

A Stochastic Approach to Fractional Diffusion

help I'm trapped in a LaTeX compiler

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Outline

- ▶ Derivation of Standard Diffusion
- ▶ Derivation of Super Diffusion
- ▶ Time Fractional Diffusion
- ▶ Applications

Central Limit Theorem and Random Walks

Random Walk

Let X_1, \dots, X_n be a sequence of random variables, then

$$S_n = \sum_{k=1}^n X_k \quad (1)$$

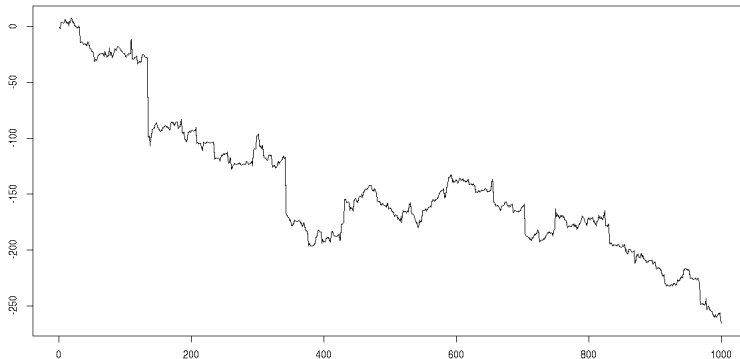
represents the position after n steps.

If $\mathbb{E}[X_i] = 0$ and $\mathbb{E}[X_i^2] = 2$ then the central limit theorem gives us that

$$\frac{S_n}{\sqrt{n}} \longrightarrow Z \quad (2)$$

weakly as $n \longrightarrow \infty$, where $Z \sim \mathcal{N}(0, 2)$

Here is what a squiggly line looks like



Central Limit Theorem and Random Walks

We can extend this idea by introducing a scaling parameter γ .

$$S_{\lfloor \gamma t \rfloor} = \sum_{k=1}^{\lfloor \gamma t \rfloor} X_k. \quad (3)$$

γ has the effect of changing the *timescale* that we are considering the process running over.

We can calculate the characteristic function of

$$\frac{S_{\lfloor \gamma t \rfloor}}{\sqrt{\gamma}}. \quad (4)$$

By the convolution theorems we can say that it is

$$\left(1 - \frac{k^2}{\gamma} + o(\gamma^{-1})\right)^{\lfloor \gamma t \rfloor} \quad (5)$$

Long Time Limit

We can rearrange

$$\left(1 - \frac{k^2}{\gamma} + o(\gamma^{-1})\right)^{\lfloor \gamma t \rfloor} = \left[\left(1 - \frac{k^2}{\gamma} + o(\gamma^{-1})\right)^{\gamma} \right]^{\frac{\lfloor \gamma t \rfloor}{\gamma}} \quad (6)$$

and then take $\gamma \rightarrow \infty$ to get that

$$\left[\underbrace{\left(1 - \frac{k^2}{\gamma} + o(\gamma^{-1})\right)^{\gamma}}_{(*)} \right]^{\frac{\lfloor \gamma t \rfloor}{\gamma}} \rightarrow e^{-tk^2} \quad (7)$$

by using the well known result

$$\lim_{n \rightarrow \infty} \left(1 + \frac{x}{n}\right)^n = e^x. \quad (8)$$

Fourier Transform and a PDE

Notice that e^{-tk^2} is just the CF of $Z_t \sim \mathcal{N}(0, 2t)$. Further we can say that $\frac{S_{\lfloor \gamma t \rfloor}}{\sqrt{\gamma}} \rightarrow Z_t$ by LCT.

We can also regard e^{-tk^2} as the FT of the density of Z_t .

