Lecture 11: More on Persistence and Self Avoiding Walk

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In the last lecture, the discussed topics were Markov Chain for Persistent Random Walk on integers, which was examined in the continuum limit with diffusive scaling. The lecture also covered the derivation of Telegraph Equation with ballistic scaling. This lecture, therefore, starts with a different way of deriving the Telegraph Equation by using Fick's Law. It, then, proceeds to solve the Telegraph Equation using the Fourier and Laplace transforms. A One-Dimensional Persistent Random Walk is also solved asymptotically using Green's Function, confirming the validity of the Central Limit Theorem once again. Eventually, the lecture introduces the concepts of Self-Avoiding Walk, which will be further examined in the next lecture.

1) Derivation of One-dimensional Persistent Random Walk by Generalizing Fick's Law

Recall that, in the last lecture, we derived the Telegraph Equation

$$\frac{\partial^2 \rho}{\partial t^2} + \frac{1}{\tau_c}\frac{\partial \rho}{\partial t} = v^2 \frac{\partial^2 \rho}{\partial x^2} \tag{1.1}$$

The derivation was from a one-dimensional persistent random walk with a "ballistic scaling" $(\rho \to 1)$

$$v = \frac{\sigma}{\tau}, \qquad \tau_c = \tau\left(\frac{-2}{\log \rho}\right) \qquad \text{(Reference: S. Goldstein)}$$

In this lecture, however, we will derive the Telegraph Equation by generalizing Fick's Law as a "continuum" constitutive equation. First, define a flux density $\vec{J}$ and the density ρ. We start the derivation by stating the Conservation Law and the Constitutive Equation or Fick's Law:

Conserivation Law $$\frac{\partial \rho}{\partial t} = -\vec{\nabla} \cdot \vec{J} \qquad (1.2)$$

Fick's Law $$\vec{J} = -D\vec{\nabla}\rho \qquad (1.3)$$

More generally, one can postulate a "relaxation time" τ_c for the flux density

$$\tau_c \frac{\partial \vec{J}}{\partial t} + \vec{J} = -D\vec{\nabla}\rho \qquad (1.4)$$

By taking the gradient of equation (4), we can easily show that

$$\tau_\tau \frac{\partial \vec{\nabla} \cdot \vec{J}}{\partial t} + \vec{\nabla} \cdot \vec{J} = -D\vec{\nabla}\rho \qquad (1.5)$$

Substituting $\frac{\partial \rho}{\partial t} = -\vec{\nabla} \cdot \vec{J}$ from equation (2) into equation (5) will show that

$$-\tau_c \frac{\partial^2 \rho}{\partial t^2} - \frac{\partial \rho}{\partial t} = -v^2 \vec{\nabla}^2 \rho \qquad (1.6)$$

which, if multiplied by τ_c on both sides, will be the telegraph equation that we derived in the last lecture and in section 1.

2) Exact Solution to a One-Dimensional Telegraph Equation in Free Space

After deriving the telegraph Equation in two different ways, we are going to solve it using the Fourier Transform and Laplace transform. From Equation (1.1), the Telegraph Equation is expressed as

$$\frac{\partial^2 \rho}{\partial t^2} + \frac{1}{\tau_c}\frac{\partial \rho}{\partial t} = v^2 \frac{\partial^2 \rho}{\partial x^2}$$

We are going to solve this second-order PDE using the Green's function with the initial conditions

$$\frac{\partial \rho}{\partial t}(x,0) = 0 \tag{2.1}$$

and

$$\rho(x,0) = \delta(x) \tag{2.2}$$

First, we Fourier-transform $\rho(x,t)$ in space and Laplace-transform it in time. As a result, we can show that

$$\hat{\tilde{\rho}} = \frac{s + \tau_c^{-1}}{s(s + \tau_c^{-1} + v^2 k^2)} \tag{2.3}$$

and by invert fourier transforming and invert laplace transforming back, we get

$$\rho(x,t) = \frac{e^{-t/2\tau_c}}{2}\left[\delta(x - vt) + \delta(x + vt) + \frac{1}{4v\tau_c}\left[I_0(z) + \frac{I_1(z)}{2\tau_c z}\right]H(vt - |x|)\right] \tag{2.4}$$

where $z = \frac{\sqrt{v^2 t^2 - x^2}}{2v\tau_c}$ and $I_n(z)$ are the modified Bessel functions.

