Lecture 16: Continuous Time Random Walks

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1 Introduction

In former lectures, we considered discrete time random walks with a constant waiting time. Here we consider continuous time random walks where the waiting time τ is a random variable. Consider the sum of random variables with random waiting time:

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

Now the sum upper limit $N(t)$, is a random function of continuous time.

We define:

$$\begin{aligned} P(x,t) &= \text{PDF for } X(t) \\ p(x) &= \text{PDF for } \Delta x_n \\ \psi(t) &= \text{PDF for the waiting time } \tau \text{ (Montroll \& Weiss)} \\ \mathcal{P}(N,t) &= \text{PDF for } N(t) \end{aligned} \tag{2}$$

We note that $\psi(t)$ and $\mathcal{P}(N,t)$ will be related and we will investigate the solution for $P(x,t)$ starting with the assumption that one of these two PDF's is known. We will first introduce some transform notation and then follow with the formalism that $\mathcal{P}(N,t)$ is known. We will then develop the relationship between $P(x,t)$ and $\psi(t)$.

As an aside, note that this continuous random walk formalism is applicable to "separable" processes that have step sizes and waiting times that are not correlated. This is usually a good model for sub-diffusive processes ($<\tau>=\infty, {\sigma_{\Delta x}}^2 < \infty$). On the other hand, this separable continuous time random walk formalism would be a poor model for continuous time Levy walks. More generally, one would define a joint PDF $\Phi(x,t)$ that a step makes a displacement x in time t:

$$\Phi(x,t) = p(x|t)\psi(t) \tag{3}$$

For now, we will only consider separable continuous time random walks.

2 $\mathcal{P}(N,t)$ Formulation and Transforms

If the PDF $\mathcal{P}(N,t)$ is known, then the overall displacement distribution is:

$$P(x,t) = \sum_{N=0}^{\infty} \mathcal{P}(N,t) p^{*N}(x) \tag{4}$$

Note that if $\mathcal{P}(N,t)$ is "localized" around $< N >= \frac{t}{<\tau>}$, then the CLT will hold, whereas if $\mathcal{P}(N,t)$ is "broad" ($< \tau >= \infty$), you can get other distributions for $P(x,t)$.

Taking the Discrete Fourier Transform of Eq. 4 yields:

$$\hat{P}(k,t) = \sum_{N=0}^{\infty} \mathcal{P}(N,t)\hat{p}^N(k) \tag{5}$$

To continue this approach, we consider several discrete transforms.

2.1 Probability generating function

The probability generating function transform yields a Taylor/power series whose coefficients are the probabilities for each N:

$$\bar{\mathcal{P}}(z,t) = \sum_{N=0}^{\infty} \mathcal{P}(N,t) z^N, \ |z| < 1 \tag{6}$$

$$\mathcal{P}(N,t) = \frac{1}{2\pi i} \oint_{|z|=1} \frac{\bar{\mathcal{P}}(z,t)}{z^{N+1}} dz \tag{7}$$

Applying this transform to Eq. 5 gives:

$$\hat{P}(k,t) = \bar{\mathcal{P}}(\hat{p}(k),t) \tag{8}$$

2.2 Moment generating function

The moment generating function transform is basically a discrete Laplace Transform.

$$\begin{aligned}\tilde{\mathcal{P}}(q,t) &= \bar{\mathcal{P}}(e^q,t) \\ &= \sum_{N=0}^{\infty} \mathcal{P}(N,t)e^{Nq}\end{aligned} \tag{9}$$

Taking the m^{th} derivative with respect to q at $q=0$ yields the m^{th} moment of N:

$$\frac{d^m\tilde{\mathcal{P}}}{dq^m}|_{q=0} =< N^m > \tag{10}$$

2.3 Cumulant generating function

The cumulant generating function transform is the logarithm of the moment generating function.

$$\check{\mathcal{P}}(q,t) = log\tilde{\mathcal{P}}(q,t) \tag{11}$$

Taking the m^{th} derivative with respect to q at $q=0$ yields the m^{th} cumulant of N:

$$\frac{d^m\check{\mathcal{P}}}{dq^m}|_{q=0} = c_m^{(N)}(t) \tag{12}$$

Recall from Lecture 3 that $\check{P}(k,t) = log\hat{P}(k,t)$ was the cumulant generating function for $X(t)$ and $\check{p}(k,t) = log\hat{p}(k,t)$ was the cumulant generating function for Δx_n.

