Lecture 17: Anomalous (Sub) Diffusion: Scaling Laws

Kevin Chu

Department of Mathematics, MIT

April 10, 2003

In this lecture, we discuss the scaling laws for anomalous diffusion. In particular, we focus on random walks that lead to sub-diffusive behavior for which the root-mean-square distance from the origin scales as t^α with $\alpha < 1/2$.

1 Montroll-Weiss Theory of Continuous-Time Random Walks

We begin by formulating a theory of CTRW from the perspective that the waiting time is the basic random variable[1]. As we saw last lecture, it is also possible to formulate a theory for CTRW that uses the number of steps taken, $N(t)$, as the basic random variable. The latter formulation tends to be bit more physically insightful. However, it is arguable that the waiting time is a more fundamnental physical quantity. In any case, it is valuable to have an understanding of both formulations.

Let $\psi(t)$ be the PDF for the waiting time between steps. We are interested in deriving the scaling laws for the moments of the total displacement

$$X(t) = \sum_{n=1}^{N} \Delta x_n, \tag{1}$$

where the Δx_n are the individual steps. Defining $P(x,t)$ to be the PDF for the $X(t)$ and $p(x,t)$ to be the PDF for the Δx_n (iid), we have that

$$P(x,t) = \sum_{N=0}^{\infty} \mathcal{P}(N,t) p^{*N}(x), \tag{2}$$

where $\mathcal{P}(N,t)$ is the probability that N steps were taken up to time t. Taking the Laplace transform with respect to time and the Fourier transform with respect to space, this equation becomes

$$\widetilde{\widehat{P}}(k,s) = \sum_{N=0}^{\infty} \widetilde{\mathcal{P}}(N,s) \left(\widehat{p}(k)\right)^N, \tag{3}$$

Recall that we can write $\mathcal{P}$ as a convolution of the waiting time density functions:

$$\mathcal{P}(t) = \left(\psi^{*N} * \Psi\right)(t), \tag{4}$$

[1] In this lecture, we consider only CTRWs for which the waiting time for a step is independent of the step size. These CTRWs are called *separable*.

where $\Psi(t) \equiv \int_t^\infty \psi(t')dt'$ is the probability that no steps are taken in the time interval $[0, t)$. Thus, we can write

$$\widetilde{\mathcal{P}}(t) = \left(\widetilde{\psi}(s)\right)^N \left(\frac{1-\widetilde{\psi}(s)}{s}\right). \tag{5}$$

Substituting this into our expression for $\widetilde{\widehat{P}}$, eq. (3), we find that

$$\begin{aligned} \widetilde{\widehat{P}}(k,s) &= \sum_{N=0}^{\infty} \left(\widetilde{\psi}(s)\right)^N \left(\frac{1-\widetilde{\psi}(s)}{s}\right) \left(\widehat{p}(k)\right)^N \\ &= \frac{1-\widetilde{\psi}(s)}{s\left(1-\widetilde{\psi}(s)\widehat{p}(k)\right)}, \end{aligned} \tag{6}$$

which is known as the Montroll-Weiss equation. With this equation, studying the distribution of $X(t)$ for various choices of $\psi(t)$ and $p(\Delta x)$ reduces to inverting equation (6).

In general, it is difficult to find exact results for $P(x,t)$, so we seek to gain some insight by examining the scaling of the moments and the qualitative shape of the distribution[2]. In this lecture, we will only focus on the scaling laws. We will address the question of shape in the next lecture.

1.1 Scaling Laws for the First and Second Moments of $X(t)$

Recall that the moments of a random variable, X, are easily related to the derivatives of the characteristic function evaluated at $k = 0$ by the formula

$$\widetilde{\langle X^n \rangle}(s) = (-i)^n \frac{\partial^n \widetilde{\widehat{P}}}{\partial k^n}(0,s). \tag{7}$$

