18.325 Topics in Applied Mathematics: Random Walks and Diffusion
Lecture 22: Continuous Time Random Walks and Anomalous Diffusion

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This lecture examines applications of continuous time random walks and moments of CTRWs. We begin with a general form for a continuous time random walk given by:

$$X_t = \sum_{n=0}^{N(t)} \Delta x_n$$

where $N(t)$ is a random process (waiting time distributions).

The probability density function is generated by taking the sum over all number of steps, n, of taking n steps in time t. That is,

$$P(x,t) = \sum_{n=0}^{\infty} \mathcal{P}(n,t) P_n(x)$$

$$\tilde{\hat{P}}(k,s) = \frac{1-\tilde{\psi}(s)}{s} \cdot \frac{1}{1-\tilde{\psi}(s)\hat{p}(k)}$$

1 Applications of Continuous Time Random Walks

1.1 Diffusion of Defects in a Crystal

$$\psi(t) = \lambda e^{-\lambda t}$$

with $\lambda = 1/\bar{\tau}$ giving the waiting time distribution for diffusion of defects in a crystal. Then, the expected motion for a single defect, neglected nearest neighbor and excluded volume effects, is given by:

$$P(x,t) = \sum_{n=0}^{\psi(t)} \Delta x_n$$

where x_n is the step size.

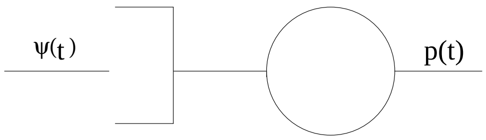

Figure 1: Standard M/M/1 queue, with poisson processes for input and output service rates.

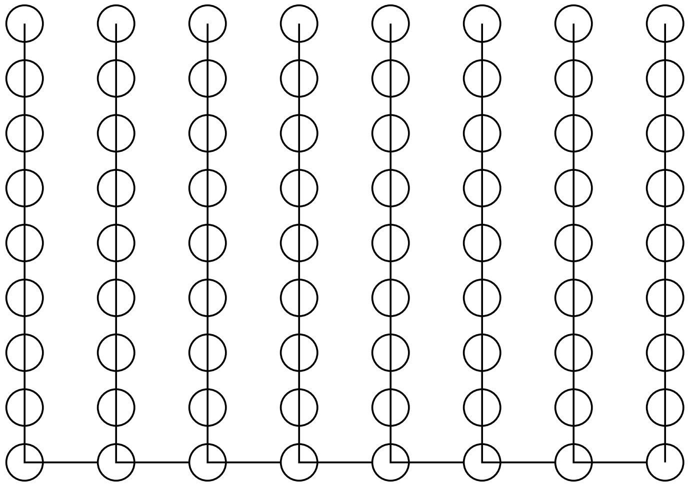

Figure 2: Comb structure. Lattice sites are represented by small circles.

1.2 Queueing Theory

Let x denote the number of people in a queue, such as Figure 1. We are interested in the dynamics of x. This is a continuous time random walk with waiting time density $\psi(t)$ to step to the right, $x \to x+1$ and another $p(t)$ to step to the left, $x \to x-1$.

We define a waiting time coming into the queue of $\psi(t) = \lambda e^{-\lambda t}$, given by a Markov (Poisson) process. We define $p(t) = \mu e^{-\mu t}$. When $\lambda < \mu$, the queue reaches steady-state. We define $\rho = \frac{\mu}{\lambda}$, the utilization of the server.

The PDF for the queue size, x, is given by

$$P(x) = \rho^x (1-\rho)$$

When the processes $p(t)$ and $\psi(t)$ are both Markov processes, the queue is called an M/M/1 Queue. These queues are useful in modeling Langmuir Surface Adsorption. In the limit where the surface has tightly bound sites and the gas is ideal, the adsorption is exactly queueing.

1.3 Anomalous Diffusion

For particular systems, such as the comb structure seen in Figure 2, the diffusion is anomalous in nature. The underlying subject is introduced here, and the particular example of the comb diffusion will be revisited later in the notes.

