

Lecture 26: Leapers and Creepers

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May 12, 2005

Introduction

This lecture considers the analysis of the non-separable CTRW in which the distributions of step size and time between steps are dependent. With such walks the issue arises of describing the walk in between *turning points*, which form a set of measure zero of the entire time-path of the process. We will first describe the general theory of such walks, following the notation of Hughes, before considering two special cases: *leapers*, which are assumed to remain at the turning point of the walk until the next step is taken, at which point the walker moves instantaneously to the next such point; and *creepers*, which are assumed to move with constant velocity between turning points.

1 Non-separable CTRW

Define $\chi(\vec{r}, t)$ the joint pdf for a step of size \vec{r} that takes time t . We can write this in terms of the conditional distributions

$$\begin{aligned}\chi(\vec{r}, t) &= p(\vec{r}|t)\psi(t) \\ &= \psi(t|\vec{r})p(\vec{r})\end{aligned}$$

and the marginal distributions are defined as:

$$\begin{aligned}\psi(t) &= \int \chi(\vec{r}, t) d\vec{r} \\ p(\vec{r}) &= \int_0^t \chi(\vec{r}, t') dt'\end{aligned}$$

The discrete points defined by the sequence of draws from χ are called the *turning points* of the random walk path, and the question arises what do we observe if we observe the walk at a time other than the occurrence of a turning point. We define the density $q(\vec{r}, t|\vec{r}', t')$, which interpolates stochastically between the current location and the next step, as the position-time

density of the *intermediate* increment of the random walk conditional on the *next* turning point being at (\vec{r}', t') . Thus between turning points we assume that the random walk follows a stochastic trajectory towards the next turning point. Once it reaches there the next turning point in space and time is selected and the walker follows the path defined by q to get there. $\chi(\vec{r}, t)$ and q define the random walk. Our goal is to write down the analog of the Bachelier equation to define the position-time density of the walker.

Define the pdf Ψ of the incremental displacement (\vec{r}, t) from the previous turning point, without reaching the next turning point where the integral is taken over all possibilities for the next turning point, in both space and time, multiplied by the conditional density q for the intermediate increment in between turning points. The integral in t' integrates over all turning points that occur later than time t .

$$\Psi(\vec{r}, t) = \int \int_t^\infty q(\vec{r}, t | \vec{r}', t') \chi(\vec{r}', t') dt' d\vec{r}'$$

The generalization of the Bachelier equation for the non-separable CTRW is then:

$$P(\vec{r}', t') = \Psi(\vec{r}, t) + \int \int P(\vec{r} - \vec{r}', t - t') \chi(\vec{r}', t') dt' d\vec{r}'$$

The first term in this equation is the density conditional on no turning point having been reached, and the second term integrates over all the possible possible locations of the first turning point and subsequent positions of the walker.

Taking the Fourier-Laplace transform (where $\tilde{}$ denotes the Laplace transform and $\hat{}$ the Fourier transform) we derive a generalization of the Montroll-Weiss equation:

$$\tilde{\hat{P}}(\vec{k}, s) = \frac{\tilde{\hat{\Psi}}(\vec{k}, s)}{1 - \tilde{\hat{\chi}}(\vec{k}, s)} \quad (1)$$

2 Leapers

Leapers are a special case of the above random walks in which the walker remains at each turning point until the next increment occurs, and then immediately leaps to the next turning point. We can describe the walk through:

$$q(\vec{r}, t | \vec{r}', t') = \delta(\vec{r}) \text{ for } 0 < t < t'$$

This is still more general than previous lecture, even though it does not feature intermediate dynamics in between turning points, since we allow (\vec{r}, t) non-separable.

Then

$$\begin{aligned}
 \Psi(\vec{r}, t) &= \int \int_t^\infty q(\vec{r}, t | \vec{r}', t') \chi(\vec{r}', t') dt' d\vec{r}' \\
 &= \delta(\vec{r}) \int_t^\infty \left(\int \chi(\vec{r}', t') d\vec{r}' \right) dt' \\
 &= \delta(\vec{r}) \int_t^\infty \psi(t') dt'
 \end{aligned}$$

