

Lecture 3: From Random Walks to Continuum Diffusion

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Overview

In the previous lecture (by Prof. Yip), we discussed how individual particles undergo complicated, apparently random motion, in a liquid or gas, which is termed “diffusion”. The same erratic motion due to collisions can be observed at the macroscopic scale in the so-called Brownian motion of a dust particle in the air. A simulation of this phenomenon (java applet), shown in lecture, can be found at

http://galileo.phys.virginia.edu/classes/109N/more_stuff/Applets/brownian/brownian.html

As this example illustrates, the phenomenon of diffusion can be simulated by molecular dynamics at the microscopic level, but it can also be modeled via simpler, more coarse-grained levels of description, which is the subject of today’s lecture. The simplest “Monte Carlo” (or probabilistic) model of diffusion is a *random walk*, where the particle is assumed to follow a trajectory of independent random displacements. We will show that after long times, the average behavior of a collection of random walkers is well-described by the *diffusion equation*, which describes diffusion at the level of a continuum, which will be the focus of the next lecture (by Prof. Rosales).

History

The erratic motion of pollen grains in water viewed under a microscope, which seemed to carry on indefinitely, was first observed by Robert Brown in 1827. It was not until 1877 that Desaulx postulated that this “Brownian motion” was due to thermal collisions with liquid molecules. Of course, molecular dynamics simulations were not available to test this hypothesis, but a mathematical theory, based on the concept of a random walk, was about to emerge.

The term “random walk” was originally proposed by Karl Pearson in 1905¹. In a letter to *Nature*, he gave a simple model to describe a mosquito infestation in a forest. At each time step, a single mosquito moves a fixed length a , at a randomly chosen angle. Pearson wanted to know the distribution of the mosquitos after many steps had been taken.

The letter was answered by Lord Rayleigh, who had already solved a more general form of this problem in 1880, in the context of sound waves in heterogeneous materials. Modeling a sound

¹See B. Hughes, *Random Walks and Random Environments*, Vol. I, Sec. 2.1 (Oxford, 1995), for excerpts and an entertaining historical discussion.

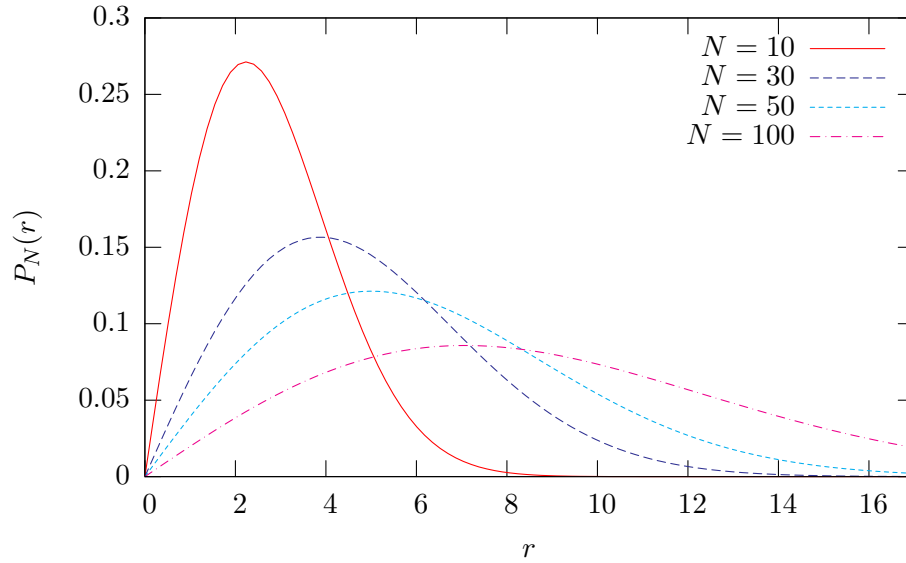


Figure 1: Rayleigh’s asymptotic approximation for $P_N(r)$ in Pearson’s random walk for several large values of N .

wave traveling through the material can be thought of as summing up a sequence of random wave-vectors \mathbf{k} of constant amplitude but random phase: sound waves in the material have roughly constant wavelength, but their directions are altered at scattering sites within the material.

