Lecture 12 : Non-identical Steps and Anomalous Diffusion

Jaehyuk Choi

Department of Mathematics, MIT

March 20, 2001

Today, we will see the anomalous diffusion cases. Consider random walks with non-identical steps which are rescaled from a common distribution $\triangle\widetilde{X_m}$.

$$X_n = \sum_{m=1}^{n} \triangle X_m = \sum_{m=1}^{n} a_m \, \triangle\widetilde{X_m}$$

Here we assume that $\triangle\widetilde{X_m}$'s are iid, the mean is zero, and the cumulants are all finite. If we let

$$c_l = l\text{th cumulant of the common step, } \triangle\widetilde{X_m}$$
$$C_{n,l} = l\text{th cumulant of position after } n \text{ steps, } X_n,$$

we know

$$C_{n,l} = c_l \sum_{m=1}^{n} a_m^l .$$

Then the cumulants of the rescaled variables are expressed as

$$\frac{C_{n,l}}{C_{n,2}^{l/2}} = \frac{c_{n,l}}{c_{n,2}^{l/2}} \, \frac{\sum_{m=1}^{n} a_m^l}{(\sum_{m=1}^{n} a_m^2)^{l/2}} = \lambda_l \, A_{n,l} \ ,$$

where $\lambda_l = c_l / c_2^{l/2}$ is the normalized cumulant.

¿From the previous lectures, we could get the CLT when $A_{n,l} \to 0$ for $l \geq 3$. In addition to this condition, if $C_{n,2} \sim n$ the diffusion was called "normal diffusion," opposed to "anomalous."

1 Example : Power-law decaying/growing steps

Suppose [1]

$$a_m = m^\alpha .$$

[1]For $\alpha < 0$, this kind of random walk has been used to model the broadening of spectral lines in single-molecule spectroscopy due to the presence of randomly situated material defects which interact with the molecule under observation via long-range power-law interactions. The power-law decaying random walk then occurs in energy, as contributions from all the defects are accumulated. For dipole interactions $\alpha = -3$. See Barkai and Silbey, Chem. Phys. Lett. **310**, 287 (1999).

Assuming $c_l = 1$ for simplicity, we get the variance :

$$C_{n,2} = \sum_{m=1}^{n} a_m^2 = \sum_{m=1}^{n} m^{2\alpha} \sim \begin{cases} n^{2\alpha+1} & \text{when } \alpha > -1/2, \\ \log n & \text{when } \alpha = -1/2, \\ \zeta(-2\alpha) & \text{when } \alpha < -1/2 \end{cases}$$

or

$$\sqrt{C_{n,2}} = \langle X_n^2 \rangle^{1/2} \sim \begin{cases} n^{\alpha+1/2} & \text{when } \alpha > -1/2, \\ \sqrt{\log n} & \text{when } \alpha = -1/2, \\ \sqrt{\zeta(-2\alpha)} & \text{when } \alpha < -1/2. \end{cases}$$

Since the variance shows qualitative differences around $-1/2$, we have a "phase transition" at $\alpha_c = -1/2$. And this is an example of "anomalous diffusion", for the variance is not scaled as n in either case.

Aside, $\zeta(z)$ is 'Reimann Zeta Function' defined as

$$\zeta(z) = \sum_{n=1}^{\infty} \frac{1}{n^z}.$$

Zeta function has a great importance in number theory in the following sense : If $p_1, p_2, \cdots$ are prime numbers in increasing order, from the fact that every integer n is factorized into the products of powers of prime numbers in a unique way,

$$\begin{aligned} \zeta(z) &= \sum_{n=1}^{\infty} \frac{1}{n^z} = \prod_{i=1}^{\infty} (1 + \frac{1}{p_i^z} + \frac{1}{p_i^{2z}} + \cdots) \\ &= \prod_{i=1}^{\infty} \frac{1}{1 - 1/p_i^z} \quad \text{for Re } z > 1. \end{aligned}$$

