Fractional diffusion on bounded domains

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Abstract

Fractional derivatives were invented in the 17th century, soon after their integer order cousins. In the past decade, an explosion of practical applications has intensified interest in the subject. Fractional differential equations are now being used in cell biology, ecology, electronics, hydrology, and medical imaging to model anomalous diffusion, where a plume of particles spreads faster than the traditional integer-order diffusion equation predicts. There now exist a variety of effective numerical methods to solve fractional diffusion equations. However, the mathematically correct specification of a well-posed fractional diffusion on a bounded domain remains an open problem. The main issue is to write appropriate boundary conditions, or their fractional analogues. In this talk, we will discuss this open problem, and one possible approach using the newly developed theory of nonlocal diffusion.

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Fractional derivatives: An old idea gets new life

Fractional derivatives $d^\alpha f(x)/dx^\alpha$ for any $\alpha > 0$ were invented by Leibniz soon after the more familiar integer derivatives.

Some derivative formulas extended to the fractional case:

$$\frac{d^\alpha}{dx^\alpha}\left[e^{\lambda x}\right] = \lambda^\alpha e^{\lambda x}$$

$$\frac{d^\alpha}{dx^\alpha}[\sin x] = \sin\left(x + \frac{\pi}{2}\alpha\right)$$

$$\frac{d^\alpha}{dx^\alpha}[x^p] = \frac{\Gamma(p+1)}{\Gamma(p-\alpha+1)} x^{p-\alpha}$$

Riemann-Liouville fractional derivatives

The Riemann-Liouville fractional derivatives are defined by

$$\mathbb{D}^{\alpha}_{x,L} f(x) = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_L^x \frac{f(u)}{(x-u)^{\alpha+1-n}} du$$

$$\mathbb{D}^{\alpha}_{-x,R} f(x) = \frac{(-1)^n}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_x^R \frac{f(u)}{(u-x)^{\alpha+1-n}} du$$

where $n-1 < \alpha \le n$.

If $f(x) = 0$ for all $x < L$ then $\mathbb{D}^{\alpha}_{x,L} f(x) = \mathbb{D}^{\alpha}_{x,-\infty} f(x) := \mathbb{D}^{\alpha}_{x} f(x)$.

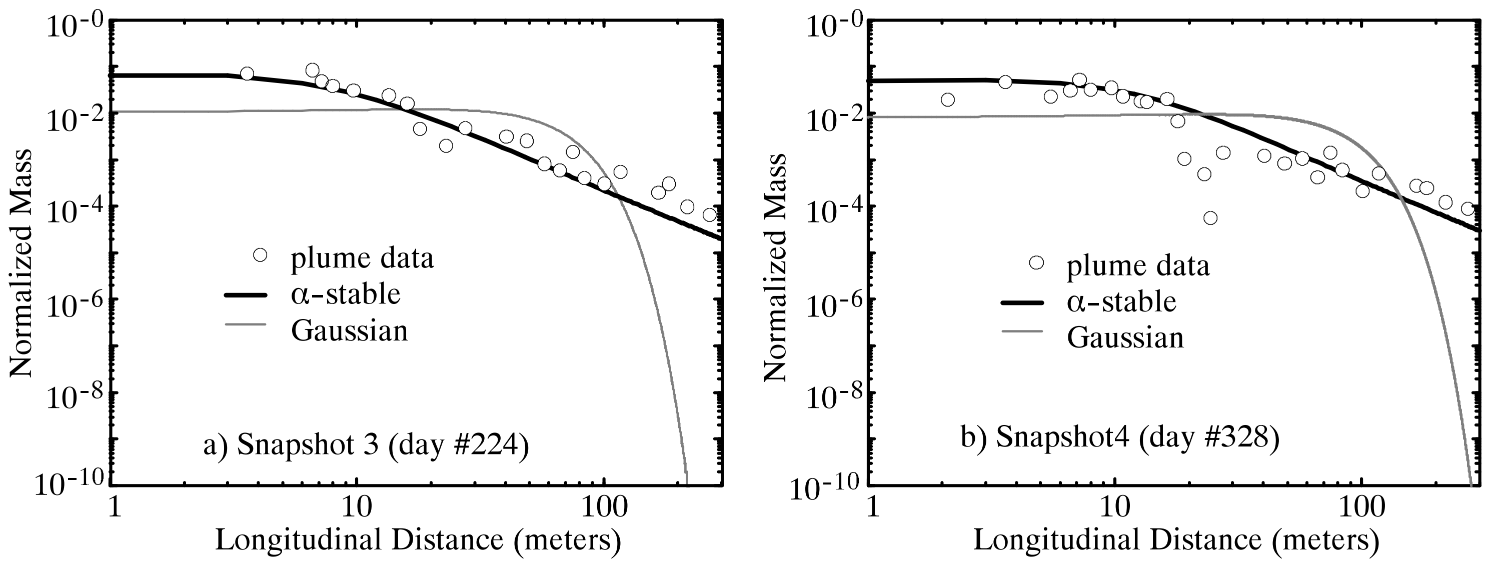
If $f(x) = 0$ for all $x > R$ then $\mathbb{D}^{\alpha}_{-x,R} f(x) = \mathbb{D}^{\alpha}_{-x,\infty} f(x) := \mathbb{D}^{\alpha}_{-x} f(x)$.

