An Invitation to Nonlocal and Fractional Models
Part two: Fractional Models

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Aim of this tutorial

I will briefly introduce:

- some differential (and integral) operators of non-integer order;
- some fractional models and motivating applications;
- some solution theory and simple numerical approximation.

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How to introduce a fractional order derivative?

There are two main approaches to generalize the order of a derivative to the fractional case:

- Generalize the difference quotient:

$$\frac{d}{dx} f(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

- With fractional integrals: recall the integration operator

$$I[f](x) = \int_0^x f(s)\,\mathrm{d}s, \qquad I^n[f](x) = I[I^{n-1}[f]](x), \quad n \geq 1.$$

  If we can define the fractional integral operator I^α with $\alpha > 0$, then a fractional derivative D^α is an inverse of I^α.

We follow the second approach in this talk.

The birth of fractional calculus

Fractional Calculus: as old as calculus!

Birthday: September 30, 1695

Leibniz and L'Hopital:

- *"Can the meaning of derivatives with integer order be generalized to derivatives with non-integer orders?"*
- *"What if the order will be 1/2?"*
- *"It will lead to a paradox, from which one day useful consequences will be drawn."*

Not a complete history:

L. Euler
(1707-1783)
1738

P.-S. Laplace
(1749-1827)
1812

J. Fourier
(1768-1830)
1822

B. Riemann
(1826-1863)
1847

J. Liouville
(1809-1882)
1832

N. Abel
(1802-1829)
1823

G. Mittag-Leffler
(1846-1927)
1903

M. Riesz
(1886-1969)
1915,1936

G. H. Hardy
(1877-1947)
1928

M. Djrbashian
(1918-1994)
1950-1970

Euler's observation (1738)

Recall the property of differentiation:

$$D^n x^m = \frac{m!}{(m-n)!} x^{m-n} = \frac{\Gamma(m+1)}{\Gamma(m-n+1)} x^{m-n}, \quad m \geq n.$$

Simple interpolation between integer cases:

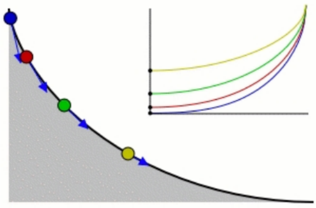
$$D^\alpha x^\beta = \frac{\Gamma(\beta+1)}{\Gamma(\alpha-\beta+1)} x^{\beta-\alpha} \qquad \alpha\text{-th order derivative}$$

$\beta - \alpha \notin \{-1, -2, -3, \ldots\}$. Here $\Gamma(z)$ denotes the Gamma function

$$\Gamma(z) = \int_0^\infty x^{z-1} e^{-x}.$$

- define fractional derivatives for polynomials;
- define fractional derivatives for all functions, which can be represented by a power series.

Abel's observation (1823): Tautochrone problem



An object slides down through a curve, only due to gravity.

Finding the curve that the total time is independent of the starting point.

- If $T(y)$ is the time of descent from height y then (tautochrone)

$$T(y) = const.$$

- At the starting position the particle is at rest

$$E(y_0) = mgy_0.$$

- At any other position

$$E(y) = mgy + \frac{1}{2}m|\mathbf{v}|^2.$$

- There is no friction, so energy is conserved. so

$$\frac{1}{2}m|\mathbf{v}|^2 = mg(y_0 - y).$$

- If s is the distance along the curve, then $\mathbf{v} = \dfrac{\mathrm{d}s}{\mathrm{d}t}$, so

$$\frac{1}{2}m\left(\frac{\mathrm{d}s}{\mathrm{d}t}\right)^2 = mg(y_0 - y).$$

- Since distance decreases with time

$$\mathrm{d}t = -\frac{1}{\sqrt{2g(y_0 - y)}}\frac{\mathrm{d}s}{\mathrm{d}y}\mathrm{d}y.$$

- Integrating

$$T(y_0) = \int_{y=y_0}^{y=0} dt = \frac{1}{\sqrt{2g}}\int_0^{y_0}\frac{1}{\sqrt{y_0 - y}}\frac{\mathrm{d}s}{\mathrm{d}y}\mathrm{d}y.$$

Recall Laplace transform

$$\hat{f}(z) = \mathcal{L}[f] = \int_0^\infty e^{-zt} f(t)\, dt.$$

If f is locally integrable on $[0, \infty)$, and if $|f(t)| \le Ce^{\lambda t}$ for $t > 0$. Then $\hat{f}(z)$ exists and is analytic for $\mathrm{R}z > \lambda$, and we have

$$f(t) = \mathcal{L}^{-1}[\hat{f}(z)] = \frac{1}{2\pi \mathrm{i}} \int_{\sigma - \mathrm{i}\infty}^{\sigma + \mathrm{i}\infty} e^{zt} \hat{f}(z)\, dz, \quad \sigma > \lambda.$$

If T is a constant, by Laplace transform, we have

$$z^{-1} T = \sqrt{\frac{\pi}{2gz}} \mathcal{L}\left[\frac{ds}{dy}\right] \Rightarrow \frac{ds}{dy} = T\frac{\sqrt{2g}}{\pi} \frac{1}{\sqrt{y}}$$

It can be shown that the cycloid obeys this equation:

$$x = T\frac{\sqrt{2g}}{\pi}(t - \sin t) \qquad y = T\frac{\sqrt{2g}}{\pi}(t - \cos t).$$

Observation: define the integral of order α $(0 < \alpha < 1)$

$$u(x) = {}_aI_x^\alpha f(x) = \frac{1}{\Gamma(\alpha)} \int_a^x (x-s)^{\alpha-1} f(s)\, ds$$

- $\alpha \to 1$: $\displaystyle \frac{1}{\Gamma(\alpha)} \int_a^x (x-s)^{\alpha-1} f(s)\, ds \to \int_a^x f(s)\, ds$
- $\alpha \to 0$:

$$\begin{aligned} &\frac{1}{\Gamma(\alpha)} \int_a^x (x-s)^{\alpha-1} f(s)\, ds \\ =& -\frac{1}{\Gamma(1+\alpha)} (x-s)^\alpha f(s)\Big|_a^x + \frac{1}{\Gamma(1+\alpha)} \int_a^x (x-s)^\alpha f'(s)\, ds \\ \to& f(a) + \int_a^x f'(s)\, ds \\ =& f(x). \end{aligned}$$

Recall that $u(x) = {}_aI_x^{\alpha} f(x)$. Note that

$$\begin{aligned}
{}_aI_x^{1-\alpha} u(x) &= {}_aI_x^{1-\alpha}\, {}_aI_x^{\alpha} f(x) \\
&= \frac{1}{\Gamma(1-\alpha)\Gamma(\alpha)} \int_a^x (x-y)^{-\alpha} \int_a^y (y-s)^{\alpha-1} f(s)\, ds\, dy \\
&= \frac{1}{\Gamma(1-\alpha)\Gamma(\alpha)} \int_a^x f(s) \int_s^x (x-y)^{-\alpha} (y-s)^{\alpha-1}\, dy\ ds \\
&= \int_a^x f(s)\, ds
\end{aligned}$$

Here we use the fact that

$$\int_s^x (x-y)^{-\alpha}(y-s)^{\alpha-1}\, dy = \int_0^{x-s} (x-s-t)^{-\alpha} t^{\alpha-1}\, dt = \Gamma(\alpha)\Gamma(1-\alpha)$$

Therefore, we derive that

$$f(x) = \frac{d}{dx}\, {}_aI_x^{1-\alpha} u(x) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_a^x (x-s)^{-\alpha} f(s)\, ds$$

This is called α-th order derivative $(0 < \alpha < 1)$

Riemann (1832) and Liouville (1847): an explicit formulation

(Left-sided) Riemann-Liouville fractional integral of order $\alpha > 0$,

$$ {}_aI_x^\alpha f(x) = \int_a^x \omega_\alpha(x-s) f(s)\, ds. $$

where the kernel $\omega_\alpha(x)$ is Gel'fand–Shilov function

$$ \omega_\alpha(x) = \frac{\max(x,0)^{\alpha-1}}{\Gamma(\alpha)} \qquad \left(\mathcal{L}[\omega_\alpha](z) = z^{-\alpha} \right) $$

Semigroup property: If $\alpha, \beta > 0$ then

$$ {}_aI_x^\alpha [\, {}_aI_x^\beta [f]](x) = {}_aI_x^{\alpha+\beta} [f](x) $$

(left-sided) Riemann-Liouville fractional derivative of order $\alpha \in (n-1, n)$

$$ {}_a^RD_x^\alpha f(x) = \frac{d^n}{dx^n} \int_a^x \omega_{n-\alpha}(x-s) f(s)\, ds. $$

Transposed Operator

Here we define the inner product

$$(f, g) = \int_a^b f(x)g(x)\,dx$$

for any functions $f, g \in L^2(a, b)$. Then we define the operator ${}_xI_b^\alpha$ by

$$({}_aI_x^\alpha f, g) = (f, {}_xI_b^\alpha g)$$

(Right-sided) R-L fractional integral of order α

$${}_xI_b^\alpha g(x) = \int_x^b \omega_\alpha(s - x)g(s)\,ds$$

(Right-sided) R-L fractional derivative of order $\alpha \in (n-1, n)$

$${}_x^RD_b^\alpha g(x) = (-1)^n \frac{d^n}{dx^n}\,{}_xI_b^{n-\alpha} g(x) = (-1)^n \frac{d^n}{dx^n} \int_x^b \omega_{n-\alpha}(s - x)g(s)\,ds$$

Remarks on R-L Derivatives

Theorem

Let $f \in W^{1,1}(a,b)$ and $\alpha \in (0,1)$. Then, for $p \in [1, 1/\alpha]$

$$ {}_a^R D_x^\alpha f(x) \in L^p(a,b) $$

and

$$ \begin{aligned} {}_a^R D_x^\alpha f(x) &= \frac{1}{\Gamma(1-\alpha)} \left[\frac{f(a)}{(x-a)^\alpha} + \int_a^x (x-y)^{-\alpha} f'(y)\, \mathrm{d}y \right] \\ &= \omega_{1-\alpha}(x-a) f(a) + {}_a I_x^{1-\alpha}[f'](x). \end{aligned} $$

- we observe that (weird)

$$ {}_a^R D_x^\alpha [1] \neq 0 $$

- If $w(a \neq 0$ we have a singularity at $t = 0$.
- ${}_a^R D_x^\alpha f(x)$ iff $f(x) = (x-a)^{\alpha-1}$.

