Lecture 3: The Long-Time Behavior of Isotropic Walks in $d \geq 1$

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February 13, 2001

Suppose that a large collection of independent random walkers takes iid steps at intervals of time τ sampled from an "isotropic" transition PDF $p_\tau(|\vec{r}|)$ which is spherically symmetric, i.e. their is no directional preference. In this general setting, the concentration $c(\vec{r}, t)$ satisfied the exact recursion

$$c(\vec{r}, t+\tau) = \int c(\vec{r}, t) p_\tau(|\vec{r} - \vec{r'}|) d\vec{r'}$$

which is essentially Bachelier's equation. The integration here is over d-dimensional space.

1 Gauss' Integral

As an aside, we seek to show that:

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$$

Proof:

$$\begin{aligned} \int_{-\infty}^{\infty} e^{-x^2} dx \int_{-\infty}^{\infty} e^{-y^2} dy &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-(x^2+y^2)} dx dy && (1) \\ &= \int_0^{\infty} 2\pi r dr e^{-r^2} && (2) \\ &= \pi && (3) \end{aligned}$$

Extending this analysis to more than one dimension,

$$\begin{aligned} \int_{-\infty}^{\infty} e^{-(x_1^2+x_2^2+\cdots+x_d^2)} dx_1 dx_2 \ldots dx_d &= \pi^{\frac{d}{2}} && (4) \\ &= \int d\Omega \int_0^{\infty} r^{d-1} e^{-r^2} dr && (5) \\ &= A_d \frac{\Gamma(\frac{d}{2})}{2} && (6) \end{aligned}$$

where A_d is the volume of the d-dimensional unit sphere, and $\Gamma(x)$ is the Gamma function, shown in Figure 1, and given by:

$$\Gamma(z) = \int_0^{\infty} e^{-t} t^{z-1} dt$$

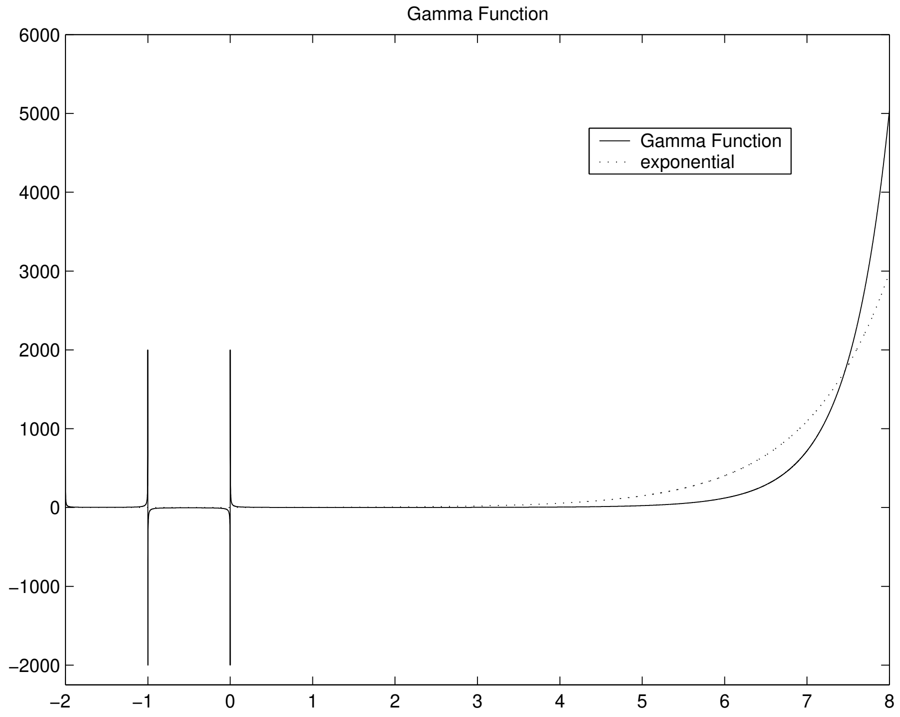

Figure 1: The Gamma function, compared with an exponential function.