Fourier transforms: $\mathbb{D}^{\alpha}_{\pm x} f(x) \Longleftrightarrow (\pm ik)^{\alpha} \widehat{f}(k)$ [Samko, (7.4)]

Here $\widehat{f}(k) := \int_{-\infty}^{\infty} e^{-ikx} f(x)\, dx$.

Application to groundwater hydrology

Fractional diffusion equation with $\alpha = 1.1$ captures power law leading tail at the MADE experimental site [BSMW01].

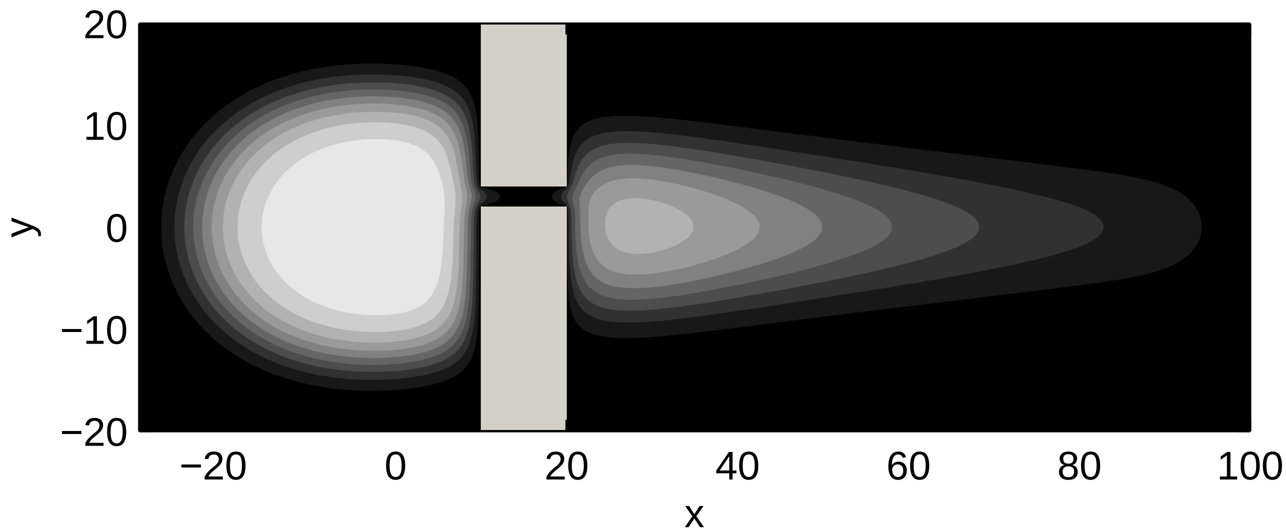


Governing equation: $$\frac{\partial c(x,t)}{\partial t} = -0.12\frac{\partial c(x,t)}{\partial x} + 0.14\frac{\partial^\alpha c(x,t)}{\partial x^\alpha}$$

Application to Ecology

Fractional derivatives model power law movements [BKM08].

$$\frac{\partial P}{\partial t} = C\frac{\partial^{1.7} P}{\partial x^{1.7}} + D\frac{\partial^2 P}{\partial y^2} + rP\left(1 - \frac{P}{K}\right)$$



Fractional diffusion jumps the barrier (nonlocal operator).

Real invasive species data shows this behavior.

Grünwald-Letnikov fractional derivatives

For any $\alpha > 0$ we can define

$$\mathbf{D}^{\alpha}_{\pm x} f(x) = \lim_{h \to 0} h^{-\alpha} \Delta^{\alpha}_{\pm h} f(x)$$

where

$$\Delta^{\alpha}_{\pm h} f(x) := \sum_{j=0}^{\infty} w_j f(x \mp jh), \quad w_j := (-1)^j \binom{\alpha}{j} = \frac{(-1)^j \Gamma(1+\alpha)}{j! \Gamma(1+\alpha-j)}$$

If f is bounded, and $f^{(k)} \in L^1(\mathbb{R})$ for $k \leq n$, for some $n > 1 + \alpha$, then $\mathbf{D}^{\alpha}_{\pm x} f(x)$ exists, and its FT is $(\pm ik)^{\alpha} \widehat{f}(k)$ [MS12, Prop 2.1].