This formula is called Euler's product. One exercise involving this function is to show that all zeros of $\zeta(z)$ lie on the line Re$z = 1/2$, which is left to the reader. (You can get the Fields Medal if you prove this. :)

Back to the diffusion problem, higher cumulants are expressed as

$$C_{n,l} = \sum_{m=1}^{n} a_m^l = \sum_{m=1}^{n} m^{l\alpha} \sim \begin{cases} n^{l\alpha+1} & \text{when } \alpha > -1/l, \\ \log n & \text{when } \alpha = -1/l, \\ \zeta(-l\alpha) & \text{when } \alpha < -1/l \end{cases}$$

1.1 Case $-1/3 < \alpha$

$$\begin{aligned}
\frac{C_{n,3}}{C_{n,2}^{l/2}} &\sim \frac{n^{3\alpha+1}}{(n^{2\alpha+1})^{3/2}} \sim \frac{1}{\sqrt{n}} \to 0 \\
\frac{C_{n,l}}{C_{n,2}^{l/2}} &\sim \frac{1}{(n^{2\alpha+1})^{3/2}}\{n^{l\alpha+1} \text{ or } \log n \text{ or } \zeta(-l\alpha) \text{ according to } \alpha\} \\
&\to 0 \text{ in either cases for } l > 3
\end{aligned}$$

Thus CLT holds in this case with the scaled variable $y = x/\sqrt{C_{n,2}} = x/n^{\alpha+1/2}$.

Furthermore if $-1/k < \alpha$, we have

$$\frac{C_{n,l}}{C_{n,2}^{l/2}} \sim \frac{1}{n^{l/2-1}} \quad \text{for } 3 < l < k$$

and we can calculate the PDF $\phi(y)$ as

$$\begin{aligned}
\log \widetilde{\phi_n}(\omega) &\sim -\frac{\omega^2}{2} + \frac{i\omega^3}{3!}\frac{\lambda_3}{\sqrt{n}} + \frac{\omega^4}{4!}\frac{\lambda_4}{n} + \cdots + \frac{\omega^k}{k!}\frac{\lambda_4}{n^{k/2}} + o(\frac{1}{n^{k/2}}) \\
\phi_n(y) &\sim \frac{e^{-y^2/2}}{\sqrt{2\pi}}\big(1 + \lambda_3\frac{f_1(y)}{\sqrt{n}} + \lambda_4\frac{f_2(y)}{n} + \cdots + \lambda_k\frac{f_k(y)}{n^{k/2}} + o(\frac{1}{n^{k/2}})\big).
\end{aligned}$$

This is the same Gram-Charlier expansion as we get from the normal diffusion cases.

1.2 Case $\alpha = -1/3$

$$\frac{C_{n,3}}{C_{n,2}^{3/2}} \sim \frac{\log n}{n^{3\alpha+3/2}} \sim \frac{\log n}{\sqrt{n}} \to 0$$

1.3 Case $-1/2 < \alpha < -1/3$

$$\begin{aligned}
\frac{C_{n,3}}{C_{n,2}^{3/2}} &\sim \frac{\zeta(-3\alpha)}{n^{3\alpha+3/2}} \to 0 \\
\frac{C_{n,l}}{C_{n,2}^{l/2}} &\sim \frac{\zeta(-l\alpha)}{n^{l\alpha+l/2}} \to 0 \quad \text{for } l > 3, \\
\phi_n(y) &\sim \frac{e^{-y^2/2}}{\sqrt{2\pi}}\big(1 + \lambda_3\frac{f_1(y)}{n^{3\alpha+3/2}} + \cdots\big)
\end{aligned}$$

1.4 Case $\alpha = -1/2$

$$\frac{C_{n,l}}{C_{n,2}^{l/2}} \sim \frac{\zeta(-l\alpha)}{(\log n)^{l/2}} \to 0 \quad \text{for } l \geq 3$$

Thus CLT holds for $\alpha \geq -1/2$.

1.5 Case $-1 < \alpha < -1/2$

$$\langle X_n^2\rangle^{1/2} \sim \sqrt{\zeta(-2\alpha)} = \text{constant}$$

We have total bounded variance though the tail is unbounded !!