Returning back to Eq. 8 and using these definitions, we arrive at:

$$\check{P}(k,t) = \check{\mathcal{P}}(\check{p}(k),t) \tag{13}$$

By differentiating at $k=0$ and performing some algebra we can determine the mean $< x >$ and the variance σ_x^2 of the total displacement (see M. Bazant Physica A, 2002):

$$\begin{aligned}< x > &=< N >< \Delta x_n > \\ \sigma_x^2 &=< N > \sigma_{\Delta x}^2 + \sigma_N^2 < \Delta x >^2\end{aligned} \tag{14}$$

Therefore, if $< \Delta x >= 0$ and $< t > \; < \infty$, then $< N > \; = \frac{t}{<\tau>}$ (Lecture 16) and $\sigma_x = \sigma_{\Delta x}\sqrt{\frac{t}{<\tau>}}$.

2.4 Example: Poisson process

For a Poisson process:

$$\mathcal{P}(N,t) = \frac{(\lambda t)^N e^{-\lambda t}}{N!}, \ \lambda = \frac{1}{<\tau>} \tag{15}$$

The probability generating function (Eq. 6) is:

$$\begin{aligned}\bar{\mathcal{P}}(z,t) &= \sum_{N=0}^{\infty} \mathcal{P}(N,t) z^N, |z| < 1 \\ &= e^{-\lambda t} \sum_{N=0}^{\infty} \frac{(\lambda t z)^N}{N!} \\ &= e^{\lambda t(z-1)}\end{aligned} \tag{16}$$

The moment generating function (Eq. 9) is:

$$\tilde{\mathcal{P}}(q,t) = e^{\lambda t(e^q - 1)} \tag{17}$$

And the cumulant generating function (Eq. 11) is:

$$\begin{aligned}\check{\mathcal{P}}(q,t) &= \lambda t(e^q - 1) \\ &= \lambda t \sum_{m=1}^{\infty} \frac{q^m}{m!}\end{aligned} \tag{18}$$

We see that the coefficient of each term of the cumulant generating function series is equal to λt. Thus (using Eq. 12) all cumulants for $N(t)$ are the same:

$$c_m^{(N)}(t) = \lambda t \text{ for all m} \tag{19}$$

3 Examples of Poisson processes

3.1 An exact result (Poisson-Bernouilli CTRW)

Starting at the origin $x_0 = 0$, take N Bernouilli steps, so we have $\Delta x_n = \pm a$ as the displacements and $\hat{p}(k) = cos(ka)$ as the characteristic function for the displacements. Assuming Poisson waiting times, we use the result from Eq. 8 to find the characteristic function of the total displacement:

$$\hat{P}(k,t) = \bar{\mathcal{P}}(\hat{p}(k),t) = e^{\lambda t(\hat{p}(k)-1)} \tag{20}$$