Caputo (1967)

(left-sided) Caputo fractional derivative of order $\alpha \in (n-1, n)$:

$$ {}_a^C D_x^\alpha f(x) = {}_a I_x^{n-\alpha} \left(\frac{d^n}{dx^n} f \right)(x) = \int_a^x \omega_{n-\alpha}(x-s) \frac{d^n}{dx^n} f(s)\, ds. $$

The adjoint operator is given by

$$ {}_x^C D_b^\alpha f(x) = (-1)^n \, {}_x I_b^{n-\alpha} \left(\frac{d^n}{dx^n} f \right)(x) = (-1)^n \int_x^b \omega_{n-\alpha}(s-x) \frac{d^n}{dx^n} f(s)\, ds. $$

The two derivatives are connected, but different. $\alpha \in (0,1)$:

$$ {}_0^R D_x^\alpha 1 = \frac{1}{\Gamma(1-\alpha)} x^{-\alpha}, \qquad {}_0^C D_x^\alpha 1 = 0. $$

Connection between two definitions

Theorem

For any $\alpha \in (n-1, n)$ *and* $x > a$,

$$ {}_a^R D_x^\alpha f(x) - {}_a^C D_x^\alpha f(x) = \sum_{k=0}^{n-1} f^{(k)}(a)\omega_{k+1-\alpha}(x-a). $$

or

$$ {}_a^R D_x^\alpha f(x) - {}_a^C D_x^\alpha f(x) = {}_a^R D_x^\alpha \Big(\sum_{k=0}^{n-1} f^{(k)}(a) \frac{(x-a)^k}{k!} \Big). $$

Alternative representation of R-L derivative

Theorem

For any $\alpha \in (0, 1)$ and $x > a$,

$$ {}_{a}^{R}D_{x}^{\alpha} f(x) = -f(x)\omega_{1-\alpha}(x-a) + \int_{a}^{x} \omega_{-\alpha}(x-y)[f(y) - f(x)]\, dy. $$

Since $\omega_{-\alpha}(x)$ is singular, the integral is defined by its principle value.

$$ \int_{a}^{x} \omega_{-\alpha}(x-y)[f(y) - f(x)]\, dy = \lim_{\epsilon \to 0} \int_{a}^{x-\epsilon} \omega_{-\alpha}(x-y)[f(y) - f(x)]\, dy $$

This is related to the nonlocal operator discussed in part I.

Laplace transform of (fractional) operators

Apply the Laplace transform on (left-sided) R-L fractional integral

$$\mathcal{L}\Big({}_0I_x^\alpha f\Big)(z) = \mathcal{L}\Big(\omega_\alpha * f\Big)(z) = \widehat{\omega}_\alpha(z)\widehat{f}(z) = z^{-\alpha}\widehat{f}(z).$$

Then for smooth f and $\alpha \in (n-1, 1)$, we have

$$\begin{aligned}\mathcal{L}\Big({}_0^CD_t^\alpha f\Big)(z) &= \mathcal{L}\Big(\omega_{n-\alpha} * D^n f\Big)(z) = \widehat{\omega}_{n-\alpha}(z)\mathcal{L}\Big(D^n f\Big)(z)\\ &= z^{\alpha-n}\left(z^n\widehat{f}(z) - \sum_{k=0}^{n-1} z^{n-z-k}D^k f(0)\right)\\ &= z^\alpha f(z) - \sum_{k=0}^{n-1} z^{\alpha-z-k}D^k f(0)\end{aligned}$$

and

$$\begin{aligned}\mathcal{L}\Big({}_0^RD_t^\alpha f\Big)(z) &= \mathcal{L}\Big(D^n[{}_0I_x^{n-\alpha} f]\Big)(z) = z^n\mathcal{L}\Big[{}_0I_x^{n-\alpha} f\Big](z)\\ &= z^n z^{\alpha-n}\widehat{f}(z) = z^\alpha\widehat{f}(z).\end{aligned}$$

Fractional relaxation equation I

Problem: for $\alpha \in (0,1)$, find u satisfying

$$ {}_0^C D_t^\alpha u(t) + \lambda u(t) = 0, \qquad \text{for } \ t > 0, \quad \text{with } \ u(0) = 1. $$

The solution can be represented by the Mittag-leffler function:

$$ u(t) = E_{\alpha,1}(-\lambda t^\alpha) = \sum_{k=0}^{\infty} \frac{(-\lambda t)^k}{\Gamma(1 + k\alpha)}. $$

where the Mittag-Leffler function is

$$ E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k\alpha + \beta)} \quad z \in \mathbb{C}, $$

By Laplace transform, we see that

$$ z^\alpha \widehat{u}(z) + \lambda \widehat{u}(z) = z^{\alpha-1} \Longrightarrow \widehat{u}(z) = z^{\alpha-1}(z^\alpha + \lambda). $$

Fractional relaxation equation II

Problem: for $\alpha \in (0,1)$, find u satisfying

$$ {}_0^C D_t^\alpha u(t) + \lambda u(t) = f(t), \qquad \text{for } \ t > 0, \quad \text{with } \ u(0) = 0. $$

Laplace transform yields that

$$ \widehat{u}(z) = (z^\alpha + \lambda)^{-1} \widehat{f}(z) \Longrightarrow u(t) = \mathcal{L}\Big[(z^\alpha + \lambda)^{-1} \Big] * f(t); $$

Note that

$$ \begin{aligned} \mathcal{L}\Big[(z^\alpha + \lambda)^{-1} \Big] &= \frac{1}{2\pi \mathrm{i}} \int_\Gamma e^{zt} (z^\alpha + \lambda)^{-1} \, dz \\ &= -\lambda^{-1} \frac{d}{dt} \frac{1}{2\pi \mathrm{i}} \int_\Gamma e^{zt} z^{\alpha-1} (z^\alpha + \lambda)^{-1} \, dz \\ &= -\lambda^{-1} \frac{d}{dt} E_{\alpha,1}(-\lambda t^\alpha). \end{aligned} $$

Simple computation yields that

$$ \mathcal{L}\Big[(z^\alpha + \lambda)^{-1} \Big] = t^{\alpha-1} E_{\alpha,\alpha}(-\lambda t^\alpha). $$

Special cases of Mittag-Leffler function.

Recall that

$$E_{1,1}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k+1)} = \sum_{k=0}^{\infty} \frac{z^k}{k!} = e^z;$$

Similarly, it is easy to check that

$$E_{1,2}(z) = \frac{e^z - 1}{z};$$

$$E_{2,1}(z) = \cosh(\sqrt{z}) = \frac{e^{\sqrt{z}} + e^{-\sqrt{z}}}{2};$$

$$E_{2,1}(-z) = \sum_{k=0}^{\infty} \frac{(-1)^k z^k}{(2k)!} = \cos(\sqrt{z});$$

$$E_{2,2}(z) = \frac{\sinh(\sqrt{z})}{\sqrt{z}}.$$

Fractional Laplacian in $\mathbb{R}^d$:

Let $s \in (0,1)$ and u: $\mathbb{R}^d \to \mathbb{R}$ belongs to Schwartz class.

- Fourier transform:

$$\mathcal{F}[(-\Delta)^s u](\xi) = |\xi|^{2s}\mathcal{F}[u](\xi)$$

- Integral representation:

$$(-\Delta)^s u(x) = c_{d,s} \int_{\mathbb{R}^d} P.V. \frac{u(x)-u(y)}{|x-y|^{d+2s}}\, dy$$

  where $c_{d,s}$ is a normalization constant.

Pointwise limits:

- $\lim\limits_{s\to 0}(-\Delta)^s u = u$
- $\lim\limits_{s\to 1}(-\Delta)^s u = \Delta u$

How to define the fractional Laplacian in a bounded domain?

Track 1: Spectral fractional Laplacian

Let Ω be a bounded domain with Lipschitz boundary $\partial\Omega$.