We wish to find the probability density function of the sound waves after many steps have been taken. We let $P_N(R)dR$ be the probability of traveling a distance between R and $R + dR$ in N steps. For steps of unit length, Lord Rayleigh showed that as $N \rightarrow \infty$,

$$P_N(R) \sim \frac{2R}{N} e^{-R^2/N}. \quad (1)$$

This function is shown in figure 1 for several values of N . We see that the expected distance traveled scales according to the square root of the number of steps, $\langle R^2 \rangle \sim N$, which is typical of “diffusion” phenomena.

Around the same time, the theory of random walks was also developed by Louis Bachelier in his truly remarkable doctoral thesis, *La Théorie de la Spéculation*, published in 1900. Bachelier proposed the random walk as the fundamental model for financial time series (e.g. stock ticks), many decades before this idea became the basis for modern theoretical finance. Bachelier also was apparently the first to see the connection between discrete random walks and the continuous diffusion (or heat) equation, which is a major theme of this class, reflected in its title.

It is curious that in the same year as Pearson’s letter, Albert Einstein also published his seminal paper on Brownian motion, which he modeled as a random walk, driven by collisions with gas molecules. Einstein did not seem to be aware of the related work of Rayleigh and Bachelier, and he focused on a different issue: the calculation of the diffusion coefficient in terms of the viscosity and temperature of the gas. Similar theoretical ideas were also published independently by Smoluchowski in 1906. The random-walk theory of Brownian motion had an enormous impact²,

²The impact was recognized by two Nobel Prizes, one to Einstein for the theory and another to Perrin for experimental confirmation.

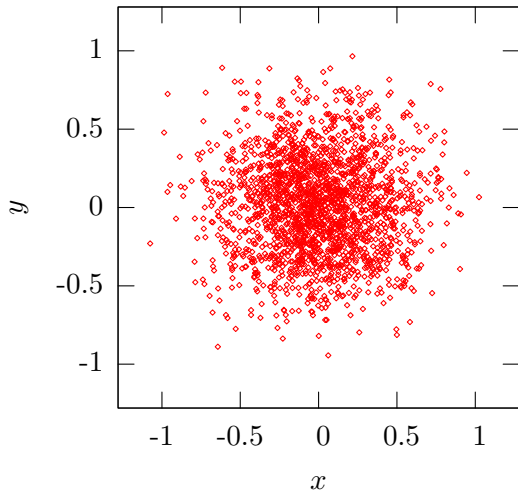


Figure 2: The positions of 2000 independent Pearson random walks released from the origin, after $N = 2000$ steps of length $a = 0.01$.

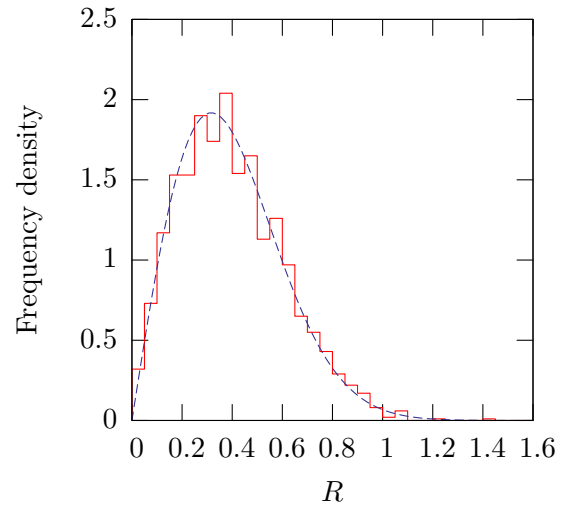


Figure 3: A normalized histogram of the distances from the origin, R_N , in Fig. 2 compared to Rayleigh's asymptotic result, Eq. (1).

because it gave strong evidence for discrete particles (“atoms”) at a time when most scientists still believed that matter was a continuum.