2 Example : Exponentially decaying/growing steps

Consider[2]

$$a_m = a^m, \quad a = \text{ constant } > 0$$

$$C_{n,l} = c_l \sum_{m=1}^{n} a^{ml} = \sum_{m=1}^{n} \frac{a^l(a - a^{nl})}{a - a^l} \sim \begin{cases} c_l \dfrac{a^l}{1-a^l} & \text{when } a < 1, \\ c_l \dfrac{a^{l(n+1)}}{a^l - 1} & \text{when } 1 < a. \end{cases}$$

2.1 Gaussian steps (with s.d. σ)

¿From the fact that the convolution of Gaussian random variables is also a Gausian, we know the exact solution of PDF of nth step :

$$\log \widehat{p}_n(k) = -\frac{k^2}{2} C_{n,2} = -\frac{k^2\sigma^2(1-a^{2n})a^2}{2(1-\sigma^2)}$$

$$\phi_n(y) = \frac{1}{2\pi} e^{-y^2/2} \quad \text{with } y = \frac{x}{\sigma\sqrt{\frac{a^2(a-a^{2n})}{1-a^2}}}$$

and the r.m.s. is given by

$$< X_n^2 >^{1/2} = \sigma\sqrt{\frac{a^2(a-a^{2n})}{1-a^2}} \sim \begin{cases} \dfrac{\sigma a}{\sqrt{1-a^2}} & \text{when } a < 1, \\ \dfrac{\sigma a^{n+1}}{\sqrt{1-a^2}} & \text{when } 1 < a \end{cases} .$$

In $a < 1$ case the position is bounded as $n \to \infty$, while $1 < a$ cases shows anomalous diffusion with exponentially growing width as $n \to \infty$.

2.2 Decaying simple walk

$$X_n = \sum_{m=1}^{n} a^m \, \varepsilon_m,$$

[2] With Bernoulli random variables and $a < 1$, this problem was first considered by Kershner and Wintner in 1935, and by Erdos in 1939-40. This general kind of decaying walk when $a < 1$ might have applications to mixing in granular media, due to the inelastic anture of collisions.

where ε_m is iid random variable taking 1 or -1 with the same probability $1/2$.

By Fourier transform we know

$$p_m(x) = \frac{1}{2}\,\delta(x + a^m) + \frac{1}{2}\,\delta(x - a^m)$$
$$\widehat{p}_m(k) = \cos(ka^m)$$

and the convolution becomes multiplication in Fourier transformed function :

$$\begin{aligned}\widehat{P}_n(k) &= \prod_{m=1}^{n} \widehat{p}_m(k) \\ &= \cos(ka)\ \cos(ka^2)\ \cdots\ \cos(ka^n)\end{aligned}$$

Specially when $a = 1/2$, we can find the exact solution.

$$\begin{aligned}\widehat{P}_n(k) &= \cos(k/2)\ \cos(k/4)\ \cdots\ \cos(k/2^n) \\ &= \frac{\sin(k)}{2\sin(k/2)}\ \frac{\sin(k/2)}{2\sin(k/4)}\ \cdots\ \frac{\sin(k/2^{n-1})}{2\sin(k/2^n)} \\ &= \frac{\sin(k/2)}{2\sin(k/2^n)} \\ &\sim \frac{\sin k}{k} \quad \text{as} \quad n \to \infty\end{aligned}$$

This is 'sinc' function and its inverse transform is uniform distribution on $[-1,\ 1]$.

$$P_\infty(x) \ = \ \begin{cases} 1/2 & \text{on } \ -1 < x < 1 \\ 0 & \text{otherwise.} \end{cases}$$