Hence $\mathbb{D}^{\alpha}_{\pm x} f(x) = \mathbf{D}^{\alpha}_{\pm x} f(x)$, since they have the same FT.

Numerical methods

Explicit/implicit Euler schemes based on the standard Grünwald approximation are unstable [MT04, Props 2.1, 2.3].

A stable, consistent implicit Euler method uses a shifted formula

$$\Delta^{\alpha}_{\pm h,s} f(x) := \sum_{j=0}^{\infty} \binom{\alpha}{j} (-1)^j f(x \mp (j+s)h),$$

and then for $f \in L^1(\mathbb{R}) \cap C^n(\mathbb{R})$ we have [MT04, Theorem 2.4]

$$\mathbf{D}^{\alpha}_{\pm x} f(x) = h^{-\alpha} \Delta^{\alpha}_{\pm h,s} f(x) + O(h).$$

The proof uses Fourier transforms.

Grünwald derivative for finite R, L

A nice trick used by Chen and Deng (2014) sets $f(x) \equiv 0$ for $x < L$ and/or $x > R$, and then applies Fourier transform methods.

Then one can prove

$$\mathbf{D}^{\alpha}_{x,L} f(x) = h^{-\alpha} \Delta^{\alpha}_{h,s} f(x) + O(h)$$

by the same arguments. This approach also leads to stable higher order methods (e.g., 4th order).

The proof (first order) using combinatorial methods is much harder [Podlubny, pp. 49–55 and 62–63].

Numerical codes for fractional diffusion

Consider the fractional diffusion equation

$$\partial_t p(x,t) = a(x,t)\mathbb{D}_x^\alpha p(x,t) + b(x,t)\mathbb{D}_{-x}^\alpha p(x,t) + c(x,t)$$

on a finite domain $L < x < R$, $0 \le t \le T$.

Shifted Grünwald approximation $\Rightarrow$ implicit Euler codes [MT04].

These codes are *mass-preserving* since $\sum_{j=0}^{\infty} \binom{\alpha}{j} (-1)^j = 0$.

Use operator splitting for 2-d [MST06] or reaction term [BKM08].

Other methods:

Finite elements [Fix and Roop, 2004; Wang and Yang, 2013]

Finite volume method [D'Elia and Gunzburger, 2013]

Spectral collocation method [Zayernouri and Karniadakis, 2014].