As in previous lectures

$$\begin{aligned}
 \tilde{\Psi}(\vec{r}, s) &= \delta(\vec{r}) \int_{t=0}^\infty \int_{t'=t}^\infty e^{-st} \psi(t') dt' dt \\
 &= \delta(\vec{r}) \int_{t'=0}^\infty \psi(t') \int_{t=0}^{t'} e^{-st} dt dt' \\
 &= \delta(\vec{r}) \int_{t'=0}^\infty \psi(t') \frac{1}{s} [1 - e^{-st'}] dt' \\
 &= \delta(\vec{r}) \frac{1 - \tilde{\psi}(s)}{s}
 \end{aligned}$$

and taking the Fourier transform of the delta function

$$\widehat{\tilde{\Psi}}(\vec{r}, s) = \frac{1 - \tilde{\psi}(s)}{s}$$

Thus

$$\tilde{P}(\vec{k}, s) = \frac{1 - \tilde{\psi}(s)}{s \left(1 - \widehat{\tilde{\chi}}(\vec{k}, s) \right)} \quad (2)$$

This general expression for the Fourier-Laplace transform of the density of the non-separable CTRW was first derived by Scher-Lax (1972). The non-separability manifests itself in the term $\widehat{\tilde{\chi}}(\vec{k}, s)$ which for a separable walk factors into $\widehat{p}(k) \tilde{\psi}(s)$

2.1 Example: Polymer Surface Adsorption (continued)

Continuing the example from Lecture 25, we can now rigorously determine the scaling of the adsorption sites, and almost completely solve the problem for the density of the random walker, up to the inversion of a Fourier transform.

Recal that time t corresponds to the number of steps taken and the diffusion coefficient $D = \frac{a^2}{6\tau_0}$ where a is the persistence length and τ_0 is the time scale which we can take as $\tau_0 = 1$. The factor $\frac{1}{6}$ arises because in d dimensions, the diffusion coefficient is related to the variance of the individual steps through $\frac{\sigma}{2d}$.

In the previous lecture we argued that the waiting time distribution is the Smirnov density

$$\psi(t) = \frac{a}{\sqrt{4\pi D_{\perp} t^3}} e^{-\frac{a^2}{4D_{\perp} t}}$$

where D_{\perp} is the diffusion coefficient of the perpendicular component of the random walk. $D_{\perp} = 3D = \frac{a^2}{2\tau_0}$ since one third of the variance is attributed to that dimension. Taking $\tau_0 = 1$, so that $\frac{a^2}{D_{\perp}} = 2$ we can simplify:

$$\psi(t) = \frac{1}{\sqrt{2\pi t^3}} e^{-\frac{1}{2t}}$$

The Laplace transform of the waiting time density is

$$\tilde{\psi}(s) = e^{-\sqrt{sa^2/D_{\perp}}} = e^{-\sqrt{2s}}$$

To proceed we need the conditional pdf of the the location of return to $z = 0$, given that the return time is at t .

$$p(\vec{r}_s | t) = \frac{1}{4\pi D_{\parallel} t} e^{-r_s^2/4D_{\parallel} t}$$

This is just 2 dimensional diffusion, once we condition on the return time and so density is given immediately as the fundamental solution to the diffusion equation. The diffusion coefficient D_{\parallel} denotes diffusion in a direction parallel to the $z = 0$ plane, and arguing as above $D_{\parallel} = \frac{a^2}{4\tau_0}$. The Fourier transform of p is

$$\hat{p}(\vec{k}_s, t) = e^{-D_{\parallel} k_s^2 t}$$

Then, since we can take the Fourier transform in the space coordinate, we can find the Fourier transform of the joint position-time step density:

$$\begin{aligned} \chi(\vec{r}_s, t) &= p(\vec{r}_s | t) \psi(t) \\ \hat{\chi}(\vec{k}_s, t) &= e^{-D_{\parallel} k_s^2 t} \psi(t) \end{aligned}$$

Note the non-separability since t appears in both terms. Taking the Laplace transform:

$$\tilde{\chi}(\vec{k}_s, t) = \int e^{-st} e^{-D_{\parallel} k_s^2 t} \frac{1}{\sqrt{2\pi t^3}} e^{-\frac{1}{2t}} dt$$

