Anomalous subdiffusion and time-fractional differential equations I

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Plan

1. (C.) Introduction: anomalous sub-diffusion and time-fractional equation
2. (Kumagai) Trap model and high dimensional scaling limits (fractional kinetic process)
3. (C.) Time-fractional parabolic equations and probabilistic representation
4. (Kumagai) Heat kernel estimates for anomalous sub-diffusions.
5. (C.) Coupled time-fractional parabolic equations and related topics
6. (Kumagai) Trap model and low dimensional scaling limit (FIN diffusion)

Random walk

Brownian motion, which is the scaling limit of simple random walk, is the building block of the modern probability theory.

Random walk model: $S_n = \sum_{k=1}^n \xi_k$, $T_n = \sum_{j=1}^n \eta_j$. where $\{\xi_k\}$ and $\{\eta_j\}$ are both i.i.d.

Counting process: $N_t = \max\{n : T_n \leq t\}$.

Continuous time random walk: $X_t = S_{N_t}$.

Key assumption for Brownian approximation: $\mathbb{E}[\xi_1] = 0$, $\sigma^2 = \mathbb{E}[\xi_1^2] < \infty$, $\mu = E[\eta_1] < \infty$.

$$\frac{1}{\sqrt{n}} S_{[nt]} \Rightarrow \sigma B_t, \quad \frac{1}{n} N_{nt} \to t/\mu.$$

For simplicity, assume $\mu = 1 = \sigma$. Then

$$\frac{1}{\sqrt{n}} X_{nt} = \frac{1}{\sqrt{n}} S_{n \frac{1}{n} N_{nt}} \Rightarrow \ B_t \quad \text{as } n \to \infty.$$

Anomalous diffusions

An increasing number of natural phenomena do not fit into the standard diffusion model. That is, either $\mathbb{E}[|\xi_k|^2] = \infty$, or $\mathbb{E}\eta_j = \infty$, or both. (E.g., Pareto-Lévy distribution.)

Superdiffusion

Another possibility for anomalous diffusion is that the random walker remains in motion without changing direction for a time that follows a Pareto-Lévy distribution.

Bird search: more effective

Measured in terms of number of stretches, this corresponds to ξ_j of Pareto-Lévy distribution and $\eta_j = 1$. The limiting process is a Lévy process. It can be described by an equation with fractional derivative in space: $\dfrac{\partial p}{\partial t} = a\Delta^{\alpha/2} p$.

Central Limit Theorem

Recall random walk $S_t = \sum_{j=1}^{[t]} \xi_j$. Assume ξ_1 is spherically symmetric.

• If $\sigma^2 := \mathbb{E}[\xi_1^2] < \infty$, then $\lambda^{-1/2} S_{\lambda t}$ converges weakly to Brownian motion σB_t.

• If $\mathbb{P}(|\xi_1| \geq \lambda) \sim C\lambda^{-\alpha}$ for some $C > 0$ and $0 < \alpha < 2$ as $\lambda \to \infty$, the (extended) CLT tells us that $\{\lambda^{-1/\alpha} S_{\lambda t}, t \geq 0\}$ converges weakly to an isotropic α-stable Lévy motion $\{Y_t\}$ with

$$\mathbb{E}[e^{i\xi \cdot Y_t}] = e^{-C_0 |\xi|^\alpha t} \qquad \text{for every } \xi \in \mathbb{R}^d \text{ and } t \geq 0,$$

where the constant C_0 depends only on C and the dimension d.

• Subordinated BM: $Y_t = B_{Z_t}$, where Z is an independent $(\alpha/2)$-subordinator.

Stable process

The α-stable process Y has scaling property $\{\lambda^{1/\alpha}Y_t, t \geq 0\}$ has the same distribution as $\{Y_{\lambda t}\}$, it represents a model for anomalous super-diffusion, where particles spread faster than Brownian particles.