Given $-\Delta$ with homogeneous Dirichlet boundary conditions, we let

$$-\Delta\varphi_k = \lambda_k\varphi_k, \quad \varphi_k|_{\partial\Omega} = 0.$$

φ_k form an orthogonal basis of $L^2(\Omega)$, i.e.,

$$u = \sum_{k=1}^{\infty}(u, \varphi_k)\varphi_k \quad \text{for any } u \in L^2(\Omega).$$

Then we define the spectral fractional Laplacian with $s \in (0, 1)$

$$(-\Delta)^s u = \sum_{k=1}^{\infty} \lambda_k^s (u, \varphi_k)\varphi_k.$$

Track 2: Integral fractional Laplacian

$$(-\Delta)^s u = c_{d,s} \int_{\mathbb{R}^d} \frac{u(x) - u(y)}{|y - x|^{2s}} \, dy.$$

We consider the following problem in $\mathbb{R}$

$$\begin{cases} (-\Delta)^s u = f, & \text{in } \Omega, \\ u = g, & \text{in } \Omega^c. \end{cases}$$

Note that the boundary value is given in Ω^c, not on $\partial\Omega$.

Concluding Remarks:

- fractional derivative evaluated at x does not only depend on all the values of the function around x (nonlocal)
- the definition of R-L and Caputo are imbalanced
- no product rule: $D^\alpha(fg) \neq (D^\alpha f)g + f(D^\alpha g)$
- composition rule works under certain conditions

$${}_0^C D_x^{0.4} x^{0.4} = \Gamma(1.4), \quad {}_0^C D_x^{0.4} \Gamma(1.4) = 0, \qquad {}_0^C D_x^{0.8} x^{0.4} = \frac{\Gamma(1.4)}{\Gamma(0.6)} x^{-0.4}.$$

$${}_0^R D_x^{0.4} x^{-0.6} = 0, \quad {}_0^R D_x^{0.4} 0 = 0, \qquad {}_0^R D_x^{0.8} x^{-0.6} = \frac{\Gamma(0.4)}{\Gamma(-0.4)} x^{-1.4}.$$

- relate to some special functions, e.g., Mittag-Leffler, Wright ...
- other types of definitions (Fourier, Grünwald, Letnikov...)

In conclusion, fractional calculus is old but requires extra care...

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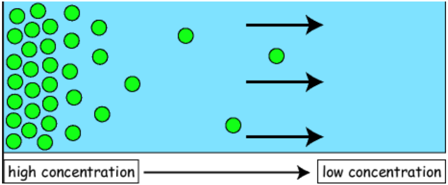
Diffusion: Adolf Fick (1855)

Adolf Fick



Diffusion

Macroscopic description: $\partial_t u = D\Delta u.$

Derivation of normal diffusion equation

:Local balance (conservation of Mass):

$$\frac{d}{dt}\int_U u\,dx = -\int_{\partial U} \mathbb{F}\cdot\nu\,dS = -\int_U \nabla\cdot\mathbb{F}\,dx \Rightarrow u_t = -\nabla\cdot\mathbb{F}$$

Linear response (Fick's first law):

$$\mathbb{F} = -D\nabla u.$$

Finally, this two physical laws lead to

$$u_t = D\Delta u.$$

Particle's Brownian motion: A. Einstain (1905), J. Perrin (1908)

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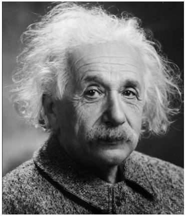
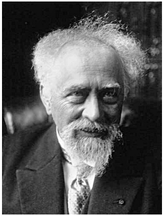




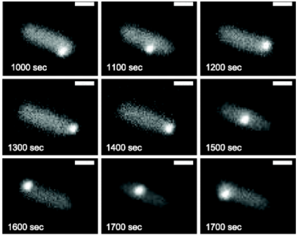
Fundamental solution: PDF to find a particle at position x and time t

$$u(x,t) = \frac{1}{(2\pi Dt)^{n/2}} e^{-\frac{|x|^2}{4Dt}}.$$

Mean square displacement of the particle:

$$\langle x^2(t) \rangle = \int_{-\infty}^{\infty} x^2 u(x,t)\, dx = 2Dt.$$

Diffusion in heterogeneous media



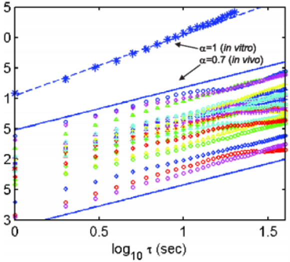
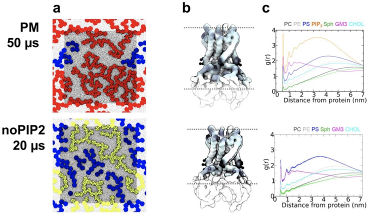


Figure: RNA movement in bacterial cytoplasm(Golding-Cox PRL 2006)

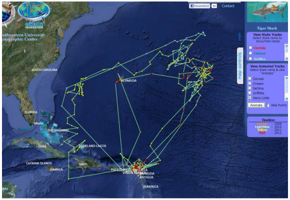
Observation:

- trajectory of target RNA is discontinuous;
- jumps are separated by random waiting times;
- MSD: $\langle x^2(t)\rangle \propto t^\alpha$.

ANOMALOUS IS NORMAL!



(a) Diffusion of proteins and lipids (Duncan etc. Sci. Rep. 2017)



(b) Migration of Tiger sharks (NSU Guy Harvey Research Inst.)

- RNA movement in bacterial cytoplasm (Golding-Cox PRL 2006),
- ultracold atoms in a polarization optical lattice (Sagi etc. PRL 2012),
- contaminants in groundwater (Kirchner-Feng-Neal Nature 2000),
- material with thermal memory(Wolfersdorf MMAS 1994),
- animals' hunting strategy (Viswanathan etc. Nature 1996, Raichlen etc. PNAS 2013)...

Generalized model: continuous time random walk (CTRW)

- the pdf of waiting time: $\psi(t)$, $t \in [0, \infty)$.
- the pdf of jump length: $\varphi(x)$, $x \in (-\infty, \infty)$.

Assumption

- a walker moves along the x-axis, starting at x_0 and $t_0 = 0$
- at time t_1, the walker jumps to position x_1
- at time t_2, the walker jumps to position x_2...

Assume that the increment satisfies

$$\Delta t_n = t_n - t_{n-1} \quad \text{and} \quad \Delta x_n = x_n - x_{n-1}$$

are i.i.d. random variables with pdf ψ and φ, respectively, i.e.,

$$P(a < \Delta t < b) = \int_a^b \psi(t)\, dt, \quad 0 < a < b < \infty$$

$$P(a < \Delta x < b) = \int_a^b \varphi(x)\, dx, \quad -\infty < a < b < \infty$$

Example

The waiting-time distribution is exponential with parameter $\tau > 0$,

$$\psi(t) = \tau^{-1} e^{-t/\tau} \quad \text{for} \quad 0 < t < \infty$$

The jump-length distribution is normal with mean 0 and variance σ^2,

$$\varphi(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{x^2}{2\sigma^2}\right)$$

Then the waiting time Δt_n and jump length Δx_n satisfy

$$\mathbb{E}(\Delta t_n) = \tau,\ \mathbb{E}(\Delta t_n^2) = \tau^2,\ \mathbb{E}(\Delta x_n) = 0,\ \mathbb{E}(\Delta x_n^2) = \sigma^2$$

The position $x(t)$ of the walker is a step function.

Trajectory of the CTRW with $\tau = 1$ and $\sigma = 1$

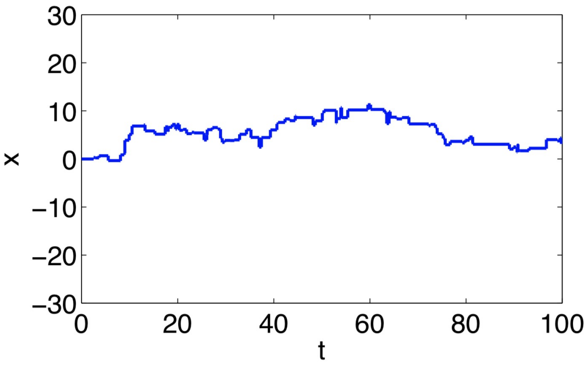


Figure: One-dimensional CTRW, with exponential waiting time distribution (with $\tau = 1$) and Gaussian jump length distribution (with $\sigma = 1$), starting from $x_0 = 0$.