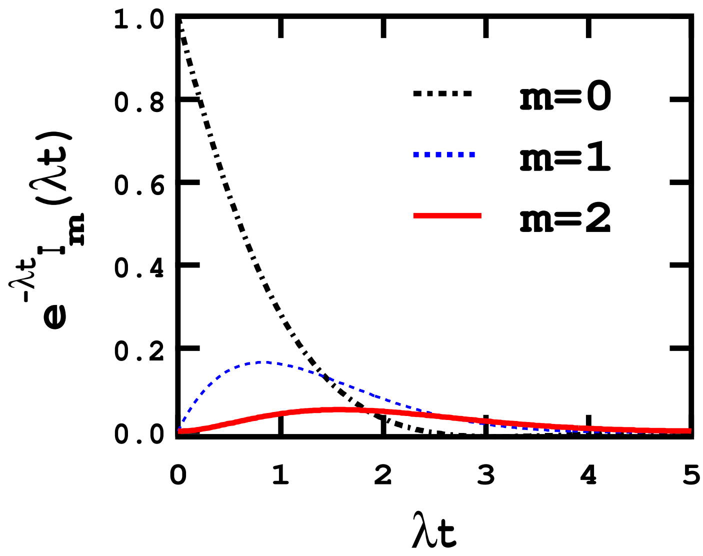

Figure 1: Probability at lattice site m ($a = 1$) after time t for a Bernouilli-Poisson CTRW.

Next we invert the Discrete Fourier Transform:

$$P(ma, t) = \int_{-\pi}^{\pi} e^{-ikma+\lambda t(cos(ka)-1)} \frac{dk}{2\pi} \tag{21}$$

In general, this integral cannot be easily performed, however this is a special case because it can be simplified using the definition of a Bessel function:

$$I_m(z) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-zcos(m\theta)} cos(m\theta) d\theta \tag{22}$$

So that we arrive at:

$$P(ma, t) = \frac{1}{a} e^{-\lambda t} I_m(\lambda t) \tag{23}$$

Figure 1 shows this distribution for $m = 0$, $m = 1$, and $m = 2$. We see that the mean of $P(ma, t)$ is located at $m < \tau >$.

3.2 A more general result (General Poisson CTRW)

So we see that the Poisson-Bernouilli Random Walk is a special case where the exact solution is available. More generally for other $p(x)$, the inverse transform integral is difficult to perform. However, by expanding the characteristic function of the displacement distribution $\hat{p}(k)$, we see the CLT in the long-time limit.

$$\hat{p}(k,t) \sim 1 - i < \Delta x > k - \frac{< \Delta x^2 > k^2}{2} + \ldots \tag{24}$$

so that:

$$\begin{aligned}\hat{P}(k,t) &= e^{\lambda t(\hat{p}(k)-1)} \\ &\sim e^{-\lambda t(i<\Delta x>k + \frac{<\Delta x^2>k^2}{2})}\end{aligned} \tag{25}$$

This expression can be inverted by completing the square, yielding the PDF for total displacement with $\frac{x}{\sqrt{\lambda t}}$ fixed and $\lambda t \to \infty$:

$$P(x,t) = \frac{e^{\frac{-(x-\lambda t<\Delta x>)^2}{2<\Delta x^2>\lambda t}}}{\sqrt{2\pi < \Delta x^2 > \lambda t}} \tag{26}$$

So we get a Gaussian distribution in the Central Region with mean:

$$< x >= \lambda t < \Delta x >=< N(t) >< \Delta x > \tag{27}$$

and variance (note $< N >= \sigma_N^2$ for the Poisson distribution):

$$\begin{aligned}\sigma_x^2 = \lambda t < \Delta x^2 > &= < N(t) >< \Delta x^2 > \\ &=< N(t) > (\sigma_{\Delta x}^2 + < \Delta x >^2) \\ &=< N(t) > \sigma_{\Delta x}^2 + \sigma_N^2 < \Delta x >^2\end{aligned} \tag{28}$$

Which are the same as the general expressions of Eq. 14.

4 Relation to the $\psi(t)$ Formulation

Now we continue by relating the above formulation to the Montroll-Weiss formulation, which assumes knowledge of $\psi(t)$, the PDF for the waiting time. The details of the Montroll-Weiss formulation will be continued in the next lecture.