The infinitesimal generator of Y is $\Delta^{\alpha/2}$: $\widehat{\Delta^{\alpha/2} f}(\xi) = -|\xi|^\alpha \widehat{f}(\xi)$. Alternatively,

$$\Delta^{\alpha/2}u(x) = \int_{\mathbb{R}^d} (u(x+z) - u(x) - \nabla u(x) \cdot z \mathbf{1}_{\{|z| \leq 1\}}) \frac{\mathcal{A}(d,-\alpha)}{|z|^{d+\alpha}} dz$$

where $\mathcal{A}(d,-\alpha) = \alpha 2^{\alpha-1}\pi^{-d/2}\Gamma(\frac{d+\alpha}{2})\Gamma(1-\frac{\alpha}{2})^{-1} \asymp \alpha(2-\alpha)$.

Space dependent non-local operator: for fundamental solutions

- Symmetric case: C.-Kumagai 2003, 2008, 2010, $\cdots$
- Non-symmetric: C.-Zhang 2016, 2018, $\cdots$

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Subdiffusion

Particle moves slower than Brownian motion, for example, due to particle sticking and trapping.

Example: (i) xerox machine, electron in amorphous media tend to get trapped by local imperfections and then released due to thermal fluctuations.

(ii) hydrology: travel times of contaminants in groundwater are much longer than that of diffusion.

(iii) biology: proteins diffuse across cell membranes.

It can be described by an equation involving fractional time derivative: $\frac{\partial^\beta p}{\partial t^\beta} = a \frac{\partial^2 p}{\partial x^2}$.

Waiting time and Subordinator

Recall that the n-th jumping time is $T_n = \sum_{k=1}^{n} \eta_k$. The number of jumps by time $t > 0$ is $N_t = \max\{n : T_n \le t\}$. So the position of the particle at time $t > 0$ is S_{N_t}.

If $\mathbb{P}(\eta_1 > t) \sim Ct^{-\beta}$ as $t \to \infty$ for some $0 < \beta < 1$, then as $c \to \infty$, $c^{-1/\beta} T_{[ct]} \Longrightarrow Z_t$: β-stable subordinator.

Scaling property: $Z_{\lambda t} = \lambda^{1/\beta} Z_t$ in distribution.

Meerschaert and Scheffler (2004) showed that $c^{-\beta} N_{ct} \Longrightarrow L_t$, where $L_t = \inf\{s : Z_s > t\}$. Thus $c^{-\beta/\alpha} S_{N_{[ct]}} \Longrightarrow Y_{L_t}$, a symmetric α-stable process time-changed by an inverse β-stable subordinator.

When $\alpha = 2$ and $0 < \beta < 1$, B_{L_t} provides a model for anomalous sub-diffusion, where particles spread slower than Brownianian particles.

Fractional-kinetics process

$$\mathbb{E}[(B_{L_t} - B_0)^2] = \frac{t^\beta}{\beta\Gamma(\beta)}.$$

B_{L_t} is called fractional-kinetics process in some literature.

It also arises

(i) (symmetric Bouchaud's trap model) as the quenched scaling limit of random walks in $\mathbb{Z}^d$ with exponential holding times at each vertices whose expected values are i.i.d random variables of power law distribution;
Ben Arous-Černý 2007: For $d \geq 3$ and $\beta \in (0,1)$,

$$\left\{n^{-\beta/2} X_{[nt]}; t \geq 0\right\} \Rightarrow \{\mathbf{BM}_{L_t}; t \geq 0\}.$$

For $d = 2$, the scaling constant is $N^{-\beta/2}(\log N)^{-(1-\beta)/2}$.

(ii) as the quenched scaling limit of constant speed random walks on $\mathbb{Z}^d$ ($d \geq 2$) with i.i.d conductances that have power law tails.
(Barlow-Černý 2011 for $d \geq 3$, Černý 2011 for $d = 2$.)

Inverse subordinator

In general, given a Markov process X_t and an independent β-subordinator Z, one can do time change to get a new process X_{L_t}, where $L_t = \inf\{r : Z_r > t\}$.

Question: What is the marginal distribution of X_{L_t}?