Note that

$$\Gamma(n+1) = n! \tag{7}$$
$$\Gamma(z+1) = z\Gamma(z) \tag{8}$$
$$\Gamma(\frac{1}{2}) = \sqrt{\pi} \tag{9}$$
$$\Gamma(\frac{3}{2}) = \frac{\sqrt{\pi}}{2} \tag{10}$$
$$\Gamma(\frac{1}{2}) = 2\int_0^\infty e^{-t^2}dt \tag{11}$$
$$= \int_{-\infty}^{\infty} e^{-t^2}dt \tag{12}$$

Rearranging the terms of Equations (4) - (6), we have the solution for A_d:

$$A_d = \frac{2\pi^{\frac{d}{2}}}{\Gamma(\frac{d}{2})}$$

Completing the aside, we now have normalization factors for an arbitrary probability distribution. Normalization of the probability distribution, $\int p_\tau(|\vec{r'}|)d\vec{r} = 1$ implies that the PDF for an arbitrary, isotropic random walk is:

$$p_\tau(\vec{r}) = \frac{\delta(|\vec{r}| - a)}{A_d a^{d-1}} \tag{13}$$

2 Diffusive Mixing in Pearson's Walk ($d = 2$)

We have from Equation (13) that for a $d = 2$ dimensional probability distribution,

$$p_\tau(\vec{r}) = \frac{\delta(|\vec{r} - a|)}{2\pi a}$$

The concentration at any time can then be found by taking the average of previous local concentrations. That is,

$$\begin{aligned} c(\vec{r}, t+\tau) &= \int c(\vec{r'}, t) p_\tau(\vec{r} - \vec{r'}) d\vec{r'} & (14) \\ &= \int c(\vec{r'}, t) \frac{\delta(|\vec{r} - a|)}{2\pi a} d\vec{r'} & (15) \\ &= \frac{1}{2\pi} \int c(\vec{r} + \hat{r}(\theta) a, t) d\theta & (16) \end{aligned}$$

which is an angular average at distance a of previous local concentrations. The result exemplifies "diffusive mixing".

This representation of diffusive mixing has a simple interpretation in terms of complex variables. Represent $c(\vec{r}, t)$ by $c(z, t)$ in the complex plane. That is,

$$c(z, t+\tau) = \frac{1}{2\pi} \int_0^{2\pi} c(z + ae^{i\theta}, t) d\theta$$

The steady state solution $c_\infty(z)$ is a function of spatial coordinates only,

$$c_\infty(z) = \frac{1}{2\pi} \int_0^{2\pi} c_\infty(z + ae^{i\theta}) d\theta$$

This is Gauss' Mean Value Theorem, which holds for any analytic function. The connection with analytic functions can be made even more clear by letting $z' = z + ae^{i\theta}$ and $dz' = iae^{i\theta} d\theta$. Substituting for $d\theta$, we have:

$$d\theta = \frac{dz'}{iae^{i\theta}} = \frac{dz'}{i(z' - z)}$$

Solving for c_∞, we have

$$c_\infty = \frac{1}{2\pi i} \oint \frac{c_\infty(z')}{z - z'} dz'$$

which is Cauchy's Integral Formula: This holds for analytic functions, of which the real and imaginary parts are harmonic, i.e. satisfy Laplace equation. Since c_∞ is real, we conclude that the steady state solution satisfies $\nabla^2 c_\infty = 0$.

Of course, we could have gotten this by setting the time derivative equal to zero in the diffusion equation, but here the connection with Gauss' Mean Value Theorem and Cauchy's formula gives further insight into the nature of diffusive mixing (or local averaging). Also, we have not yet made the approximations of the Kramers-Moyal moment expansion which leads to the diffusion equation (see below).