Once an exact solution is known for a value of a, we can find other solution related to it. If we define $P_\infty(X, a)$ and $\widehat{P}_\infty(k, a)$ as PDF and structure function of X_∞ with stepsize varying with the factor of a, we know the following property by regrouping terms :

$$\begin{aligned}\widehat{P}_\infty(k, a) &= \prod_{n=1}^{\infty} \cos(ka^n) \\ &= \cos(ka)\ \cos(ka^3)\cdots\cos(ka^2)\ \cos(ka^4)\cdots \\ &= \widehat{P}_\infty(\frac{k}{a}, a^2)\ \widehat{P}_\infty(k, a^2) \\ \text{or } &= \widehat{P}_\infty(\frac{k}{a^2}, a^3)\ \widehat{P}_\infty(\frac{k}{a}, a^3)\ \widehat{P}_\infty(k, a^3) \\ &\cdots\end{aligned}$$

Since $\widehat{P}_\infty(k, \frac{1}{2})$ is known, we can get $\widehat{P}_\infty(k, \frac{1}{2^{1/m}})$ for $m = 1,\ 2,\ \cdots$. For example if $a = 1/\sqrt{2}$,

$$\widehat{P}_\infty(k, \frac{1}{\sqrt{2}}) = \widehat{P}_\infty(\sqrt{2}k, \frac{1}{2})\ \widehat{P}_\infty(k, \frac{1}{2})$$
$$P_\infty(x, \frac{1}{\sqrt{2}}) = P_\infty(\frac{x}{\sqrt{2}}, \frac{1}{2})\ *\ P_\infty(x, \frac{1}{2}),$$

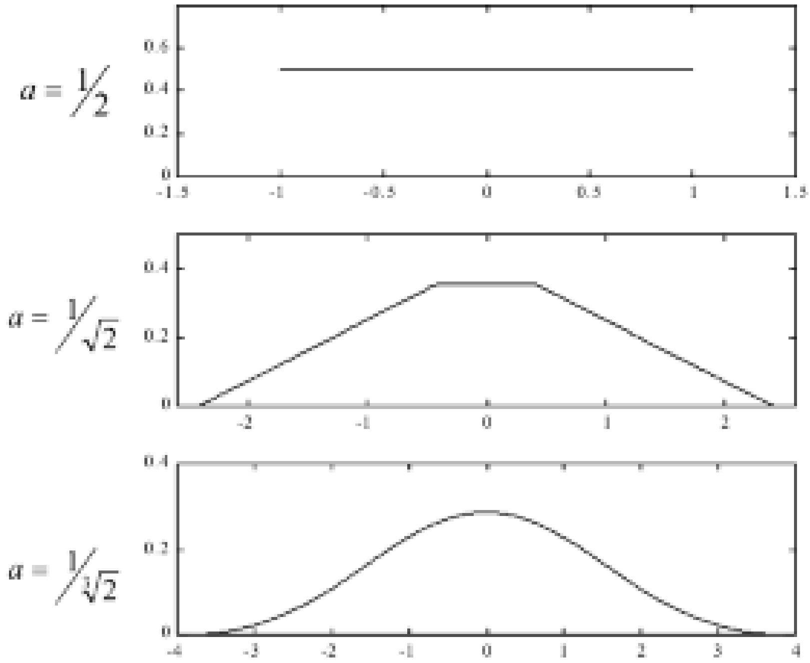

Figure 1: PDF of exponentially decaying step when $a = 1/n^{1/k}$

which is the convolution of two unit distributions on intervals $[-1, 1]$ and $[-\sqrt{2}, \sqrt{2}]$.

We also have another approach which goes without Fourier transform. If we let $P_\infty^{sm}(x)$ the PDF when walkers started their step as a^2 instead of a (thus stepsize goes like $a^2, a^3, \cdots$), the distribution will look like $P_\infty(x)$ except that every distance scale is multiplicated by a. The the probability of the walker settling within dx around point x has the relation :

$$P_\infty^{sm}(x)\ dx = P_\infty(\frac{x}{a})\ \frac{dx}{a}.$$

Now then, $P_\infty(x)$ is nothing but the average of two P_∞^{sm}'s centered at a and $-a$,since after the first step the walker is at either a or $-a$ with probability $1/2$ and their next step size is a^2. Thus we have the functional equation $P_\infty(x)$ satisfy :

$$\begin{aligned} P_\infty(x) &= \frac{1}{2}\ (P_\infty^{sm}(x-a) + P_\infty^{sm}(x+a)) \\ &= \frac{1}{2a}\ (P_\infty(\frac{x-a}{a}) + P_\infty(\frac{x+a}{a})). \end{aligned}$$