As its historical origins demonstrate, the concept of the random walk has incredibly broad applicability, and today, a century later, it is nearly ubiquitous in science and engineering.

Simulations of Pearson's Random Walk

In lecture, a demo `rr` was shown³ of 10,000 particles undergoing Pearson's random walk in the plane. The demo shows the time-evolution of the radial distribution, as well as the scaling of the variance of the radial distance with time (on a log-log plot) to test the “square-root” dependence ($x \propto \sqrt{t}$) discussed in the previous lecture on molecular diffusion.

Results from similar simulations (by Chris Rycroft) in Fig. 3 demonstrate that Lord Rayleigh's result rather accurate in describing the distribution of walkers at long times, roughly beyond 100 steps. It is impressive how the complicated collection of random walkers tends toward a simple, smooth distribution, at least in the central region.

From Random Walks to Continuum Diffusion

We now present a simple derivation of a generalization of Lord Rayleigh's result. (In class this derivation was done in $d = 1$ dimension, but these notes consider the more general case of $d \geq 1$.) The analysis proceeds by taking the “continuum limit” of long-time statistics, which yields the classical partial differential equation for diffusion.

Consider a random walker, who initially starts at the origin in d dimensions. At each step, the walker moves by an amount $\Delta \mathbf{X}_N$, chosen from a probability distribution $p_N(\mathbf{r})$. For this derivation, which shall consider the case of independent, identically distributed (IID) steps, so that

³Written in C++ by Bob Sumner with OpenGL graphics.

$p_N(\mathbf{r}) = p(\mathbf{r})$. Furthermore, we shall assume that the steps are isotropic, so that $p(\mathbf{r})$ is a function of the radial distance $r = |\mathbf{r}|$ only. This condition also automatically eliminates any drift, so that $\langle \Delta \mathbf{X}_N \rangle = 0$.

Let \mathbf{X}_N be the position of the walker after N steps, and let $P_N(\mathbf{R})$ be the associated probability density function (PDF). For IID displacements, we have the following recursion for the PDF:

$$P_{N+1}(\mathbf{R}) = \int p(\mathbf{r}) P_N(\mathbf{R} - \mathbf{r}) d^d \mathbf{r}. \quad (2)$$

In one dimension ($d = 1$), this is Bachelier's Equation. The key assumption is the *independence* of the steps, which allows the probability of a transition from $\mathbf{R} - \mathbf{r}$ to \mathbf{R} in the N th step to be factored into the two terms in the integrand.

Starting from Eq. (2), we can formally take the continuum limit to quickly arrive at Rayleigh's solution (1) to Pearson's problem. In subsequent lectures we will gain a better understanding of this approximation, but here we just give simple arguments. As $N \rightarrow \infty$, $P_N(\mathbf{r})$ varies on length scales which are much larger than a typical \mathbf{r} , and therefore we Taylor expand inside the integral to obtain

$$\begin{aligned} P_{N+1}(\mathbf{R}) &= \int p(\mathbf{r}) \left[P_N(\mathbf{R}) - \mathbf{r} \cdot \nabla P_N(\mathbf{R}) + \frac{1}{2} \mathbf{r} \cdot \nabla \nabla P_N \cdot \mathbf{r} + \dots \right] d^d \mathbf{r} \\ &= P_N(\mathbf{R}) - 0 + \frac{1}{2} \sum_i \sum_j \langle r_i r_j \rangle \frac{\partial^2 P_N}{\partial R_i \partial R_j} + \dots \\ &= P_N(\mathbf{R}) + \frac{\langle \mathbf{r} \cdot \mathbf{r} \rangle}{2d} \nabla^2 P_N(\mathbf{R}) + \dots \end{aligned}$$

We assume that steps are taken at intervals of Δt , and defining time by $t = N \Delta t$ we obtain

$$\frac{P_{N+1}(\mathbf{R}) - P_N(\mathbf{R})}{\Delta t} = \frac{\langle r^2 \rangle}{2d \Delta t} \nabla^2 P_N + \dots$$