Rather usefully we have also have that e^{-tk^2} is a solution to

$$\frac{d\hat{u}}{dt} = -k^2 \hat{u} \quad (9)$$

We can actually use a analogous result from last week's homework to invert the Fourier transform of u to get

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \quad (10)$$

A More General Result

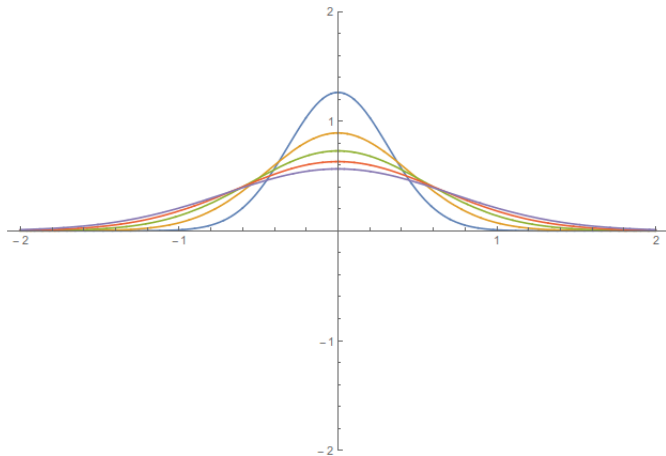
We can generalize this result a bit and say that if $\mathbb{E}[X_i^2] = \sigma^2$ then $\frac{S_{\lfloor \gamma t \rfloor}}{\sqrt{\gamma}} \longrightarrow Z_t$, but now $Z_t \sim \mathcal{N}(0, 2\sigma^2 t)$.

Further the Fourier transform of the density of Z_t is $e^{-t\sigma^2 k^2}$ which means the density is now a solution to

$$\frac{\partial u}{\partial t} = \underbrace{\frac{\sigma^2}{2}}_D \frac{\partial^2 u}{\partial x^2}. \quad (11)$$

What this says is that as particles jump around more, they diffuse more rapidly.

A Plot



Recap

- ▶ All we have done to get this result is require that the random variables that represent the *jumps* fulfill the requirements of the CLT.
- ▶ What if we relax the *finite second moment* condition?

Pareto Distribution

- ▶ Consider a random variable P with density $Cx^{-\alpha-1}$ for some normalizing constant C .
- ▶ If we require $1 < \alpha < 2$ then we have $\mathbb{E}[P]$ exists but $\mathbb{E}[P^2] = \infty$ does not.
- ▶ It can be shown (with very lengthy computation) that the FT of the density of P is $1 + (ik)^\alpha + O(k^2)$.
- ▶ The idea is to setup a sequence of random variables Y_1, \dots, Y_n , all iid with Pareto distribution with parameter α and use these as the *jumps* in the random walk.

Pareto Distribution

Setup $S_n = \sum_{k=1}^n Y_k$ as before.

By the convolution theorems for FTs we can calculate the FT of the density of $\frac{S_n}{n^{\frac{1}{\alpha}}}$ to be

$$\left(1 + \frac{(ik)^\alpha}{n} + O(n^{-\frac{2}{\alpha}})\right)^n \quad (12)$$

Notice that as $n \rightarrow \infty$ this has limit $e^{(ik)^\alpha}$.

The LCT implies that $\frac{S_n}{n^{\frac{1}{\alpha}}} \rightarrow Z$ where Z has FT $e^{(ik)^\alpha}$.

Notice that in some way this is an *Extended Central Limit Theorem*.

