Fractional Diffusion Equations

IMPA November 1 2017

William Rundell
Texas A&M University

Historical Classical Diffusion

$$\left.\begin{array}{c}\text{Robert Brown (1828)}\\ \text{Thomas Graham (1827)}\end{array}\right\}\quad \text{Experimental observation of diffusion}$$

Adolf Fick (1855): Macro derivation of the heat equation

$$J = -K\nabla u, \quad u_t = \mathrm{div}\, J, \;\Rightarrow\; u_t - K\mathrm{div}\nabla u = 0$$

Einstein (1905): Gave accepted notion of diffusion - particles pushed around by the thermal motion of atoms.

Brownian Random Walk and Classical Diffusion

In one space dimension this can be modeled by the master equation

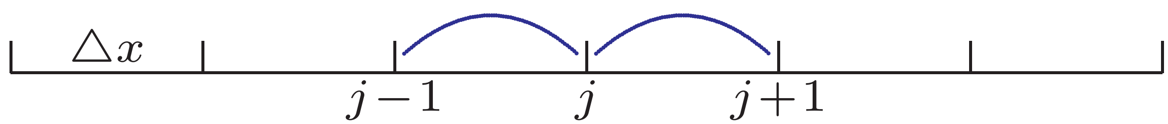
$$p_j(t + \Delta t) = \tfrac{1}{2} p_{j-1}(t) + \tfrac{1}{2} p_{j+1}(t),$$

the index j denotes the position on the underlying 1-dim lattice.

It defines the probability density function (PDF) $p(t)$ to be at position j at time $t + \Delta t$ and to depend on p at the two adjacent sites $j \pm 1$ at time t.

$\frac{1}{2} \Rightarrow$ directional isotropy; jumps to the left and right are equally likely.

Δt is a fixed time step. Δx is a fixed jump distance.



Brownian Random Walk and Classical Diffusion

In one space dimension this can be modeled by the master equation

$$p_j(t+\Delta t) = \tfrac{1}{2} p_{j-1}(t) + \tfrac{1}{2} p_{j+1}(t),$$

the index j denotes the position on the underlying 1-dim lattice.

It defines the probability density function (PDF) $p(t)$ to be at position j at time $t+\Delta t$ and to depend on p at the two adjacent sites $j \pm 1$ at time t.

$\frac{1}{2} \Rightarrow$ directional isotropy; jumps to the left and right are equally likely.

Δt is a fixed time step. Δx is a fixed jump distance.

Rearranging : $$\frac{p_j(t+\Delta t) - p_j(t)}{\Delta t} = \frac{(\Delta x)^2}{2\Delta t} \frac{p_{j-1}(t) - 2p_j(t) + p_{j+1}(t)}{(\Delta x)^2}$$

Brownian Random Walk and Classical Diffusion

In one space dimension this can be modeled by the master equation

$$p_j(t+\Delta t) = \tfrac{1}{2} p_{j-1}(t) + \tfrac{1}{2} p_{j+1}(t),$$

the index j denotes the position on the underlying 1-dim lattice.

It defines the probability density function (PDF) $p(t)$ to be at position j at time $t+\Delta t$ and to depend on p at the two adjacent sites $j \pm 1$ at time t.

$\frac{1}{2} \Rightarrow$ directional isotropy; jumps to the left and right are equally likely.

Δt is a fixed time step. Δx is a fixed jump distance.

Rearranging : $$\frac{p_j(t+\Delta t) - p_j(t)}{\Delta t} = \frac{(\Delta x)^2}{2\Delta t} \frac{p_{j-1}(t) - 2p_j(t) + p_{j+1}(t)}{(\Delta x)^2}$$

leads to the diffusion equation $$\frac{\partial}{\partial t} u(x,t) = K \frac{\partial^2}{\partial x^2} u(x,t),$$

Brownian Random Walk and Classical Diffusion

In one space dimension this can be modeled by the master equation

$$p_j(t+\Delta t) = \tfrac{1}{2} p_{j-1}(t) + \tfrac{1}{2} p_{j+1}(t),$$

the index j denotes the position on the underlying 1-dim lattice.

It defines the probability density function (PDF) $p(t)$ to be at position j at time $t+\Delta t$ and to depend on p at the two adjacent sites $j \pm 1$ at time t.

$\frac{1}{2} \Rightarrow$ directional isotropy; jumps to the left and right are equally likely.

Δt is a fixed time step. Δx is a fixed jump distance.

Rearranging : $$\frac{p_j(t+\Delta t) - p_j(t)}{\Delta t} = \frac{(\Delta x)^2}{2\Delta t} \frac{p_{j-1}(t) - 2p_j(t) + p_{j+1}(t)}{(\Delta x)^2}$$

leads to the diffusion equation $$\frac{\partial}{\partial t} u(x,t) = K \frac{\partial^2}{\partial x^2} u(x,t),$$

The continuum limit is taken such that $K = \lim_{\Delta x \to 0, \Delta t \to 0} \frac{(\Delta x)^2}{2\Delta t}$ is a positive constant – the diffusion coefficient – it couples the spatial and time scales.

Suppose now the jump length Δx has a PDF given by $\lambda(x)$ so that

$$P(a < \Delta x < b) = \int_a^b \lambda(x)\, dx.$$

If $\lambda(x)$ decays sufficiently fast as $x \to \pm\infty$, the Fourier transform gives

$$\widetilde{\lambda}(\xi) = \int_{-\infty}^{\infty} e^{-i\xi x} \lambda(x) dx = \int_{-\infty}^{\infty} \left(1 - i\xi x - \tfrac{1}{2}\xi^2 x^2 + \ldots\right) \lambda(x) dx$$

$$= 1 - i\xi\mu_1 - \tfrac{1}{2}\xi^2 \mu_2 + \ldots,$$

where μ_j is the j th moment $\mu_j = \int_{-\infty}^{\infty} x^j \lambda(x) dx$ – provided these exist

Suppose now the jump length Δx has a PDF given by $\lambda(x)$ so that

$$P(a < \Delta x < b) = \int_a^b \lambda(x)\, dx.$$

If $\lambda(x)$ decays sufficiently fast as $x \to \pm\infty$, the Fourier transform gives

$$\widetilde{\lambda}(\xi) = \int_{-\infty}^{\infty} e^{-i\xi x} \lambda(x) dx = \int_{-\infty}^{\infty} \left(1 - i\xi x - \tfrac{1}{2}\xi^2 x^2 + \ldots\right) \lambda(x) dx$$

$$= 1 - i\xi\mu_1 - \tfrac{1}{2}\xi^2\mu_2 + \ldots,$$

where μ_j is the j th moment $\mu_j = \int_{-\infty}^{\infty} x^j \lambda(x) dx$ – provided these exist

Assume $\lambda(x)$ is normalized and even: $\mu_1 = 0$, $\mu_2 = 1$ and $\mu_3 = 0$. Then

$$\widetilde{f}(\xi) = 1 - \tfrac{1}{2}\xi^2 + O(\xi^4).$$

Suppose now the jump length Δx has a PDF given by $\lambda(x)$ so that

$$P(a < \Delta x < b) = \int_a^b \lambda(x)\, dx.$$

If $\lambda(x)$ decays sufficiently fast as $x \to \pm\infty$, the Fourier transform gives

$$\widetilde{\lambda}(\xi) = \int_{-\infty}^{\infty} e^{-i\xi x} \lambda(x) dx = \int_{-\infty}^{\infty} \left(1 - i\xi x - \tfrac{1}{2}\xi^2 x^2 + \ldots\right) \lambda(x) dx$$
$$= 1 - i\xi\mu_1 - \tfrac{1}{2}\xi^2\mu_2 + \ldots,$$

where μ_j is the j th moment $\mu_j = \int_{-\infty}^{\infty} x^j \lambda(x) dx$ – provided these exist
Assume $\lambda(x)$ is normalized and even: $\mu_1 = 0$, $\mu_2 = 1$ and $\mu_3 = 0$. Then

$$\widetilde{f}(\xi) = 1 - \tfrac{1}{2}\xi^2 + O(\xi^4).$$

Theorem. *If X and Y are independent random variables with a* PDF *given by f and g, respectively, then the sum $Z = X + Y$ has the* PDF $f * g$.

Suppose now the jump length Δx has a PDF given by $\lambda(x)$ so that

$$P(a<\Delta x<b) = \int_a^b \lambda(x)\,dx.$$

If $\lambda(x)$ decays sufficiently fast as $x \to \pm\infty$, the Fourier transform gives

$$\begin{aligned}\widetilde{\lambda}(\xi) &= \int_{-\infty}^{\infty} e^{-i\xi x}\lambda(x)dx = \int_{-\infty}^{\infty}\left(1 - i\xi x - \tfrac{1}{2}\xi^2 x^2 + \ldots\right)\lambda(x)dx \\ &= 1 - i\xi\mu_1 - \tfrac{1}{2}\xi^2\mu_2 + \ldots,\end{aligned}$$

where μ_j is the jth moment $\mu_j = \int_{-\infty}^{\infty} x^j\lambda(x)dx$ – provided these exist. Assume $\lambda(x)$ is normalized and even: $\mu_1 = 0$, $\mu_2 = 1$ and $\mu_3 = 0$. Then

$$\widetilde{f}(\xi) = 1 - \tfrac{1}{2}\xi^2 + O(\xi^4).$$

Theorem. *If X and Y are independent random variables with a* PDF *given by f and g, respectively, then the sum $Z = X + Y$ has the* PDF *$f * g$.*

Assume the steps ΔX_1, ΔX_2, $\ldots$ are independent. Then $X_n = \Delta X_1 + \ldots + \Delta X_n$ gives the position of the walker after n steps.