We define:

$$\begin{aligned}\psi(t) &= \text{PDF for the waiting time } \tau \text{ between steps} \\ \psi_N(t) &= \text{PDF for waiting time of } N^{th}\text{step, } = \psi(t)^{*N}(t) \\ \Psi(t) &= \text{Probability that no step was taken in } 0 \le t' \le t\end{aligned} \tag{29}$$

So that:

$$\Psi(t) = 1 - \int_0^t \psi(t')dt' = \int_t^\infty \psi(t')dt' \tag{30}$$

Now we can relate $\mathcal{P}(N,t)$ to $\psi(t)$, realizing that $\mathcal{P}(N,t)$ is the convolution that the N^{th} step was taken in the interval $[0,t]$ AND no steps were taken afterward.

$$\begin{aligned}\mathcal{P}(N,t) &= \int_0^t \psi_N(t')\Psi(t-t')dt' \\ &= (\psi_N * \Psi)(t) \\ &= (\psi_1 * \psi_2 * \ldots * \psi_N * \Psi)(t)\end{aligned} \tag{31}$$

Taking the Laplace transform simplifies the convolution formula:

$$\tilde{\mathcal{P}}(N,s) = \tilde{\psi}^N(s)\tilde{\Psi}(s) = \tilde{\psi}^N(s)\left(\frac{1-\tilde{\psi}(s)}{s}\right) \tag{32}$$

Here we've used the definition of $\Psi(t)$ (Eq. 30) and performed its Laplace transform by integration by parts. This result directly relates the PDF's for the two approaches to continuous time random walks.

We can calculate the average number of steps as a function of time in terms of $\psi(t)$.

$$< N > (t) = \sum_{N=0}^{\infty} N\mathcal{P}(N,t) \tag{33}$$

Taking the Laplace transform and inserting Eq. 32 gives:

$$\begin{aligned}< \tilde{N} >(s) &= \sum_{N=0}^{\infty} N\tilde{\mathcal{P}}(N,s) \\ &= (\frac{1-\tilde{\psi}(s)}{s})\sum_{N=0}^{\infty} N\tilde{\psi}^N(s) \\ &= (\frac{1-\tilde{\psi}(s)}{s})\tilde{\psi}(s)\frac{d}{d\tilde{\psi}}\sum_{N=0}^{\infty}\tilde{\psi}^N(s) \\ &= (\frac{1-\tilde{\psi}(s)}{s})\frac{\tilde{\psi}(s)}{(1-\tilde{\psi}(s))^2} \\ &= \frac{\tilde{\psi}(s)}{s(1-\tilde{\psi}(s))}\end{aligned} \tag{34}$$

4.1 Example of the relation between $\mathcal{P}(N,t)$ and $\psi(t)$

Assume we have an exponential waiting time distribution, $\psi(t) = \frac{e^{-\frac{t}{<\tau>}}}{<\tau>} = \lambda e^{-\lambda t}$.

The Laplace transform is:

$$\tilde{\psi}(s) = \lambda \int_0^\infty e^{-st} e^{-\lambda t} dt = \frac{\lambda}{s+\lambda} \tag{35}$$

Using Eq. 32, we see that:

$$\begin{aligned} \tilde{\mathcal{P}}(N,s) &= \left(\frac{\lambda}{s+\lambda}\right)^N \left(\frac{1-\frac{\lambda}{s+\lambda}}{s}\right) \\ &= \frac{\lambda^N}{(s+\lambda)^{N+1}} \end{aligned} \tag{36}$$

Invert the Laplace transform:

$$\mathcal{P}(N,t) = \frac{1}{2\pi i} \oint_{c-i\infty}^{c+i\infty} e^{st} \frac{\lambda^N}{(s+\lambda)^{N+1}} ds \tag{37}$$

This integral has a $N+1$ order pole at $s = -\lambda$. The Residue Theorem implies that this integral evaluates to $2\pi i Res(-\lambda)$.

$$\begin{aligned} \mathcal{P}(N,t) &= Res(-\lambda) \\ &= \frac{\lambda^N}{N!} \left(\frac{d^N}{ds^N} e^{st}\right) |_{s=-\lambda} \\ &= \frac{(\lambda t)^N}{N!} e^{-\lambda t} \end{aligned} \tag{38}$$

So this $\psi(t)$ PDF for an exponential waiting time corresponds to a Poisson PDF for $N(t)$.