In addition, from $\hat{\tilde{\rho}}(k,s)$, we can obtain moments $\langle x^n(t)\rangle$ by inverting the derivative $\frac{\partial^n \hat{\tilde{\rho}}}{\partial k^n}$. For instance, by inverting $\frac{\partial^2 \hat{\tilde{\rho}}}{\partial k^2}(k = 0, s)$, we can show that

$$\langle x^2(t)\rangle = 2v^2\tau_c^2\left[\frac{t}{\tau_c} + (e^{-\frac{t}{\tau_c}} - 1)\right] \tag{2.5}$$

with $\frac{N}{n_c} = \frac{t}{\tau_c}$ as $n_c \gg 1$

3) Exact Solution to a Persistent Random Walk in One-Dimension

Recall from the previous lecture that we have considered a one-dimensional persistent random walk with a probability α of stepping to the right, and a probability $\beta = 1 - \alpha$ of stepping to the left. In the last lecture, we have defined

$$A_{n+1}(m) = P(X_{n+1} = m \mid X_n = m-1)P(X_n = m-1) \tag{3.1}$$

$$B_{n+1}(m) = P(X_{n+1} = m \mid X_n = m+1)P(X_n = m+1) \tag{3.2}$$

and we have also shown that

$$A_{n+1}(m) = \alpha A_n(m-1) + \beta B_n(m-1) \tag{3.3}$$

$$B_{n+1}(m) = \beta A_n(m+1) + \alpha B_n(m+1) \tag{3.4}$$

Please note that each step of a one-dimensional persistent random walk is only depended upon its previous step without any dependence on any other earlier steps. Therefore, we can conclude that the one-dimensional persistent random walk is a "Markov Chain". For simplicity, we also assume that the "walker" does not have a velocity at the starting point

Initial conditions

$$A_0(m) = \frac{1}{2}\delta_{m,0} \tag{3.5}$$

$$B_0(m) = \frac{1}{2}\delta_{m,0} \tag{3.6}$$

We will start solving Equation (3.3) and (3.4) with the initial conditions (3.5) and (3.6) by first using the discrete Fourier transform (See the appendix.)

$$\hat{A}_n(k) = \sum_{m=-\infty}^{\infty} \exp(imk) A_n(m) \tag{3.7}$$

which has an invert function defined as following

$$A_n(m) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \exp(-imk)\, \hat{A}_n(k)dk\,. \tag{3.8}$$

After the Fourier transforms, we can write Equation (3.3) and (3.4) in the matrix form as following

$$\begin{bmatrix} \hat{A}_{n+1}(k) \\ \hat{B}_{n+1}(k) \end{bmatrix} = \begin{bmatrix} \alpha\exp(ik) & \beta\exp(ik) \\ \beta\exp(-ik) & \alpha\exp(-ik) \end{bmatrix} \begin{bmatrix} \hat{A}_n(k) \\ \hat{B}_n(k) \end{bmatrix} \tag{3.9}$$

Now, with the assumption that each step is identical and independent, we can write Equation (3.9) in terms of the initial conditions

$$\begin{bmatrix} \hat{A}_n(k) \\ \hat{B}(k) \end{bmatrix} = \begin{bmatrix} \alpha \exp(ik) & \beta \exp(ik) \\ \beta \exp(-ik) & \alpha \exp(-ik) \end{bmatrix}^n \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix}. \qquad (3.10)$$

For simplicity, we will re-write equation (3.10) as following

$$\begin{bmatrix} \hat{A}_n(k) \\ \hat{B}(k) \end{bmatrix} = M^n \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} \qquad (3.11)$$

In order to further-simplify the problem, we notice that equation (3.11) is a system of eigenvalue equations and a matrix ***M*** can be written as

$$\mathbf{MS} = \mathbf{\Lambda S} \qquad (3.12)$$

where $\mathbf{S}$ is a matrix whose columns are the eigenvectors corresponding to the eigenvalues in the diagonal matrix $\mathbf{\Lambda}$. Multiply both sides by the inverse of $\mathbf{S}$, we get

$$\mathbf{M} = \mathbf{S\Lambda S}^{-1} \qquad (3.13)$$

and

$$\mathbf{M}^n = (\mathbf{S\Lambda S}^{-1})^n = \mathbf{S\Lambda}^n\mathbf{S}^{-1} \qquad (3.14)$$