3 Isotropic Functions

Let $p_\tau(|\vec{r}|)$ be the PDF of the random displacement of a walker taking independent, identical steps. Assume all moments of p_τ exist, and in particular, that the second moment is nonzero and the function has zero mean. Then we have,

$$c(\vec{r}, t+\tau) = \int p_\tau(|\vec{r}-\vec{r'}|)c(\vec{r}, t)d\vec{r'} \tag{17}$$

Let $\vec{y} = \vec{r} - \vec{r'}$. Then $d\vec{y} = -d\vec{r'}$. By substitution, we have

$$c(\vec{r}, t+\tau) = \int p_\tau(|\vec{y}|)c(\vec{r}-\vec{y})d\vec{y} \tag{18}$$

In the long time limit, due to diffusive mixing, the concentration will vary very slowly on the relatively short length scale over which the transition probability is significant. Therefore, expanding in a Taylor Series about $\vec{r}$, we have

$$c(\vec{r}+\vec{y}, t) = c(\vec{r}, t) - \vec{y}\cdot\nabla c(\vec{r}, t) + \frac{1}{2}\sum_{i,j}\frac{\partial^2 c(\vec{r}, t)}{\partial x_i \partial x_j}\cdot y_i y_j$$

where $\vec{r} = (x_1, x_2, \cdots, x_d)$ and $\vec{y} = (y_1, y_2, \cdots, y_d)$. Rewrite terms in the RHS of the equation as:

$$\frac{1}{2}\sum_{i,j}\frac{\partial^2 c(\vec{r}, t)}{\partial x_i \partial x_j}\cdot y_i y_j = \frac{1}{2}\left(\frac{\partial^2 c}{\partial x_1^2}y_1^2 + \frac{\partial^2 c}{\partial x_2^2}y_2^2 + \cdots + \frac{\partial^2 c}{\partial x_d^2}y_d^2\right) + mixed\ partials$$

Neglecting the mixed partials terms, as p_τ is isotropic and since $< y_i y_j >= 0$ for $i \neq j$.

$$c(\vec{r}, t+\tau) = c(\vec{r}, t)\int p_\tau(|\vec{y}|)d\vec{y} - \nabla c(\vec{r}, t)\cdot\int \vec{y}p_\tau(|\vec{y}|)d\vec{y} + \frac{1}{2}\left(\frac{\partial^2 c}{\partial x_1^2} < y_1^2 > + \frac{\partial^2 c}{\partial x_2^2} < y_2^2 > + \cdots \frac{\partial^2 c}{\partial x_d^2} < y_d^2 >\right)$$

of which the RHS includes terms that are precisely d one-dimensional integrals. The first term on the RHS is a multiple of the first moment (which we took to be zero). Since the PDF is isotropic, $< y_1^2 >=< y_2^2 >$ and so on. The equation reduces to:

$$\frac{c(\vec{r}, t+\tau) - c(\vec{r}, t)}{\tau} = \frac{\int d\vec{y}y_1^2 p_\tau(\vec{y})}{2\tau}\nabla^2 c \tag{19}$$

$$= \frac{\int d\vec{y}|\vec{y}|^2 p_\tau(|\vec{y}|)}{2\tau d}\nabla^2 c \tag{20}$$

Note that the equation reduced to d identical integral terms in second moments. As $\tau \to 0$, the equation yields the result:

$$\frac{\partial c}{\partial t} = D\nabla^2 c + O(\tau^{1/2})$$

The terms of $O(\tau^{1/2})$ terms come from doing the Taylor expansion about t, which has been neglected here. D is given by:

$$D = \frac{\int d\vec{r}|\vec{r}|^2 p_\tau(|\vec{r}|)}{2\tau d} = \frac{\int d\vec{y}y_1^2 p_\tau(\vec{y})}{2\tau}$$

This formula will allow us to get the long-time behavior of any isotropic walk from the Green function of the associated diffusion equation.