Using this formula to compute the first moment of $\widetilde{X}(s)$, we find that

$$\begin{aligned} \widetilde{\langle X \rangle}(s) &= -i\frac{\partial \widetilde{\widehat{P}}}{\partial k}(0,s) \\ &= \left[\frac{1-\widetilde{\psi}(s)}{s}\right] \left[\frac{\widetilde{\psi}(s)\left(-i\frac{\partial \widehat{p}}{\partial k}(0)\right)}{\left(1-\widetilde{\psi}(s)\widehat{p}(0)\right)^2}\right] \\ &= \frac{\langle \Delta x \rangle \widetilde{\psi}(s)}{s\left(1-\widetilde{\psi}(s)\right)} \\ &= \widetilde{\langle N \rangle}(s) \langle \Delta x \rangle, \end{aligned} \tag{8}$$

where we have made use of formula for $\widetilde{\langle N \rangle}(s)$ from last lecture. Inverting the Laplace transform, we obtain

$$\langle X \rangle (t) = \langle N \rangle (t) \langle \Delta x \rangle, \tag{9}$$

which is the same expression we derived last lecture starting with the N as the basic random variable.

[2] Recall the analysis of the Poisson-Bernoulli random walk discussed in the last lecture

Similarly, we can compute the second moment for $\tilde{X}(s)$ as[3]

$$\begin{aligned}
\widetilde{\langle X^2\rangle}(s) &= -\frac{\partial^2 \tilde{\hat{P}}}{\partial k^2}(0,s) \\
&= \frac{\tilde{\psi}(s)\left\langle(\Delta x)^2\right\rangle}{s\left(1-\tilde{\psi}(s)\right)} + \frac{2\left(\tilde{\psi}(s)\right)^2\langle\Delta x\rangle^2}{s\left(1-\tilde{\psi}(s)\right)^2} \\
&= \widetilde{\langle N\rangle}(s)\left\langle(\Delta x)^2\right\rangle + \left[\widetilde{\langle N^2\rangle} - \widetilde{\langle N\rangle}\right]\langle\Delta x\rangle^2 .
\end{aligned} \tag{10}$$

To arrive at the last equality, we calculate $\widetilde{\langle N^2\rangle}$ in the same manner as we $\widetilde{\langle N\rangle}$ in the last lecture:

$$\begin{aligned}
\widetilde{\langle N^2\rangle} &= \sum_{N=0}^{\infty} N^2 \tilde{\mathcal{P}}(N,s) \\
&= \frac{1-\tilde{\psi}(s)}{s}\sum_{N=0}^{\infty} N^2\left(\tilde{\psi}(s)\right)^N \\
&= \frac{1-\tilde{\psi}(s)}{s}\left(\tilde{\psi}\frac{d}{d\tilde{\psi}}\right)^2\sum_{N=0}^{\infty}\left(\tilde{\psi}(s)\right)^N \\
&= \frac{1-\tilde{\psi}(s)}{s}\left(\tilde{\psi}\frac{d}{d\tilde{\psi}}\right)^2\frac{1}{1-\tilde{\psi}} \\
&= \frac{2\left(\tilde{\psi}\right)^2}{s\left(1-\tilde{\psi}\right)^2} + \frac{\tilde{\psi}}{s\left(1-\tilde{\psi}\right)}.
\end{aligned} \tag{11}$$

Upon inverting the Laplace transform, we find that the second moment of $X(t)$ is given by

$$\left\langle X^2\right\rangle(t) = \langle N\rangle(t)\left\langle(\Delta x)^2\right\rangle + \left[\left\langle N^2\right\rangle(t) - \langle N\rangle(t)\right]\langle\Delta x\rangle^2 . \tag{12}$$

Finally, combining the results from equations (9) and (12), we find that the variance for $X(t)$ is given by

$$\sigma^2_{X(t)} = \langle N\rangle(t)\sigma^2_{\Delta x} + \langle\Delta x\rangle^2\sigma^2_{N(t)}. \tag{13}$$

Physically, this equation tells us that the variance of the walker's position at time t arises from two sources: variations in the step size and variations in the number of steps taken. It is important to note that latter variation only matters when the individual steps have a mean drift.

While equation (13) is a nice theoretical result, inversion of the Laplace transforms to compute the first and second moments often poses some difficulties. Fortunately, when deriving scaling laws, we primarily care about the long time behavior, $t \to \infty$, which corresponds to the limit $s \to 0$.