The next calculation is to find the eigenvalues (λ), which requires that they satisfy the following equation

$$\det(\lambda \mathbf{I} - \mathbf{M}) = 0 \qquad (3.15)$$

with matrix **I** as an identity matrix. The solutions (or the eigenvalues) of equation (3.15) are expressed in the quadratic equation

$$\lambda^2 - 2\lambda\alpha\cos(k) + (\alpha^2 - \beta^2) = 0. \qquad (3.16)$$

The solutions of this quadratic equation are

$$\lambda_\pm = \alpha\cos(k) \pm \sqrt{\alpha^2\cos^2(k) - (\alpha^2 - \beta^2)} = \alpha\cos(k) \pm \sqrt{\beta - \alpha^2\sin^2(k)} \qquad (3.17)$$

with the help from the geometric identity $\sin^2(k) + \cos^2(k) = 1$. When k is asymptotically small, we can Taylor expand

$$\cos(k) \sim 1 - \frac{k^2}{2} \qquad (3.18)$$

and

$$\sin(k) \sim \mathrm{k}.$$

We can write the approximated eigenvalues as

$$\lambda_{\pm} \approx \alpha\left(1-\frac{k^2}{2}\right) \pm \beta\left[1-\left(\frac{\alpha k}{\beta}\right)^2\right]^{1/2} \qquad (3.19)$$

and we can further made use of the asymptotically small k by stating the asymptotic expansion

$$\sqrt{1-\varepsilon^2} \sim 1-\frac{\varepsilon^2}{2} \qquad (3.20)$$

and re-write the eigenvalues once again as

$$\lambda_{\pm} \sim (\alpha \pm \beta) - \frac{\alpha k^2}{2\beta}(\beta \pm \alpha). \qquad (3.21)$$

We have defined from the beginning that $(\alpha + \beta) = 1$

$$\therefore \lambda_{+} = 1 - \frac{\alpha k^2}{2\beta} \qquad (3.22)$$

and

$$\lambda_{+}^{n} = (1-\frac{\alpha k^2}{2\beta})^n = \exp(-\frac{\alpha \omega^2}{2\beta}).$$

(3.23)

Here, we define $\omega = k\sqrt{n}$ and make use of the asymptotic expansion $\left(1+\frac{\varepsilon}{n}\right)^n \sim \exp(\varepsilon)$.

Next, we proceed to find the other eigenvalue, using the similar techniques.

$$\lambda_{-} \sim (\alpha - \beta) - \frac{\alpha k^2}{2\beta}(\beta - \alpha) \qquad (3.24)$$

$$\lambda_{-}^{n} \sim (\alpha - \beta)^n \exp(\frac{\alpha \omega^2}{2\beta}) \qquad (3.25)$$

Notice that $(\alpha - \beta)$<0 and, in the limit of n approaching infinity, $\lambda_{-}^{n} \to 0$. Substituting the two eigenvalues back into equation (3.12), we obtain

$$\mathbf{MS} = \begin{bmatrix} \exp(-\frac{\alpha\omega^2}{2\beta}) & 0 \\ 0 & 0 \end{bmatrix} \mathbf{S} \tag{3.26}$$

We then compute the non-trivial eigenvector (columns of S), using the expression $(\lambda \mathbf{I} - \mathbf{M})\mathbf{S} = \mathbf{0}$, and get

$$\mathbf{S} = \begin{bmatrix} 1 & -\beta \\ \alpha & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{S}^{-1} = \begin{bmatrix} \alpha & \beta \\ -1 & 1 \end{bmatrix} \tag{3.27}$$

Substituting the eigenvalues and newly-obtained eigenvectors into Equation (3.14), we can show that asymptotically

$$\mathbf{M}^n \sim \begin{bmatrix} 1 & -\beta \\ 1 & \alpha \end{bmatrix} \begin{bmatrix} \exp(\frac{-\alpha\omega^2}{2\beta}) & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \alpha & \beta \\ -1 & 1 \end{bmatrix} \sim \exp(\frac{-\alpha\omega^2}{2\beta}) \begin{bmatrix} \alpha & \beta \\ \alpha & \beta \end{bmatrix}. \tag{3.28}$$