Denote by $g_\beta(u)$ the density of Z_1. Then by scaling, Z_s has density $s^{-1/\beta} g_\beta(s^{-1/\beta} u)$ for any $s > 0$. Using the inverse relation $\mathbb{P}(L_t \leq s) = \mathbb{P}(Z_s \geq t)$ and taking derivatives, it follows that L_t has the density

$$f_t(s) = \frac{d}{ds}\mathbb{P}(Z_s \geq t) = t\beta^{-1} s^{-1-1/\beta} g_\beta(ts^{-1/\beta}).$$

Marginal distribution

For $\phi \geq 0$,

$$\begin{aligned} u(t,x) &:= \mathbb{E}_x\left[\phi(X_{L_t})\right] \\ &= \int_0^\infty \mathbb{E}_x[\phi(X_s)]\mathbb{P}(L_t \in ds) = \int_0^\infty P_s\phi(x)f_t(s)ds \\ &= \int_0^\infty P_{(t/s)^\beta}\phi(x)g_\beta(s)ds. \end{aligned}$$

Time fractional equation

Suppose that $\mathcal{L}$ is the generator of a strong Markov process X.

Theorem (Baeumer-Meerschaert, 2001; Meerschaert-Scheffler, 2004): $u(t,x) = \mathbb{E}_x[f(X_{L_t})]$ solves

$$\frac{\partial^\beta u(t,x)}{\partial t^\beta} = \mathcal{L}_x u(t,x), \quad u(0,x) = f(x).$$

where Caputo fractional derivative:

$$\frac{\partial^\beta \psi(t)}{\partial t^\beta} := \frac{1}{\Gamma(1-\beta)} \int_0^t (t-r)^{-\beta} \psi'(r) dr.$$

Tools used: Mittag-Leffer functions, and the self-similarity of the β-subordinator.

- For $p > 0$, $\partial_t^\beta (t^p) = \frac{\Gamma(p+1)}{\Gamma(p+1-\beta)} t^{p-\beta}$.

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Fractional derivative: a brief history

Letter from l'Hôpital to Leibniz (1695): What if n be $1/2$ in $\frac{d^n}{dx^n}$?

Leibiniz: It will lead to a paradox. $\cdots$ From this apparent paradox, one day useful consequences will be drawn.

S. F. Lacroix (1819): defined $\frac{d^{1/2}}{dx^{1/2}}(x^p) = \frac{\Gamma(p+1)}{\Gamma(p+1/2)} x^{p-1/2}$, motivated by the identity $\frac{d^k}{dx^k}(x^n) = \frac{n!}{(n-k)!} x^{n-k} = \frac{\Gamma(n+1)}{\Gamma(n+1-k)} x^{n-k}$.

Liousville: attempted a first logical definition of fractional derivative. Three long memoirs in 1832 and several more through 1855.
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Time-fractional calculus

Time-fractional calculus has been widely used since late last century in various fields to model sub-diffusive phenomena, ranging from physics, chemistry, signal processing to biology, economics and social sciences.

See B. Ross (1975) for a survey on fractional calculus, and the book by M. M. Meerschaert and A. Sikorskii (2011).

Classical Caputo fractional derivative

$$\begin{aligned}\frac{\partial^\beta g(t)}{\partial t^\beta} &= \int_0^t \frac{1}{\Gamma(1-\beta)}(t-s)^{-\beta} g'(s)ds \quad \text{if } g \text{ is Lipschitz} \\ &= \frac{d}{dt}\int_0^t \frac{1}{\Gamma(1-\beta)}(t-s)^{-\beta}\left((g(s)-g(0)\right)ds,\end{aligned}$$

where $\Gamma(\lambda)=\int_0^\infty t^{\lambda-1}e^{-t}dt$. (A. N. Kochubei)

Connection to β-stable subordinator: S_t has no drift (i.e. $\kappa=0$) and its Lévy measure is $\nu(dx)=\frac{\beta}{\Gamma(1-\beta)}x^{-(1+\beta)}dx$.

$$w(x):=\nu[x,\infty)=\int_x^\infty \frac{\beta}{\Gamma(1-\beta)}y^{-(1+\beta)}dy=\frac{x^{-\beta}}{\Gamma(1-\beta)}.$$

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General time-fractional derivative

