III. RANDOM WALKS.

1905 Karl Pearson poses the problem of the random walk, being interested in the dynamics how mosquito populations invade cleared jungle regions:
"Can any of your readers refer me to a work wherein I should find the solution to the following problem [...]:
A man starts from a point O and walks l yards in a straight line; he then turns through any angle whatever and walks l yards in a second 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 $r+dr$ from his starting point, O."

Lord Rayleigh pointed out one week later that in the limit of large n the solution is a Gaussian.

Consider a jump process on a one-dimensional lattice with spacing a. At each step the probability to jump left or right is equal.
$\rightsquigarrow$ Probability to reach site m after N steps ($N \pm m$ are always even!)

$$g(m,N) = \left(\frac{1}{2}\right)^N \frac{N!}{\underbrace{\left[\frac{1}{2}(N-m)\right]!}_{\frac{N-m}{2}\text{ jumps to left}}\,\underbrace{\left[\frac{1}{2}(N+m)\right]!}_{\frac{N+m}{2}\text{ jumps to right}}}$$

Stirling's formula: $\log N! = \left(N+\frac{1}{2}\right)\log N - N + \frac{1}{2}\log 2\pi + \mathcal{O}\left(N^{-1}\right)$

Expansion of log: $\log(1+z) \sim z - \frac{z^2}{2}, \quad z \ll 1.$

$$\Rightarrow \log g(m,N) \approx -\frac{1}{2}\log N + \log 2 - \frac{1}{2}\log 2\pi - \frac{m^2}{2N}$$

$$g(m,N) \simeq \sqrt{\frac{2}{\pi N}}\,\exp\left(-\frac{m^2}{2N}\right)$$

m is either always even (N even) or always odd (N odd)

$\Rightarrow$ probability to meet the walker at site m:

$$P(m,N) = \frac{1+(-1)^{N-m}}{2}\, g(m,N) \approx \frac{1+(-1)^{N-m}}{\sqrt{2\pi N}} \exp\left(-\frac{m^2}{2N}\right). \quad (*)$$

Note that $P(m,N)=0$ for $|m|>N$ for exact expression, but not for approximation.
This result is one form of the central limit theorem (CLT): the (normalised) sum of independent random variables with finite variance is well approximated by a random variable with a Gaussian distribution in the limit of large numbers.

Even for $N=10$ the approximation $(*)$ containing the Gaussian is almost exact (normalisation is 0.999594).

The factor $\frac{1+(-1)^{N-m}}{2}$ is essential for the normalisation.

Continuum limit:

Position of the walker is $x=ma$:

$$P(x,N) \approx \sqrt{\frac{1}{2\pi N a^2}} \exp\left(-\frac{x^2}{2Na^2}\right)$$

from Jacobian

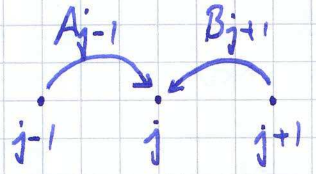
Time $t=N\Delta t$ and diffusion constant $K=\frac{a^2}{2\Delta t}$

$$\Rightarrow P(x,t) \approx \sqrt{\frac{1}{4\pi K t}} \exp\left(-\frac{x^2}{4Kt}\right).$$

IV. THE FOKKER-PLANCK EQUATION.

Let us start from a random walk, but now the probability to jump left or right depends on the walker's position: we start from the discrete master equation

$$W_j(t+\Delta t) = A_{j-1}\, W_{j-1}(t) + B_{j+1}\, W_{j+1}(t)$$ Pr to find walker at j at $t+\Delta t$



$A_j + B_j = 1$ jump w Pr $= 1$.

