Anomalous Diffusion Coefficient via Simple Particle Hopping Analysis

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Presentation Skeleton

- How to introduce coefficient of anomalous diffusion?
- Classical diffusion in $\mathbb{R}$
- Anomalous diffusion in $\mathbb{R}$
- Hopping model in $\mathbb{Z}$
- How to obtain Einstein diffusion law without CLT?
- Relationship between time step and spacing
- Existence of proporcionality limit
- Main result: Anomalous diffusion coefficient without GCLT
- Tools: Fourier transform, l'Hospital rule, Riemann integral

Classical Diffusion in Onedimensional Continuum

$$\frac{\partial \mathrm{c}(x,t)}{\partial t} = D\nabla \mathrm{c}(x,t), \quad D>0, t>0, x\in\mathbb{R} \tag{1}$$

$$\mathrm{c}(x,0+) = \delta(x) \tag{2}$$

How to obtain Fourier image of fundamental solution?

$$\mathrm{c}(x,t) \xrightarrow{\mathcal{L}} \hat{\mathrm{c}}(x,s) \xrightarrow{\mathcal{F}} \tilde{\mathrm{c}}(\omega,s) \xrightarrow{\mathcal{L}^{-1}} \mathrm{C}(\omega,t) \tag{3}$$

$$s\ \hat{\mathrm{c}}(x,s) - \delta(x) = D\nabla\hat{\mathrm{c}}(x,s) \tag{4}$$

$$\tilde{\mathrm{c}}(\omega,s) = \frac{1}{s+D\omega^2} \tag{5}$$

$$\mathrm{C}(\omega,t) = \exp(-Dt\omega^2) \tag{6}$$

Anomalous Diffusion in Onedimensional Continuum

$$\frac{\partial \mathrm{c}(x,t)}{\partial t} = D\nabla^{(\alpha)}\mathrm{c}(x,t), \quad \alpha \in (1,2), D > 0, t > 0, x \in \mathbb{R} \tag{7}$$

$$\mathrm{c}(x,0+) = \delta(x) \tag{8}$$

How to obtain Fourier image of fundamental solution?

$$\mathrm{c}(x,t) \xrightarrow{\mathcal{L}} \hat{\mathrm{c}}(x,s) \xrightarrow{\mathcal{F}} \tilde{\mathrm{c}}(\omega,s) \xrightarrow{\mathcal{L}^{-1}} \mathrm{C}(\omega,t) \tag{9}$$

$$s\ \hat{\mathrm{c}}(x,s) - \delta(x) = D\nabla^{(\alpha)}\hat{\mathrm{c}}(x,s) \tag{10}$$

$$\tilde{\mathrm{c}}(\omega,s) = \frac{1}{s + D|\omega|^{\alpha}} \tag{11}$$

$$\mathrm{C}(\omega,t) = \exp(-Dt|\omega|^{\alpha}) \tag{12}$$

Onedimensional Hopping Model as Stochastic Tool

$$x_k = hk, \quad \Delta t = t/N > 0, h > 0, k \in \mathbb{Z}, N \in \mathbb{N} \tag{13}$$

$$\mathrm{prob}(X = x_k) = p_k, \quad p_0 = 0, p_{-k} = p_k \tag{14}$$

$$\mathrm{f}(x) = \sum_{k=1}^{\infty} (\delta(x + hk) + \delta(x - hk)) p_k \tag{15}$$

$$\mathrm{F}(\omega) = \mathcal{F}\{\mathrm{f}(x)\} = 2 \sum_{k=1}^{\infty} p_k \cos(hk\omega) \tag{16}$$

$$\mathrm{F}_N(\omega) = \left(2 \sum_{k=1}^{\infty} p_k \cos(h_N k\omega) \right)^N \to \mathrm{C}(\omega, t) \tag{17}$$

$$\mathrm{G}(\omega) = \lim_{N\to\infty} \ln \mathrm{F}_N(\omega) = \lim_{N\to\infty} N \ln \mathrm{F}(\omega) = \ln \mathrm{C}(\omega, t) \tag{18}$$

Onedimensional Brownian Motion as Simple Hopping

$$p_1 = p_{-1} = 1/2 \tag{19}$$

$$\mathrm{F}(\omega) = \cos h\omega \tag{20}$$

$$\mathrm{F}_N(\omega) = \cos^N h_N\omega \tag{21}$$

Hypothesis to be proven

$$\Delta t = Q h_N^2 \tag{22}$$

Substitution $\xi = h_N|\omega| \to 0+$ produces

$$N = \frac{t}{Q h_N^2} = \frac{t\omega^2}{Q\xi^2} \to \infty \tag{23}$$

Therefore

$$\mathrm{G}(\omega) = \lim_{N\to\infty} N \ln \cos h_N\omega = \frac{t\omega^2}{Q} \lim_{\xi\to 0+} \frac{\ln \cos \xi}{\xi^2} \tag{24}$$