But we can evaluate this immediately since it is just the Laplace transform of the Smirnov evaluated at $s + D_{\parallel} k_s^2$ instead of s :

$$\tilde{\chi}(\vec{k}_s, t) = e^{-\sqrt{2(s + D_{\parallel} k_s^2)}}$$

Thus applying the generalized Montrol-Weiss equation (2)

$$\tilde{\tilde{P}}(\vec{k}, s) = \frac{1 - e^{-\sqrt{2}s}}{s \left(1 - e^{-\sqrt{2(s + D_{\parallel} k_s^2)}} \right)}$$

We can study the long-time behavior in the "central region" by considering the limits $k_s \rightarrow 0$ and $s \rightarrow 0$. Expanding the exponentials around $s = 0$

$$\tilde{\tilde{P}}(\vec{k}, s) \sim \frac{1}{\sqrt{s^2 + D_{\parallel} k_s^2 s}}$$

Noting that the transform can be written:

$$\tilde{\tilde{P}}(\vec{k}, s) \sim \frac{1}{\sqrt{\left(s + \frac{1}{2} D_{\parallel} k_s^2\right)^2 - \left(\frac{D_{\parallel} k_s^2}{2}\right)^2}}$$

and noting that $[Le^{-\alpha t} f(t)](s) = \tilde{f}(s + \alpha)$

$$\hat{P}(\vec{k}, s) \sim e^{-\frac{1}{2} D_{\parallel} k_s^2 t} L^{-1} \frac{1}{\sqrt{s^2 - \left(\frac{D_{\parallel} k_s^2}{2}\right)^2}}$$

But this Laplace transform can be inverted in terms of the modified Bessel function of the first kind $I_0(x)$ - see Appendix for derivation.

$$\hat{P}(\vec{k}, t) \sim e^{-\frac{1}{2} D_{\parallel} k_s^2 t} I_0\left(\frac{D_{\parallel} k_s^2 t}{2}\right)$$

Inverting the Fourier transform in space we derive an integral expression for the density:

$$P(\vec{r}_s, t) \sim \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{i\vec{k}_s \cdot \vec{r}_s} e^{-\frac{1}{2} D_{\parallel} \|\vec{k}_s\|^2 t} I_0\left(\frac{D_{\parallel} \|\vec{k}_s\|^2 t}{2}\right) \frac{d\vec{k}_s}{(2\pi)^2}$$

This is clearly not a Gaussian distribution, but the scaling is still square root, i.e. $\frac{\langle r_s \rangle}{\sqrt{t}} \rightarrow$ non-degenerate limiting pdf. This can be seen if we change the variable to $\vec{\zeta} = \frac{\vec{r}_s}{\sqrt{t}}$ we can write $P(\vec{\zeta}, t) = tP(\vec{r}_s, t)$ and defining $\vec{\kappa}_s = \vec{k}_s \sqrt{t}$ so that $d\vec{\kappa}_s = t d\vec{k}_s$

$$P(\vec{\zeta}, t) \sim \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{i\vec{\kappa}_s \cdot \vec{\zeta}} e^{-\frac{1}{2} D_{||} \|\kappa_s\|^2} I_0 \left(\frac{D_{||} \|\vec{\kappa}_s\|^2}{2} \right) \frac{d\vec{\kappa}_s}{(2\pi)^2}$$

and it is clear that $\vec{\zeta}$ has a non-degenerate limiting distribution which is nevertheless not Gaussian.

3 Creepers

The second special case that we consider is that of *creepers*, which move with constant velocity between turning points. We can define the creeper in terms of the q distribution:

$$q(\vec{r}, t | \vec{r}', t') = \delta \left(\vec{r} - \vec{r}' \frac{t}{t'} \right) \text{ for } 0 < t < t'$$

Thus a creeper moves non-stochastically between turning points.

$$\Psi(\vec{r}, t) = \int_t^{\infty} \chi \left(\vec{r} \frac{t'}{t}, t' \right) dt'$$

and

$$\begin{aligned} \chi(\vec{r}, t) &= p(\vec{r}) \psi(t | \vec{r}) \\ &= p(\vec{r}) \delta(t - \tau(\vec{r})) \end{aligned}$$

where

$$v(\vec{r}) = \frac{\vec{r}}{\tau(\vec{r})}$$

is the constant velocity for step size \vec{r} that will occur after time $\tau(\vec{r})$. $\tau(\vec{r}) = v/c$ for a single constant speed c

If $p(\vec{r})$ has a Lévy distribution this is called a Lévy walk, although Hughes discourages the terminology.