Numerical example

The fractional diffusion equation

$$\partial_t p(x,t) = a(x)\mathbb{D}_x^{1.8} p(x,t) + c(x,t)$$

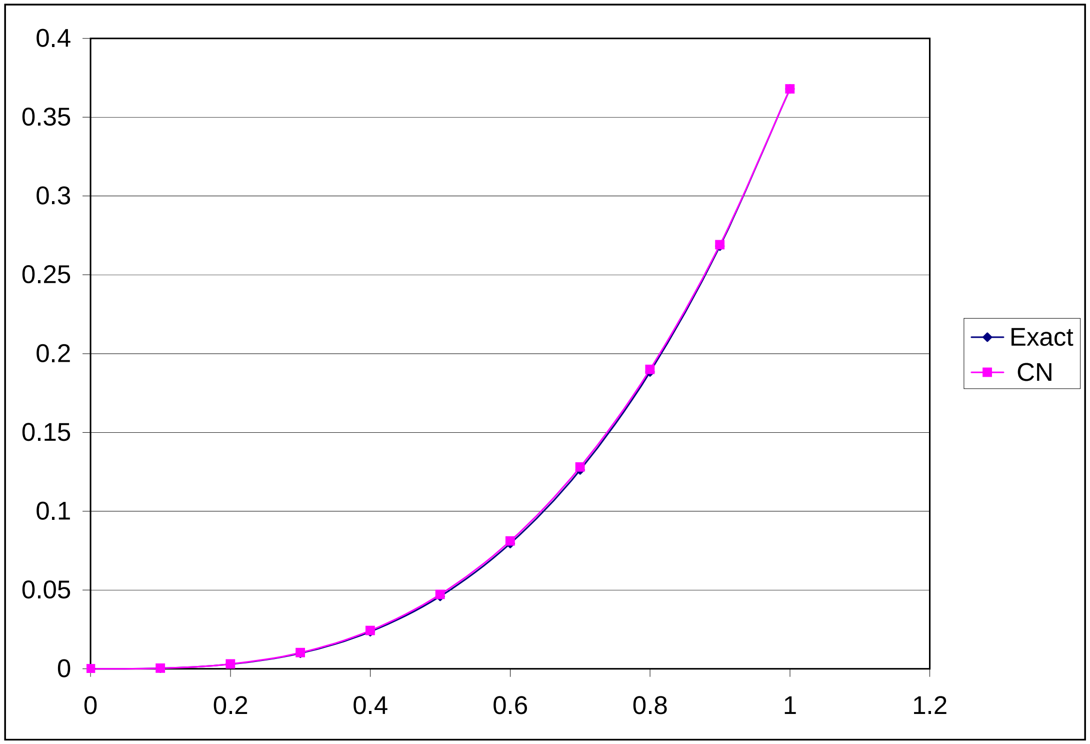
on the bounded domain $0 < x < 1$, with

$$\begin{aligned} p(x,0) &= x^3 \\ p(0,t) &= 0 \\ p(1,t) &= e^{-t} \\ a(x) &= \frac{\Gamma(2.2)}{8} x^{2.8} \\ c(x,t) &= -(1+x)e^{-t}x^3 \end{aligned}$$

has exact solution $p(x,t) = e^{-t}x^3$ for all $t > 0$ [MT06].

Numerical solution

Crank-Nicolson solution at time $t = 1.0$ with $\Delta t = 1/10$ and $\Delta x = h = 1/10$ matches the exact solution [MT06].



Error analysis

Crank-Nicolson method is first-order accurate. Richardson extrapolation yields a second order method [MT06].

Δt	Δx	CN Error	Rate	RE Error	Rate
1/10	1/10	1.82×10^{-3}	–	1.77×10^{-4}	–
1/15	1/15	1.17×10^{-3}	$\approx 15/10$	7.85×10^{-5}	$\approx (15/10)^2$
1/20	1/20	8.64×10^{-4}	$\approx 20/15$	4.41×10^{-5}	$\approx (20/15)^2$
1/25	1/25	6.85×10^{-4}	$\approx 25/20$	2.83×10^{-5}	$\approx (25/20)^2$

Computing the exact solution

Not hard to check that

$$\mathbb{D}^{\alpha}_{x,L}(x-L)^p = \frac{\Gamma(p+1)}{\Gamma(p+1-\alpha)}(x-L)^{p-\alpha}$$

$$D^{\alpha}_{-x,R}(R-x)^p = \frac{\Gamma(p+1)}{\Gamma(p+1-\alpha)}(R-x)^{p-\alpha}$$

If $p(x,t) = e^{-t}x^3$ then

$$\partial_t p(x,t) = -e^{-t}x^3 \quad \text{and} \quad \mathbb{D}^{1.8}_x p(x,t) = \frac{\Gamma(4)}{\Gamma(2.2)}\, e^{-t}x^{1.2}$$

Plug into $\partial_t p(x,t) = a(x)\mathbb{D}^{1.8}_x p(x,t) + c(x,t)$ to get $c(x,t)$.

Existence and uniqueness

There exists a solution $p(x,t) = e^{-t}x^3$ to the fractional PDE

$$\partial_t p(x,t) = a(x)\mathbb{D}_x^{1.8} p(x,t) + c(x,t)$$

on $0 < x < 1$, with $p(x,0) = x^3$, $p(0,t) = 0$, $p(1,t) = e^{-t}$, $c(x,t) = -(1+x)e^{-t}x^3$, and $a(x) = \Gamma(2.2)x^{2.8}/6$.

Question: Is this solution unique?

We assume $p(x,t) = 0$ for $x \le 0$ to make $\mathbb{D}_x^{1.8} p(x,t) = \mathbb{D}_{x,0}^{1.8} p(x,t)$.

Suppose for example that $p(x,t) = 1$ for $-1 < x < 0$. Then

$$\begin{aligned}\mathbb{D}_x^{1.8} p(x,t) &= \frac{\Gamma(4)}{\Gamma(2.2)}\, e^{-t}x^{1.2} + \frac{1}{\Gamma(0.2)}\frac{d^2}{dx^2}\int_{-1}^{0} \frac{1}{(x-\xi)^{0.8}} d\xi \\ &= \frac{3}{\Gamma(2.2)}\, e^{-t}x^{1.2} + \frac{0.8}{\Gamma(0.2)}\left[x^{-1.8} - (x+1)^{-1.8}\right]\end{aligned}$$

and then $c(x,t)$ must change. BC $p(0,t) = 0$ is under-specified.