Probability Density

Let $p(x,t)$ denote the pdf for the position of the particle at time t, that is,

$$P(a < x(t) - x_0 < b) = \int_a^b p(x,t)\,dx.$$

Then in the Laplace-Fourier domain

$$\widehat{\widetilde{p}}(\xi,z) = \frac{1-\widehat{\psi}(z)}{z}\frac{1}{1-\widetilde{\varphi}(\xi)\widehat{\psi}(z)}$$

Example

$$\psi(t) = \tau^{-1}e^{-t/\tau} \quad \text{and} \quad \varphi(x) = \frac{1}{\sigma\sqrt{2\pi}}\exp\left(-\frac{x^2}{2\sigma^2}\right)$$

Direct computation leads to

$$\widehat{\psi}(z) = \frac{1}{1+\tau z} \quad \text{and} \quad \widetilde{\varphi}(\xi) = e^{-\sigma^2\xi^2/2}$$

and hence

$$\widehat{\widetilde{p}}(\xi,z) = \frac{\tau}{1+\tau z - \exp(-\sigma^2\xi^2/2)}.$$

Classification of CTRW

Different types of CTRW processes can be categorized by

the characteristic waiting time

$$T = \mathbb{E}[\Delta t_n] = \int_0^\infty t\psi(t)\,dt$$

and the jump length variance

$$\Sigma^2 = \mathbb{E}[(\Delta x_n)^2] = \int_{-\infty}^\infty x^2\varphi(x)\,dx$$

being finite or diverging.

In the rest of this section, we shall discuss the following three scenarios:

(i) Finite T and Σ^2

(ii) Diverging T and finite Σ^2

(iii) Diverging Σ^2 and finite T.

Case (i) Finite T and Σ^2 (Brownian Motion)

Let the pdfs $\psi(t)$ and $\varphi(x)$ be normalized to satisfy

$$\int_0^\infty t\psi(t)\,dt = 1, \quad \int_{-\infty}^\infty x\varphi(x)\,dx = 0, \quad \int_{-\infty}^\infty x^2\varphi(x)\,dx = 1.$$

Two physical parameters $\tau > 0$ and $\sigma > 0$.

Let the random variables Δt_n and Δx_n follow the rescaled pdfs

$$\psi_\tau = \frac{1}{\tau}\psi\left(\frac{t}{\tau}\right) \quad \text{and} \quad \varphi_\sigma = \frac{1}{\sigma}\varphi\left(\frac{x}{\sigma}\right)$$

a simple computation shows

$$\mathbb{E}(\Delta t_n) = \tau,\ \mathbb{E}(\Delta t_n^2) = \tau^2,\ \mathbb{E}(\Delta x_n) = 0,\ \mathbb{E}(\Delta x_n^2) = \sigma^2$$

Case (i) Finite T and Σ^2

By the scaling rules for the Fourier and Laplace transformations:

$$\widehat{\psi}_\tau(z) = \widehat{\psi}(\tau z) \quad \text{and} \quad \widetilde{\varphi}_\sigma(\xi) = \widetilde{\varphi}(\sigma\xi)$$

and hence

$$\widehat{\widetilde{p}}(\xi, z; \sigma, \tau) = \frac{1 - \widehat{\psi}(\tau z)}{z} \frac{1}{1 - \widehat{\psi}(\tau z)\widetilde{\varphi}(\sigma\xi)}.$$

We shall study the diffusion limit, i.e., as $\tau, \sigma \to 0$. The Taylor expansion

$$\widehat{\psi}(z) = \widehat{\psi}(0) + \widehat{\psi}'(0)z + O(z^2) = 1 - z + O(z^2).$$

and

$$\widehat{\varphi}(\xi) = 1 - \frac{1}{2}\xi^2 + O(\xi^4).$$

Then simple algebra (left as an exercise) gives

$$\widehat{\widetilde{p}}(\xi, z; \sigma, \tau) = \frac{\tau}{\tau z + \frac{1}{2}\sigma^2\xi^2} \times \frac{1 + O(\tau z)}{1 + O(\tau z + \sigma^2\xi^2)}.$$

Case (i) Finite T and Σ^2

Now let $\sigma \to 0$ and $\tau \to 0$ with the scaling $\dfrac{\sigma^2}{2\tau} = D$ for a fixed number $D > 0$ and obtain that

$$\widehat{\widetilde{p}}(\xi, z) = \lim_{\sigma,\tau\to 0} \frac{\tau}{\tau z + \frac{1}{2}\sigma^2\xi^2} = \frac{1}{z + D\xi^2}.$$

Inverting the Laplace transform, we have

$$\widetilde{p}(\xi, t) = \frac{1}{2\pi \mathrm{i}} \int_\Gamma \frac{e^{zt}\, dz}{z + D\xi^2} = e^{-D\xi^2 t}.$$

Then inverting the Fourier transform we obtain that

$$p(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-D\xi^2 t} e^{\mathrm{i}\xi x}\, d\xi = \frac{1}{\sqrt{4\pi D t}} \exp\left(-\frac{x^2}{4Dt}\right)$$

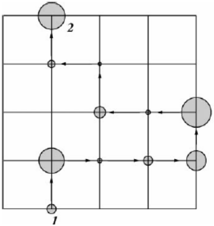
which satisfies the normal diffusion equation

$$\partial_t p(x, t) - \partial_{xx} p(x, t) = 0 \quad \text{for} \quad t \in (0, \infty),\ x \in (-\infty, \infty)$$

Case (ii) Divergent T and finite Σ^2

- the characteristic waiting time T diverges
- jump length variance Σ^2 is still kept finite

This occurs for example when the particle might be trapped in a certain potential well, and it takes a long time to leave.



To model such phenomena, we employ a heavy-tailed waiting time pdf with the asymptotic behaviour for some $\alpha \in (0, 1)$

$$\psi(t) \sim At^{-\alpha-1} \quad \text{as} \quad t \to \infty$$

Case (ii) Divergent T and finite Σ^2

One example of such pdfs is

$$\psi(t) = A/(1+t)^{\alpha+1}$$

Remark

- The (asymptotic) power law decay is heavy tailed, and allows occasional very large waiting time between consecutive walks.
- Again, the specific form of $\psi(t)$ is irrelevant, and only the power law decay at large time matters.
- The parameter α determines the asymptotic decay of the pdf $\psi(t)$.
- The mean waiting time is divergent:

$$\int_0^\infty t\psi(t)\,dt = \infty$$

Case (ii) Divergent T and finite Σ^2

the assumption on $\varphi(x)$ remains unchanged, i.e.,

$$\int_{-\infty}^{\infty} x\varphi(x)\,dx = 0 \quad \text{and} \quad \int_{-\infty}^{\infty} x^2\varphi(x)\,dx = 1.$$

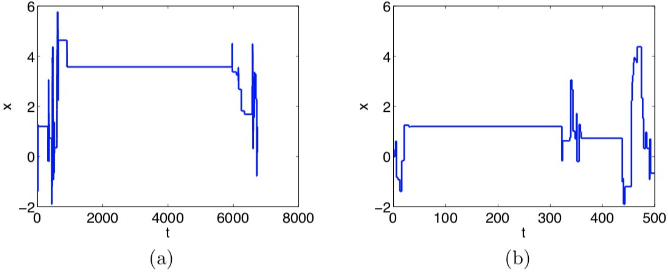


Figure: CTRW with a power law waiting time pdf. Panel (a) is one sample trajectory with waiting time pdf $\psi(t) = \alpha/(1+t)^{\alpha}$ $\alpha = 3/4$, and standard Gaussian jump length pdf; Panel (b) is a zoom-in of the first cluster of Panel (a).

Case (ii) Divergent T and finite Σ^2

As previously, now we introduce the following rescaled pdfs

$$\psi_\tau = \frac{1}{\tau}\psi\left(\frac{t}{\tau}\right) \quad \text{and} \quad \varphi_\sigma = \frac{1}{\sigma}\varphi\left(\frac{x}{\sigma}\right)$$

and the Laplace-Fourier transform yields

$$\widehat{\widetilde{p}}(\xi, z; \sigma, \tau) = \frac{1 - \widehat{\psi}(\tau z)}{z} \frac{1}{1 - \widehat{\psi}(\tau z)\widetilde{\varphi}(\sigma\xi)}.$$

Next we apply the expansion

$$\widehat{\psi}(z) = 1 - B_\alpha z^\alpha + O(z) \quad \text{and} \quad \widehat{\varphi}(\xi) = 1 - \frac{1}{2}\xi^2 + O(\xi^4),$$

Case (ii) Divergent T and finite Σ^2

Consequently, simple algebraic manipulations give

$$\widehat{\widetilde{p}}(\xi, z; \sigma, \tau) = \frac{B_\alpha \tau^\alpha z^{\alpha-1}}{B_\alpha \tau^\alpha z^\alpha + \frac{1}{2}\sigma^2 \xi^2} \times \frac{1 + O(\tau^{1-\alpha} z^{1-\alpha})}{1 + O(\tau^{1-\alpha} z^{1-\alpha} + \tau^\alpha z^\alpha + \sigma^2 \xi^2)}.$$

Consider the diffusion limit by sending $\sigma \to 0$ and $\tau \to 0$ while keeping

$$\frac{\sigma^2}{2B_\alpha \tau^\alpha} = D_\alpha$$

for some fixed $D_\alpha > 0$. Thus we obtain

$$\widehat{\widetilde{p}}(\xi, z) = \frac{z^{\alpha-1}}{z^\alpha + D_\alpha \xi^2}$$

Notice that we recover the earlier formula by putting $\alpha = 1$.