Taylor expansions: $W_j(t+\Delta t) \approx W_j(t) + \Delta t \frac{\partial}{\partial t} W_j(t)$

$$A_{j-1} W_{j-1} \approx A(x) W(x) - \Delta x \frac{\partial}{\partial x} A(x) W(x) + \frac{(\Delta x)^2}{2} \frac{\partial^2}{\partial x^2} A(x)\, W(x)$$

$$B_{j+1} W_{j+1} \approx B(x)\, W(x) - \Delta x \frac{\partial}{\partial x} B(x) W(x) + \frac{(\Delta x)^2}{2} \frac{\partial^2}{\partial x^2} B(x)\, W(x)$$

$$\Rightarrow W(x,t) + \Delta t \frac{\partial W}{\partial t} = \underbrace{\left[A(x) + B(x)\right]}_{\equiv 1} W(x,t) + \Delta x \frac{\partial}{\partial x}\left(B(x) - A(x)\right) W(x,t)$$
$$+ \frac{(\Delta x)^2}{2} \frac{\partial^2}{\partial x^2}\left[A(x) + B(x)\right] W(x,t)$$

$$\frac{\partial}{\partial t} W(x,t) = \frac{\Delta x}{\Delta t} \frac{\partial}{\partial x}\left[B(x) - A(x)\right] W(x,t) + \frac{(\Delta x)^2}{2\Delta t} \frac{\partial^2}{\partial x^2} W(x,t)$$

Continuum limit $\Delta x \to 0$, $\Delta t \to 0$:

$$\frac{\partial}{\partial t} P(x,t) = \frac{\partial}{\partial x} \frac{V'(x)}{m\eta} P(x,t) + K \frac{\partial^2}{\partial x^2} P(x,t)$$ Fokker-Planck equation

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$$\lim_{\Delta x \to 0, \Delta t \to 0} \frac{\Delta x}{\Delta t}\left[B(x) - A(x)\right] \equiv \frac{V'(x)}{m\eta}$$

$$\lim_{\Delta x \to 0, \Delta t \to 0} \frac{(\Delta x)^2}{2\Delta t} = K$$

for proper limit we must have that $B(x) - A(x) \approx \Delta x$

$F(x) = -V'(x)$ is the external force. η is the friction coefficient.

In a confining potential the long-time limit of $P(x,t)$ reaches the equilibrium distribution:

$$P_{eq}(x) = \mathcal{N} \exp\left(-\frac{V(x)}{k_B T}\right).$$

$$\frac{\partial}{\partial t} P(x,t) = 0 \Rightarrow 0 = \left(\frac{\partial}{\partial x} \frac{V'(x)}{m\eta} + K \frac{\partial^2}{\partial x^2}\right) P(x,\cancel{t})$$

$$\rightsquigarrow \quad 0 = \left(\frac{V'(x)}{m\eta} + K \frac{\partial}{\partial x}\right) P_{eq}(x)$$

$$\Rightarrow \quad P_{eq}(x) = \mathcal{N} \exp\left(-\frac{V(x)}{K m\eta}\right)$$

$$\Rightarrow \quad \underline{\underline{K = \frac{k_B T}{m\eta}}}$$ Einstein - Stokes - Smoluchowski relation (fluctuation - dissipation relation).

<u>Constant external force F_0:</u>

$$\frac{\partial}{\partial t} P(x,t) = -\frac{F_0}{m\eta} \frac{\partial}{\partial x} P(x,t) + K \frac{\partial^2}{\partial x^2} P(x,t)$$ sometimes called diffusion-advection eq.

(i.) <u>Similarity solution</u> with Galilei (wave) variable $\xi = x - \frac{F_0}{m\eta} t$

$$P(x,t) = G\left(x - \frac{F_0}{m\eta} t, t\right) \therefore G(x,t) = \frac{1}{\sqrt{4\pi K t}} \exp\left(-\frac{x^2}{4Kt}\right).$$

(ii.) <u>Second Einstein relation (linear response):</u>

$$\frac{d}{dt}\langle x(t)\rangle = \frac{F_0}{m\eta} \quad \Rightarrow \langle x(t)\rangle = \frac{F_0}{m\eta} t = \frac{F_0 K}{k_B T} t$$

w/o force we know that: $\langle x^2(t)\rangle_0 = 2Kt$

$$\Rightarrow \underline{\underline{\langle x(t)\rangle_{F_0} = \frac{F_0}{2 k_B T} \langle x^2(t)\rangle_0 .}}$$

V. The continuous time random walk process

EW Montroll, GH Weiss, J Math Phys 6, 167 (1965).
H Scher, M Lax, Phys Rev B 7, 4502 (1973).
MF Shlesinger, J Stat Phys 10, 421 (1974).
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J Klafter, R Silbey, Phys Rev Lett 44, 55 (1980).