Symmetric case

Theorem. For any $p_0 \in V_c := \{v \in V : v(x) = 0 \; \forall \; x \notin (L, R)\}$ (V defined in next slide), the fractional diffusion problem

$$\begin{aligned} \partial_t p(x,t) &= \mathbb{D}_x^\alpha p(x,t) + \mathbb{D}_{-x}^\alpha p(x,t) \\ p(x,0) &= p_0(x) \quad \text{for all } L < x < R \\ p(x,t) &= 0 \quad \text{for all } x \notin (L,R) \text{ and all } t \in [0,T] \end{aligned}$$

has a unique solution in $L^\infty([0,T], V_c) \cap H^1([0,T], L^2(\mathbb{R}))$ [DDGLM14].

Open problems:

Non-symmetric case $a\,\mathbb{D}_x^\alpha p(x,t) + b\,\mathbb{D}_{-x}^\alpha p(x,t)$.

Variable coefficients $a(x,t)$, $b(x,t)$, forcing term, reaction term.

Higher dimensions.

Non-Dirichlet boundary conditions.

Proof [DDGLM14, Theorem 4.1]

The *nonlocal diffusion equation*

$$\partial_t p(x,t) = Lp(x,t) := \int \Big[p(y,t) - p(x,t)\Big]\gamma(y,x)\,dy$$

with kernel $\gamma(y,x) = C|y-x|^{-\alpha-1}$ is a fractional diffusion equation

$$\partial_t p(x,t) = \mathbb{D}_x^\alpha p(x,t) + \mathbb{D}_{-x}^\alpha p(x,t)$$

where $C = 1/\Gamma(1-\alpha)$ and $\alpha \in (0,1)$ [MS12, Example 3.24].

Define the nonlocal energy semi-norm

$$|||v||| := \frac{1}{2}\int_{\mathbb{R}\times\mathbb{R}} |v(x) - v(y)|^2 \gamma(y,x)\,dy\,dx,$$

the nonlocal energy space $V := \{v \in L^2(\mathbb{R}) : |||v||| < \infty\}$, and recall that the nonlocal volume-constrained energy space is

$$V_c := \{v \in V : v(x) = 0 \ \forall\ x \notin (L,R)\}.$$

Proof, continued [DDGLM14, Theorem 4.1]

V_c is a Hilbert space, and a closed subspace of $L^2(\mathbb{R})$.

The bilinear form

$$a(u,v) = \int_{\mathbb{R}\times\mathbb{R}} \Big(u(x) - u(y)\Big)\Big(v(x) - v(y)\Big)\gamma(y,x)\,dy\,dx$$

is coercive and continuous on $V_c \times V_c$, and $a(u,v) = (L(u), v)$.

L generates a continuous semigroup.

Invoke the standard theory [Pazy, 1983].

Reflected stable process

Take a stable Lévy process Y_t with

$$\mathbb{E}[e^{ikY_t}] = e^{t(ik)^\alpha}$$

for some $1 < \alpha \leq 2$, with no positive jumps.