This is also a random variable, and has a Fourier transform $p_n(\xi) = (\widetilde{\lambda}(\xi))^n$, and the normalized sum $X_n/\sqrt{n}$ has the Fourier transform

$$(\widetilde{p}_n(\xi/\sqrt{n}))^n = \left(1 - \frac{1}{2n}\xi^2 + O(n^{-2})\right)^n .$$

The limit $n \to \infty$ gives $\widetilde{p}(\xi) = e^{-\frac{\xi^2}{2}}$ and inverting the Fourier transform gives a Gaussian distribution $p(x) = \frac{1}{\sqrt{4\pi}} e^{-\frac{x^2}{4}}$.

This is also a random variable, and has a Fourier transform $p_n(\xi) = (\widetilde{\lambda}(\xi))^n$, and the normalized sum $X_n/\sqrt{n}$ has the Fourier transform

$$(\widetilde{p}_n(\xi/\sqrt{n}))^n = \left(1 - \tfrac{1}{2n}\xi^2 + O(n^{-2})\right)^n .$$

The limit $n \to \infty$ gives $\widetilde{p}(\xi) = e^{-\frac{\xi^2}{2}}$ and inverting the Fourier transform gives a Gaussian distribution $p(x) = \frac{1}{\sqrt{4\pi}} e^{-\frac{x^2}{4}}$.

This is a statement of the central limit theorem that the long term averaged behavior of i.i.d. variables is a Gaussian density.

This is also a random variable, and has a Fourier transform $p_n(\xi) = (\widetilde{\lambda}(\xi))^n$, and the normalized sum $X_n/\sqrt{n}$ has the Fourier transform

$$(\widetilde{p}_n(\xi/\sqrt{n}))^n = \left(1 - \frac{1}{2n}\xi^2 + O(n^{-2})\right)^n .$$

The limit $n \to \infty$ gives $\widetilde{p}(\xi) = e^{-\frac{\xi^2}{2}}$ and inverting the Fourier transform gives a Gaussian distribution $p(x) = \frac{1}{\sqrt{4\pi}} e^{-\frac{x^2}{4}}$.

This is a statement of the central limit theorem that the long term averaged behavior of i.i.d. variables is a Gaussian density.

One requirement for the whole procedure to work is that the second moment μ_2 of $\lambda(x)$ be finite.

Now we interpret X_n as the particle position after n steps at the time t. We correlate the time step size Δt with the variance of Δx, following the coupling ansatz and rescaling the variance of $\lambda(x)$ to Kt.

Now we interpret X_n as the particle position after n steps at the time t. We correlate the time step size Δt with the variance of Δx, following the coupling ansatz and rescaling the variance of $\lambda(x)$ to Kt.

By the scaling rule for the Fourier transform, the Fourier transform $\widetilde{p}_n(\xi)$ is

$$p_n(\xi) = (1 - n^{-1} K t \xi^2 + O(n^{-2}))^n$$

Taking the limit of a large number of steps $n \to \infty$, we arrive at the Fourier transform $\widetilde{p}(\xi) = e^{-\xi^2 K t}$.

Now we interpret X_n as the particle position after n steps at the time t. We correlate the time step size Δt with the variance of Δx, following the coupling ansatz and rescaling the variance of $\lambda(x)$ to Kt.

By the scaling rule for the Fourier transform, the Fourier transform $\widetilde{p}_n(\xi)$ is

$$p_n(\xi) = (1 - n^{-1}Kt\xi^2 + O(n^{-2}))^n$$

Taking the limit of a large number of steps $n \to \infty$, we arrive at the Fourier transform $\widetilde{p}(\xi) = e^{-\xi^2 Kt}$.

Inverting this gives the PDF of being at a certain position x at time t, is governed by the diffusion equation and has the Gaussian PDF

$$p(x,t) = \frac{1}{\sqrt{4\pi Kt}} e^{-x^2/4Kt}.$$

This is the fundamental solution of the heat/diffusion equation

Now we interpret X_n as the particle position after n steps at the time t. We correlate the time step size Δt with the variance of Δx, following the coupling ansatz and rescaling the variance of $\lambda(x)$ to Kt.

By the scaling rule for the Fourier transform, the Fourier transform $\widetilde{p}_n(\xi)$ is

$$p_n(\xi) = (1 - n^{-1} K t \xi^2 + O(n^{-2}))^n$$

Taking the limit of a large number of steps $n \to \infty$, we arrive at the Fourier transform $\widetilde{p}(\xi) = e^{-\xi^2 K t}$.

Inverting this gives the PDF of being at a certain position x at time t, is governed by the diffusion equation and has the Gaussian PDF

$$p(x,t) = \frac{1}{\sqrt{4\pi K t}} e^{-x^2/4Kt}.$$

This is the fundamental solution of the heat/diffusion equation

For fixed time $t > 0$, $p(x,t)$ is a Gaussian distribution in x with mean zero and variance $2Kt$. It scales linearly with the time t. $\langle x^2 \rangle \propto t$.

Now we interpret X_n as the particle position after n steps at the time t. We correlate the time step size Δt with the variance of Δx, following the coupling ansatz and rescaling the variance of $\lambda(x)$ to Kt.

By the scaling rule for the Fourier transform, the Fourier transform $\widetilde{p}_n(\xi)$ is

$$p_n(\xi) = (1 - n^{-1}Kt\xi^2 + O(n^{-2}))^n$$

Taking the limit of a large number of steps $n \to \infty$, we arrive at the Fourier transform $\widetilde{p}(\xi) = e^{-\xi^2 Kt}$.

Inverting this gives the PDF of being at a certain position x at time t, is governed by the diffusion equation and has the Gaussian PDF

$$p(x,t) = \frac{1}{\sqrt{4\pi Kt}} e^{-x^2/4Kt}.$$

This is the fundamental solution of the heat/diffusion equation

For fixed time $t > 0$, $p(x,t)$ is a Gaussian distribution in x with mean zero and variance $2Kt$. It scales linearly with the time t. $\langle x^2 \rangle \propto t$.

The linear scaling with t is one characteristic feature of classical diffusion.

This is the essential content of Einstein's 1905 paper.

A (slightly) more general case

A walker moves along the x-axis, starting at a position x_0 at time $t_0 = 0$.

At time t_1, the walker jumps to x_1, then at time t_2 jumps to x_2, $\ldots$.

Assume that the temporal and spatial increments

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

are iid random variables, with PDFs $\psi(t)$ and $\lambda(x)$, – the waiting time and jump length distribution, respectively..

A (slightly) more general case

A walker moves along the x-axis, starting at a position x_0 at time $t_0 = 0$.

At time t_1, the walker jumps to x_1, then at time t_2 jumps to x_2, $\ldots$.

Assume that the temporal and spatial increments

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

are iid random variables, with PDFs $\psi(t)$ and $\lambda(x)$, – the waiting time and jump length distribution, respectively..

The probability of Δt_n lying in any interval $[a, b] \subset (0, \infty)$ is

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

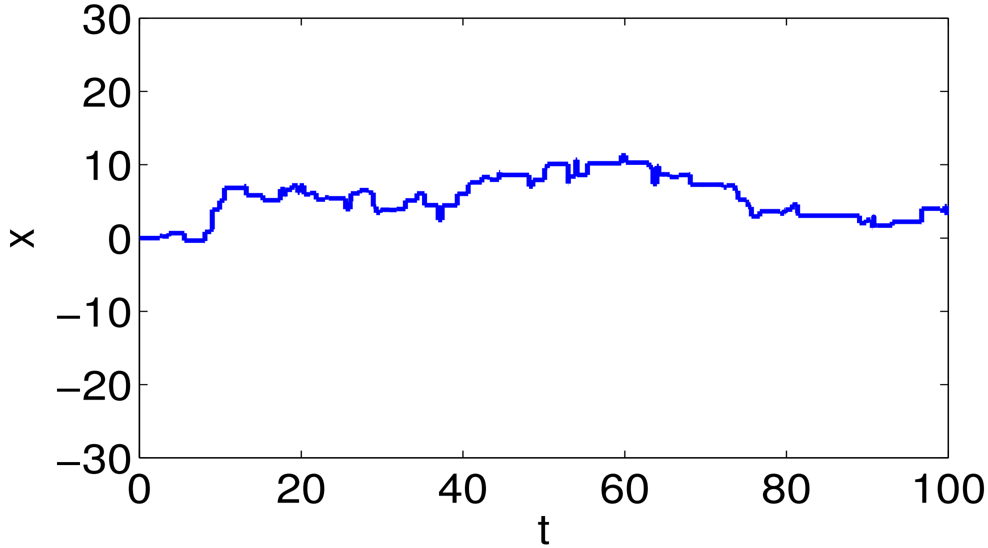
and the probability of Δx_n lying in any interval $[a, b] \subset \mathbb{R}$ is

$$P(a < \Delta x_n < b) = \int_a^b \lambda(x)\, dx.$$

Goal: determine $P($the walker lies in a given spatial interval at time $t)$.