Substituting the asymptotic expression for $\mathbf{M}^n$, Equation (3.11) becomes

$$\begin{bmatrix} \hat{\mathbf{A}}_n(k) \\ \hat{\mathbf{B}}_n(k) \end{bmatrix} = \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} \exp(\frac{-\alpha\omega^2}{2\beta}). \tag{3.29}$$

We then proceed into finding the Fourier transform of the probability density function (PDF) which is the sum of the probability of going to the left and to the right

$$\hat{\mathbf{P}}_n(k) = \hat{\mathbf{A}}_n(k) + \hat{\mathbf{B}}_n(k). \tag{3.30}$$

The asymptotic value for the characteristic function (or the Fourier transform of PDF) is

$$\hat{\mathbf{P}}_n(k) \sim \exp(\frac{-\alpha\omega^2}{2\beta}) \tag{3.31}$$

Inverting the Fourier Transform, we eventually arrive at the answer of

$$\mathbf{P}_n(m) \sim (2\pi \frac{\alpha n}{\beta})^{-1/2} \exp(-\frac{m^2 \beta}{2\alpha n}) \ . \tag{3.32}$$

Please note that this is a value of the PDF in the limit of $n \to \infty$, which is in a Gaussian form, confirming that the Central Limit Theorem still holds. As a last notice of this section, one can also observe that the variance of this Gaussian is $\frac{n\alpha}{\beta}$. Then, we can conclude that

$$\frac{D}{D_0} = \frac{\alpha}{\beta} \tag{3.33}$$

with $D_0 = \sigma^2 / 2T$

4) Introduction to Self-Avoiding Walk

We would like to finish this lecture by introducing the idea of Self-Avoiding Walk, which will be discussed further in the next lecture. Roughly defined, Self-Avoding Walk (SAW) of length N is a set of random walks of length N that do not "self-intersect". For instance, if a random walker is on a lattice, it does not visit the same site twice. For a continuum random variable, it cannot get too close to the path it has travel through.

<u>Some Interesting Facts about SAW</u> (Reference: Hughes, volume 1)

1) Define d = surface/volume = constant. The variance of the displacement the random walker travels from the starting point will be

$$\left\langle R_n^{\ 2} \right\rangle \sim K(d) N^{2v} \tag{4.1}$$

where v =1 when d = 1
=3/4 when d = 2
=0.593 when d = 3
½ when $d \geq 4$

or $v = \dfrac{3}{d+2}$ "Fisher-Flory"

2) Let C_n = numbers of SAW of length N

$$C_n \sim AN^g \mu^N \tag{4.2}$$

Please note that $\log C_n \sim N$ where N is the length of the walk which is a constant. If $C_n = z^n$ where z = coordinate. For instance, z = 2d for a cubic. We can find the connectivity constant $\mu < z$ as following

$\mu =$ 4.1515 when d =2
2.683 when d=3
4.683 when d=4

3) "Mass Distribution"

$$P(\vec{r}, N) \cong \frac{C_1}{N^{d\nu}} \left(\frac{r}{N^\nu} \right)^t \exp[-c_2 \left(\frac{r}{N^\nu} \right)^\delta] \tag{4.3}$$

where $\delta = \dfrac{1}{1-\nu} \geq 2$

The discussion on Self-avoiding Walk will be resumed in the next lecture.

Appendix : Discrete Fourier Transform

The discrete fourier transform we have applied in equation (3.7) and (3.8) can also be viewed as the coefficients of a Laurent series in the complex plane.

$$\widetilde{A}_n(z) = \sum_{m=-\infty}^{\infty} A_n(m) z^m$$

and its inverse

$$A_n(m) = \frac{1}{2\pi i} \oint \frac{\widetilde{A}_n(z)dz}{z^{m+1}}$$

If we set z= exp(ik) with k being a real number, or on the other hand, take the contour integral to be that of the unit circle, we will get the discrete Fourier transform as in Section 3.