Basic ingredient: Waiting time distribution $\psi(t)$

After each jump the walker waits for a random time drawn from the probability density function $\psi(t)$. We use $\psi(u) = \langle e^{-ut} \rangle$

Sticking probability for not moving:

$$\phi(t) = \int_t^\infty \psi(t')\,dt' = 1 - \int_0^t \psi(t')\,dt' \Rightarrow \phi(u) = \frac{1}{u} - \frac{\psi(u)}{u} = \frac{1-\psi(u)}{u}$$

PDF of occurrence of ith step at time $t = t_1 + t_2 + \ldots + t_i$

$$\mathcal{L}\{\psi_i(t)\} = \underline{\psi_i(u)} = \langle e^{-ut} \rangle = \underset{\text{independent}}{\underline{\langle e^{-u(t_1+t_2+\ldots+t_i)} \rangle}^{\,t_i}}$$

$$= \langle e^{-ut_1} \rangle \langle e^{-ut_2} \rangle \cdots \langle e^{-ut_i} \rangle = \langle e^{-ut} \rangle^i = \underline{\underline{\psi^i(u)}}$$

$\Rightarrow$ Probability that the walker has jumped exactly i times up to time t:

$$Q_i(t) = \int_0^t \psi_i(t')\,\phi(t-t')\,dt'$$

$$\rightsquigarrow Q_i(u) = \psi_i(u)\,\phi(u) = \frac{1-\psi(u)}{u}\,\psi^i(u).$$

$\Rightarrow$ Probability to find walker at site n at time t:

$$P(n,t) = \sum_{i=0}^\infty p_i(n)\,Q_i(t) \quad \therefore \quad p_i(n) \text{ is probability at site } n \text{ after } i\text{th step.}$$

$$\rightsquigarrow P(n,u) = \frac{1-\psi(u)}{u} \sum_{i=0}^\infty p_i(n)\,\psi^i(u) = \frac{1-\psi(u)}{u}\,p_0(n) + \frac{1-\psi(u)}{u} \sum_{i=1}^\infty p_i(n)\,\psi^i(u)$$

(**)

Continuum limit:

$p_0(x) = \delta(x)$ initial condition

$p_{i+1}(x) = p_i(x) + \frac{a^2}{2}\frac{\partial^2}{\partial x^2} p_i(x) + \dots$ according to our results from chapter IV.

$$\Rightarrow \mathcal{P}(x,u) = \frac{1-\psi(u)}{u}\delta(x) + \frac{1-\psi(u)}{u}\sum_{i=1}^{\infty}\left(p_{i-1}(x) + \frac{a^2}{2}\frac{\partial^2}{\partial x^2} p_{i-1}(x)\right)\psi^i(u)$$

but from (**) $\frac{1-\psi(u)}{u}\sum_{i=1}^{\infty} p_{i-1}(x)\psi^i(u) = \frac{1-\psi(u)}{u}\sum_{i=0}^{\infty} p_i(x)\psi^{i+1}(u)$

$$= \mathcal{P}(x,u)\,\psi(u)$$

$$\Rightarrow \mathcal{P}(x,u) = \frac{1-\psi(u)}{u}\delta(x) + \psi(u)\left(\mathcal{P}(x,u) + \frac{a^2}{2}\frac{\partial^2}{\partial x^2}\mathcal{P}(x,u)\right)$$

$$\underline{\underline{\mathcal{P}(x,u) - \frac{\delta(x)}{u} = \frac{\psi(u)}{1-\psi(u)}\frac{a^2}{2}\frac{\partial^2}{\partial x^2}\mathcal{P}(x,u)}}$$ CTRW with arbitrary $\psi(t)$ in the continuous space approximation.