Case (ii) Divergent T and finite Σ^2

Invert the Fourier-Laplace transform back into the space-time domain.

$$\widetilde{p}(\xi, t) = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma} e^{zt} \frac{z^{\alpha-1}}{z^{\alpha} + D_{\alpha}\xi^2} \, dz = E_{\alpha,1}(-D_{\alpha}\xi^2 t^{\alpha})$$

Next applying the Fourier transform of the M-Wright function

$$p(x, t) = \frac{1}{2\sqrt{D_{\alpha} t^{\alpha}}} M_{\alpha/2}\left(\frac{|x|}{\sqrt{D_{\alpha} t^{\alpha}}}\right).$$

With $\alpha = 1$, this formula recovers the Gaussian density.

It is easy to check that the pdf $p(x, t)$ satisfies the following time fractional diffusion equation

$$\partial_t^{\alpha} p(x, t) = D_{\alpha} \partial_{xx} p(x, t) \quad \text{for} \ \ t \in (0, \infty), \ x \in (-\infty, \infty)$$

∂_t^{α} denotes the (left sided) Caputo fractional derivative starting from 0.

Case (ii) Divergent T and finite Σ^2

Now let us compute the mean square displacement

$$m(t) = \int_{-\infty}^{\infty} x^2 p(x,t)\, dx, \quad t > 0.$$

To derive an explicit formula, we resort to the Laplace transform

$$\begin{aligned} \widehat{m}(z) &= \int_{-\infty}^{\infty} x^2 \widehat{p}(x,z)\, dx = -\frac{d^2}{d\xi^2}\widehat{\widehat{p}}(\xi,z)\Big|_{\xi=0} \\ &= -\frac{d^2}{d\xi^2}\frac{z^{\alpha-1}}{z^\alpha + D_\alpha \xi^2}\Big|_{\xi=0} = 2D_\alpha z^{-1-\alpha} \end{aligned}$$

which upon inverse Laplace transform yields

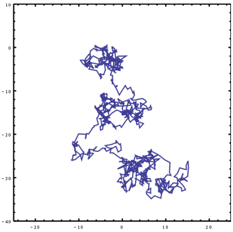
$$m(t) = \frac{2D_\alpha}{\Gamma(1+\alpha)} t^\alpha \qquad \text{subdiffusion}$$

the MSD grows only sublinearly with the time t, which, at large time t, is slower than that in the Gaussian diffusion case.

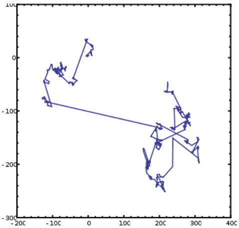
Case (iii) Finite T and Divergent Σ^2

- the characteristic waiting time T is kept finite
- jump length variance Σ^2 is divergent

To be specific, we assume an exponential waiting time $\psi(t)$, and that the jump length follows a (possibly asymmetric) Lévy distribution.



(a) Brownian motion



(b) Levy Flight

Case (iii) Finite T and Divergent Σ^2

Standard Lévy stable random variables via their characteristic function

$$\ln \widetilde{\varphi}(\xi;\mu,\beta) = \begin{cases} -|\xi|^\mu(1 - \mathrm{i}\beta \mathsf{sign}(\xi)\tan(\frac{\mu\pi}{2})), & \mu \neq 1, \\ -|\xi|^\mu(1 + \mathrm{i}\beta \mathsf{sign}(\xi)\frac{2}{\pi}\ln|\xi|), & \mu = 1, \end{cases}$$

where $\mu \in (0,2)$, $\beta \in [-1,1]$.

Remark on μ

- μ determines the decay rate at which the tails of the pdf taper off.

  $$\varphi(x) \sim A_{\mu,\beta}|x|^{-1-\mu}, \quad \text{as} \quad |x| \to \infty$$

  The second moment diverges.
- When $\mu = 2$, it recovers a Gaussian distribution.
- $\mu = 1$ and $\beta = 0$, the density is identical to the Cauchy distribution

  $$\varphi(x) = \frac{1}{\pi(1+x^2)}.$$

Case (iii) Finite T and Divergent Σ^2

Remark on β

- β lies in the range $[-1, 1]$, and determines the degree of asymmetry of the distribution.
- When β is negative (respectively positive), the distribution is skewed to the left (respectively right).
- In the symmetric case $\beta = 0$, the expression simplifies to

$$\widetilde{\varphi}(\xi; \mu) = e^{-|\xi|^{\mu}}.$$

Case (iii) Finite T and Divergent Σ^2

By similar argument, we have

$$\widehat{\widetilde{p}}(\xi, z) = \lim_{\sigma,\tau\to 0} \widehat{\widetilde{p}}(\xi, z; \sigma, \tau) = \frac{1}{z + D_\mu |\xi|^\mu (1 - \mathrm{i}\beta \operatorname{sign}(\xi) \tan \frac{\mu\pi}{2})}$$

where we keep the scaling

$$D_\mu = \frac{\sigma^\mu}{\tau}$$

for some positive constant $D_\mu > 0$, which represents the diffusion coefficient in the stochastic process.

However, an explicit expression is unavailable.

One can verify by Fourier and Laplace inversion, the pdf satisfies

$$\partial_t p(x,t) = \frac{D_\mu}{2} \left((1-\beta)\, {}_{-\infty}^{\;R}D_x^\mu + (1+\beta)\, {}_{x}^{R}D_\infty^\mu p(x,t) \right).$$

for $t \in (0, \infty)$ and $x \in (-\infty, \infty)$

Case (iii) Finite T and Divergent Σ^2

In particular, $\beta = 0$, it further simplifies to

$$\partial_t p(x,t) = D_\mu \nabla_x^\mu p(x,t),$$

were ∇_x^μ denotes the Riesz fractional operator

$$D_\mu \nabla_x^\mu f = \frac{1}{2}\left({}_{-\infty}^{\ R}D_x^\mu + {}_{x}^{R}D_\infty^\mu \right) f$$

The solution in this case can be obtained using the Fox functions.

Further, we have the power-law asymptotics as

$$p(x,t) \sim \frac{D_\mu t}{|x|^{1+\mu}}, \quad \text{as} \ \ |x| \to \infty.$$

Therefore, the mean squared displacement diverges (superdiffusion).

Remark

- the divergent mean squares displacement has caused some controversy in practice, and various modifications have been proposed.
- boundary value problems for superdiffusion are much more involved than for the subdiffusive case, as the long jumps make the very definition of a boundary condition actually quite intricate.
- if $\Omega = \mathbb{R}$, the Riesz fractional operator is equivalent to both the spectral fractional Laplacian and regional fractional Laplacian, which can be easily checked by it Fourier transform. However, in the bounded domain, it is identical to the regional fractional Laplacian.

R. Metzler, J. Klafter, The random walk's guide to anomalous diffusion: a fractional dynamics approach, (339) (1), 2000, 1–77. (7427 google scholar citations)

Artificial boundary condition

Consider the IBVP of one-dimensional heat equation

$$\begin{cases} \partial_t u - \partial_{xx} u = f, & (x,t) \in (-1,\infty) \times (0,T), \\ u(x,0) = u_0, & x \in (-1,\infty), \\ u(-1,t) = 0, & t \in (0,T), \\ u(x,t) \to 0, & x \to \infty. \end{cases}$$

Note that the problem is posed on the infinite domain $(-1,\infty)$.

Assume that both of u_0 and f have compact supports in $(-1,0)$.

Our goal is to compute the solution in a finite domain $(-1,0)$.

However, we need the boundary condition on $x=0$.

Artificial boundary condition

To this end, we consider the following exterior problem.

$$\begin{cases} \partial_t u - \partial_{xx} u = 0, & (x,t) \in (0,\infty) \times (0,T), \\ u(x,0) = 0, & x \in (0,\infty), \\ u(0,t) \ \text{ is given}, & t \in (0,T), \\ u(x,t) \to 0, & x \to \infty. \end{cases}$$

Applying Laplace transform, it is easy to have

$$z\widehat{u}(x,z) - \partial_{xx} u(x,z) = 0.$$

Then the general solution can be written as

$$\widehat{u}(x,z) = c_1(z) e^{\sqrt{z}x} + c_2(z) e^{-\sqrt{z}x}$$

Artificial boundary condition

Meanwhile, since $\mathrm{Re}\sqrt{z} > 0$, we apply the boundary condition at infinity

$$\widehat{u}(x, z) = c_2(z)e^{-\sqrt{z}x}.$$

where $c_2(z)$ is the Laplace transform of the boundary condition:

$$c_2(z) = \widehat{u}(0, z).$$

Then a simple computation yields that

$$\widehat{u}_x(0, z) = -\sqrt{z}\widehat{u}(0, z).$$

On the other hand, noting that $u(0, 0) = 0$, we have

$$\mathcal{L}[\partial_t^{\frac{1}{2}} u(0, t)](z) = \sqrt{z}\widehat{u}(0, z).$$

As a result, we have that

$$-\mathcal{L}[\partial_t^{\frac{1}{2}} u(0, t)] = \mathcal{L}[u_x(0, t)]$$

Artificial boundary condition

After the inverse transform, we have

$$u_x(0,t) = -\partial_t^{\frac{1}{2}} u(0,t).$$

This supply a dynamic boundary condition at $x = 0$.