In applications and numerical approximations, there is a need to consider more general fractional-time derivatives, for example where its value at time t may depend only on the finite range of the past from $t-\delta$ to t such as

$$\frac{d}{dt}\int_{(t-\delta)^+}^{t}(t-s)^{-\beta}\left(f(s)-f(0)\right)ds.$$

Given a decreasing left-continuous function $w \in L^1_{loc}[0,\infty)$ with $\lim_{x\to\infty} w(x) = 0$, define

$$\partial_t^w f(t) := \frac{d}{dt} I_t^w f := \frac{d}{dt}\int_0^t w(t-s)\left(f(s)-f(0)\right)ds.$$

Such w determines a measure ν on $(0,\infty)$ by $\nu[x,\infty) = w(x)$. By Fubini, $\int_0^a w(x)dx = \int_0^\infty (z\wedge a)\nu(dz)$.

Thus $w \in L^1_{loc}[0,\infty) \Longleftrightarrow \nu$ on $\mathbb{R}_+$ with $\int_0^\infty (1\wedge z)\nu(dz) < \infty$.

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General time-fractional derivative

Generalized Riemann-Liouville type integral

$$I_t^w f := \int_0^t w(t-s)\,(f(s)-f(0))\,ds.$$

$$\partial_t^w f(t) := \frac{d}{dt} I_t^w f.$$

Lemma (C. '24)

If f is a local Lipschitz function on $[0,\infty)$, then $\partial_t^w f(t)$ exists for almost every $t>0$ and

$$\partial_t^w f(t) = \int_0^t w(t-s) f'(s) ds.$$

Subordinator

Suppose $S = \{S_t; t \geq 0\}$ is a subordinator independent of X with Laplace exponent ϕ:

$$\mathbb{E}\left[e^{-\lambda S_t}\right] = e^{-t\phi(\lambda)}.$$

There is a unique $\kappa \geq 0$ and a measure $\nu(dx)$ with $\int_0^\infty (1 \wedge x)\nu(dx) < \infty$ so that

$$\phi(\lambda) = \kappa\lambda + \int_0^\infty (1 - e^{-\lambda x})\nu(dx) =: \kappa\lambda + \phi_0(\lambda)$$

$$S_t = \kappa t + \overline{S}_t.$$

β-stable subordinator: if $\phi(\lambda) = \lambda^\beta$ for $0 < \beta < 1$.

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Generator

Given a Markov process $(X, \mathbb{P}_x, x \in \mathcal{X})$ on $\mathcal{X}$, its transition semigroup $\{P_t; t \geq 0\}$ is given by

$$P_t\phi(x) = \mathbb{E}_x[\phi(X_t)].$$

The infinitesimal generator $\mathcal{L}$ of X is

$$\mathcal{L}\phi(x) = \lim_{t \to 0} \frac{P_t\phi(x) - \phi(x)}{t}.$$

Hence $u(t,x) = P_t\phi(x)$ solves $\frac{\partial u}{\partial t} = \mathcal{L}u$ with $u(0,x) = \phi(x)$.

- When X is Brownian motion on $\mathbb{R}^d$, $\mathcal{L} = \frac{1}{2}\Delta$.
- When X is an absorbing (or reflecting) Brownian motion in $D \subset \mathbb{R}^d$, $\mathcal{L}$ is the Dirichlet (or Neumann) Laplacian in D.
- When X is an isotropic α-stable procese, $\mathcal{L} = -(-\Delta)^{\alpha/2}$.

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Questions

(i) Existence and uniqueness for solution of

$$(\kappa\partial_t + \partial_t^w)\, u = \mathcal{L}u \quad \text{with } u(0,x) = f(x),$$

and its probabilistic representation.

(ii) Given a strong Markov process X and subordinator S, what equation does $u(t,x) = \mathbb{E}_x\left[f(X_{L_t})\right] = \mathbb{E}P_{L_t}f(x)$ satisfy? Here

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Framework

From now on, we assume S_t is a subordinator that is not compounded Poisson; i.e. either ν is infinite or $\kappa > 0$. Define $w(x) = \nu[x, \infty)$.

Facts: (i) $t \mapsto S_t$ is strictly increasing so its inverse subordinator L_t is continuous in t.

(ii) $\mathbb{E}\left[e^{\lambda L_t}\right] < \infty$ for any $\lambda \geq 1$.