Long Time Limit

Like before we can introduce a time scale parameter γ and write

$$S_{[\gamma t]} = \sum_{k=1}^{[\gamma t]} Y_k. \quad (13)$$

Again by considering the FT of

$$\frac{S_{[\gamma t]}}{\gamma^{\frac{1}{\alpha}}} \quad (14)$$

which is

$$\left(1 + \frac{(ik)^\alpha}{\gamma} + o(\gamma^{\frac{-2}{\alpha}})\right)^{[\gamma t]}. \quad (15)$$

Long Time Limit

$$\left(1 + \frac{(ik)^\alpha}{\gamma} + o(\gamma^{\frac{-2}{\alpha}})\right)^{\lfloor \gamma t \rfloor} \quad (16)$$

By taking $\gamma \rightarrow \infty$ we get that the Fourier transform converges to

$$e^{t(ik)^\alpha} \quad (17)$$

and by the LCT this gives us that

$$\frac{S_{\lfloor \gamma t \rfloor}}{\gamma^{\frac{1}{\alpha}}} \rightarrow Z_t \quad (18)$$

where Z_t has FT $\hat{u}(k) = e^{t(ik)^\alpha}$.

Notice that this is a stable distribution (check against the definition in the notes).

It is clear that $\hat{u}(t) = e^{t(ik)^\alpha}$ is a solution to

$$\frac{d\hat{u}}{dt} = (ik)^\alpha \hat{u}. \quad (19)$$

Unfortunately we can't use *last week's homework* to invert this FT and this is where we introduce fractional calculus.

Motivations

Cauchy Formula for Repeated Integration

$$\int_a^x \int_a^{y_1} \cdots \int_a^{y_{n-1}} f(y_n) dy_n \cdots dy_2 dy_1 = \frac{1}{(n-1)!} \int_a^x (x-t)^{n-1} f(t) dt$$

Motivations

Cauchy Formula for Repeated Integration

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The idea is to replace the factorials with gamma functions to define an integral of arbitrary order

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Riemann-Liouville Fractional Integral

$$(I_a^\alpha f)(x) = \frac{1}{\Gamma(\alpha)} \int_a^x (x-t)^{\alpha-1} f(t) dt$$

Motivations (Derivatives)

Riemann-Liouville Fractional Derivative

$$\begin{aligned}(\mathcal{D}_a^\alpha f)(x) &= \frac{d^n}{dx^n} (I_a^{n-\alpha} f)(x) \\ &= \frac{1}{\Gamma(1-\alpha)} \frac{d^n}{dx^n} \int_a^x \frac{f(t)dt}{(x-t)^{\alpha-n+1}}\end{aligned}$$

where $n = \lfloor \alpha \rfloor + 1$.

Motivations (Derivatives)

Caputo Fractional Derivative

$$\begin{aligned}({}^C\mathcal{D}_a^\alpha f)(x) &= \left(I_a^{n-\alpha} \frac{d^n}{dx^n} f\right)(x) \\ &= \frac{1}{\Gamma(1-\alpha)} \int_a^x \frac{\frac{d^n}{dt^n} f(t) dt}{(x-t)^{\alpha-n+1}}\end{aligned}$$

where $n = \lfloor \alpha \rfloor + 1$.

Riemann-Liouville vs Caputo Derivative

- ▶ The Caputo derivative is often used in fractional differential equations because it can be coupled with integer order initial conditions, whereas often the Riemann-Liouville derivative can't be coupled with integer order initial conditions.
- ▶ When we set $a = -\infty$ for a large class of functions these derivatives are the same.

Fractional Derivative Fourier Transform

It can be shown that

$$\mathcal{F}\{-\infty \mathcal{D}^\alpha f(x)\} = (ik)^\alpha \mathcal{F}\{f(x)\} \quad (20)$$

and it is precisely this result that we use to *invert* the Fourier transform we had before. That is we can say that

$$\frac{\partial u}{\partial t}(x, t) = -\infty \mathcal{D}_x^\alpha u(x, t) \quad (21)$$

where u is the density of $Z_t = \lim_{\gamma \rightarrow \infty} \frac{Y_1 + Y_2 + \dots + Y_{\lfloor \gamma t \rfloor}}{\gamma^{\frac{1}{\alpha}}}$.

It can be shown that $u(x, t) = Ax^{-\alpha-1} + o(x^{-\alpha-1})$ as $x \rightarrow \infty$ with A depending on t and α .