Then the reflected process

$$Z_t = Y_t - \inf\{Y_s : 0 \leq s \leq t\}$$

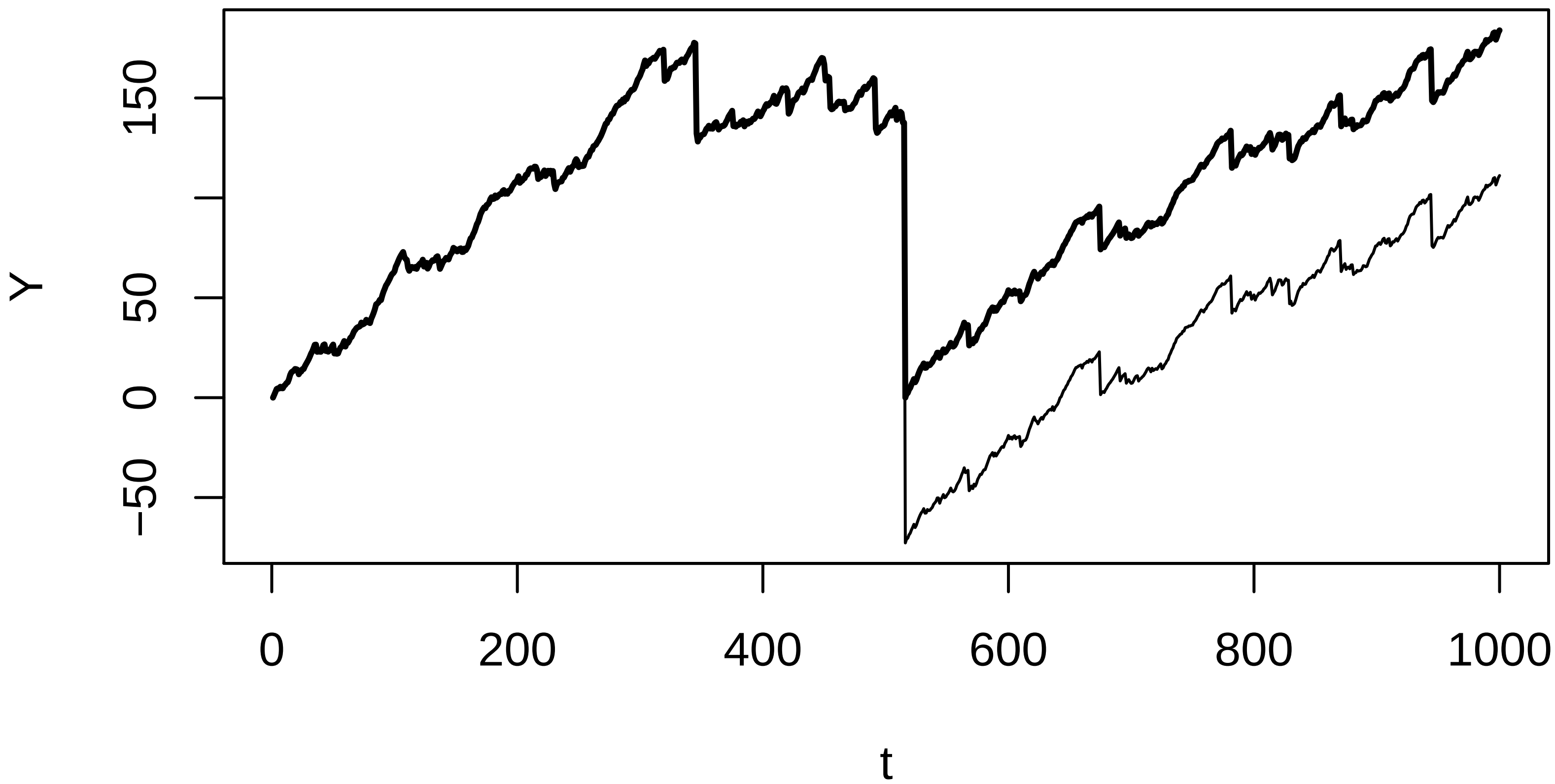
is a Markov process on the real line [BKMSS14, Theorem 2.1].

Application: If $\partial_t p = Lp$ governs the Markov process $X(t)$, then $\partial_t^\beta p = Lp$ governs $X(Z_t)$ for $\beta = 1/\alpha$ [BKMSS14, Theorem 4.1].

Here L generates the C_0 semigroup $T_t f(x) = \mathbb{E}[f(X_t)|X_0 = x]$.

Reflected stable sample path

Stable process Y_t (thin line) with $\alpha = 1.3$ and reflected stable Z_t (thick line). See Appendix for R code.



Fractional reflecting boundary condition

The probability densities $p(x,t)$ of the reflected stable process $x = Z_t$ solve [BKMSS14, Theorem 2.3]

$$\partial_t p(x,t) = \mathbb{D}^{\alpha}_{-x} p(x,t); \quad \mathbb{D}^{\alpha-1}_{-x} p(0,t) = 0.$$

Without the reflecting boundary condition $\mathbb{D}^{\alpha-1}_{-x} p(0,t) = 0$, the fractional PDE $\partial_t p(x,t) = \mathbb{D}^{\alpha}_{-x} p(x,t)$ governs the stable process Y_t on the entire real line.

The BC $\mathbb{D}^{\alpha-1}_{-x} p(0,t) = 0$ is a no-flux boundary condition, just like the $\alpha = 2$ case where Y_t is a Brownian motion.