As $N \rightarrow \infty$, the limiting distribution $\rho(\mathbf{R}, t)$, defined by $P_N(\mathbf{R}) = \rho(\mathbf{R}, N \Delta t)$, satisfies

$$\frac{\partial \rho}{\partial t} = D \nabla^2 \rho \quad (3)$$

where $D = \langle r^2 \rangle / 2d \Delta t$, which is the *diffusion equation*. Since the walker starts from the origin, we have the initial condition $\rho(\mathbf{R}, 0) = \delta(\mathbf{R})$.

In lecture, we simply quoted a basic exact solution to the diffusion equation (below), but in these notes we sketch a derivation (which requires some more advanced concepts). We make use of the Fourier Transform, defined for this class to be

$$\begin{aligned} \hat{\rho}(\mathbf{k}, t) &= \int e^{-i\mathbf{k} \cdot \mathbf{x}} \rho(\mathbf{x}, t) d^d \mathbf{x} \\ \rho(\mathbf{x}, t) &= \frac{1}{(2\pi)^d} \int e^{i\mathbf{k} \cdot \mathbf{x}} \hat{\rho}(\mathbf{k}, t) d^d \mathbf{k}. \end{aligned}$$

Thus we obtain the ordinary differential equation

$$\frac{\partial \hat{\rho}}{\partial t} = -D k^2 \hat{\rho}$$

which has solution

$$\hat{\rho}(\mathbf{k}, t) = e^{-Dk^2t} \hat{\rho}(\mathbf{k}, 0) = e^{-Dk^2t}.$$

Taking the inverse Fourier Transform gives

$$\rho(\mathbf{R}, t) = \frac{e^{-R^2/4Dt}}{(4\pi Dt)^{d/2}}.$$

Thus in the corresponding discrete problem, as $N \rightarrow \infty$,

$$P_N(\mathbf{R}) \sim \frac{e^{-dR^2/2\langle r^2 \rangle N}}{(2\pi \langle r^2 \rangle N/d)^{d/2}}. \quad (4)$$

This is the long time limit of $P_N(\mathbf{R})$ for an isotropic random walk in d dimensions. The PDF for the position tends to a Gaussian (or normal) distribution, whose width depends only on the variance of the individual displacements. Our derivation predicts the same asymptotic result for any PDF so long as $\langle r^2 \rangle$ exists.

For an isotropic walk, we can easily calculate the PDF of the distance R from the origin via

$$P_N(R) = A_d R^{d-1} P_N(\mathbf{R})$$

where A_d is the surface area of the unit sphere in d dimensions ($A_1 = 1$, $A_2 = 2\pi$, $A_3 = 4\pi, \dots$). For Pearson's problem, we have $\langle r^2 \rangle = a^2$ and $d = 2$, so Equation (4) gives the asymptotic result:

$$\begin{aligned} P_N(\mathbf{R}) &\sim \frac{e^{-R^2/a^2N}}{\pi a^2 N} \\ P_N(R) &\sim \frac{2R}{a^2 N} e^{-R^2/a^2N} \end{aligned}$$

which agrees with Lord Rayleigh's solution, Eq. (1), for $a = 1$.

More General Situations

This brief section supplements the lecture to mention more general situations of random walks and diffusion. For further reading (at a more advanced level), see the online notes for 18.366 Random Walks and Diffusion, <http://www.ocw.mit.edu/OcwWeb/Mathematics/18-366Spring-2005/CourseHome/index.htm>.

Normal Diffusion

As our simple derivation suggests, the statistical properties of random walks tend toward universal distributions after large numbers of steps. In the case of the PDF for the final position, our result for isotropic random walks is a multi-dimensional generalization of the Central Limit Theorem (CLT) for sums of independent, identically distributed random variables. As long as a finite second moment $\langle r^2 \rangle$ exists for the random displacements, the asymptotic form of $P_N(\mathbf{R})$ is given by Eq. (4), or, more generally, by a solution to the continuum diffusion equation.