Suppose that $\{T_t; t \geq 0\}$ is a strongly continuous semigroup with infinitesimal generator $(\mathcal{L}, \mathcal{D}(\mathcal{L}))$ in some Banach space $(\mathbb{B}, \|\cdot\|)$. Note $\|T_t\| \leq c\, e^{\alpha t}$ for some $c, \alpha > 0$.

E.g. Markov transition semigroups; Schrödinger semigroups.

E.g. $(\mathbb{B}, \|\cdot\|) = L^p(\mathcal{X}; \mu)$ for $p \geq 1$ or $(C_\infty(\mathcal{X}), \|\cdot\|_\infty)$.

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From now on, we assume S_t is a subordinator that is not compounded Poisson; i.e. either ν is infinite or $\kappa > 0$. Define $w(x) = \nu[x, \infty)$.

Facts: (i) $t \mapsto S_t$ is strictly increasing so its inverse subordinator L_t is continuous in t.

(ii) $\mathbb{E}\left[e^{\lambda L_t}\right] < \infty$ for any $\lambda \geq 1$.

Suppose that $\{T_t; t \geq 0\}$ is a strongly continuous semigroup with infinitesimal generator $(\mathcal{L}, \mathcal{D}(\mathcal{L}))$ in some Banach space $(\mathbb{B}, \| \cdot \|)$. Note $\|T_t\| \leq c\, e^{\alpha t}$ for some $c, \alpha > 0$.

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Main result

Theorem (C. CSF '17, CJAPS '24)

For every $f \in \mathcal{D}(\mathcal{L})$, $u(t,x) := \mathbb{E}\left[T_{L_t} f(x)\right]$ is the unique solution in $(\mathbb{B}, \|\cdot\|)$ to

$$\left(\kappa \partial_t + \partial_t^w\right) u(t,x) = \mathcal{L}u(t,x) \quad \text{with } u(0,x) = f(x)$$

in the following sense:

1. $u(t) \in \mathcal{D}(\mathcal{L})$, $\|u(t)\| + \|\mathcal{L}u(t)\| \le c\, e^{\alpha t}$, *and* $t \mapsto u(t)$ *is continuous in* $(\mathbb{B}, \|\cdot\|)$;
2. *for every* $t > 0$, $I_t^w(u) := \int_0^t w(t-s)(u(s) - f(x))ds$ *converges absolutely in* $(\mathbb{B}, \|\cdot\|)$ *and*

$$\lim_{\delta \to 0} \frac{1}{\delta}\left(\kappa(u(t+\delta) - u(t)) + I_{t+\delta}^w(u) - I_t^w(u)\right) = \mathcal{L}u(t)$$

in $(\mathbb{B}, \|\cdot\|)$.

Main result

Theorem (C. '17 & '24 (continued))

In addition, $t \mapsto \mathcal{L}u(t)$ are continuous in $(\mathbb{B}, \|\cdot\|)$. When $\kappa > 0$, $t \mapsto u(t)$ is globally Lipschitz continuous in $(\mathbb{B}, \|\cdot\|)$, and both $\partial_t u(t)$ and $\frac{d}{dt} I_t^w(u)$ exists as a continuous function taking values in $(\mathbb{B}, \|\cdot\|)$.

Conversely, if $u(t)$ is a solution in the sense of (i) and (ii) above with $f \in \mathcal{D}(\mathcal{L})$, then $u(t) = \mathbb{E}\left[T_{L_t} f(x)\right]$ in $\mathbb{B}$ for every $t \geq 0$.

Remarks

(i) The assumption that $f \in \mathcal{D}(\mathcal{L})$ in the Theorem is to ensure that all the integrals involved in the proof are absolutely convergent in the Banach space $\mathbb{B}$. This condition can be relaxed if we formulate the time fractional equation in the weak sense when the strongly continuous semigroup $\{T_t; t \geq 0\}$ is symmetric in a Hilbert space $L^2(E; m)$ and so its quadratic form can be used to formulate weak solutions.
[C.-Kim-Kumagai-Wang, 2018]

(ii) Special cases or related work: Meerschaert and Scheffler (2008) and Kolokoltsov (2011).

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Thank you!