(1.) Back to the diffusion equation:

Sharp waiting time PDF: $\psi(t) = \delta(t-\tau) \Rightarrow \psi(u) = e^{-u\tau} \approx 1 - u\tau + \dots$

many step $\equiv$ long time corresponds to short $u \rightsquigarrow$ powers in $(u\tau)^2 \dots$ neglected

Same result for Poissonian $\psi(t)$:

$$\psi(t) = \tau^{-1}e^{-t/\tau} \Rightarrow \psi(u) = \frac{1}{u+\tau^{-1}} \approx 1 - u\tau + \dots$$

In fact, this behaviour is universal, as long as the characteristic waiting time ~~___~~ remains finite:

$$\langle\tau\rangle = \int_0^{\infty}\psi(t)\,t = \int_0^{\infty} t\,\psi(t)\,e^{-ut}\,dt\Big|_{u=0} = -\frac{d\psi(u)}{du}\Big|_{u=0}$$

$\Rightarrow$ for finite $\langle\tau\rangle$ we have $\psi(u) \doteq 1 - \langle\tau\rangle u + \dots$

Up to first order in τ: $\dfrac{\psi(u)}{1-\psi(u)} = \dfrac{1-u\tau}{u\tau} = \dfrac{1}{u\tau} - 1$

$$\Rightarrow P(x,u) - \frac{\delta(x)}{u} = \left(\frac{1}{u\tau} - 1\right) \frac{a^2}{2} \frac{\partial^2}{\partial x^2} P(x,u)$$

The diffusion constant is $K = \lim\limits_{a \to 0, \tau \to 0} \dfrac{a^2}{2\tau}$

$\Rightarrow$ the term $\lim\limits_{a \to 0, \tau \to 0} a^2 \longrightarrow 0$

$$\Rightarrow P(x,u) - \frac{\delta(x)}{u} = \frac{1}{u} K \frac{\partial^2}{\partial x^2} P(x,u)$$

After inverse Laplace transformation:

$$P(x,t) - \delta(x) = \int_0^t K \frac{\partial^2}{\partial x^2} P(x,t')\, dt' \quad \text{integral form of diffusion eq.}$$

$$\rightsquigarrow \frac{\partial}{\partial t} P(x,t) = K \frac{\partial^2}{\partial x^2} P(x,t) \ \checkmark.$$

(2) Diverging characteristic waiting time:

Assume the form $\psi(u) = e^{-(u\tau)^\alpha}$, $0<\alpha<1$ for the waiting time PDF. This is actually the characteristic function of a one-sided Lévy stable law, resulting from a generalisation of the CLT for random variables with diverging variance. The leading order of the Laplace inversion is $\psi(t) \sim \tau^\alpha / t^{1+\alpha}$.

In particular, we see that $\langle \tau \rangle = \int_0^\infty t\, \psi(t)\, dt = -\dfrac{d\psi(u)}{du}\Big|_{u=0} = \tau^\alpha u^{\alpha-1} e^{-(u\tau)^\alpha}\Big|_0 \to \infty$.

This process is scale-free, i.e. there is no time scale separating single jump events from the limit of a large number of jumps $\rightsquigarrow$ ageing, non-ergodicity.

In Laplace space, we find

$$P(x,u) - \frac{\delta(x)}{u} = \frac{1}{u^\alpha} K_\alpha \frac{\partial^2}{\partial x^2} P(x,t) \ \therefore\ K_\alpha = \lim_{a \to 0, \tau \to 0} \frac{a^2}{2\tau^\alpha} \ \therefore\ [K_\alpha] = \frac{cm^2}{sec^\alpha}. \quad (*)$$