1.2 Useful Tauberian Theorems

Before turning to an analysis of some important classes of anomalous diffusion, we record a few Tauberian theorems which will prove useful. These theorems relate the leading order behavior

[3]In this analysis, we implicitly assume that the variance of an individual step is finite, but not necessarily nonzero.

of various Laplace transforms around $s = 0$ to the leading order behavior of the inverse Laplace transforms for large t:

$$\begin{aligned}
s \to 0 \quad & \qquad t \to \infty \\
\tilde{\psi}(s) \sim 1 - \langle \tau \rangle s \quad & \Longleftrightarrow \quad \psi(t) = o\left(\frac{1}{t^2}\right) && (14) \\
\tilde{\psi}(s) \sim 1 - A s^{\alpha} \quad & \Longleftrightarrow \quad \psi(t) \sim \frac{1}{t^{1+\alpha}} \quad (0 < \alpha < 1) && (15) \\
\tilde{\psi}(s) \sim s^{-\beta} \quad & \Longleftrightarrow \quad \psi(t) \sim \frac{t^{\beta-1}}{\Gamma(\beta)} \quad (\beta > 0). && (16)
\end{aligned}$$

The first case arises whenever $\tilde{\psi}(s)$ is differentiable in the real direction at $s = 0$ ($\tilde{\psi}(s)$ need not be analytic). The second case is common when $\tilde{\psi}(s)$ depends exponentially on s to some power. As an example, recall the Lévy flights whose PDFs have Laplace transforms of the form

$$\tilde{l}_{\alpha,1}(s) = e^{-s^{\alpha}} \sim 1 - s^{\alpha}. \tag{17}$$

Finally, the last case arises in the scaling of moments (which grow with time). Note that this case can also be generalized as the 'Strong Tauberian Theorem' (Hughes, p.249),

$$\tilde{\psi}(s) \sim L(s^{-1}) s^{-\beta} \Longleftrightarrow \psi(t) \sim \frac{L(t)\, t^{\beta-1}}{\Gamma(\beta)} \quad (\beta > 0) \tag{18}$$

for any slowly varying function $L(t)$ (satifying $L(\lambda t)/L(t) \to 1$ for all $\lambda > 0$) such as $L(t) = \log t$.

2 Normal Diffusion ($\langle \tau^2 \rangle < \infty,\ 0 < \sigma_{\Delta x}^2 < \infty$)

Before turning our attention towards anomalous diffusion, we apply the formal theory derived above to the case of normal diffusion. Since the second moment of τ is finite, we can approximate $\tilde{\psi}(s)$ by the following asymptotic expansion

$$\tilde{\psi}(s) \sim 1 - \langle \tau \rangle s + \frac{\langle \tau^2 \rangle}{2} s^2 \tag{19}$$

Using this approximation in equation (8), we obtain

$$\begin{aligned}
\widetilde{\langle X \rangle}(s) \quad & \sim \quad \frac{1 - \langle \tau \rangle s + \frac{\langle \tau^2 \rangle}{2} s^2}{s\left(\langle \tau \rangle s - \frac{\langle \tau^2 \rangle}{2} s^2\right)} \langle \Delta x \rangle \\
& \sim \quad \frac{\langle \Delta x \rangle}{s^2 \langle \tau \rangle} + \frac{1}{s}\left(\frac{\langle \tau^2 \rangle}{2 \langle \tau \rangle^2} - 1\right) \langle \Delta x \rangle . && (20)
\end{aligned}$$

Therefore,

$$\begin{aligned}
\langle X \rangle (t) \quad & \sim \quad \left(\frac{t}{\langle \tau \rangle}\right) \langle \Delta x \rangle + \left(\frac{\langle \tau^2 \rangle}{2 \langle \tau \rangle^2} - 1\right) \langle \Delta x \rangle \\
& \sim \quad \langle N \rangle \langle \Delta x \rangle && (21)
\end{aligned}$$

which is the same leading order advective behavior as we would see in a diffusion process arising from a discrete-time mechanism with a fixed time $\langle \tau \rangle$ between steps.