Fractional Derivative Fourier Transform

Actually this isn't entirely the case... In space we will often use a *Riesz* or *Riesz-Feller* fractional derivative.

The Riesz fractional derivative of a function f is defined as

$$\mathcal{F}^{-1}\{-|k|^\alpha \hat{f}(k)\}(x). \quad (22)$$

The reason one does this is because $e^{(ik)^\alpha}$ isn't really well defined for non-integer α and $k < 0$.

In the lecture notes we define

$$(ik)^\alpha = |k|^\alpha \left(\cos\left(\frac{\alpha\pi}{2}\right) + i \operatorname{sgn}(k) \sin\left(\frac{\alpha\pi}{2}\right) \right) \quad (23)$$

Generalisation To Higher Dimensions

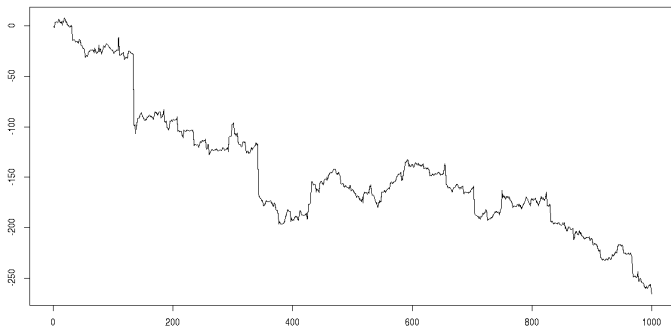
- ▶ It's this definition

$$\mathcal{D}^\alpha f(x) = \mathcal{F}^{-1}\{-\|k\|^\alpha \hat{f}(k)\}(x) \quad (24)$$

which naturally generalises to higher dimensions.

- ▶ This allows us to define things like a fractional Laplacian.
- ▶ Just like in the *normal* case we can use a change of coordinates to get a Laplacian in other coordinates (say on the surface of a sphere). This gets very complicated very quickly.

A Plot



Time Fractional Diffusion

- ▶ A similar idea can be applied to the *time* between steps.
- ▶ This is done by considering something called a continuous time random walk.
- ▶ If we choose the distribution to be the *exponential* distribution we get normal diffusion.
- ▶ If we choose something different, say the *Mittag-Leffler* distribution, then we can get time-fractional diffusion.
- ▶ This is where the time derivative is fractional.
- ▶ Because we don't run into problems with negative time its actually quite natural to use the RL or Caputo fractional derivatives here. (We work in Laplace space quite often).

Coupled Continuous Time Random Walks

- ▶ One can go even further with space and time derivatives.
- ▶ If we assume that the waiting times between jumps and time size of the jumps are independent then we get a *decoupled* random walk.
- ▶ If we don't assume this then we get a coupled random walk. This has particularly interesting applications in finance.

Applications

Finance

- ▶ Raberto, M., Scalas, E., Gorenflo, R., & Mainardi, F. (2000). The waiting-time distribution of LIFFE bond futures. arXiv preprint cond-mat/0012497
- ▶ Scalas, E., Gorenflo, R., & Mainardi, F. (2000). Fractional calculus and continuous-time finance. *Physica A: Statistical Mechanics and its Applications*, 284(1), 376-384.

Biology

- ▶ Goychuk, I., & Hnggi, P. (2004). Fractional diffusion modeling of ion channel gating. *Physical Review E*, 70(5), 051915.

Chemistry

- ▶ Bazelyansky, M., Robey, E., & Kirsch, J. F. (1986). Fractional diffusion-limited component of reactions catalyzed by acetylcholinesterase. *Biochemistry*, 25(1), 125-130.

Acknowledgement

This talk was partly based off ideas outlined in

- ▶ Meerschaert, M. M., & Sikorskii, A. (2011). Stochastic models for fractional calculus (Vol. 43). Walter de Gruyter.
- ▶ the lecture notes for this course.