We can also understand this as the inverse Fourier transform of $\widehat{P}_\infty(k)$ taking out one $\cos(ka)$:

$$\begin{aligned} \widehat{P}_\infty(k) &= \cos(ka)\ \left[\cos(ka^2)\cos(ka^3)\ \cdots\ \right] \\ &= \cos(ka)\widehat{P}_\infty(ka) = \frac{1}{2}(e^{ika} + e^{-ika})\widehat{P}_\infty(ka) \end{aligned}$$

¿From the analysis of this equation, we can infer the exact solution of $a = 1/2$ or $a = 1/\sqrt{2}$. For numerical scheme, this functional relation can be modified as an recursion formula to get $P_\infty(x)$,

$$P^{(k+1)}(x) = \frac{1}{2a}(P^{(k)}(\frac{x-a}{a}) + P^{(k)}(\frac{x+a}{a})) \quad \text{where} \quad \lim_{k\to\infty} P^{(k)}(x) = P_\infty(x)$$

2.3 Growing simple walk

¿From the relation

$$\widehat{P}_n(k,a) \;=\; \cos(ka^n)\;\cos(ka^{n-1})\cdots\cos(ka) \;=\; \widehat{P}_n(ka^{n+1},\frac{1}{a}),$$

we infer that $a \leftrightarrow 1/a$ shows equivalent limiting distribution. The r.m.s. is

$$\langle X_n^2\rangle^{1/2} \;=\; \sigma_{m=1}^n a^{2m} \;=\; a^2\frac{a^{2n}-1}{a^2-1} \sim \frac{a^{2(n+1)}}{a^2-1},$$

and we can scale as

$$\zeta = \frac{\sqrt{a^2-1}}{a^{n+1}}x$$

to get the same limiting distribution as the $1/a$ case. The diffusion is anomalous with exponentially growing width.

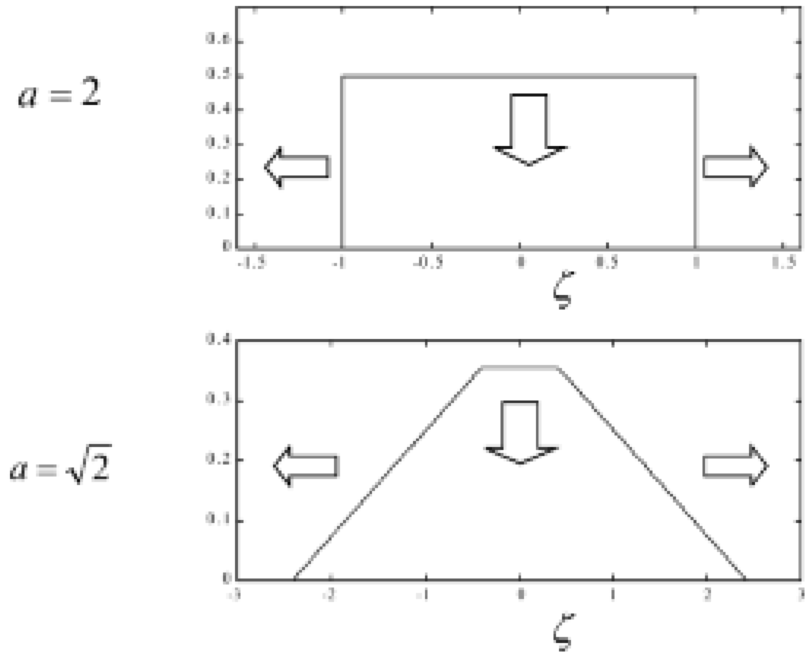

Figure 2: PDF of exponentially growing step scaled as as described in the main text.