Substituting (19) into equation (10) and carrying out some algebra, we see that the variance for $X(t)$ is

$$\sigma_X^2 \sim \frac{t}{\langle\tau\rangle}\left(\sigma_{\Delta x}^2 + \frac{\langle\Delta x\rangle^2}{\langle\tau\rangle^2}\sigma_\tau^2\right). \tag{22}$$

Notice that when there is a mean drift, *i.e* $\langle\Delta x\rangle \neq 0$, then diffusion is enhanced from the randomness in the number of steps. Intuitively, in the absence of drift, σ_X^2 is independent of the variation in the number of steps because the contribution from walks with a few extra steps balances against the contribution from walks that are short a few steps. An interesting consequence of equation (22) is that knowledge of the diffusion coefficient alone (*e.g.* from experiment) is not sufficient to distinguish between continuous- and discrete-time random walk mechanisms for diffusion. A discrete-time random walk with fixed step time, τ, and step variance, $\sigma_{\Delta x}^2$, given by the right hand side of equation (22) would leads to the same diffusion coefficient. However, differences between continuous- and discrete-time mechanisms would show up in the higher order moments.

A comparison of equation (22) with equation (13) shows how variation in number of steps is related to variations in step size:

$$\begin{aligned}\sigma_N^2(t) &\sim \frac{\sigma_\tau^2 t}{\langle\tau\rangle^3}\\ &= \frac{\sigma_\tau^2}{\langle\tau\rangle^2}\langle N\rangle,\end{aligned} \tag{23}$$

which implies that

$$\sigma_N(t) \propto \sqrt{t} \propto \sqrt{\langle N\rangle}\ . \tag{24}$$

So, for normal diffusion, the fluctuations in the number of steps taken in an interval $[0, t)$ is not too big and shows the typical square root dependence that we expect.

3 Anomalous Diffusion

In this section, we focus on anomalous diffusion processes that break the usual $t^{1/2}$ dependence for the root-mean-square displacement of the walker.

3.1 Dispersion ($\langle\tau\rangle < \infty,\ \langle\tau^2\rangle = \infty,\ \langle\Delta x\rangle \neq 0,\ \sigma_{\Delta x}^2 = 0$)

In this case, all step sizes are the same, so the randomness in the process is due solely to the randomness in the waiting time between steps. These dispersive processes are active areas of interest and have many applications in chemistry and soft condensed-matter physics. Typically, the waiting time density scales like

$$\psi(t) \sim \frac{1}{t^{1+\alpha}}, \tag{25}$$

with $1 < \alpha < 2$.

An example application is gel electrophoresis of polymers (*e.g.* DNA). In this system, the gel forms a "frozen" interconnected network of chain molecules soaked in electrolyte (see figure 1). The DNA is placed in wells at one end of the gel and an electric field, E, is applied to drive the DNA through the gel. Because the gel network is so tangled, the DNA strands get trapped in the gel

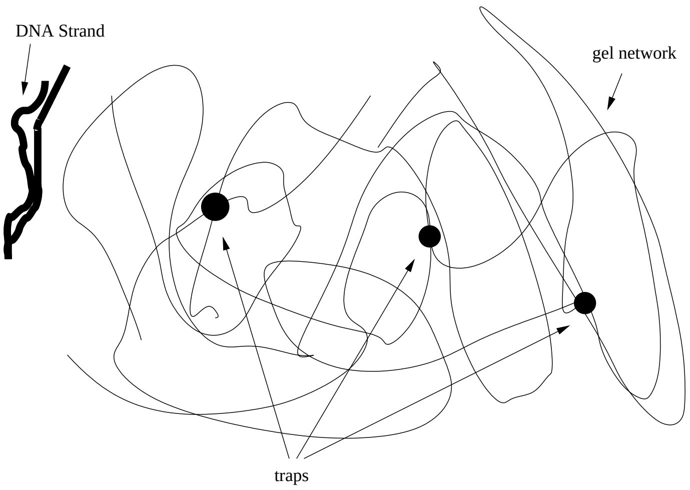

Figure 1: Cartoon of DNA strand in a gel network.

from time to time. As a simple model, we can assume that the distance between trapping points is a constant, Δx. Then the mean distance travelled by a DNA strand of length, L, is given by

$$\Delta x \left(\frac{t}{\langle \tau \rangle_L} \right) \tag{26}$$

where the average waiting time between steps depends on the length of the DNA strand.