Let $\psi(t)$ be the return time of a $d = 1$ walker.

$$\psi(t) \sim \frac{1}{t^{3/2}}$$

for $(\bar{\tau} = \infty)$

The width scales as

$$\sigma_x^2(t) \sim t^{\frac{1}{2}}$$

and

$$\sigma_x(t) \sim t^{\frac{1}{4}}$$

which yields anomalous diffusion.

This 1D model is also useful for diffusion in a random environment (fractal) or for diffusion of a large bead on the structure of a liquid polymer.

2 Moments of CTRW

Montroll-Weiss Equation

$$\tilde{\hat{P}}(k,s) = \frac{1-\tilde{\psi}(s)}{s} \cdot \frac{1}{1-\tilde{\psi}(s)\widehat{p}(k)}$$

$$\tilde{\overline{X}}(s) = i\frac{d}{dk}\tilde{\hat{P}}|_{k=0} = \frac{1-\tilde{\psi}(s)}{s}\frac{\tilde{\psi}(s)}{i}\frac{d\hat{p}}{dk}(1-\tilde{\psi}(s)\hat{p}(k))^2\big|_{k=0}$$

This is the Laplace Transform of the expected position. Continuing the development and noting that normalization/conservation of mass requires $\widehat{p(0)} = 1$ and defining $i\frac{d\widehat{p}}{dk}(0) = \overline{\Delta X}$,

$$\tilde{\bar{X}}(s) = \frac{1-\tilde{\psi}(s)}{s} \cdot \frac{\tilde{\psi}(s)\overline{\Delta X}}{(1-\tilde{\psi}(s))^2} = \frac{\tilde{\psi}(s)\overline{\Delta X}}{s(1-\tilde{\psi}(s))} = \tilde{\bar{n}}(s)\overline{\Delta X}$$

with

$$\bar{(}X(t)) = \bar{n}(t)\overline{\Delta X}$$

as expected.

Similarly,

$$X\bar{(s)}^2 = \frac{\overline{\Delta X}^2\tilde{\psi}(s)}{s\,(1-\tilde{\psi}(s))} + \frac{2\overline{\Delta X^2}\tilde{\psi}(s)^2}{s\,(1-\tilde{\psi}(s))^2}$$

3 Tauberian Theorems (for Laplace Transforms)

For functions of the form:

$$\tilde{f}(s) = \frac{L(\frac{1}{s})}{s^\alpha}$$

$s \to 0$, where

$$\frac{L(\alpha t)}{L(t)} = 1$$

as $t \to \infty$, we are interested in properties of the long time behavior (or vice-versa for functions defined as $s \to \infty$). This effectively restricts L to slowly varying functions such as $\log$.

Then, we have that

$$\int_0^t f(\tau)d\tau \sim \frac{t^\alpha L(t)}{\Gamma(1+\alpha)}$$

If $f(t)$ also asymptotically monotonic as $t \to \infty$ (no oscillatory behavior at large t), then we can differentiate, yielding

$$f(t) \sim \frac{d}{dt}\left(\frac{t^{\alpha}L(t)}{\Gamma(1+\alpha)}\right)$$

as $t \to \infty$.

The simplest case is

$$\tilde{f}(s) \sim s^{-\alpha}$$

as $s \to 0$ (monotonic).

Then

$$f(t) \sim \frac{t^{\alpha-1}}{\Gamma(\alpha)}$$

as $t \to \infty$.

This is similar to

$$\hat{f}(k) \sim 1 - |k|^{\alpha}$$

for $k \to 0$ leads to

$$f(x) \sim \frac{const}{x^{1+\alpha}}$$

for $|x| \to \infty$ (for Fourier Transforms), with $0 \le \alpha \le 2$.

In general, Tauberian theorems allow information about the long-time behavior of the function to provide information regarding the small s behavior in the Laplace domain or the small k behavior in Fourier domain. Similarly, short-time behavior can provide long s or k behavior in the Laplace or Fourier domains, respectively.

3.1 Normal Diffusion

Given $\bar{\tau} < \infty$ and $\bar{\tau^2} < \infty$.

