A Stochastic Approach to Fractional Diffusion

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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 $X_1, \ldots X_n$ be a sequence of random variables, then

$$S_n = \sum_{k=1}^{n} X_n \tag{1}$$

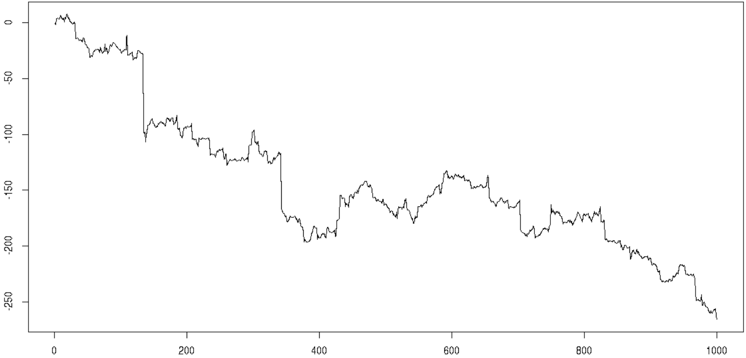
represents the position after n steps.

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

$$\frac{S_n}{\sqrt{n}} \longrightarrow Z \tag{2}$$

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.

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

γ has the effect of changing the *timescale* that we are considering the process running over.
We can calculate the characteristic function of

$$\frac{S_{\lfloor \gamma t \rfloor}}{\sqrt{\gamma}}. \tag{4}$$

By the convolution theorems we can say that it is

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

Long Time Limit

We can rearrange

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

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

$$\Bigg[\underbrace{\left(1-\frac{k^2}{\gamma}+o(\gamma^{-1})\right)^{\gamma}}_{\circledast}\Bigg]^{\frac{\lfloor\gamma t\rfloor}{\gamma}}\longrightarrow e^{-tk^2} \tag{7}$$

by using the well known result

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

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 $\frac{S_{\lfloor \gamma t \rfloor}}{\sqrt{\gamma}} \longrightarrow Z_t$ 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

$$\frac{d\hat{u}}{dt} = -k^2 \hat{u} \tag{9}$$

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

$$\frac{\partial u}{dt} = \frac{\partial^2 u}{\partial x^2} \tag{10}$$

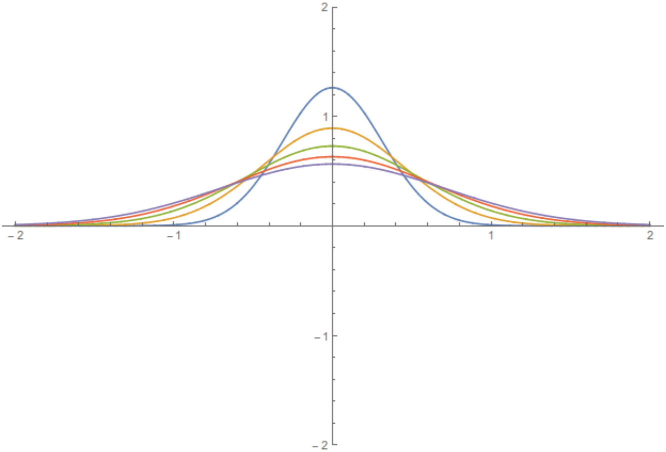
A More General Result

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

$$\frac{\partial u}{\partial t} = \underbrace{\frac{\sigma^2}{2}}_{D} \frac{\partial^2 u}{\partial x^2}. \tag{11}$$

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 $Y_1, \ldots Y_n$, all iid with Pareto distribution with parameter α and use these as the *jumps* in the random walk.

Pareto Distribution

Setup $S_n = \sum_{k=1}^{n} Y_n$ 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

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

Notice that as $n \longrightarrow \infty$ this has limit $e^{(ik)^\alpha}$.
The LCT implies that $\frac{S_n}{n^{\frac{1}{\alpha}}} \longrightarrow Z$ 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

$$S_{\lfloor \gamma t \rfloor} = \sum_{k=1}^{\lfloor \gamma t \rfloor} Y_k. \tag{13}$$

Again by considering the FT of

$$\frac{S_{\lfloor \gamma t \rfloor}}{\gamma^{\frac{1}{\alpha}}} \tag{14}$$

which is

$$\left(1 + \frac{(ik)^{\alpha}}{\gamma} + o(\gamma^{\frac{-2}{\alpha}})\right)^{\lfloor \gamma t \rfloor}. \tag{15}$$

Long Time Limit

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

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

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

and by the LCT this gives us that

$$\frac{S_{\lfloor \gamma t \rfloor}}{\gamma^{\frac{1}{\alpha}}} \longrightarrow Z_t \tag{18}$$

where Z_t has FT $\hat{u}(k) = e^{t(ik)^\alpha}$.
Notice that this is a stable distribution.

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

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

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

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

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

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

Motivations (Derivatives)

Caputo Fractional Derivative

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

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

$$\mathcal{F}\left\{{}_{-\infty}\mathcal{D}^{\alpha} f(x)\right\} = (ik)^{\alpha}\mathcal{F}\{f(x)\} \tag{20}$$

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

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

where u is the density of $Z_t = \lim_{\gamma\longrightarrow\infty} \frac{Y_1+Y_2+\cdots+Y_{\lfloor\gamma t\rfloor}}{\gamma^{\frac{1}{\alpha}}}$.
It can be shown that $u(x,t) = Ax^{-\alpha-1} + o(x^{-\alpha-1})$ as $x \longrightarrow \infty$ with A depending on t and α.

Fractional Derivative Fourier Transform

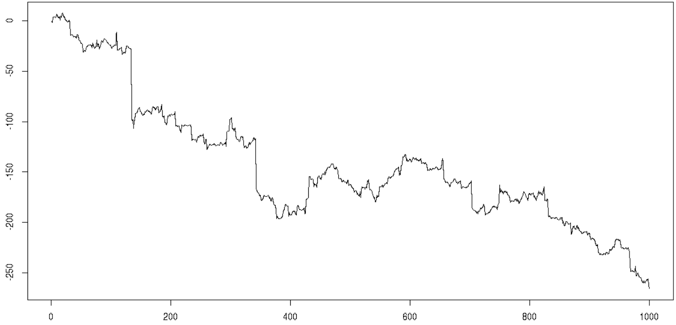
Actually this isn't entirely the case... In space we will often use a *Riesz* or *Riesz-Feller* fractional derivative.

The Riesz fractional derivative of a function f is defined as

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

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

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.

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.