Therefore, it suffices to find the solution of the following IBVP:

$$\begin{cases} \partial_t u - \partial_{xx} u = f, & (x,t) \in (-1,0) \times (0,T), \\ u(x,0) = u_0, & x \in (-1,0), \\ u_x(0,t) = -\partial_t^{\frac{1}{2}} u(0,t), & t \in (0,T) \\ u(-1,t) = 0, & t \in (0,T), \end{cases}$$

Dirichlet to Neumann Map (DtN):

Let $\Omega \in \mathbb{R}^d$ be a bounded domain with Lipschitz boundary $\partial\Omega$.

$U(x_1, x_2, \ldots, x_d, y)$ is the solution to the following BVP:

$$\begin{cases} \operatorname{div}(\nabla U) = 0, & \text{in } \Omega \times \mathbb{R}^+, \\ U = 0, & \text{on } \partial\Omega \times \mathbb{R}^+, \\ -\lim\limits_{y \to 0} \partial_y U = f, & \text{on } \Omega \times \{0\}, \end{cases}$$

Question: what is the value of U on Ω (i.e., $y = 0$)?

Let Δ be the standard Laplacian on Ω, with the homogenenous Dirithlet boundary condition. Then the elliptic equation is equivalent to

$$-\Delta U - \partial_{yy} U = 0.$$

$\{\lambda_n\}$ denote the eigenvalues of such $-\Delta$, and $\{\varphi_n\}$ are correspondition normalized eigenfunctions.

Dirichlet to Neumann Map (DtN):

Take inner product with φ_n in $L^2(\Omega)$, we have

$$\lambda_n(U(\cdot,y),\varphi_n) - \partial_{yy}(U(\cdot,y),\varphi_n) = 0,$$

where $(\cdot,\cdot)$ denotes the inner product in $L^2(\Omega)$, i.e.,

$$(f,g) = \int_\Omega f(x)g(x)\,dx.$$

Then the general solution can be written as

$$(U(\cdot,y),\varphi_n) = c_{1,n}e^{\sqrt{\lambda_n}y} + c_{2,n}e^{-\sqrt{\lambda_n}y}.$$

Using the decay condition at infinity, we know that $c_{1,n} = 0$.

Now apply the boundary condition at $y = 0$, we have

$$(\partial_y U(\cdot,y),\varphi_n)\Big|_{y=0} = -c_{2,n}\sqrt{\lambda_n} = -(f,\varphi_n).$$

Dirichlet to Neumann Map (DtN):

Therefore,

$$c_{2,n} = \frac{1}{\sqrt{\lambda_n}}(f, \varphi_n).$$

If we let

$$u(x) = U(x,y)\Big|_{y=0} = c_{2,n}e^{-\sqrt{\lambda_n}y}|_{y=0} = c_{2,n}.$$

Then, we have derived that

$$\sqrt{\lambda_n}(u, \varphi_n) = (f, \varphi_n), \quad \text{for all} \quad n \in \mathbb{N}^+.$$

This is equivalent to

$$(-\Delta)^{\frac{1}{2}}u = f \qquad \text{in } \Omega,$$

where Δ is the Laplacian on Ω with the homog. Dirichlet BC.

Fractional Dirichlet-to-Neumann map: L. Caffarelli and L. Silvestre. An extension problem related to the fractional Laplacian. Communications in Partial Differential Equations, (2007) (1887 google scholar citations).

Table of Contents

Time-fractional diffusion equation

Initial-boundary value problem: $0 < \alpha < 1$, for $u(x,t)$ for $T \geq t > 0$:

$$\begin{aligned} \partial_t^\alpha u - \Delta u &= f, \quad \text{in } \Omega \qquad T \geq t > 0, \\ u &= 0, \quad \text{on } \partial\Omega \quad T \geq t > 0, \\ u(0) &= v, \quad \text{in } \Omega. \end{aligned}$$

Ω: bounded, convex polygonal domain in $\mathbb{R}^d$

∂_t^α: the left-sided Caputo fractional derivative of order $\alpha \in (0,1)$

$$\partial_t^\alpha u(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-\tau)^{-\alpha} \frac{d}{d\tau} u(\tau)\, d\tau.$$

The model is known to capture well the dynamics of sub-diffusion.

Smoothing property

Fractional diffusion: $(f \equiv 0, \quad v \neq 0)$:

$$\|u(t)\|_{\dot{H}^p(\Omega)} \leq Ct^{-\frac{p-q}{2}\alpha}\|v\|_{\dot{H}^q(\Omega)}, \quad 0 \leq q \leq p+2, \quad \ell \geq 0.$$

Spatial regularity restriction (order 2)!!!

The estimate is sharp in sense that Sakamoto-Yamamoto JMAA 2011

$$c_1\|v\|_{L^2} \leq \|u(t)\|_{H^2} \leq c_2\|v\|_{L^2}.$$

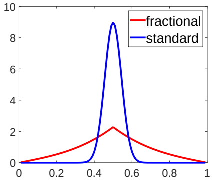
Standard diffusion: $(f \equiv 0, \quad v \neq 0)$:

$$\|u(t)\|_{\dot{H}^p(\Omega)} \leq Ct^{-\frac{p-q}{2}}\|v\|_{\dot{H}^q(\Omega)}, \quad 0 \leq q \leq p, \quad \ell \geq 0.$$

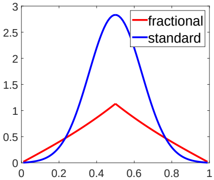
Smoothing property

1-D example: $\partial_t^\alpha u - u_{xx} = 0$, $v(x) = \delta_{1/2}(x) \in \dot{H}^{-1/2-\epsilon}(\Omega)$

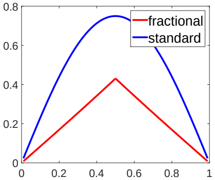
Plot of $u(t)$ at $t = 10^{-1}$, 10^{-2} and 10^{-3};



(c) $t = 10^{-3}$



(d) $t = 10^{-2}$



(e) $t = 10^{-1}$

$\alpha \in (0,1)$: continuous and piecewise smooth for all $t > 0$

$\alpha = 1$: infinitely differentiable for all $t > 0$

Galerkin FE Approx.

$\mathcal{T}_h$: regular partitions of Ω into d-simplexes.

$$X_h = \left\{\chi \in H_0^1(\Omega) : \ \chi \ \text{ is a linear function over } \ \tau, \quad \forall \tau \in \mathcal{T}_h\right\}.$$

The semidiscrete Galerkin FEM: find $u_h(t) \in X_h$ such that

$$\begin{gathered}(\partial_t^\alpha u_h, \chi) + (\nabla u_h, \nabla \chi) = (f, \chi), \quad \forall \chi \in X_h, \ T \geq t > 0, \\ u_h(0) = v_h,\end{gathered}$$

- choice of v_h depends on the regularity of v;
- solution can be expressed by Mittag-Leffler function.

Nonsmooth data, $v \in H^{-s}(\Omega)$ with $s \in [0,1)$: Jin-Lazarov-Z 2013

$$\|u_h(t) - u(t)\|_{L^2(\Omega)} \leq ch^{2-s} t^{-\alpha} \|v\|_{H^{-s}(\Omega)}.$$

Question: develop a high-order method in case of nonsmooth data?

Time discretization

- history mechanism: storage issue
- limited smoothing property: low accuracy

Popular schemes:

- collocation method (L1, L1-2...) Lin-Xu 2007, Sun-Wu 2006...
- convolution quadrature using BDF Lubich 1986, 1988...
- spectral methods Chen-Xu-Hesthaven 2015, Chen-Shen-Zhang-Z 2020...,
- DG methods Mustapha-McLean 2013, Mustapha-Abdallah-Furati 2014...

Piecewise linear collocation method (L1 scheme)

Step size τ and $t_n = n\tau$:

$$\begin{aligned}
\partial_t^\alpha u(t_n) &= \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{n-1} \int_{t_j}^{t_{j+1}} \frac{\partial u(s)}{\partial s} (t_n - s)^{-\alpha}\, ds \\
&\approx \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{n-1} \frac{u(t_{j+1}) - u(t_j)}{\tau} \int_{t_j}^{t_{j+1}} (t_n - s)^{-\alpha} ds \\
&= \tau^{-\alpha}[b_0 u(t_n) - b_n u(t_0) + \sum_{j=1}^{n} (b_j - b_{j-1}) u(t_{n-j})] =: \bar{\partial}_\tau^\alpha u^n,
\end{aligned}$$

where the weights b_j are given by $b_j = ((j+1)^{1-\alpha} - j^{1-\alpha})/\Gamma(2-\alpha)$.

Fully discrete: Given u_h^k, $k = 0, 1, \ldots, n-1$, we compute u^n by

$$\bar{\partial}_\tau^\alpha u_h^n - \Delta u_h^n = f_h(t_n).$$

This yields a clean time-stepping scheme.