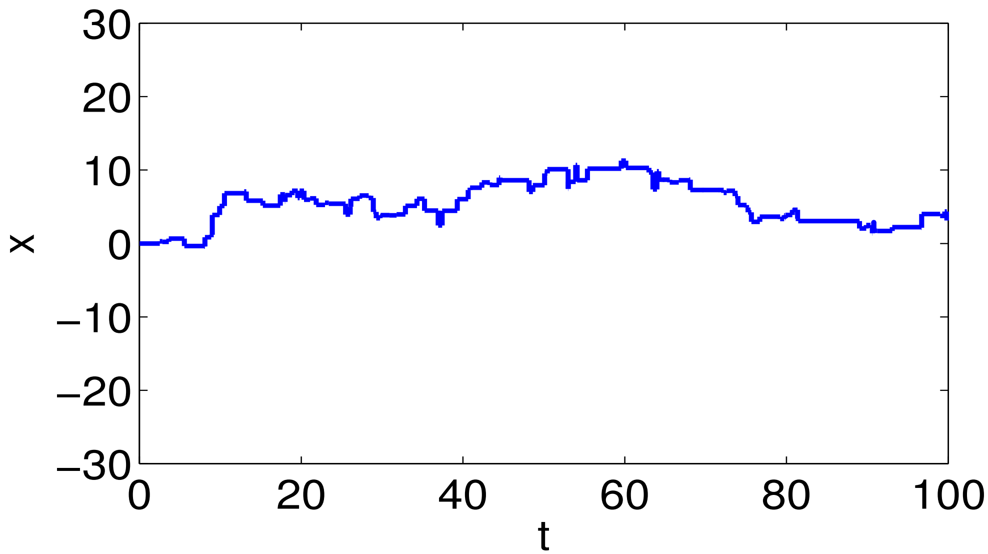
For given ψ and λ, the position x can be regarded as a step function of t.

For given ψ and λ, the position x can be regarded as a step function of t.



Random walk with exponentially decaying $\psi(t)$ and Gaussian $\lambda(x)$.

For given ψ and λ, the position x can be regarded as a step function of t.

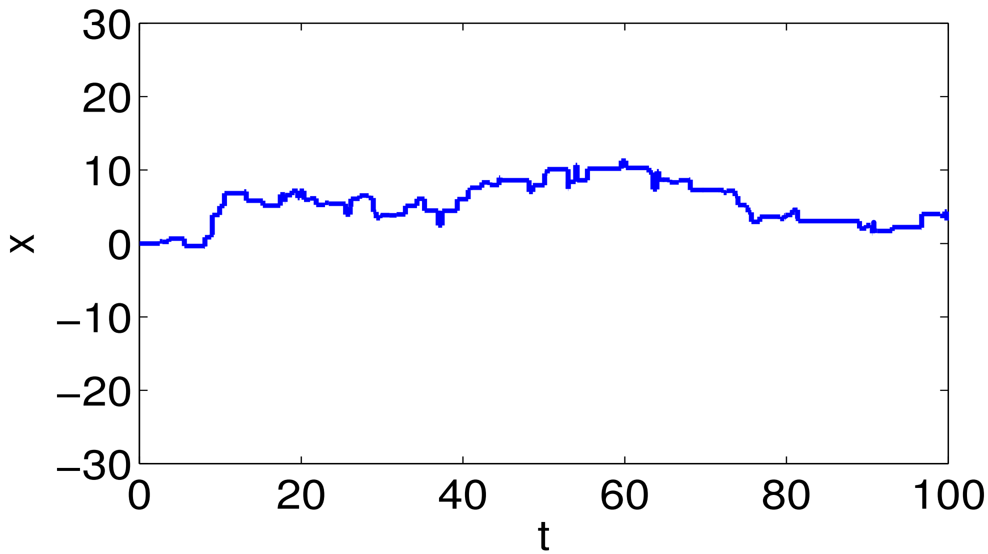


Random walk with exponentially decaying $\psi(t)$ and Gaussian $\lambda(x)$.

Different CTRW processes can be categorized by the characteristic waiting time T and the jump length variance Σ^2 being finite or diverging.

$$T =: E[\Delta t_n] = \int_0^\infty t\psi(t)dt \quad \Sigma^2 =: E[(\Delta x_n)^2] = \int_{-\infty}^\infty x^2\lambda(x)dx.$$

For given ψ and λ, the position x can be regarded as a step function of t.



Random walk with exponentially decaying $\psi(t)$ and Gaussian $\lambda(x)$.

Different CTRW processes can be categorized by the characteristic waiting time T and the jump length variance Σ^2 being finite or diverging.

$$T =: E[\Delta t_n] = \int_0^\infty t\psi(t)dt \quad \Sigma^2 =: E[(\Delta x_n)^2] = \int_{-\infty}^\infty x^2\lambda(x)dx.$$

If both T and Σ are finite, the long-time limit corresponds to Brownian motion, and thus the CTRW does not lead to anything new.

Fractional Calculus

Fractional Calculus

History of generalizing from the integers $\mathbb{N} \to \mathbb{R},\ \mathbb{C}$

Bernoulli, Euler, (1730s): $n! \to \Gamma(z+1)$

Fractional Calculus

History of generalizing from the integers $\mathbb{N} \to \mathbb{R},\ \mathbb{C}$

Bernoulli, Euler, (1730s): $n! \to \Gamma(z+1)$

Attempts to do the same for differentiation formulae; (1740 - today)

To compute the fractional derivative of order α use the n^{th} formulae and replace $n \to \alpha$.

EXAMPLES:

$$D^{(n)}x^m = \frac{m!}{(m-n)!}x^{m-n} \to D^{\alpha}x^m = \frac{m!}{\Gamma(m-\alpha+1)!}x^{m-\alpha}$$

$$D^{(n)}e^{\lambda x} = \lambda^n e^{\lambda x} \to D^{\alpha}e^{\lambda x} = \lambda^{\alpha}e^{\lambda x}$$

$$D^{(n)}\sin(x) = \sin(x + n\frac{\pi}{2}) \to D^{\alpha}\sin(x) = \sin(x + \alpha\frac{\pi}{2})$$

The Abel integral operator

The integral operator $A^\alpha f = \dfrac{1}{\Gamma(\alpha)} \displaystyle\int_a^t \dfrac{f(\tau)\,d\tau}{(t-\tau)^{1-\alpha}} \quad \alpha > 0$ arose in Abel's 1823 solution of the more general tautochrone and brachistochrone problems which were originally posed and solved in a simpler form by Huygens in 1659 and Bernoulli in 1695 respectively.

The Abel integral operator

The integral operator $A^\alpha f = \dfrac{1}{\Gamma(\alpha)} \displaystyle\int_a^t \frac{f(\tau)\,d\tau}{(t-\tau)^{1-\alpha}}$ $\alpha > 0$ arose in Abel's 1823 solution of the more general tautochrone and brachistochrone problems which were originally posed and solved in a simpler form by Huygens in 1659 and Bernoulli in 1695 respectively.

In these particular applications $\alpha = 1/2$ and the solution to $A^{1/2}y = f$ is given by the well-known formula

$$f(x) = \frac{1}{\pi}\frac{d}{dx}\int_a^x \frac{f(s)\,ds}{(x-s)^{1/2}}.$$

As was shown by Abel, for general α, $0 < \alpha < 1$ this becomes

$$f(x) = \frac{\sin(\pi(1-\alpha))}{\pi}\frac{d}{dx}\int_a^x \frac{f(s)\,ds}{(x-s)^{\alpha}}.$$

The Abel integral operator

The integral operator $A^\alpha f = \dfrac{1}{\Gamma(\alpha)}\displaystyle\int_a^t \dfrac{f(\tau)\,d\tau}{(t-\tau)^{1-\alpha}} \quad \alpha > 0$ arose in Abel's 1823 solution of the more general tautochrone and brachistochrone problems which were originally posed and solved in a simpler form by Huygens in 1659 and Bernoulli in 1695 respectively.

In these particular applications $\alpha = 1/2$ and the solution to $A^{1/2}y = f$ is given by the well-known formula

$$f(x) = \frac{1}{\pi}\frac{d}{dx}\int_a^x \frac{f(s)\,ds}{(x-s)^{1/2}}.$$

As was shown by Abel, for general α, $0 < \alpha < 1$ this becomes

$$f(x) = \frac{\sin(\pi(1-\alpha))}{\pi}\frac{d}{dx}\int_a^x \frac{f(s)\,ds}{(x-s)^{\alpha}}.$$

The important point here is that in his solution of the integral equation Abel had shown the way to rigorously define a fractional integral and, by his inversion of this, how to define a fractional derivative.

The Abel integral operator

The integral operator $A^\alpha f = \dfrac{1}{\Gamma(\alpha)} \displaystyle\int_a^t \frac{f(\tau)\,d\tau}{(t-\tau)^{1-\alpha}}$ $\alpha > 0$ arose in Abel's 1823 solution of the more general tautochrone and brachistochrone problems which were originally posed and solved in a simpler form by Huygens in 1659 and Bernoulli in 1695 respectively.