It turns out that for "short" DNA strands, the waiting time seems to have a finite mean and variance so that the initial DNA well propagates in the direction of applied field and spreads out as it would in normal diffusion and relative fluctuations decay like $1/\sqrt{t}$ (see figure 2). However, for "long" DNA strands, the waiting time distribution has a much fatter tail and the initial DNA well propagates in such a way that the mean and standard deviation both scale linearly with time, and thus relative fluctuations do not decay (see figure 3) The theoretical and experimental details can be found in the reference

- E. Yarmola, *et. al.*. J. Chem. Phys. B, **101**, 2381 (1997).

3.2 Infinite Mean Waiting Time ($\langle \tau \rangle = \infty,\ 0 < \sigma^2_{\Delta x} < \infty$)

In this case, the randomness in the step size and the randomness in the number of steps both play a significant role in the scaling laws for $\langle X \rangle$ and $\langle X^2 \rangle$. The typical large t asymptotic behavior for $\psi(t)$ for this kind of diffusion is

$$\psi(t) \propto \frac{1}{t^{1+\alpha}} \tag{27}$$

with $0 < \alpha < 1$. The corresponding Laplace transform has the following form as $s \to 0$

$$\tilde{\psi}(s) \sim 1 - A s^{\alpha}. \tag{28}$$

First, we examine the average displacement of the walker. Using formulas derived earlier, we find that

$$\widetilde{\langle N \rangle}(s) = \frac{\tilde{\psi}(s)}{s\left(1 - \tilde{\psi}(s)\right)}$$

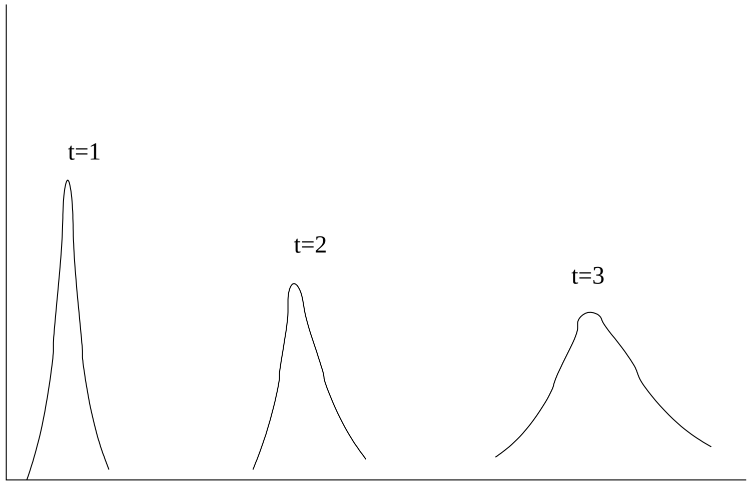

Figure 2: DNA concentration profile as a function of time for short DNA strands.

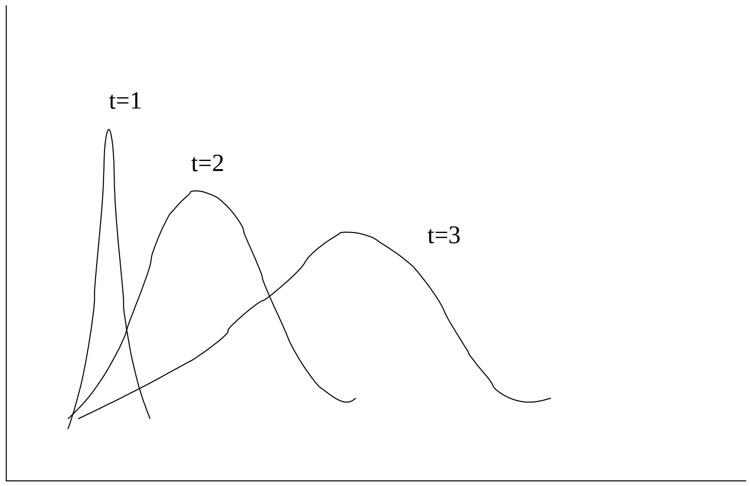

Figure 3: DNA concentration profile as a function of time for long DNA strands.