Error estimate

Truncation error:

$$\max_{n=1,2,\ldots N} |\partial_t^\alpha u(t_n) - \bar\partial_\tau^\alpha u^n| \le c\tau^{2-\alpha}\|u\|_{C^2[0,T]}$$

Y. Lin, C. Xu. Finite difference/spectral approximations for the time-fractional diffusion equation. J. Comput. Phys. 225, 1533–1552. (1050 Google Scholar citation)

In general, piecewise kth order polynomial approximation:

$$\max_{n=1,2,\ldots N} |\partial_t^\alpha u(t_n) - \bar\partial_\tau^\alpha u^n| \le c\tau^{k+1-\alpha}\|u\|_{C^{k+1}[0,T]}$$

M. Stynes. Too much regularity may force too much uniqueness. Fract. Calc. Appl. Anal. 19 (2016), no. 6, 1554–1562.

$$E_{\alpha,1}(-t^\alpha) = 1 - t^\alpha/\Gamma(1-\alpha) + O(t^{2\alpha}).$$

- In general, $u \in C^\alpha([0,T];L^2(\Omega))$;
- the low regularity leads to the bad approximation.

Time discretization with graded mesh

One can (should?) consider graded meshes

- M. Stynes, E. O'Riordan, Eugene, J.L. Gracia. Error analysis of a finite difference method on graded meshes for a time-fractional diffusion equation. SIAM J. Numer. Anal. 55 (2017) 1057–1079.
- H. Liao, W. McLean, J. Zhang. A discrete Grönwall inequality with applications to numerical schemes for subdiffusion problems. SIAM J. Numer. Anal. 57 (2019), 218–237
- N. Kopteva. Error analysis of the L1 method on graded and uniform meshes for a fractional-derivative problem in two and three dimensions. Math. Comp. 88 (2019), 2135–2155.
- K. Mustapha, B. Abdallah, K. Furati. A discontinuous Petrov-Galerkin method for time-fractional diffusion equations. SIAM J. Numer. Anal. 52 (2014), 2512–2529.
- S. Chen, J. Shen, Z. Zhang, Z, A spectrally accurate approximation to subdiffusion equations using the log orthogonal functions. SIAM J. Sci. Comput. 42 (2020), A849–A877.

Convolution quadrature (CQ)

C. Lubich NM 1986, SIMA 1988

For $u(t) = 0$ for $t \le 0$, apply Laplace transform

$$\mathcal{L}[\partial_t^\alpha u](z) = z^\alpha \mathcal{L}[u](z)$$

We want the numerical scheme by discrete convolution

$$\bar\partial_\tau^\alpha u(t) = \tau^{-\alpha} \sum_{j=0}^{\infty} \omega_j u(t - j\tau)$$

Then apply Laplace transform

$$\mathcal{L}[\bar\partial_\tau^\alpha u(t)](\xi) = \tau^{-\alpha} \sum_{j=0}^{\infty} \omega_j \int_0^\infty u(t - j\tau) e^{zt}\, dt = \tau^{-\alpha} \sum_{j=0}^{\infty} \omega_j e^{jz\tau} \mathcal{L}[u](z)$$

Backward Euler scheme:

$$\sum_{j=0}^{\infty} \omega_j \xi^j = (1 - \xi)^\alpha.$$

Convolution quadrature (CQ)

Taylor's expansion:

$$\tau^{-\alpha}\sum_{j=0}^{\infty}\omega_j e^{jz\tau} = \Big[\frac{1-e^{-z\tau}}{\tau}\Big]^{\alpha} = z^{\alpha} + cz^{1+\alpha}\tau + o(\tau)$$

is the first order approximation of z^{α}.

Fully discrete scheme:

Given u_h^k, $k = 0,\, 1,\, \ldots,\, n-1$, we compute u^n by

$$\bar\partial_\tau^{\alpha}(u_h^n - u_h^0) - \Delta u_h^n = f_h(t_n).$$

Advantage: inherit the stability and accuracy of backward Euler scheme.

Apply generating functions of high-order schemes (with extra correction)

- Backward Differentiation Formula (BDF): Jin-Li-Z 2017
- Runge-Kutta scheme: Banjai, López-Fernández 2019, Fischer 2019
- L1 scheme: Yan-Khan-Ford 2018

Remark

Open problems:

- time-dependent diffusion coefficients;
- high-order spatial approximations;
- nonlinear models and high-order approximation ...

Other relevent works:

- fast algorithms: Achim-LopezFernandez-Lubich 2006, Mclean 2013, Zhang-Zhang-Jiang-Zhang 2017
- inverse problem: Cheng-Nakagawa-Yamamoto-Yamazaki 2009, Zheng-Wei 2010, Jin-Rundell 2015, Liu-Li-Yamamoto 2019 ...
- optimal control: Zhou-Gong 2016, Jin-Li-Z 2017

Space-fractional superdiffusion models

Defined by fractional derivatives: with $\alpha \in (1,2)$ and $\theta \in (0,1)$:

$$-[\theta\, {}_0D_x^\alpha + (1-\theta)\, {}_xD_1^\alpha]u + bu' + qu = f, \quad x \in D = (0,1),$$
$$u(0) = u(1) = 0,$$

- two-point boundary value problem.
- two different types: Caputo (C) or Riemann-Liouville (RL).
- different choices give different solution behaviors.
- in particular, if $b = q = 0$ and $\theta = 1/2$, RL fractional derivatives is equivalent to the integral fractional Laplacian $(-\Delta)^{\alpha/2}$.
- RL, boundary singularity... Ervin-Heuer-Roop 2018

$$\begin{cases} x^{\alpha-1} + \ldots, & \theta > \frac{1}{2}, \\ (1-x)^{\alpha-1} + \ldots, & \theta < \frac{1}{2}, \\ \text{dist}(x, \partial D)^{\alpha/2} + \ldots, & \theta = \frac{1}{2}. \end{cases}$$

Fractional Sturm-Liouville problem

For $\alpha \in (1,2)$, we consider the 1-D fractional Sturm-Liouville problem:

$$
\begin{aligned}
-{}_0D_x^{\alpha} u + qu &= \lambda u, \quad x \in D = (0,1), \\
u(0) = u(1) &= 0,
\end{aligned}
$$

- $q \in L^{\infty}(\Omega)$ or a suitable subspace
- ${}_0D_x^{\alpha}$: left-sided Riemann-Liouville or Caputo fractional derivative
- $\alpha \to 2$, it reduces to Classical Sturm-Liouville problem
- space fractional (super)-diffusion: Levy Flight

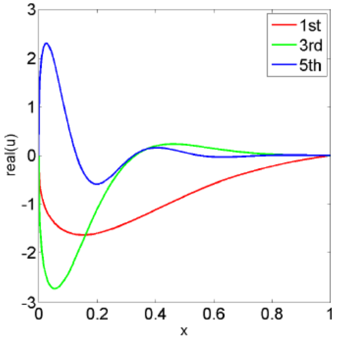
Comparison for the case $q = 0$

	classical, $\alpha = 2$	R.-L. case	Caputo case
λ_n=zeros of	$E_{2,2}(-\lambda)$	$E_{\alpha,\alpha}(-\lambda)$	$E_{\alpha,2}(-\lambda)$
eigenfcn	$\sin\sqrt{\lambda_n}x$	$x^{\alpha-1}E_{\alpha,\alpha}(-\lambda_n x^\alpha)$	$xE_{\alpha,2}(-\lambda_n x^\alpha)$
asymptotic	$\lambda_n = n^2\pi^2$,	$\lvert\lambda_n\rvert \sim (n\pi)^\alpha$	$\lvert\lambda_n\rvert \sim (n\pi)^\alpha$
asymptotic	$\arg(\lambda_n) = 0$	$\arg(\lambda_n) \sim \frac{2-\alpha}{2}\pi$	$\arg(\lambda_n) \sim \frac{2-\alpha}{2}\pi$

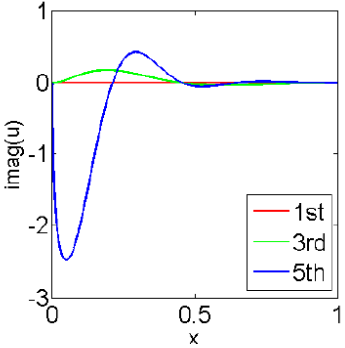
- $\alpha = 2$ is the limit case
- R.-L. case is more singular, numerically more challenging
- both cases genuinely complex: equally (more) informative?

Plot of eigenfunctions

$\alpha = 4/3$: eigenfunctions for Riemann-Liouville case



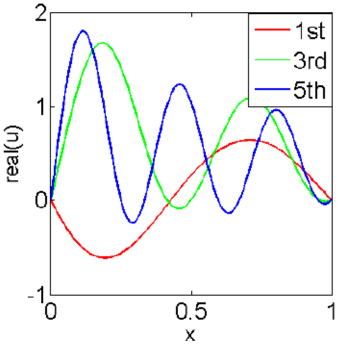
(a) real part



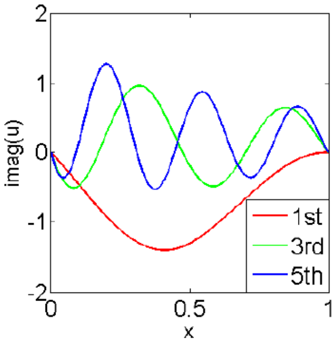
(b) imaginary part

Plot of eigenfunctions

$\alpha = 4/3$: eigenfunctions for Caputo case



(a) real part



(b) imaginary part

Questions: are these two cases equally (more) informative???