4 Green Functions

The Green function is a solution (in this case) to the diffusion equation, $G(\vec{r},t)$ subject to the initial condition $G(\vec{r},0)=\delta(\vec{r})$. A more general solution to the diffusion equation can be constructed by taking the convolution of the Green's Function solution with arbitrary initial condition, $c(\vec{r},0)$.

$$c(\vec{r},t)=\int c(\vec{r},0)G(\vec{r}-\vec{r'},t)d\vec{r'}$$

This reduces function the c to a weighted sum of responses to δ functions. Note that the solution $G(\vec{r},t)$ is the leading order approximation of the solution of a single random walker starting at the origin with steps of time τ and variance $2D\tau$.

The solution for G can be found via (at least) two methods: Fourier Transforms and Similarity Solutions. Here we analyze the method of Fourier Transforms.

4.1 Derivation of the Green Function via Fourier Transform

The Fourier Transform is defined by:

$$\hat{G}(\vec{k},t)=\int e^{-i\vec{k}\cdot\vec{r}}G(\vec{r},t)d\vec{r}$$

and the inversion formula states

$$G(\vec{r},t)=\frac{1}{(2\pi)^d}\int e^{-i\vec{k}\cdot\vec{r}}\hat{G}(\vec{k},t)d\vec{k}$$

Fourier Transforms effectively yield a superposition of weighted plane wave states.

A property of the Fourier Transform is

$$\nabla^{\hat{2}}G=(-k_1^2+-k_2^2+\cdots)\hat{G}$$

which can be derived using integration by parts. Taking the Fourier Transform of the diffusion equation, we have:

$$\frac{\partial\hat{G}}{\partial t}=-D|\vec{k}|^2\hat{G}$$

The solution is given by:

$$\begin{aligned}\hat{G}(\vec{k},t) &= \hat{G}(k,0)e^{-D|\vec{k}|^2t} && (21)\\ &= e^{-t/\tau(\vec{k})} && (22)\end{aligned}$$

since $\hat{G}(\vec{k},0)=1$ for $G(\vec{x},0)=\delta x$, where $\tau(\vec{k})$ defined by

$$\tau(\vec{k})=\frac{1}{D|\vec{k}^2|}$$

is the decay rate for the Fourier mode $\vec{k}$. Higher Fourier modes decay quicker than lower Fourier modes. This leads to Diffusive Mixing. Peaky behavior is quickly smoothed.

Comments on Green's Function Solutions:

- As $t/\tau \to \infty$, large $\vec{k}$ values decay
- Small $\vec{k}$ near $\vec{0}$ dominate
- $\hat{G}(\vec{0}, t) = \hat{G}(\vec{0}, 0) = 1$ doesn't decay at origin

The last condition corresponds to a conservation equation (either mass conservation or probability conservation). That is

$$\hat{G}(\vec{0}, t) = \int G(\vec{r}, t) d\vec{r}$$

Via the inverse Fourier Transform, we have:

$$\begin{aligned} G(\vec{r}, t) &= \frac{1}{(2\pi)^d} \int e^{i\vec{k}\cdot\vec{r} - D|\vec{k}|^2 t} d\vec{k} \qquad (23) \\ &= \frac{1}{(2\pi)^d} \int e^{-Dt[(\vec{k} - \frac{i\vec{r}}{2Dt})^2 + \frac{\vec{r}^2}{4(Dt)^2}]} d\vec{k} \qquad (24) \\ &= \frac{1}{(2\pi)^d} e^{-\frac{\vec{r}^2}{4Dt}} \int e^{-Dt|\vec{k}|^2} d\vec{k} \qquad (25) \end{aligned}$$

Therefore:

$$G(\vec{r}, t) = \frac{e^{-\vec{r}^2/4Dt}}{(4\pi Dt)^{d/2}}$$

Since we have already argued that the long-time asymptotics of a random walk is governed by the diffusion equation, this result for the Green function gives the exact leading order behavior of the random walk, technically in the "intermediate limit" $t/\tau \to \infty$ with $x/\sqrt{t}$ held fixed. (More on this in the next lecture.)