Reflected Brownian motion

The PDF of a reflected Brownian motion solves the diffusion equation $\partial_t p = \partial_x^2 p$ with a reflecting boundary condition:

$$\frac{\partial}{\partial x} p(x,t)\bigg|_{x=0+} := \lim_{h \to 0+} \frac{p(x+h,t) - p(x,t)}{h}\bigg|_{x=0} = 0$$

In the stable case, the reflecting boundary condition is

$$D_{-x}^{\alpha-1} p(x,t)\bigg|_{x=0+} := \lim_{h \to 0+} \frac{1}{h^{\alpha-1}} \sum_{k=0}^{\infty} w_k^{\alpha-1} p(x+kh,t)\bigg|_{x=0} = 0$$

where

$$w_k^{\alpha} := (-1)^k \frac{\Gamma(\alpha+1)}{k!\Gamma(\alpha-k+1)}$$

When $\alpha = 2$, $w_0^{\alpha-1} = 1$, $w_1^{\alpha-1} = -1$, and $w_k^{\alpha-1} = 0$ for $k > 1$.

Tempered fractional derivatives

The tempered fractional derivatives

$$\partial_x^{\alpha,\lambda} f(x) := \frac{\alpha(\alpha-1)}{\Gamma(2-\alpha)} \int_0^\infty \Big(f(x-y) - f(x) + y f'(x) \Big) e^{-\lambda y} y^{-\alpha-1} dy$$

$$\partial_{-x}^{\alpha,\lambda} f(x) := \frac{\alpha(\alpha-1)}{\Gamma(2-\alpha)} \int_0^\infty \Big(f(x+y) - f(x) - y f'(x) \Big) e^{-\lambda y} y^{-\alpha-1} dy$$

for any $1 < \alpha < 2$ and $\lambda > 0$ [SMC14, (16) and (17)].

Fourier transforms [BM10, Sec 2]:

$$\partial_{\pm x}^{\alpha,\lambda} f(x) \Longleftrightarrow \Big[(\lambda \pm ik)^\alpha - \lambda^\alpha \mp ik\alpha\lambda^{\alpha-1} \Big] \widehat{f}(k).$$

$\lambda = 0 \Rightarrow$ Riemann-Liouville fractional derivative.

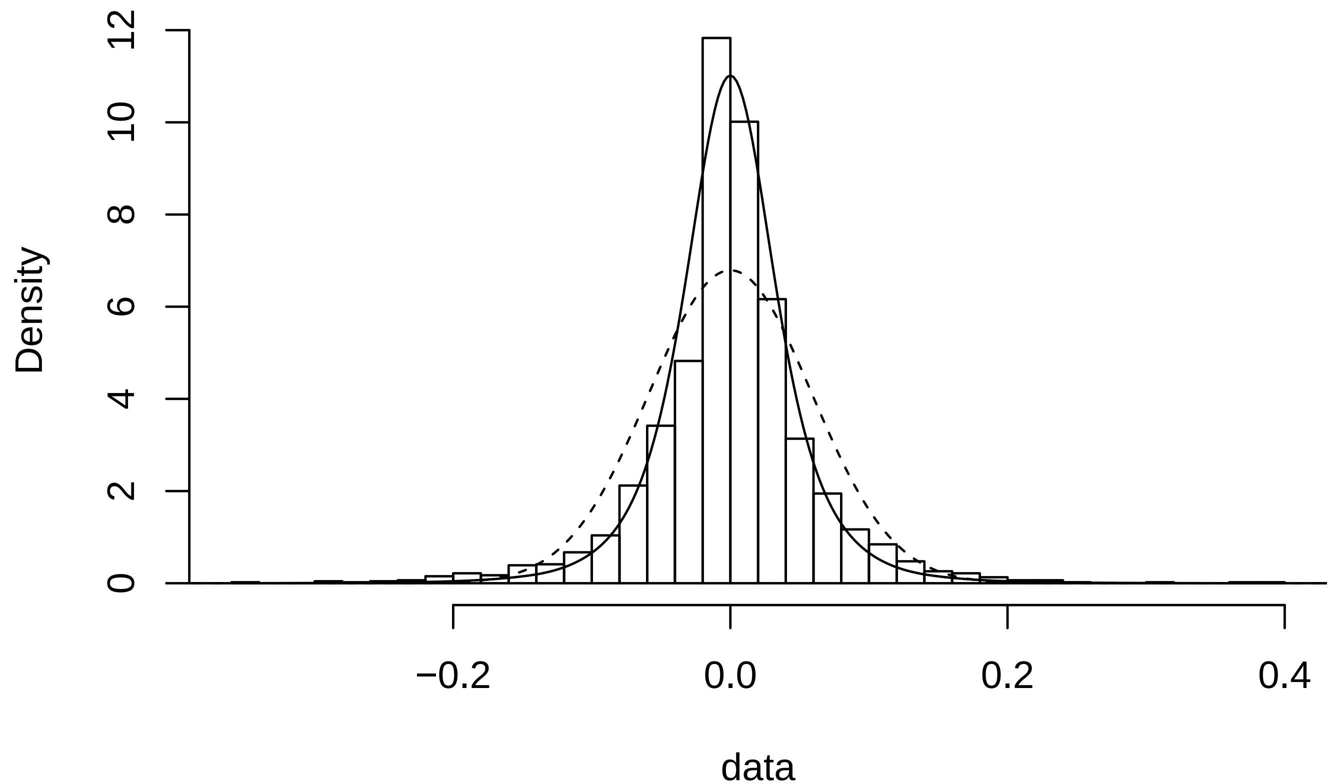
$0 < \alpha < 1 \Rightarrow$ simpler formula [MS12, (7.17) and (7.25)]