In these particular applications $\alpha = 1/2$ and the solution to $A^{1/2}y = f$ is given by the well-known formula

$$f(x) = \frac{1}{\pi}\frac{d}{dx}\int_a^x \frac{f(s)\,ds}{(x-s)^{1/2}}.$$

As was shown by Abel, for general α, $0 < \alpha < 1$ this becomes

$$f(x) = \frac{\sin(\pi(1-\alpha))}{\pi}\frac{d}{dx}\int_a^x \frac{f(s)\,ds}{(x-s)^{\alpha}}.$$

In this sense Abel is the true mathematical founder of the concept although later work by Liouville and by Riemann have dominated the nomenclature.

Definition. *The Riemann-Liouville fractional derivative* ${}^{R}D_x^{\alpha}u(x)$ *is defined for* $a \in \mathbb{R}$ *by*

$$ {}_a^R D_x^{\alpha} u(x) = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_a^x (x-s)^{n-1-\alpha} u(s)\, ds. $$

This is clearly based on Abel's integral and suggests that the fractional derivative of f is the n^{th} integer derivative of the fractional integral $I_x^{\alpha} f(x) = \frac{1}{\Gamma(n-\alpha)} \int_0^x (x-s)^{-\alpha} f(s)\, ds$ of f where $n-1 < \alpha \leq n$.

Definition. *The Riemann-Liouville fractional derivative* ${}^{R}D_x^{\alpha}u(x)$ *is defined for* $a \in \mathbb{R}$ *by* ${}^{R}_{a}D_x^{\alpha}u(x) = \dfrac{1}{\Gamma(n-\alpha)} \dfrac{d^n}{dx^n} \displaystyle\int_a^x (x-s)^{n-1-\alpha} u(s)\, ds.$

This is clearly based on Abel's integral and suggests that the fractional derivative of f is the n^{th} integer derivative of the fractional integral $I_x^{\alpha} f(x) = \frac{1}{\Gamma(n-\alpha)} \int_0^x (x-s)^{-\alpha} f(s)\, ds$ of f where $n-1 < \alpha \le n$.

There is another version that reverses the above order; the Djrbashyan-Caputo derivative:- ${}^{C}_{a}D_x^{\alpha}u(x) = \dfrac{1}{\Gamma(n-\alpha)} \displaystyle\int_a^x (x-s)^{n-1-\alpha} u^{(n)}(s)\, ds$

Definition. *The Riemann-Liouville fractional derivative* ${}^{R}D_x^{\alpha}u(x)$ *is defined for* $a \in \mathbb{R}$ *by*

$$ {}_a^R D_x^{\alpha} u(x) = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_a^x (x-s)^{n-1-\alpha} u(s)\, ds. $$

This is clearly based on Abel's integral and suggests that the fractional derivative of f is the n^{th} integer derivative of the fractional integral $I_x^{\alpha} f(x) = \frac{1}{\Gamma(n-\alpha)} \int_0^x (x-s)^{-\alpha} f(s)\, ds$ of f where $n-1 < \alpha \leq n$.

There is another version that reverses the above order; the Djrbashyan-Caputo derivative:-

$$ {}_a^C D_x^{\alpha} u(x) = \frac{1}{\Gamma(n-\alpha)} \int_a^x (x-s)^{n-1-\alpha} u^{(n)}(s)\, ds $$

This version was studied extensively by the Armenian mathematician M . M. Djrbashyan, in his 1966 book. However, there was a considerable amount of earlier work on this version of the integral, but only available in the Russian literature.

Definition. *The Riemann-Liouville fractional derivative* ${}^{R}D_x^{\alpha}u(x)$ *is defined for* $a \in \mathbb{R}$ *by* ${}_{a}^{R}D_x^{\alpha}u(x) = \dfrac{1}{\Gamma(n-\alpha)}\dfrac{d^n}{dx^n}\displaystyle\int_a^x (x-s)^{n-1-\alpha}u(s)\,ds.$

This is clearly based on Abel's integral and suggests that the fractional derivative of f is the n^{th} integer derivative of the fractional integral $I_x^{\alpha}f(x) = \frac{1}{\Gamma(n-\alpha)}\int_0^x (x-s)^{-\alpha}f(s)\,ds$ of f where $n-1 < \alpha \leq n$.

There is another version that reverses the above order; the Djrbashyan-Caputo derivative:- ${}_{a}^{C}D_x^{\alpha}u(x) = \dfrac{1}{\Gamma(n-\alpha)}\displaystyle\int_a^x (x-s)^{n-1-\alpha}u^{(n)}(s)\,ds$

This version was studied extensively by the Armenian mathematician M . M. Djrbashyan, in his 1966 book. However, there was a considerable amount of earlier work on this version of the integral, but only available in the Russian literature.

The geophysicist Michele Caputo rediscovered this version in 1967 as a tool for understanding seismological phenomenon, and later with Francesco Mainardi in viscoelasticity where the memory effect of the fractional derivative were crucial.

THE POWER FUNCTION: Differentiating the fractional integral and using $\Gamma(z+1) = z\Gamma(z)$ gives

$$ {}_{0}^{R}D_x^{\alpha}(x-a)^{\gamma} = \frac{\Gamma(\gamma+1)}{\Gamma(\gamma+1-\alpha)}(x-a)^{\gamma-\alpha} \quad x > a, \quad \gamma > -1 $$

THE POWER FUNCTION: Differentiating the fractional integral and using $\Gamma(z+1) = z\Gamma(z)$ gives

$$ {}_0^R D_x^\alpha (x-a)^\gamma = \frac{\Gamma(\gamma+1)}{\Gamma(\gamma+1-\alpha)}(x-a)^{\gamma-\alpha} \quad x > a, \quad \gamma > -1 $$

This implies ${}_0^R D_x^\alpha 1 = \frac{1}{\Gamma(1-\alpha)}(x-a)^{-\alpha}$. This is particularly inconvenient for practical applications involving initial/boundary conditions

THE POWER FUNCTION: Differentiating the fractional integral and using $\Gamma(z+1) = z\Gamma(z)$ gives

$$ {}_0^R D_x^\alpha (x-a)^\gamma = \frac{\Gamma(\gamma+1)}{\Gamma(\gamma+1-\alpha)} (x-a)^{\gamma-\alpha} \quad x > a, \quad \gamma > -1 $$

This implies ${}_0^R D_x^\alpha \, 1 = \frac{1}{\Gamma(1-\alpha)} (x-a)^{-\alpha}$. This is particularly inconvenient for practical applications involving initial/boundary conditions

We compute ${}_0^R D_x^\alpha e^{\lambda x}$ by fractionally differentiating the series term-by-term:

$$ {}_0^R D_x^\alpha e^{\lambda x} = {}_0^R D_x^\alpha \sum_{k=0}^{\infty} \frac{(\lambda x)^k}{\Gamma(k+1)} = \sum_{k=0}^{\infty} \lambda^k \frac{{}_0^R D_x^\alpha x^k}{\Gamma(k+1)} = \sum_{k=0}^{\infty} \frac{\lambda^k x^{k-\alpha}}{\Gamma(k+1-\alpha)} $$

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

where $E_{\alpha,\beta}(z)$ will be defined shortly.

These examples show:

The product rule ${}_0^R D_x^\alpha (fg) \neq ({}_0^R D_x^\alpha f)g + f\,{}_0^R D_x^\alpha g,$ fails!

Thus in addition, no integration by parts, . . . Green's Theorem . . .]
– major PDE tool gone!.

Djrbashian-Caputo fractional derivative

For $f \in L^1(D)$, the left-sided Djrbashian-Caputo fractional derivative of order α, denoted by ${}_0^C D_x^\alpha f$, is defined by

$${}_0^C D_x^\alpha f(x) := ({}_a I_x^{n-\alpha} f^{(n)})(x) = \frac{1}{\Gamma(n-\alpha)} \int_a^x (x-s)^{n-\alpha-1} f^{(n)}(s) ds,$$

if the integral on the right hand side exists

The Djrbashian-Caputo derivative is more restrictive than the Riemann-Liouville since it requires the nth order classical derivative to be absolutely integrable.

Note that in general

$$({}_0^R D_x^\alpha f)(x) \neq ({}_0^C D_x^\alpha f)(x),$$

even when both derivatives are defined.

[But they do agree if $f^{(k)}(0) = 0$ for $k = \lfloor \alpha \rfloor$].

$${}_0^C D_x^\alpha f(x) = {}_0^R D_x^\alpha \left(f(x) - \sum_{k=0}^{n-1} \frac{(x-a)^k}{k!} f^{(k)}(a^+) \right)$$

Djrbashian-Caputo fractional derivative

For $f \in L^1(D)$, the left-sided Djrbashian-Caputo fractional derivative of order α, denoted by ${}_0^C D_x^\alpha f$, is defined by

$${}_0^C D_x^\alpha f(x) := ({}_a I_x^{n-\alpha} f^{(n)})(x) = \frac{1}{\Gamma(n-\alpha)} \int_a^x (x-s)^{n-\alpha-1} f^{(n)}(s) ds,$$

if the integral on the right hand side exists

The Djrbashian-Caputo derivative is more restrictive than the Riemann-Liouville since it requires the nth order classical derivative to be absolutely integrable.

