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18.325 Professor Bazant

Lecture 1: Historical Introduction to Random Walks and Diffusion 02/06/01

I. Introduction

Pearson (1905) introduced the term "random walk"

He was interested in describing the spatial/temporal evolution of mosquito populations invading cleared jungle regions. He found it too complex to model deterministically, so he conceptualized a simple random model

Pearson posed his problem in a letter to *Nature*:

If a "random walker" begins at the origin taking steps of length, l, each in a random direction, what is the probability, $P(r < |\mathbf{x}_n| < r + \delta r)$ of being located at $r + \delta r$ after n steps

Lord Rayleigh replied one week later with the answer to Pearson's problem (He had already solved this problem (1888) while investigating wave fields of constant amplitude and random phase):

$$P_n(\mathbf{x})d\mathbf{x} \sim \frac{2}{n} e^{-\frac{r^2}{n}} r dr \quad \text{(essentially the Central Limit Theorem)}$$

(Gaussian behavior)

Rayleigh had also found the solution for a random walk in 1-D, with steps of unit length

$$P_n(x)dx = \frac{1}{\sqrt{2\pi n}} e^{-\frac{x^2}{2n}} dx \qquad \text{(Gaussian process with } \sigma^2 \equiv n\text{)}$$

So, spreading about the origin ~ σ (standard deviation) ~ $\sqrt{n}$

II. Bachelier (1900)

Wrote Ph.D. thesis on stock market speculation (under Poincarè);

No single trend for stock value is expected over another, so Bachelier formulated fluctuations in value as a random walk--steps (fluctuations) are independent and given by transition probabilities,

$$P_1(x-x') \text{ (discrete steps)}$$

$$P(x-x',\tau) \text{ (continuous time)}$$

which represent the probability distributions for step size, $\Delta x = x - x'$, in a single step (discrete case) or time interval, τ (continuous case)

Bachelier gave the probability distribution of walkers after n steps (discrete) or time, t (continuous) as:

$$P_{n+1}(x) = \int_{-\infty}^{\infty} P_1(x-x')P_n(x')dx' \qquad \text{or}$$

$$P(x,t+\tau) = \int P(x-x',\tau)P(x',t)dx'$$

He also found the solution (continuous)

$$P(x,t) = \frac{1}{\sqrt{2\pi\sigma^2 t}} e^{\frac{x^2}{2\sigma^2 t}} \qquad \text{(Gaussian function)}$$

(Bachelier used an unusual normalization of the Gaussian function to allow only positive values of x instead of $x \in (-\infty,\infty)$ as allowed by transitions)

Gaussian behavior: spreading about the origin ~ σ ~ $\sqrt{t}$

Bachelier noted also that his solution satisfied Fourier's Equation of heat conduction,

$$\frac{\partial p}{\partial t} = D\frac{\partial^2 p}{\partial x^2}$$

which also happens to be the Diffusion Equation (Fick).

Despite Bachelier's insights, his work has been often-neglected, and suffered in relative obscurity until economists "discovered" it decades later.

III. Diffusion

Macroscopic process (net movement of mass from higher to lower concentration) derived from random molecular motions

Fick's (1855) law (observed): flux of mass is proportional to and directionally opposite concentration gradient,

$$\text{flux} = \mathbf{J} = -D\nabla C$$

Applying conservation of mass to a differential control volume (the net rate of flux through the surface into the control volume must equal the time rate of change of mass in the control volume),

$$\frac{\partial}{\partial t}\int_V C dV = \int_V \frac{\partial C}{\partial t} dV \qquad \text{(rate of change of mass in the control volume)}$$

$$= -\oint_S \mathbf{J}\cdot\mathbf{n} ds = \oint_S D\nabla C \cdot \mathbf{n} \qquad \text{(net flux into the control volume through the surface)}$$

(Applying Gauss' Divergence Theorem)

$$= \oint_V \nabla\cdot(D\nabla C) dV$$

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \qquad \text{(Differential Control Volume)}$$

Fourier (1822) did the same analysis for Temperature in place of Concentration

IV. Einstein (1905)

Gave a physical description of Brownian motion; Later experimentally verified by Perrin (1909)--Both sets of work received Nobel Prize for providing proof for the atomic nature of matter

Einstein's assumptions (similar to Bachelier):

- Many *Independent* random walkers
- Each takes steps that, after some very small time interval, τ, can be considered *Independent* in time

He used a continuum approach rather than discrete:

Each particle has a transition probability for step length, $p(\delta x, \tau)$ in the time interval, τ

and C(x,t) = Concentration of particles at x at time, t is expressed (similar to Bachelier) as,

$$C(x,t+\tau) \approx \int_{-\infty}^{\infty} p(\delta x, \tau) C(x-\delta x, t) d\delta x$$

He normalized the transition pdf, such that $\int p(\delta x, \tau) d\delta x = 1$

and assumed that the step size, given by the transition pdf, was small compared with the typical length scale for variations in the concentration distribution,

$\delta x <<$ characteristic length scale for variations in C(x,t)

And Taylor-expanded around C(x,t):

$$C(x-\delta x, t) = C(x,t) - \delta x \frac{\partial C(x,t)}{\partial x} + \frac{\delta x^2}{2}\frac{\partial^2 C(x,t)}{\partial x^2} - \frac{\delta x^3}{3!}\frac{\partial^3 C(x,t)}{\partial x^3} + \ldots$$

Substituting $C(x-\delta x, t)$ (no longer expressed as a function of δx) into the previous expression for $C(x,t+\tau)$,

$$C(x,t+\tau) \approx C(x,t)\int_{-\infty}^{\infty} p(\delta x,\tau) d\delta x + \frac{\partial C(x,t)}{\partial x}\int_{-\infty}^{\infty} p(\delta x,\tau)\delta x d\delta x + \frac{\partial^2 C(x,t)}{\partial x^2}\int_{-\infty}^{\infty} p(\delta x,\tau)\frac{\delta x^2}{2} d\delta x$$

$$-\frac{\partial^3 C(x,t)}{\partial x^3}\int_{-\infty}^{\infty} p(\delta x,\tau)\frac{\delta x^3}{3!} d\delta x + \ldots$$

Noting that $\left\langle \delta x^n \right\rangle \equiv \int_{-\infty}^{\infty} p(\delta x, \tau) \frac{\delta x^n}{n!} d\delta$ is the n$^{\text{th}}$ moment of the transition probability distribution, that the zeroth moment = $\int_{-\infty}^{\infty} p(\delta x, \tau) d\delta x = 1$,

and dividing through by τ,

$$\frac{C(x,t+\tau) - C(x,t)}{\tau} = \frac{\partial C}{\partial t} \qquad \text{and}$$

$$\frac{\partial C}{\partial t} + \frac{\langle \delta x \rangle}{\tau} \frac{\partial C}{\partial x} = \frac{\left\langle \delta x^2 \right\rangle}{2\tau} \frac{\partial^2 C}{\partial x^2} - \frac{\left\langle \delta x^3 \right\rangle}{3!\tau} \frac{\partial^3 C}{\partial x^3} \cdots$$

Also, *if the second moment(variance) of the transition pdf is finite,*

$$\lim_{\tau \to 0} \frac{\langle \delta x \rangle}{\tau} \qquad \text{and} \qquad \lim_{\tau \to 0} \frac{\left\langle \delta x^2 \right\rangle}{2\tau}$$

are constants and can be defined as

$$v \equiv \lim_{\tau \to 0} \frac{\langle \delta x \rangle}{\tau} \qquad \text{and} \qquad D \equiv \lim_{\tau \to 0} \frac{\left\langle \delta x^2 \right\rangle}{2\tau}$$

where v is a net drift (advection) of the distribution of walkers and D is the diffusion constant

For small time, t ~ τ, the characteristic length scale of the distribution, based on diffusion,

$$\delta x \sim \sqrt{2D\tau} = O(\tau^{1/2})$$

is much greater than the characteristic scale based on advection

$$\delta x \sim v\tau$$

since $\tau^{1/2} >> \tau$

So, with

$$\delta x \sim \tau^{1/2}$$

it follows that

$$\langle \delta x^n \rangle \sim \tau^{n/2}$$

and

$$\frac{\partial C}{\partial t} + \frac{\langle \delta x \rangle}{\tau}\frac{\partial C}{\partial x} = \frac{\langle \delta x^2 \rangle}{2\tau}\frac{\partial^2 C}{\partial x^2} + O(\tau^{1/2})$$

For small t, $\tau^{1/2}$ >> (t ~ τ) so the $O(\tau^{1/2})$ term is significant and the fluctuations are dominant;

But as $\frac{t}{\tau} \to \infty$, the fluctuations become insignificant and the $O(\tau^{1/2})$ and higher order terms are negligible (*if the second moment is finite)*

After neglecting the higher order terms, the diffusion equation with the drift term is obtained,

$$\frac{\partial C}{\partial t} + v\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2}$$

So Einstein has introduced drift into the random walk and begins to address the behavior for small-time