4.2 Applications to Isotropic Random Walks

4.2.1 Simple Bernoulli Walk on Integers ($d = 1$)

The transition PDF for a simple walk is

$$p_\tau(x) = \frac{1}{2}(\delta(x-a) + \delta(x+a))$$

where

$$D = \frac{a^2}{2\tau}$$

Let $t = n\tau$ for n steps and τ time per step. Let $x = ma$.

The discrete probability of walker being at location m at step n is given by $p_n(m)$ which after long times behaves like

$$p_n(m) \sim aG(ma, n\tau)$$

Therefore,

$$p_n(m) \sim \frac{e^{-\frac{m^2}{2n}}}{\sqrt{2\pi n}}$$

as $n \to \infty$, with $\frac{m}{\sqrt{n}}$ held constant. This is the deMoivre-Laplace Central Limit Theorem, because the random walk simply amounts to an addition of random variables:

$$x_n = \sum_{i=1}^{n} \delta x_i$$

$$\mathrm{Var}(x_n) = n\mathrm{Var}(\delta x_i) = n$$

The Central Limit Theorem says the sum of a large number of identical independently distributed random variables with finite variances is well approximated by a single random variable with Gaussian distribution.

4.2.2 Isotropic Random Walk with Fixed Step Length in d-Dimensions

The isotropic PDF, p_τ, with a fixed step length is given by:

$$p_\tau(\vec{r}) = \frac{\delta(|\vec{r}| - a)}{A_d a^{d-1}}$$

with

$$D = \frac{a^2}{2\tau d}$$

The probability of being at $\vec{r}$ after n steps is

$$p_n(\vec{r}) \sim e^{-\frac{d|\vec{r}|^2}{2a^2 n}} \left(\frac{d}{2\pi a^2 n}\right)^{\frac{d}{2}}$$

in the intermediate limit $n \to \infty$ with $r/\sqrt{n}$ fixed.

We also introduce a one-dimensional radial analog to each of these probability density functions. Let $R_n(r)$ be the radial probability density, such that $R_1(r) = \delta(r - a)$. That is, $R_n(r)\Delta r$ is the probability of finding the walker at a radius between r and $r + \Delta r$. For proper normalization, the radial probability density and the volume probability density are related via

$$R_n(r) = A_d r^{d-1} p_n(|\vec{r}|).$$

so that

$$\int_0^\infty R_n(r)dr = \int p_n(|\vec{r}|)d\vec{r} = 1.$$

For the special case $d = 2$, Pearson's Walk:

$$p_n(\vec{r}) \sim \frac{e^{-\frac{|\vec{r}|^2}{a^2 n}}}{\pi a^2 n}$$

and

$$R_n(r) \sim \frac{2r}{a^2 n} e^{-\frac{r^2}{a^2 n}}$$

This was Rayleigh's solution to Pearson's problem in *Nature*.

For the special case d=3, Rayleigh's Walk (also sometimes called an Isotropic Random Flight):

$$p_n(\vec{r}) \sim \left(\frac{3}{\pi a^2 n}\right)^{\frac{3}{2}} e^{-\frac{3|\vec{r}|^2}{2a^2 n}}$$

and

$$R_n(r) \sim 4\pi r^2 \left(\frac{3}{\pi a^2 n}\right)^{\frac{3}{2}} e^{-\frac{3|\vec{r}|^2}{2a^2 n}}$$

4.2.3 Polya's Walk in d Dimensions

Polya's walk is a d-dimensional non-isotropic walk on an integer (or hypercubic) lattice. In this case, we have

$$D = \frac{a^2}{2\tau}$$

and

$$p_n(\vec{r}) \sim (\frac{d}{2\pi a^2 n})^{\frac{d}{2}} e^{-\frac{|\vec{r}|^2}{2a^2 n}}$$

Note the difference with Pearson's isotropic walk discussed above.