Just as in the Riemann-Liouville case, neither the composition rule nor the product rule hold for the Djrbashian-Caputo fractional derivative.

Djrbashian-Caputo fractional derivative

For $f \in L^1(D)$, the left-sided Djrbashian-Caputo fractional derivative of order α, denoted by ${}_0^C D_x^\alpha f$, is defined by

$$ {}_0^C D_x^\alpha f(x) := ({}_a I_x^{n-\alpha} f^{(n)})(x) = \frac{1}{\Gamma(n-\alpha)} \int_a^x (x-s)^{n-\alpha-1} f^{(n)}(s) ds, $$

if the integral on the right hand side exists

The Djrbashian-Caputo derivative is more restrictive than the Riemann-Liouville since it requires the nth order classical derivative to be absolutely integrable.

Laplace transforms:

$$ \mathcal{L}[{}_0^R D_x^\alpha f](z) = z^\alpha \mathcal{L}[f](z) - \sum_{k=0}^{n-1} z^{n-k-1} ({}_0^R D_x^{\alpha+k-n} f)(0^+). $$

$$ \mathcal{L}[{}_0^C D_x^\alpha f](z) = z^\alpha \mathcal{L}[f](z) - \sum_{k=0}^{n-1} z^{\alpha-k-1} \mathcal{L}[f]^{(k)}(0). $$

More members of the fractional derivative zoo

A combination of left and right Riemann-Liouville derivatives

$$D_x^{\beta} = (\theta)\, {}^{R}_{a^+}D_x^{\alpha} + (1-\theta)\, {}^{R}_{b^-}D_x^{\alpha}$$

is called the *Riesz fractional derivative.*

The case $\beta = \frac{1}{2}$ is the *symmetric Riesz derivative.*

The case $a = -\infty$, $b = \infty$ is the *symmetric Weyl derivative*.

The fractional power of $(-\triangle)$ can be defined as the pseudodifferential operator with symbol $\xi^{2\alpha}$.

These are most commonly used for space fractional derivatives.

Important message

- There are many different definitions of “fractional derivative”; we have looked at only two, but will briefly mention one or two others.
  One must specify which derivative is being used!!
- All of these derivatives are nonlocal - they have a history mechanism. This will cause considerable anxiety with the analysis (and outcomes).
- Different derivatives and different “fractional orders” α will lead to quite different domains of definition and mapping properties.
- All these derivatives have a starting point. This must be included or one gets different answers!

The Mittag-Leffler and Wright functions

The two-parameter Mittag-Leffler function $E_{\alpha,\beta}(z)$ is defined by

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

for $\alpha > 0$, and $\beta \in \mathbb{R}$. The function $E_{\alpha,1}(z)$, is often denoted by $E_\alpha(z)$.

The two-parameter Mittag-Leffler function $E_{\alpha,\beta}(z)$ is defined by

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

for $\alpha > 0$, and $\beta \in \mathbb{R}$. The function $E_{\alpha,1}(z)$, is often denoted by $E_\alpha(z)$.

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

Theorem.
For $\alpha > 0$ and $\beta \in \mathbb{R}$, $E_{\alpha,\beta}(z)$ is an entire function of order $\frac{1}{\alpha}$ type 1.
$E_{\alpha,\beta}(-x)$ is completely monotone on $\mathbb{R}^+$ for $\alpha \in (0,1)$ and $\beta \geq \alpha$.

Recursion, differentiation/integral representation formulae $\ldots$ and

$$\mathcal{L}E_\alpha(-\lambda t^\alpha) = \frac{z^{\alpha-1}}{\lambda + z^\alpha}$$

For our purposes, the most interesting and important properties of the function $E_{\alpha,\beta}(z)$ are associated with its asymptotic behavior as $z \to \infty$ in various sectors of the complex plane $\mathbb{C}$. This result is due to Djrbashian

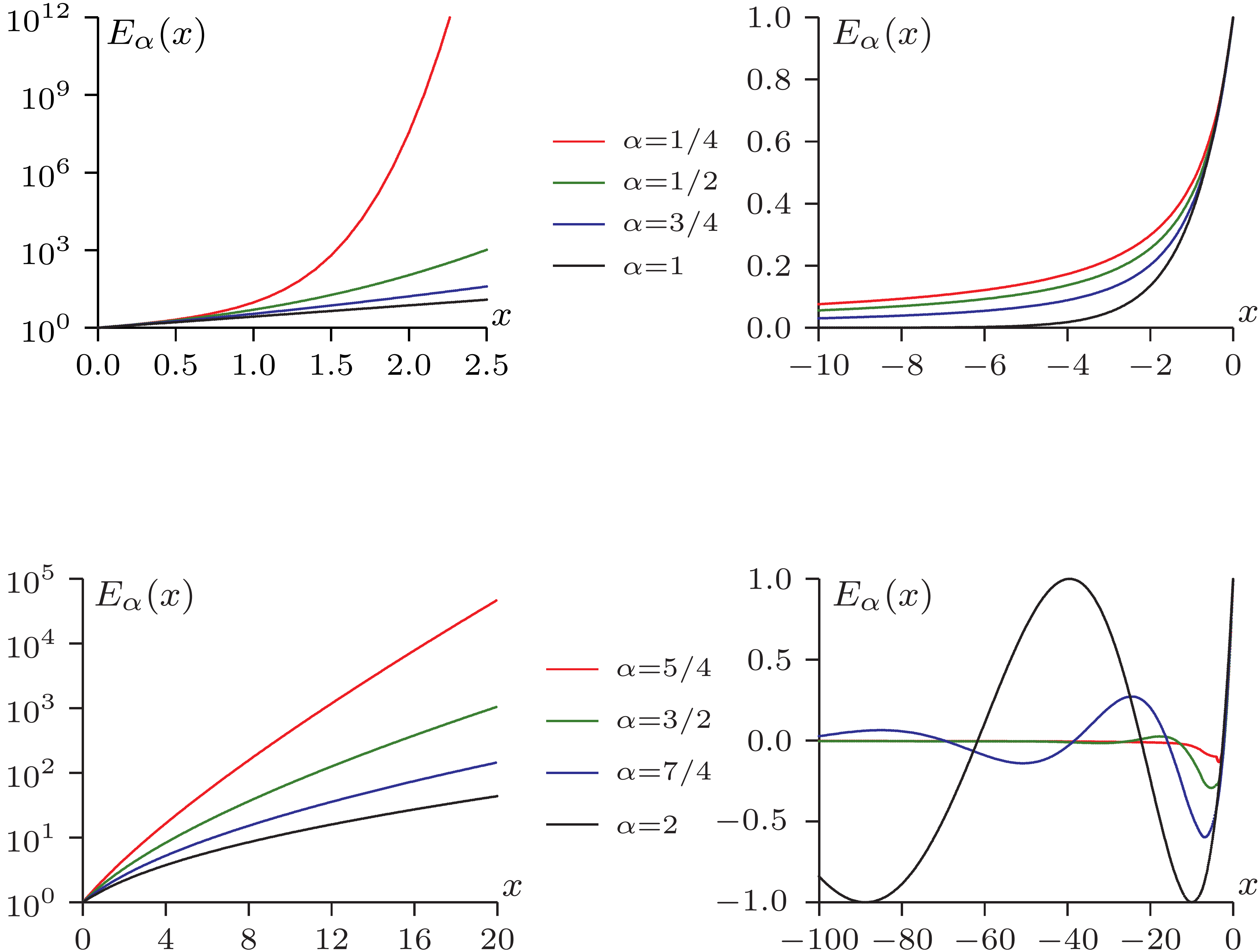
Theorem. *Let* $\alpha \in (0, 2)$, $\beta \in \mathbb{R}$, *and* $\mu \in (\alpha\pi/2, min(\pi, \alpha\pi))$, *and* $N \in \mathbb{N}$. *Then for* $|\text{arg}(z)| \leq \mu$ *with* $|z| \to \infty$,

$$E_{\alpha,\beta}(z) \sim \frac{1}{\alpha} z^{\frac{1-\beta}{\alpha}} e^{z^{\frac{1}{\alpha}}}$$

and for $\mu \leq |\arg(z)| \leq \pi$ with $|z| \to \infty$

$$E_{\alpha,\beta}(z) = -\sum_{k=1}^{N} \frac{1}{\Gamma(\beta-\alpha k)} \frac{1}{z^k} + O\left(\frac{1}{z^{N+1}}\right).$$

- On the positive real axis it grows exponentially, and the growth rate increases with decreasing α.
- The important message is: $E_{\alpha,\beta}(z)$, with $\alpha \in (0, 2)$ and $\beta - \alpha \notin -\mathbb{N}$ decays only linearly on the negative real axis.