$$\Psi(\vec{r}, t) = p \left(\frac{\tau(\vec{r})}{t} \vec{r} \right)$$

Hughes advocates the use of Mellin transforms to analyze this type of random walk, through which it is possible to show:

$$\text{If } p(\vec{r}) \sim \frac{A}{|\vec{r}|^{d+\alpha}}$$

where $\alpha > 0$ and $\alpha < 2$ is a Lévy distribution and $\alpha > 2$ has finite variance

$$\text{and } \tau(\vec{r}) \propto |\vec{r}|^{1-\beta} \text{ so that velocity } v(\vec{r}) \propto |\vec{r}|^\beta$$

where $\beta = 0$ corresponds to a single constant velocity c and $\beta = 1$ is a discrete RW with a constant time step.

Then the mean-square displacement is

$$\langle \vec{r}^2 \rangle \propto t^{2\nu} \text{ as } t \rightarrow \infty$$

where

$$2\nu = \begin{cases} 1 & \alpha > \max(2, 1 - \beta) \\ \frac{\alpha}{1-\beta} & 2 < \alpha < 1 - \beta \\ 1 + \frac{2-\alpha}{1-\beta} & 1 - \beta < \alpha < 2 \\ \frac{2}{1-\beta} & \alpha < \min(2, 1 - \beta) \end{cases}$$

3.1 Application: Schlesinger, West, Klafter

Creepers provide a microscopic model of turbulence.

Richardson (1926) observed that in turbulent flow the mean-square position of a particle obeys the following law: $\langle r^2 \rangle \propto t^3$. This is a superdiffusion that is even faster than ballistic motion for a single typical velocity, in which $\langle r^2 \rangle \propto t^2$. Turbulent flow does not have a single characteristic velocity, but the question remains, what kind of random walk could a microscopic particle be performing that would be consistent with this empirical observation?

According to Richardson’s observation, the random walk must satisfy $\tau(r) \sim r^{2/3}$, which suggests $\beta = \frac{1}{3}$ in the creeper model, and from the result above, if $\alpha < \frac{2}{3}$ we derive $\langle \vec{r}^2 \rangle \propto t^{2\nu}$ as $t \rightarrow \infty$ where $2\nu = \frac{2}{1-\beta} = 3$ as required. The step distribution with $\alpha < \frac{2}{3}$ is a Lévy flight with tails which are even broader than the Cauchy distribution.

This model also correctly predicts the Kolmogorov energy spectrum, which is essentially the Fourier transform of the velocity spectrum:

At frequency k

$$E(k) \propto \frac{v^2}{2} = \frac{\left(r^{\frac{1}{3}}\right)^2}{1/r} = r^{5/3} = k^{-5/3}$$

4 References

Shlesinger, West, Klafter. Physics Review Letters, 1987

5 Appendix: Laplace Transform of the Modified Bessel Function of the First Kind $I_0(x)$

The modified Bessel function $I_0(x)$ can be defined as:

$$I_0(x) = \sum_{n=0}^{\infty} \frac{(x/2)^{2n}}{(n!)^2}$$

An alternative integral definition is:

$$I_0(x) = \frac{1}{\pi} \int_0^{\pi} e^{x \cos \theta} d\theta$$

Consider the transform of $I_0(\alpha t)$ and change the variable to $y = st$ in the integral

$$\begin{aligned} [LI_0(\alpha t)](s) &= \sum_{n=0}^{\infty} \frac{(\alpha/2)^{2n}}{(n!)^2} \int_0^{\infty} e^{-st} t^{2n} dt \\ &= \frac{1}{s} \sum_{n=0}^{\infty} \frac{(\alpha/2)^{2n} s^{-2n}}{(n!)^2} \int_0^{\infty} e^{-y} y^{2n} dy \\ &= \frac{1}{s} \sum_{n=0}^{\infty} \frac{(\alpha/2)^{2n} s^{-2n}}{(n!)^2} (2n)! \\ &= \frac{1}{s} \sum_{n=0}^{\infty} \frac{(\alpha/s)^{2n}}{n!} \frac{(2n-1)!!}{2^n} \\ &= \frac{1}{s} \left(1 - \left(\frac{\alpha}{s} \right)^2 \right)^{-\frac{1}{2}} \\ &= \frac{1}{\sqrt{s^2 - \alpha^2}} \end{aligned}$$