Application to finance

Bilinear ARMA forecast errors for annual inflation rates fit

$$\partial_t p(x,t) = \frac{D}{2}\left[\partial_x^{\alpha,\lambda} p(x,t) + \partial_{-x}^{\alpha,\lambda} c(x,t)\right]$$

at $t = 1$ (solid line) with $\alpha = 1.1, \lambda = 12, D = 0.1$. Diffusion equation (dotted line, $\alpha = 2$) misses sharp data peak [SMC14].



Numerical solution [SMC14, Example 5.3]

Exact solution $u(x,t) = x^\beta e^{-\lambda x - t}/\Gamma(1+\beta)$ vs implicit Euler for

$$\partial_t p(x,t) = a(x)\partial_x^{\alpha,\lambda} p(x,t) + c(x,t)$$

on $x \in [0,1]$, with $\alpha = 1.5$, $\lambda = 0.5$, $\beta = 2.5$, boundary conditions $p(0,t) = 0$ and $p(1,t) = e^{-\lambda - t}/\Gamma(\beta+1)$, initial condition $p(x,0) = x^\beta e^{-\lambda x}/\Gamma(\beta+1)$, diffusion coefficient $a(x) = x^\alpha \Gamma(1+\beta-\alpha)/\Gamma(\beta+1)$, and forcing function

$$c(x,t) = e^{-\lambda x - t}\frac{\Gamma(1+\beta-\alpha)}{\Gamma(\beta+1)} \cdot \left(\frac{(1-\alpha)\lambda^\alpha x^{\alpha+\beta}}{\Gamma(\beta+1)} + \frac{\alpha\lambda^{\alpha-1}x^{\alpha+\beta-1}}{\Gamma(\beta)} - \frac{2x^\beta}{\Gamma(1+\beta-\alpha)}\right)$$

Δt	Δx	Max error	Error rate
.05000	.05000	.003560	–
.02500	.02500	.001900	1.87
.01250	.01250	.000982	1.94
.00625	.00625	.000499	1.97

Numerical method [SMC14, Theorem 5.2]

Stable, consistent implicit Euler codes for $1 < \alpha < 2$: use

$$\partial_x^{\alpha,\lambda} f(x) + \alpha\lambda^{\alpha-1} f'(x) = \lim_{h\to 0} h^{-\alpha} \sum_{j=0}^{\infty} g_j f(x-(j-1)h),$$

where the exponentially tempered Grünwald weights are

$$g_j = \begin{cases} w_j e^{-(j-1)h\lambda} & \text{for } j \neq 1, \\ w_1 - e^{h\lambda}(1-e^{-h\lambda})^\alpha & \text{for } j = 1. \end{cases}$$

Codes are mass-preserving since (by the Binomial formula)

$$\sum_{j=0}^{\infty} w_j e^{-\lambda j h} = \left(1 - e^{-h\lambda}\right)^\alpha$$

Question: Are solutions unique? This is a nonlocal diffusion with kernel $\gamma(y,x) = C(y-x)^{-\alpha-1} e^{-\lambda(y-x)} H(y-x)$.

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R code for reflected stable sample path

```
# Plot stable Y_t with characteristic function exp(t(ik)^a)
# and the reflected stable process Z_t=Y_t-inf{Y_u:0<=u<=t}
#
# You need to install the fBasics package on your R platform.
# Try Packages > Load package to see if fBasics is available.
# If not then use Packages > Install package(s)
 library(fBasics)
 t=seq(1:1000)
 a=1.3
 g=(abs(cos(pi*a/2)))^(1/a)
 y=rstable(t,alpha=a,beta=-1.0,gamma=g,delta=0.0,pm=1)
 Y=cumsum(y)
 Z=Y-cummin(Y)
 plot(t,Y,type="l",ylim=c(min(Y),max(Z)))
 lines(t,Z,lwd=2)
```