$E_\alpha(x)$
10^{12}
10^{9}
10^{6}
10^{3}
10^{0}
0.0
0.5
1.0
1.5
2.0
2.5
x
α=1/4
α=1/2
α=3/4
α=1
$E_\alpha(x)$
1.0
0.8
0.6
0.4
0.2
0.0
−10
−8
−6
−4
−2
0
x
$E_\alpha(x)$
10^{5}
10^{4}
10^{3}
10^{2}
10^{1}
10^{0}
0
4
8
12
16
20
x
α=5/4
α=3/2
α=7/4
α=2
$E_\alpha(x)$
1.0
0.5
0.0
−0.5
−1.0
−100
−80
−60
−40
−20
0
x

The initial value problem for the fractional ordinary differential equation

$$ {}_0D_t^{\alpha} u(t) + \lambda u(t) = 0 \quad x > 0, \quad u(0) = 1 \qquad 0 < \alpha < 1 $$

has solution $u(t)$ given by $\quad u(t) = E_{\alpha}(-\lambda t^{\alpha}) = \sum_{k=0}^{\infty} \frac{(-\lambda t^{\alpha})^k}{\Gamma(k\alpha + 1)}$

The initial value problem for the fractional ordinary differential equation

$$ {}_0D_t^{\alpha} u(t) + \lambda u(t) = 0 \quad x > 0, \quad u(0) = 1 \qquad 0 < \alpha < 1 $$

has solution $u(t)$ given by $\quad u(t) = E_{\alpha}(-\lambda t^{\alpha}) = \sum_{k=0}^{\infty} \frac{(-\lambda t^{\alpha})^k}{\Gamma(k\alpha + 1)}$

We want the fundamental solution for

$$ {}_0^C D_t^{\alpha} p(x,t) - u_{xx} \qquad \text{on} \;\; \mathbb{R} \times \mathbb{R}^+ $$

First take a Fourier transform in space,

$$ {}_0^C D_t^{\alpha} \tilde{p}(\xi, t) + \xi^2 \tilde{p}(\xi, t) \quad \Rightarrow \quad p(\xi, t) = E_{\alpha}(-\xi^2 t^{\alpha}) $$

[To invert we need the inverse Laplace transform of the Mittag Leffler function]

For $\mu,\ \rho \in \mathbb{R}$ with $\rho > -1$, the Wright function $W_{\rho,\mu}(z)$ is defined by

$$W_{\rho,\mu}(z) = \sum_{k=0}^{\infty} \frac{z^k}{k!\Gamma(\rho k + \mu)} \quad z \in \mathbb{C}.$$

For $\mu,\ \rho \in \mathbb{R}$ with $\rho > -1$, the Wright function $W_{\rho,\mu}(z)$ is defined by

$$W_{\rho,\mu}(z) = \sum_{k=0}^{\infty} \frac{z^k}{k!\Gamma(\rho k + \mu)} \quad z \in \mathbb{C}.$$

There is a particular version we need $M_\mu(z) = W_{-\mu,1-\mu}(-z)$.

For $\mu,\ \rho \in \mathbb{R}$ with $\rho > -1$, the Wright function $W_{\rho,\mu}(z)$ is defined by

$$W_{\rho,\mu}(z) = \sum_{k=0}^{\infty} \frac{z^k}{k!\Gamma(\rho k + \mu)} \quad z \in \mathbb{C}.$$

There is a particular version we need $M_\mu(z) = W_{-\mu,1-\mu}(-z)$.

The Laplace transform of a Wright function is a Mittag-Leffler function

$$\mathcal{L}[W_{\rho,\mu}(x)](z) = \frac{1}{z} E_{\rho,\mu}(z^{-1})$$

For $\mu,\ \rho \in \mathbb{R}$ with $\rho > -1$, the Wright function $W_{\rho,\mu}(z)$ is defined by

$$W_{\rho,\mu}(z) = \sum_{k=0}^{\infty} \frac{z^k}{k!\Gamma(\rho k + \mu)} \quad z \in \mathbb{C}.$$

There is a particular version we need $M_\mu(z) = W_{-\mu,1-\mu}(-z)$.

The Laplace transform of a Wright function is a Mittag-Leffler function

$$\mathcal{L}[W_{\rho,\mu}(x)](z) = \frac{1}{z} E_{\rho,\mu}(z^{-1})$$

Theorem. $\mathcal{L}[M_\mu(x)](z) = E_\mu(-z),\ \mathcal{F}[M_\mu(|x|)](\xi) = 2E_{2\mu}(-\xi^2)$

For $\mu,\ \rho \in \mathbb{R}$ with $\rho > -1$, the Wright function $W_{\rho,\mu}(z)$ is defined by

$$W_{\rho,\mu}(z) = \sum_{k=0}^{\infty} \frac{z^k}{k!\Gamma(\rho k + \mu)} \quad z \in \mathbb{C}.$$

There is a particular version we need $M_\mu(z) = W_{-\mu,1-\mu}(-z)$.

The Laplace transform of a Wright function is a Mittag-Leffler function

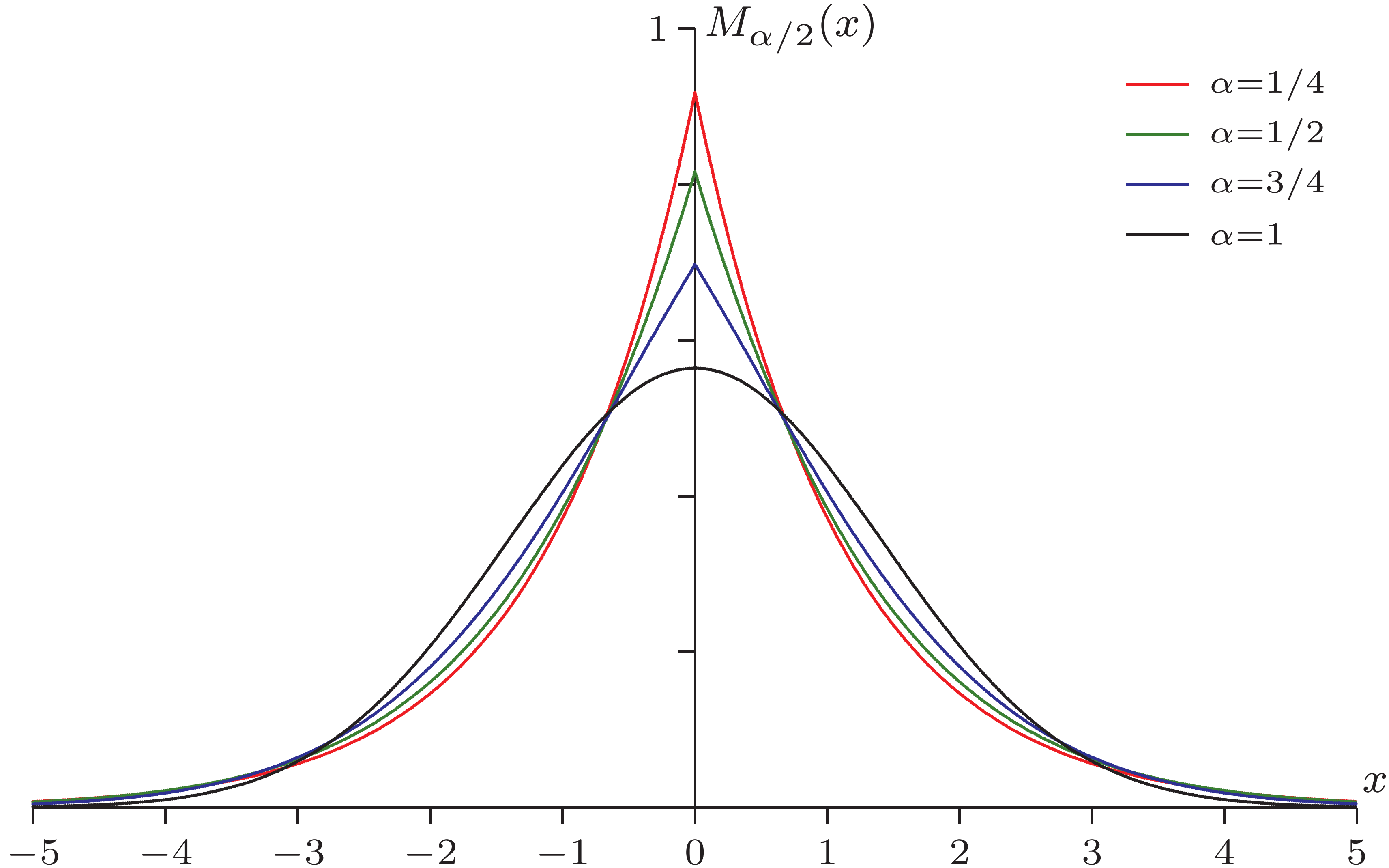
$$\mathcal{L}[W_{\rho,\mu}(x)](z) = \frac{1}{z} E_{\rho,\mu}(z^{-1})$$

Theorem. $\mathcal{L}[M_\mu(x)](z) = E_\mu(-z),\ \mathcal{F}[M_\mu(|x|)](\xi) = 2E_{2\mu}(-\xi^2)$

Combining all of this, the Fundamental Solution is

$$p(x,t) = \frac{1}{\sqrt{4K\,t^\alpha}} M_{\frac{\alpha}{2}}\left(\frac{|x|}{\sqrt{Kt^\alpha}}\right)$$

The Fundamental Solution of $\partial_t^\alpha - u_{xx} = 0$



Random Walks leading to Anomolous Diffusion

Now we consider the situation where the characteristic waiting time T diverges, but the jump length variance Σ^2 is still kept finite.

