg_n(x-1) + qg_n(x+1).$$

When $p = q = 1/2$,

$$g_{n+1}(x) = \frac{1}{2}g_n(x-1) + \frac{1}{2}g_n(x+1).$$

Subtract $g_n(x)$ on both sides:

$$g_{n+1}(x) - g_n(x) = \frac{1}{2}\left[g_n(x-1) + g_n(x+1) - 2g_n(x)\right].$$

In the continuum limit, it corresponds to the diffusion equation

$$\frac{\partial g(x,t)}{\partial t} = D\frac{\partial^2 g(x,t)}{\partial x^2}. \tag{14}$$

where $D = \frac{1}{2}\frac{(\Delta x)^2}{\Delta t}$.

Central Limit Theorem: Convolution

The distribution of sum of two random variables:

$$g_n(x) = \int g_{n-1}(x - x')g_1(x')dx'.$$

Fourier transform of the equation is

$$\begin{aligned}
&\frac{1}{\sqrt{2\pi}} \int \int g_{n-1}(x - x')g_1(x')e^{ikx}dx'dx \\
&= \frac{1}{\sqrt{2\pi}} \int g_1(x') \int g_{n-1}(x - x')e^{ikx}dxdx' \\
&= \frac{1}{\sqrt{2\pi}} \int g_1(x')e^{ikx'} \int g_{n-1}(x - x')e^{ik(x-x')}dxdx' \\
&= \frac{1}{\sqrt{2\pi}} Q(k) \times Q_{n-1}(k) = \frac{1}{\sqrt{2\pi}} Q(k)^n
\end{aligned}$$

Applying inverse transformation:

$$g(x) = \frac{1}{2\pi} \int dk e^{-ikx} Q(k)^n.$$

Gaussian (Normal) Distribution

The Gaussian distribution with the mean x_0 and the standard deviation σ is given by

$$g(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x-x_0)^2}{2\sigma^2}\right]. \tag{15}$$

- Gaussian approximation to the Binomial Distribution
- Central limit theorem:

  Sum of independent and identically distributed random variables (convolution) with finite variance σ^2 is converging to the normal distribution in the limit $N \to \infty$.

Where to go next...

Let us go to equilibrium statistical mechanics.