Inverse fractional Sturm-Liouville problem

Recover $q(x)$ from its spectrum $\{\lambda_n\}$:

$$
\begin{aligned}
-{}_0D_x^\alpha u + qu &= \lambda u, \quad x \in D = (0,1), \\
u(0) &= u(1) = 0,
\end{aligned}
$$

Classical case $\alpha = 2$ (Rundell 1998)

$$-u'' + qu = \lambda u, \quad x \in D = (0,1).$$

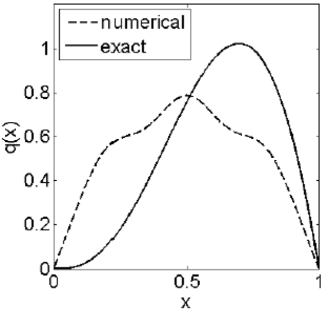
- $\{\lambda_n\}$ only determines an even potential $q(x)$ w.r.t. $x = \frac{1}{2}$

  $q(x)$ is the potential $\Longrightarrow q(1-x)$ is also a potential

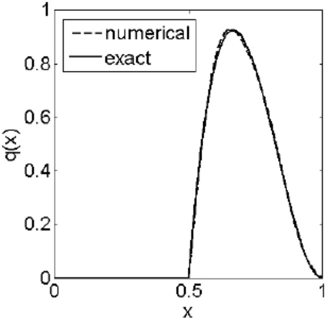
- $\{\lambda_n\}$ determines $q(x)$ if it is known on $[0, \frac{1}{2}]$
- to uniquely determine $q(x)$, need a second $\{\lambda_n\}$

Question: what about the fractional case??

Riemann-Liouville case



(a) nonsymmetric potential



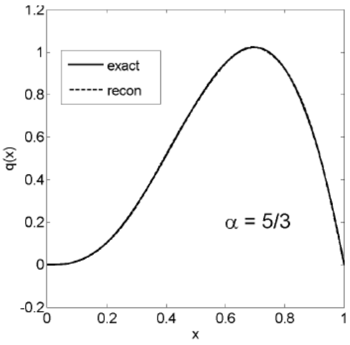
(b) potential on $[\frac{1}{2}, 1]$

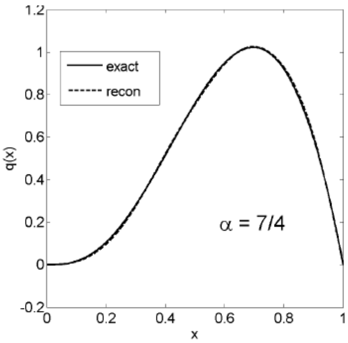
observations:

- one single spectrum only determines the even potential
- it determines the potential on a half interval

it is as informative as the case $\alpha = 2$

Caputo case





observations: one spectrum uniquely determines the potential!!!

- it is more informative than the case of Riemann-Liouville and $\alpha = 2$
- the reason is still not clear...

Numerical treatment

FEM:

- Ervin-Roop 2006, Ervin-Roop 2018
- Jin-Lazarov-Z 2014, 2016, Jin-Lazarov-Pasciak-Rundell 2015...
- Wang-Yang 2015, 2016, Du-Wang 2016...

Spectral Method:

- Zayernouri-Ainsworth-Karniadakis 2015, 2017, Zhang-Zeng-Karniadakis 2015...
- Chen-Shen-Wang 2015, Mao-Shen 2016

Finite difference Method:

- Kopteva-Stynes 2017, Stynes-O'Riordan-Gracia 2016, Stynes-Gracia 2015
- Hao-Zhao 2017, Tian-Zhou-Deng 2015, Ding-Li-Chen 2015...

Question: convinced high-dimensional model?

Spectral fractional Laplacian

Let Ω be a bounded domain with Lipschitz boundary $\partial\Omega$.

Given $-\Delta$ with homogeneous Dirichlet boundary conditions, we let

$$-\Delta\varphi_k = \lambda_k\varphi_k, \quad \varphi_k|_{\partial\Omega} = 0.$$

φ_k form an orthogonal basis of $L^2(\Omega)$, i.e.,

$$u(x) = \sum_{k=1}^{\infty}(u,\varphi_k)\varphi_k(x) \quad \text{for any } u \in L^2(\Omega).$$

Then we define the spectral fractional Laplacian with $s \in (0,1)$

$$(-\Delta)^s u = \sum_{k=1}^{\infty}\lambda^s(u,\varphi_k)\varphi_k.$$

Now we consider the fractional diffusion problem

$$(-\Delta)^s u = f, \qquad \text{in } \ \Omega,$$

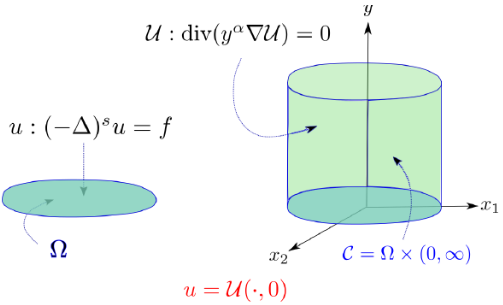
We have to represent the operator in some computable forms.

Method 1: DtN map

$(-\Delta)^s$ can be realized as a Dirichlet to Neumann Mapping (DtN)

$$\begin{cases} \operatorname{div}(y^\alpha \nabla U) = 0, & \text{in } \Omega \times \mathbb{R}^+, \\ U = 0, & \text{on } \partial\Omega \times \mathbb{R}^+, \\ -\lim\limits_{y \to 0} y^\alpha \partial_y U = c_s f, & \text{on } \Omega \times \{0\}, \end{cases}$$

where $\alpha = 1 - 2s$ and $c_s = 2^{1-2s}\Gamma(1-s)/\Gamma(s)$.



Method 1: DtN map

Fractional DtN: Caffarelli-Silvestre 2007, Stinga-Torrea 2010, Cabre-Tan 2010...

Numerical analysis:

- FEM, a priori and posteriori error: Otarola-Salgodo-Nochetto 2015, Chen-Otarola-Salgodo-Nochetto 2015
- multilevel: Chen-Otarola-Salgodo-Nochetto 2015
- spectral method: Chen-Mao-Shen 2017, Ainsworth-Glusa 2019
- redial basis method: Antil-Chen-Narayan 2019
- sparse tensor product FEM: Banjai-Melenk-Nochetto-Otárola-Salgado-Schwab 2019

Method 2: integral expression

Balakrishnan Formula: deforming the contour of a Dunford Integral:

$$u = (-\Delta)^{-s} f = \frac{\sin(\pi s)}{\pi} \int_0^\infty z^{-s}(zI - \Delta)^{-1} f \, ds$$

Numerical Approximation:

- step 1: approximate the integral by quadrature. (fast convergence)
- step 2: solve several elliptic problems in parallel. (FEM analysis)

Relevant results:

- SINC quadrature + a priori error Bonito-Pasciak 2015
- A^s for a sectorial operator A Bonito-Pasciak 2016

A survey paper:

A. Bonito, J.P. Borthagaray, R.H. Nochetto, E. Otárola, A.J. Salgado, Numerical methods for fractional diffusion. Comput. Vis. Sci. 19 (2018), no. 5-6, 19–46.

Integral fractional Laplacian

We consider the following nonlocal boundary value problem:

$$\begin{cases} (-\Delta)^s u = f, & \text{in } \Omega, \\ u = 0, & \text{in } \Omega^c. \end{cases}$$

where

$$(-\Delta)^s u = c_{d,s} \int_{\mathbb{R}^d} \frac{u(x) - u(y)}{|y - x|^{d+2s}} \, dy.$$

Note that the boundary value is given in Ω^c, not on $\partial\Omega$.

The trace boundary condition is replaced with a volume constraint.

Define the Sobolev spave $\widetilde{H}^s(\Omega)$ by

$$\widetilde{H}^s(\Omega) = \{u = U|_\Omega : U \in H^s(\mathbb{R}^d), U|_{\Omega^c} = 0.\}$$

Integral fractional Laplacian

Variational Problem: find $u \in \widetilde{H}^s(\Omega)$ such that for any $v \in \widetilde{H}^s(\Omega)$

$$a(u,v) := \frac{c_{d,s}}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{(u(x)-u(y))(v(x)-v(y))}{|y-x|^{d+2s}} \, dy \, dx = \int_\Omega f v \, ds$$

Then well-posedness follows from the Lax-Milgram lemma

Boundary layers: Grubb 2015, Ros-Oton & Serra 2014

$$u(x) \approx \mathrm{dist}(x, \partial\Omega)^s + v(x), \quad \text{with a smoother} v.$$

Numerical approximation:

- FDM: Huang -Oberman 2014, Del Teso-Endal-Jakobsen 2018, 2019
- FEM: Acosta-Borthagaray 2017, Ainsworth-Glusa 2017
- applying Dunford integral: Bonito-Lei-Pasciak 2019

A recent survey

D'Elia, Du, Glusa, Gunzburger, Tian, Zhou, Numerical methods for nonlocal and fractional models, Acta Numerica, 2020. arXiv:2002.01401.

Thanks for your attention !!!

Questions???