Random Walks leading to Anomolous Diffusion

Now we consider the situation where the characteristic waiting time T diverges, but the jump length variance Σ^2 is still kept finite.

To model such phenomena, we employ a heavy-tailed waiting time PDF with the asymptotic behaviour $\psi(t) \sim \dfrac{A}{t^{1+\alpha}}$ as $t \to \infty$, $\alpha \in (0,1)$, $A > 0$.

The specific form of $\psi(t)$ is irrelevant; large time decay matters.

The parameter α determines the asymptotic decay of the PDF; the closer is α to zero, the slower the decay and the more likely a long waiting time.

Random Walks leading to Anomolous Diffusion

Now we consider the situation where the characteristic waiting time T diverges, but the jump length variance Σ^2 is still kept finite.

To model such phenomena, we employ a heavy-tailed waiting time PDF with the asymptotic behaviour $\psi(t) \sim \dfrac{A}{t^{1+\alpha}}$ as $t \to \infty\,,\ \alpha \in (0,1)\,,\ A > 0\,.$

The specific form of $\psi(t)$ is irrelevant; large time decay matters.

The parameter α determines the asymptotic decay of the PDF; the closer is α to zero, the slower the decay and the more likely a long waiting time.

For this power law decay the mean waiting time is divergent: $\int_0^\infty t\psi(t)dt = +\infty$ and the preceding analysis breaks down. But, the assumption on $\lambda(x)$ remains unchanged, i.e., $\int_{-\infty}^{\infty} x\lambda(x)\,dx = 0$ and $\int_{-\infty}^{\infty} x^2\lambda(x)\,dx = 1\,.$

Random Walks leading to Anomolous Diffusion

Now we consider the situation where the characteristic waiting time T diverges, but the jump length variance Σ^2 is still kept finite.

To model such phenomena, we employ a heavy-tailed waiting time PDF with the asymptotic behaviour $\psi(t) \sim \dfrac{A}{t^{1+\alpha}}$ as $t \to \infty$, $\alpha \in (0,1)$, $A > 0$.

The specific form of $\psi(t)$ is irrelevant; large time decay matters.

The parameter α determines the asymptotic decay of the PDF; the closer is α to zero, the slower the decay and the more likely a long waiting time.

For this power law decay the mean waiting time is divergent: $\int_0^\infty t\psi(t)dt = +\infty$ and the preceding analysis breaks down. But, the assumption on $\lambda(x)$ remains unchanged, i.e., $\int_{-\infty}^{\infty} x\lambda(x)\,dx = 0$ and $\int_{-\infty}^{\infty} x^2\lambda(x)\,dx = 1$.

Take the rescaled PDFs for the waiting time Δt_n and jump length Δx_n:

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

The Laplace-Fourier transform $\widehat{\widetilde{p}}(\xi, z; \sigma, \tau)$ is

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

The Laplace-Fourier transform $\widehat{\widetilde{p}}(\xi, z; \sigma, \tau)$ is

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

Several algebraic manipulations later $\ldots$ compute the Fourier-Laplace transform $\widehat{\widetilde{p}}(\xi, z)$ by sending $\substack{\sigma \to 0 \\ \tau \to 0}$, keeping $\frac{\sigma^2}{2B_\alpha \tau^\alpha} = K_\alpha$ fixed

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

The Laplace-Fourier transform $\widehat{\widetilde{p}}(\xi, z; \sigma, \tau)$ is

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

Several algebraic manipulations later $\ldots$ compute the Fourier-Laplace transform $\widehat{\widetilde{p}}(\xi, z)$ by sending $\substack{\sigma \to 0 \\ \tau \to 0}$, keeping $\frac{\sigma^2}{2B_\alpha \tau^\alpha} = K_\alpha$ fixed

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

Invert the Fourier-Laplace transform $\widehat{\widetilde{p}}(\xi, z)$ back into space-time using the Laplace transform formula of the Mittag-Leffler function $E_\alpha(z)$,

$$\widetilde{p}(\xi, t) = E_\alpha(-K_\alpha t^\alpha \xi^2)$$

and next applying the Fourier transform of the M-Wright function we get $p(x, t)$ in the physical domain

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

Thus the fractional time derivative of order α corresponds to a particular decay choice of the time PDF $\psi(t)$.

Thus the fractional time derivative of order α corresponds to a particular decay choice of the time PDF $\psi(t)$.

Now compute the mean square displacement $\mu_2(t) = \int_{-\infty}^{\infty} x^2 p(x,t)\,dx$. by taking the Laplace transform

$$\widehat{\mu}_2(z) = \int_{-\infty}^{\infty} x^2 \widehat{p}(x,z)dx = -\frac{d^2}{d\xi^2}\widehat{\widetilde{p}}(\xi,z)|_{\xi=0}$$

$$= -\frac{d^2}{d\xi^2}(z + K_\alpha z^{1-\alpha}\xi^2)^{-1}|_{\xi=0} = 2K_\alpha z^{-1-\alpha},$$

and taking the inverse Laplace transform yields

$$\langle x^2 \rangle := \mu_2(t) = \frac{2K_\alpha}{\Gamma(1+\alpha)} t^\alpha \propto t^\alpha$$

Thus the fractional time derivative of order α corresponds to a particular decay choice of the time PDF $\psi(t)$.

Now compute the mean square displacement $\mu_2(t) = \int_{-\infty}^{\infty} x^2 p(x,t)\, dx$. by taking the Laplace transform

$$\widehat{\mu}_2(z) = \int_{-\infty}^{\infty} x^2 \widehat{p}(x,z) dx = -\frac{d^2}{d\xi^2} \widehat{\widehat{p}}(\xi, z)|_{\xi=0}$$

$$= -\frac{d^2}{d\xi^2} (z + K_\alpha z^{1-\alpha} \xi^2)^{-1} |_{\xi=0} = 2K_\alpha z^{-1-\alpha},$$

and taking the inverse Laplace transform yields

$$\langle x^2 \rangle := \mu_2(t) = \frac{2K_\alpha}{\Gamma(1+\alpha)} t^\alpha \propto t^\alpha$$

Thus the mean square displacement grows only sublinearly with the time t. Such a diffusion process is often called *subdiffusive*.

If we retain the finite mean assumption on $\psi(t)$ but similarily relax the finite variance condition on $\lambda(x)$,

$$\lambda(x) \sim \frac{B}{x^{2+\beta}} \quad \text{as } x \to \infty$$

we obtain a space fractional derivative of order β.

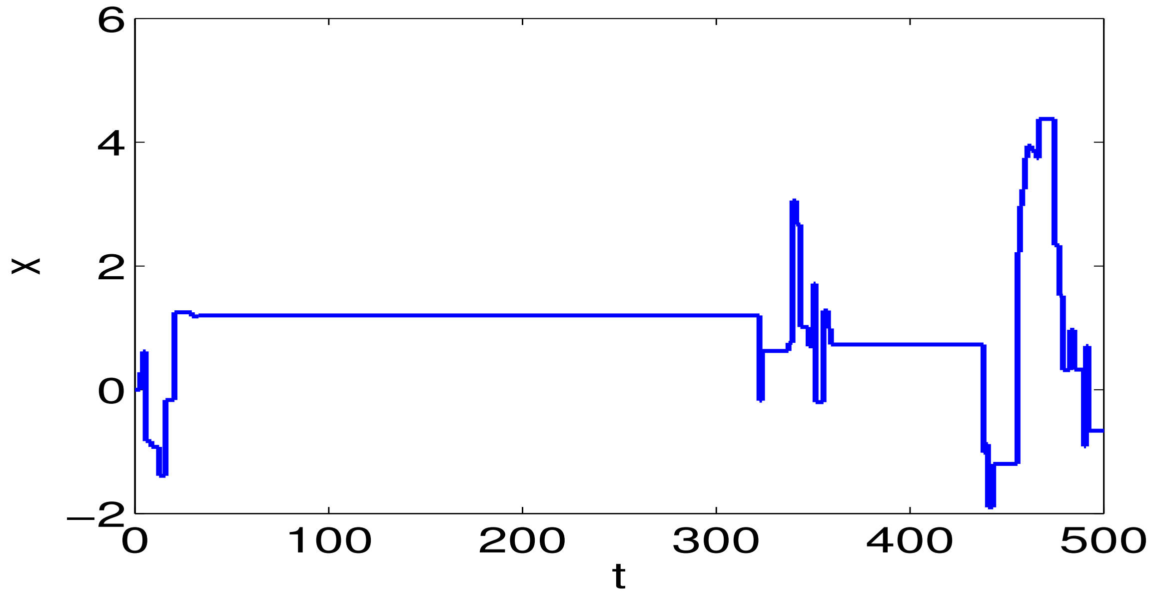
If we retain the finite mean assumption on $\psi(t)$ but similarily relax the finite variance condition on $\lambda(x)$,