$$\sim \frac{1}{As^{1+\alpha}}. \tag{29}$$

Using the Tauberian theorems, this implies that as $t \to \infty$,

$$\langle N \rangle (t) \sim \frac{t^\alpha}{A\Gamma(1+\alpha)}. \tag{30}$$

Thus, the scaling for the average displacement is given by

$$\langle X \rangle (t) \sim \frac{\langle \Delta x \rangle t^\alpha}{A\Gamma(1+\alpha)}. \tag{31}$$

Note that since $\alpha < 1$, the drift is sublinear. Also, the "velocity" of the mean displacement tends towards zero as for long times because

$$\frac{d\langle X \rangle}{dt} \to 0 \tag{32}$$

as $t \to \infty$.

Next, we look at the mean square displacement of the walker. Using equation (10), we obtain

$$\begin{aligned} \widetilde{\langle X^2 \rangle}(s) &= \frac{\tilde{\psi}(s)\langle (\Delta x)^2 \rangle}{s\left(1-\tilde{\psi}(s)\right)} + \frac{2\left(\tilde{\psi}(s)\right)^2 \langle \Delta x \rangle^2}{s\left(1-\tilde{\psi}(s)\right)^2} \\ &\sim \frac{\langle (\Delta x)^2 \rangle}{As^{1+\alpha}} + \frac{2\langle \Delta x \rangle^2}{A^2 s^{1+2\alpha}}. \end{aligned} \tag{33}$$

From this expression, we see that if there is a non-zero mean drive, then the randomness in the number of steps taken dominates the behavior of $\widetilde{\langle X^2 \rangle}(s)$ because it makes the more singular contribution.

We consider the two cases separately.

1. $\langle \Delta x \rangle = 0$.

   In this case, the Laplace transform of the mean square displacement is

   $$\widetilde{\langle X^2 \rangle}(s) \sim \frac{\langle (\Delta x)^2 \rangle}{As^{1+\alpha}}, \tag{34}$$

   so

   $$\left\langle X^2 \right\rangle (t) \sim \frac{\langle (\Delta x)^2 \rangle t^\alpha}{A\Gamma(1+\alpha)}. \tag{35}$$

   Since $\langle X \rangle (t) = 0$ in this case,

   $$\sigma_X^2(t) \sim \frac{\langle (\Delta x)^2 \rangle t^\alpha}{A\Gamma(1+\alpha)}, \tag{36}$$

   which means that

   $$\sigma_X(t) \propto t^{\alpha/2} \propto \sqrt{\langle N \rangle (t)} \tag{37}$$

   Notice that while we have retained the square root scaling with the number of steps, we have lost the usual square root scaling with time.

2. $\langle \Delta x \rangle \neq 0$.

   In this case, we obtain

$$\widetilde{\langle X^2 \rangle}(s) \sim \frac{2 \langle \Delta x \rangle^2}{A^2 s^{1+2\alpha}}, \tag{38}$$

   which can be inverted to give

$$\left\langle X^2 \right\rangle (t) \sim \frac{2 \langle \Delta x \rangle^2 t^{2\alpha}}{A^2 \Gamma(1+2\alpha)} \propto \langle X \rangle^2 . \tag{39}$$

   Therefore,

$$\sigma_X^2(t) \sim \frac{2 \langle \Delta x \rangle^2 t^{2\alpha}}{A^2 \Gamma(1+2\alpha)} - \frac{\langle \Delta x \rangle^2 t^{2\alpha}}{A^2 \left(\Gamma(1+\alpha)\right)^2} \tag{40}$$

   so that

$$\sigma_X(t) \sim \frac{\langle \Delta x \rangle t^{\alpha}}{A} \sqrt{\frac{2}{\Gamma(1+2\alpha)} - \frac{1}{\left(\Gamma(1+\alpha)\right)^2}}. \tag{41}$$

   From this formula, we see that when there is a mean drift for the individual steps, the width of the distribution scales like $t^{\alpha} \propto \langle N \rangle (t)$. Thus, this case breaks both the square root scaling with time and with the number of steps taken.