Note the “square-root scaling” of the width of the PDF, which grows like

$$R \propto \sqrt{\langle r^2 \rangle N}.$$

which is characteristic of spreading by “normal diffusion”. More generally, we will see that the variance of the position is given by

$$\text{Var}(\mathbf{R}_N) = N \text{Var}(\vec{r}).$$

for independent, identically distributed random displacements.

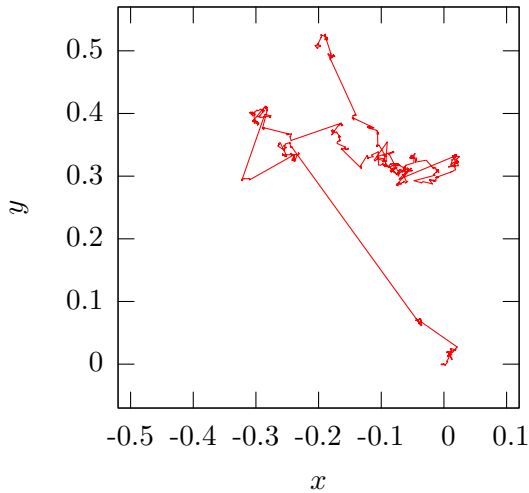


Figure 4: Two thousand steps of a random walk based on the Cauchy distribution.

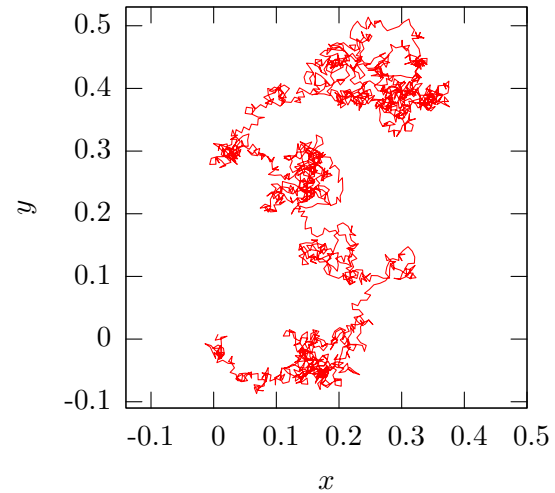


Figure 5: Two thousand steps of Pearson's random walk, with $a = 0.01$.

Anomalous Diffusion

When the assumptions of the CLT break down, random walks can exhibit rather different behavior. For example, the limiting distribution for the position may not be Gaussian, and the scaling of its width,

$$R \propto N^\nu,$$

is generally “anomalous” with $\nu \neq 1/2$. The second part of this class is devoted to various cases of anomalous diffusion.

One way to violate the CLT with IID displacements is via “fat-tailed” probability distributions, which assign sufficient probability to very large steps that the variance is infinite. An example is PDF for a Cauchy random variable,

$$p(x) = \frac{b}{\pi(b^2 + x^2)}.$$

Since the probability density function decays like x^{-2} as $x \rightarrow \infty$, the variance is infinite. Figure 4 shows an example of a two dimensional, isotropic random walk, where the distances of the steps are chosen from a Cauchy distribution. We see that the walk mostly takes small steps, but occasionally makes very large jumps, comparable to the total displacement. This is rather different from the case of Pearson's walk, shown in Figure 5, where the step size is constant and normal diffusion occurs.

Other ways to achieve anomalous diffusion include highly non-uniform step distributions, strong correlations between steps, and interactions between multiple random walkers. In such cases, the continuum limit is more subtle and leads to various generalizations of the diffusion equation.

In the next lecture (by Prof. Rosales), the diffusion equation will be derived by purely continuum arguments (Fick's Law) without any reference to particles undergoing random walks, but it is

helpful to always keep in mind the microscopic mechanism behind a continuum model. Following the continuum section of the class, we will return to random walks and related topics in a section on “Monte Carlo simulation,” which involves the random motion of discrete particles (or more general objects).