Then,

$$\tilde{\psi}(s) \sim 1 - \bar{\tau}s + \frac{\overline{\tau^2}}{2}s^2 - \cdots$$

for $s \to 0$.

$$\tilde{\bar{X}}(s) \sim \frac{(1-\bar{\tau}s + \frac{\overline{\tau^2}}{2}s^2)\overline{\Delta X}}{s(\bar{\tau} - \frac{\overline{\tau^2}s^2}{2})} \sim \frac{\overline{\Delta X}}{\bar{\tau}}\frac{1}{s^2} + \frac{\overline{\Delta X}}{s}\left(\frac{\overline{\tau^2}}{2\bar{\tau}^2} - 1\right) + \cdots$$

Yields the most singular part of the Laplace Transform at the origin. The first term is effectively the mean displacement over the mean waiting time. Using the Tauberian theorem, we have:

$$\overline{X(t)} \sim \overline{\Delta X}\frac{t}{\bar{\tau}} + \overline{\Delta X}\left(\frac{\overline{\tau^2}}{2\bar{\tau}^2} - 1\right) + \cdots$$

for $t \to \infty$.

Similarly, it can be shown that

$$\sigma_x^2(t) = \left[\sigma_{\Delta X}^2 + \sigma_{\tau}^2(\frac{\overline{\Delta X}^2}{\bar{\tau}})\right]\frac{t}{\bar{\tau}}$$

The extra terms on the right act to enhance diffusion.

Note:

$$X = \sum_{m=1}^{N} \Delta X_m$$

where ΔX_m are iid.

Since,

$$\bar{X} = \bar{N}\overline{\Delta X}$$

$$\sigma_x(t)^2 \sim \sigma_{\Delta X}^2 + \sigma_\tau^2 \left(\frac{\bar{X}}{\bar{\tau}}\right)^2 \left(\frac{t}{\bar{\tau}}\right)$$

as $t \to \infty$.

3.2 CLT for drifting CTRW

If $\bar{\tau} < \infty$ and $\Delta\bar{X} \neq 0$,

$$P(x,t) \to \frac{e^{-\frac{x-\bar{x}(t)^2}{2\sigma_x^2(t)}}}{\sqrt{2\pi\sigma_x^2(t)}}$$

3.3 Anomalous Diffusion

$\bar{\tau} = \infty$ infinite mean waiting time, one-sided stable laws.

$$\psi(t) \sim \ell_{\alpha,1}(t) \sim \frac{T^\alpha}{t^{\alpha+1}}$$

$$\psi_n(t) \sim \ell_{\alpha,1}\left(\frac{t}{n^{\frac{1}{\alpha}}}\right)$$

for $0 < \alpha < 1$.

Assume

$$\tilde{\psi(s)} \sim 1 - (sT)^\alpha$$

$s \to 0$

Then we have

$$\bar{X}(t) \ll \sigma_x(t)$$

If $\overline{\Delta X} = 0$ (no net drift), then

$$\sigma_x^2(t) = \frac{\sigma_{\Delta X}^2}{\Gamma(1-\alpha)\Gamma(1+\alpha)}\left(\frac{t}{T}\right)^\alpha$$

when $\overline{\Delta X} = 0$ and $t \to \infty$.

The width of the distribution $P(x,t)$ is given by

$$\sigma_x(t) \sim t^{\frac{\alpha}{2}}$$

when $\alpha < 1$, because the waiting time between terms is so long, the result is anomalous sub diffusion.

If $\overline{\Delta X} \neq 0$ (drift),

$$\sigma_x^2(t) \sim \frac{\overline{\Delta X}^2}{\Gamma(1-\alpha)^2}\left[\frac{2}{\Gamma(1+2\alpha)} - \frac{1}{\Gamma(1+\alpha)^2}\right]\left(\frac{t}{T}\right)^{2\alpha}$$

where the width of the distribution $P(x,t)$ is given by

$$\sigma_x(t) \sim t^\alpha$$

4 Shape of the Limiting Distribution

4.1 Poisson-Bernoulli CTRW

Poisson refers to waiting times and Bernoulli refers to the steps.

For this CTRW, we have

$$\psi(t) = \lambda e^{-\lambda t}$$

and

$$p(\hat{k}) = cos(ak)$$

So,

$$P(ma, t) = \frac{e^{-\lambda t}}{a} I_m(\lambda t)$$

with

$$I_m(x) = \frac{1}{2\pi} \int_{-\pi}^{\pi} cos(m\theta) e^{x \cos(\theta)} d\theta$$

being the modified bessel function.