Einstein Diffusion Law as the First Result

After double application of l'Hospital rule

$$\mathrm{G}(\omega) = -\frac{t\omega^2}{2Q} = -Dt\omega^2 \tag{25}$$

Resulting formula for diffusion coefficient

$$D = \frac{1}{2Q} = \frac{h_N^2}{2\Delta t} \tag{26}$$

But the variance $\mathrm{var}X = \sigma^2 = h_N^2$ and therefore

$$\sigma^2 = 2D\Delta t \tag{27}$$

Onedimensional Hopping with Heavy Tails

$$p_k = p_{-k} = C^*/|k|^{\alpha+1}, \quad k \in \mathbb{N} \tag{28}$$

$$C^* = \frac{1}{2\zeta_{\alpha+1}} \tag{29}$$

$$\mathrm{F}(\omega) = \frac{1}{\zeta_{\alpha+1}} \sum_{k=1}^{\infty} \frac{\cos kh\omega}{k^{\alpha+1}} \tag{30}$$

$$\mathrm{F}_N(\omega) = \left(\frac{1}{\zeta_{\alpha+1}} \sum_{k=1}^{\infty} \frac{\cos kh_N\omega}{k^{\alpha+1}} \right)^N \tag{31}$$

Hypothesis to be proven

$$\Delta t = Qh_N^{\alpha} \tag{32}$$

Substitution $\xi = h_N|\omega| \to 0+$ produces

$$N = \frac{t}{Qh_N^{\alpha}} = \frac{t|\omega|^{\alpha}}{Q\xi^{\alpha}} \to \infty \tag{33}$$

Simple Result with Nontrivial Limit

Therefore

$$\mathrm{G}(\omega) = \lim_{N\to\infty} N \ln\left(\frac{1}{\zeta_{\alpha+1}}\sum_{k=1}^{\infty}\frac{\cos kh_N\omega}{k^{\alpha+1}}\right) = \frac{t|\omega|^{\alpha}}{Q}\mathrm{L}(\alpha) \tag{34}$$

$$\mathrm{L}(\alpha) = \lim_{\xi\to 0+}\frac{-\ln\zeta_{\alpha+1} + \ln\sum_{k=1}^{\infty}\frac{\cos k\xi}{k^{\alpha+1}}}{\xi^{\alpha}} \tag{35}$$

Supposing the existency and finiteness of $\mathrm{L}(\alpha) < 0$ we have

$$D = -\mathrm{L}(\alpha)/Q > 0 \tag{36}$$

But how to evaluate the limit ?

Analysis for $\alpha \in (1,2) \cap \mathbb{Q}$: Part I.

We express the exponent of anomalous diffusion

$$\alpha = u/v, \quad u, v \in \mathbb{N}, v \geq 2, v < u < 2v \tag{37}$$

and apply the substitution

$$\xi = \eta^v, \quad \xi^\alpha = \eta^u, \eta \to 0+ \tag{38}$$

The first application of l'Hospital rule

$$\mathrm{L}(\alpha) = \lim_{\eta \to 0+} \frac{-\ln \zeta_{\alpha+1} + \ln \sum_{k=1}^{\infty} \frac{\cos k\eta^v}{k^{\alpha+1}}}{\eta^u} \tag{39}$$

$$\mathrm{L}(\alpha) = \lim_{\eta \to 0+} \frac{-\sum_{k=1}^{\infty} \frac{v\eta^{v-1} k \sin k\eta^v}{k^{\alpha+1}}}{u\eta^{u-1} \sum_{k=1}^{\infty} \frac{\cos k\eta^v}{k^{\alpha+1}}} = \frac{-1}{\alpha \zeta_{\alpha+1}} \lim_{\eta \to 0+} \frac{\sum_{k=1}^{\infty} \frac{\sin k\eta^v}{k^\alpha}}{\eta^{u-v}} \tag{40}$$

Analysis for $\alpha \in (1,2) \cap \mathbb{Q}$: Part II.

The second application of l'Hospital rule

$$\mathrm{L}(\alpha) = \frac{-1}{\alpha\zeta_{\alpha+1}} \lim_{\eta\to 0+} \frac{\sum_{k=1}^{\infty} \frac{v\eta^{v-1} k \cos k\eta^v}{k^\alpha}}{(u-v)\eta^{u-v-1}} \tag{41}$$

$$\mathrm{L}(\alpha) = \frac{-1}{\alpha(\alpha-1)\zeta_{\alpha+1}} \lim_{\eta\to 0+} \left(\eta^{2v-u} \sum_{k=1}^{\infty} \frac{\cos k\eta^v}{k^{\alpha-1}} \right) \tag{42}$$

Comming back to $\xi = \eta^v \to 0+$

$$\mathrm{L}(\alpha) = \frac{-1}{\alpha(\alpha-1)\zeta_{\alpha+1}} \lim_{\xi\to 0+} \left(\xi \sum_{k=1}^{\infty} \frac{\cos k\xi}{(k\xi)^{\alpha-1}} \right) \tag{43}$$

we recognize Riemann integral with spacing ξ

$$\mathrm{L}(\alpha) = \frac{-1}{\alpha(\alpha-1)\zeta_{\alpha+1}} \int_0^\infty \frac{\cos y \mathrm{d}y}{y^{\alpha-1}} \tag{44}$$

which includes relative convergent positive integral

Final Formula for Anomal Diffusion Coefficient

$$D = \frac{\Gamma(2-\alpha)\cos\frac{\pi}{2}(2-\alpha)}{Q\alpha(\alpha-1)\zeta_{\alpha+1}} \tag{45}$$

Conclusion:

- Understanding diffusion process without CLT
- Understanding anomalous diffusion without GCLT
- Determination of factor Q for stochastic simulations
- $\alpha, D \Rightarrow Q$
- $Q, h, \alpha \Rightarrow \Delta t$

Thank you for your attention.