That this shape yields a Gaussian (CLT) is left as an exercise to the reader.

4.1.1 Anomalous Diffusion

e.g. comb diffusion, where $\alpha < 1$.

As $\tau \to \infty$,

$$\psi \sim \frac{1}{t^{\alpha+1}}$$

$$\psi_n(t) \sim \ell_{\alpha,1}(\frac{x}{n^{\frac{1}{\alpha}}})$$

$$\tilde{\psi}_n(s) = \tilde{\psi}(s)^n = \tilde{\psi}(n^{\frac{1}{\alpha}} s)$$

$$\tilde{\mathcal{P}}(n, s) = \tilde{\psi}(s)^n \left(\frac{1 - \tilde{\psi(s)}}{s} \right) = \frac{\tilde{\psi}(s)^n}{s} - \frac{\tilde{\psi}(s)^{n+1}}{s} = \frac{\tilde{\psi}(n^{1/\alpha} s)}{s} - \frac{\tilde{\psi}((n+1)^{1/\alpha} s)}{s}$$

for $s \neq 0$.

$$\mathcal{P}(n, t) = L_\alpha \left(\frac{t}{n^{1/\alpha}} \right) - L_\alpha \left(\frac{t}{(n+1)^{1/\alpha}} \right) + (1 - L_\alpha(t))\delta(x)$$

where $L_\alpha(t) = \int_0^t \ell_{\alpha,1}(t)dt$

Then, treating n as a continuous variable, we have

$$\mathcal{P}(n, t) \sim -\frac{d}{dn} L_{\alpha,1} \left(\frac{t}{n^\alpha} \right) = \frac{t}{\alpha n^{1/\alpha - 1}} \ell_{\alpha,1} \left(\frac{t}{n^{1/\alpha}} \right)$$

$$P(n, t) = \sum_{n=1}^{\infty} \left[L_\alpha(\frac{t}{n^{1/\alpha}} - L_\alpha(\frac{t}{(n+1)^{1/\alpha}}) \right] \cdot P_n(x) + (1 - L_\alpha(t))\delta(x)$$

where the last term comes from the probability that the walker never took a step in the given time interval.

That is,

$$(1 - L_\alpha(t))\delta(x) = \int_t^\infty \ell_{\alpha,1}(\tau) d\tau$$

If $n \to \infty$, and ignoring the $\delta(x)$ term, we have

$$P(x,t) \sim \int_0^\infty dn \left[-\frac{d}{dn} L_{\alpha,1}(\frac{t}{n^{1/\alpha}}) \right] \frac{e^{-\frac{(x-n\overline{\Delta X})^2}{2n\sigma^2_{\Delta X}}}}{\sqrt{2\pi n \sigma^2_{\Delta X}}}$$

For the comb problem ($\alpha = 1/2$), the waiting time distribution is given by the Smirnov density, which is a one-sided stable-law,

$$\psi = \ell_{\alpha,1}(t) = \left(\frac{1}{4\pi t^3} \right)^{1/2} e^{-1/4t}$$

$$\psi \sim t^{\frac{-3}{2}}$$

as $t \to 0$ and $\alpha = 1/2$.

Using Laplace's Method $x \gg t^{1/4}$ (in the tail of the distribution),

$$P(x,t) \sim \int_0^\infty dn \frac{t}{\alpha n^{\frac{1}{\alpha}-1}}$$

$$P(x,t) \sim \frac{At^{1/6}}{|x|^{1/3}} e^{-|x|^{4/3}/t^{1/3}}$$

Letting $\zeta = \frac{x}{t^{\frac{1}{4}}}$, and holding ζ constant, we have $x = \zeta t^{1/4}$. The tails are given by

$$P(x,t) \sim \Phi(\zeta) t^{-1/4} \sim \frac{At^{1/12}}{\zeta^{1/3}} e^{-\zeta^{1/3}}$$

Gives stretched/compressed exponentials. There is no power law dependence in the tails of the distribution (no Gaussian behavior either).