$$\lambda(x) \sim \frac{B}{x^{2+\beta}} \quad \text{as } x \to \infty$$

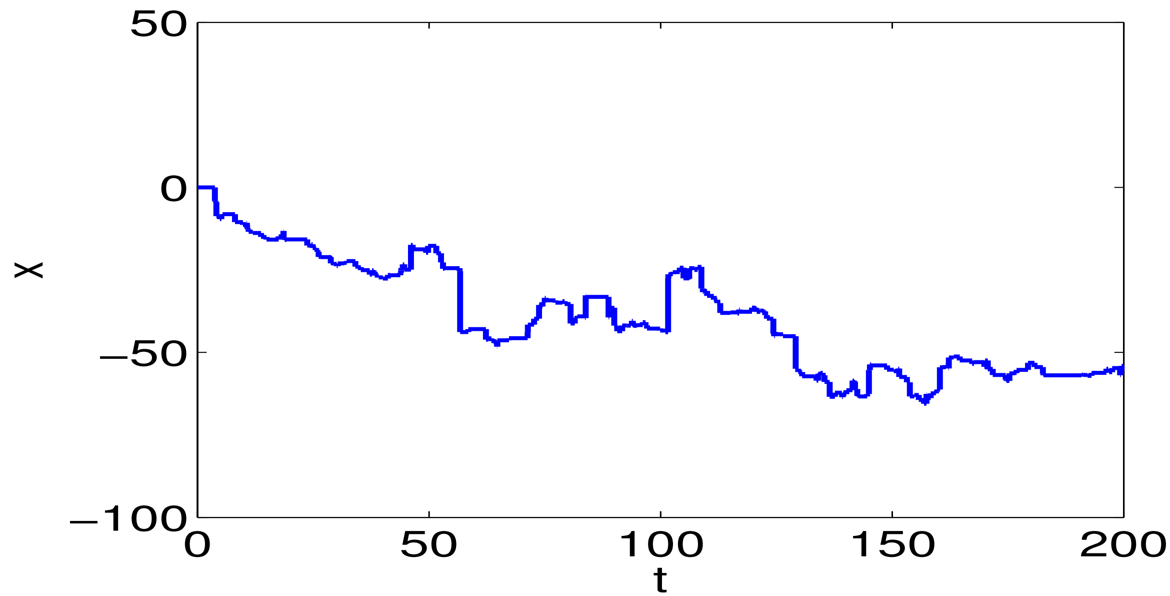
we obtain a space fractional derivative of order β.

Naturally, we can do those in both space and time.

Infinite mean in $\psi(t)$



Infinite variance in $\lambda(x)$



Subdiffusion Model

A is a strongly elliptic partial differential operator in Ω.
$\partial_t^\alpha u$ is the Djrbashian-Caputo derivative of u of order $\alpha \in (0, 1)$.

$$\begin{aligned} \partial_t^\alpha u(x,t) &= Au(x,t) + f(x,t) \quad (x,t) \in \Omega \times (0,T], \\ u(x,t) &= 0 \quad (x,t) \in \partial\Omega \times (0,T], \\ u(x,0) &= u_0(x) \quad x \in \Omega \end{aligned} \tag{$**$}$$

Subdiffusion Model

A is a strongly elliptic partial differential operator in Ω.
$\partial_t^\alpha u$ is the Djrbashian-Caputo derivative of u of order $\alpha \in (0,1)$.

$$\begin{aligned} \partial_t^\alpha u(x,t) &= Au(x,t) + f(x,t) \quad (x,t) \in \Omega \times (0,T], \\ u(x,t) &= 0 \quad (x,t) \in \partial\Omega \times (0,T], \\ u(x,0) &= u_0(x) \quad x \in \Omega \end{aligned} \tag{**}$$

Is the single fractional exponent the only possibility?

Subdiffusion Model

A is a strongly elliptic partial differential operator in Ω.
$\partial_t^\alpha u$ is the Djrbashian-Caputo derivative of u of order $\alpha \in (0, 1)$.

$$\begin{aligned} \partial_t^\alpha u(x,t) &= Au(x,t) + f(x,t) \quad (x,t) \in \Omega \times (0,T], \\ u(x,t) &= 0 \quad (x,t) \in \partial\Omega \times (0,T], \\ u(x,0) &= u_0(x) \quad x \in \Omega \end{aligned} \qquad (**)$$

Is the single fractional exponent the only possibility?

- The "multi-term model": $\partial_t^\alpha = \sum_{j=1}^m q_j \partial_t^{\alpha_j}$ where $\alpha_j \in (0, 1]$.

  This arises from assuming the relevant probability density function has m terms of the form $q_j/t^{1+\alpha_j}$, $1 \le j \le m$.

Subdiffusion Model

A is a strongly elliptic partial differential operator in Ω.
$\partial_t^\alpha u$ is the Djrbashian-Caputo derivative of u of order $\alpha \in (0,1)$.

$$\begin{aligned} \partial_t^\alpha u(x,t) &= Au(x,t) + f(x,t) \quad (x,t) \in \Omega \times (0,T], \\ u(x,t) &= 0 \quad (x,t) \in \partial\Omega \times (0,T], \\ u(x,0) &= u_0(x) \quad x \in \Omega \end{aligned} \tag{$**$}$$

Is the single fractional exponent the only possibility?

- The "multi-term model": $\partial_t^\alpha = \sum_{j=1}^m q_j \partial_t^{\alpha_j}$ where $\alpha_j \in (0,1]$.

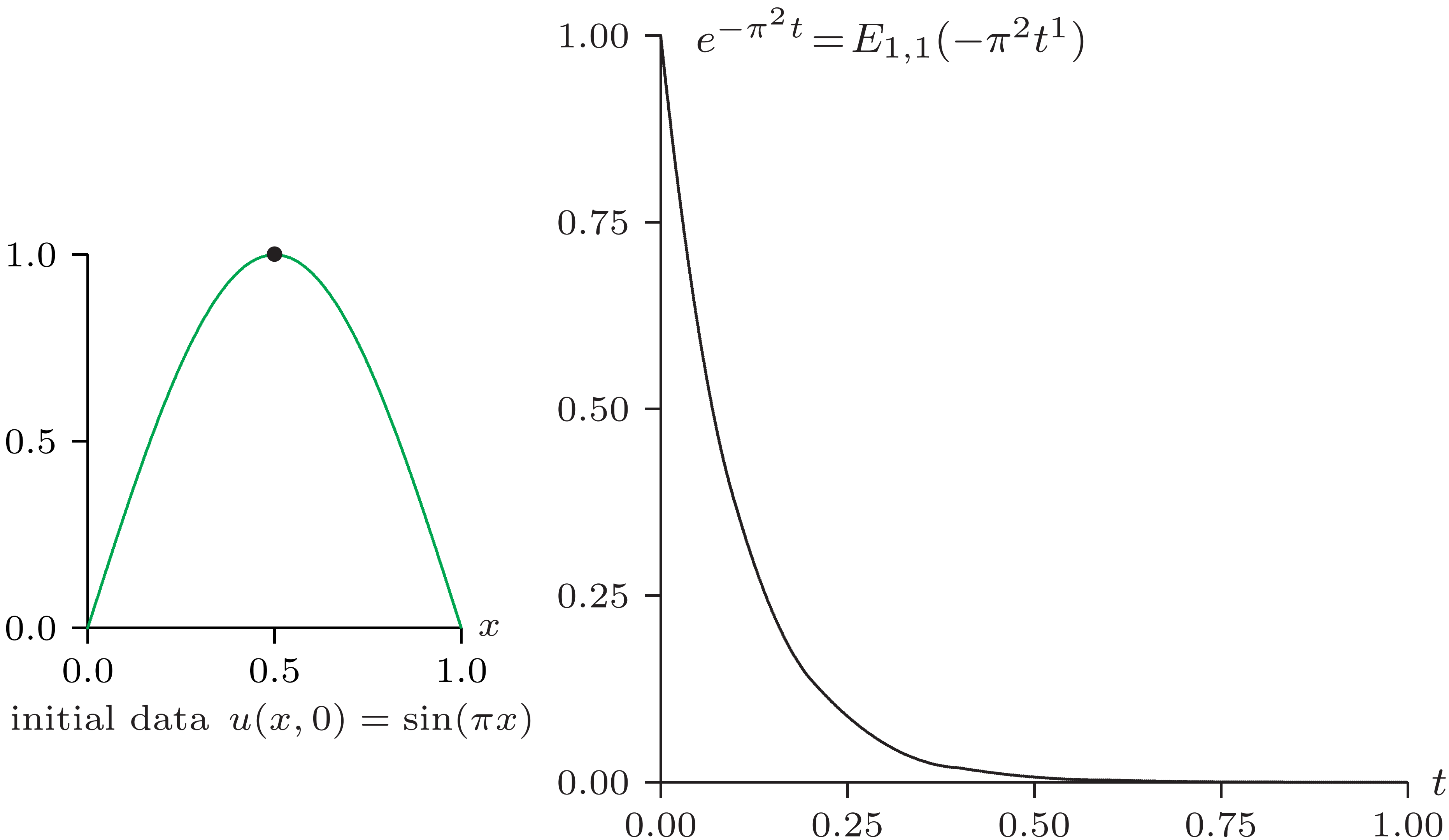
  This arises from assuming the relevant probability density function has m terms of the form $q_j/t^{1+\alpha_j}$, $1 \le j \le m$.

- The fully distributed model: $\partial^i(\mu)u(t) = \int_0^1 \mu(\alpha)\partial_t^\alpha \, d\alpha$

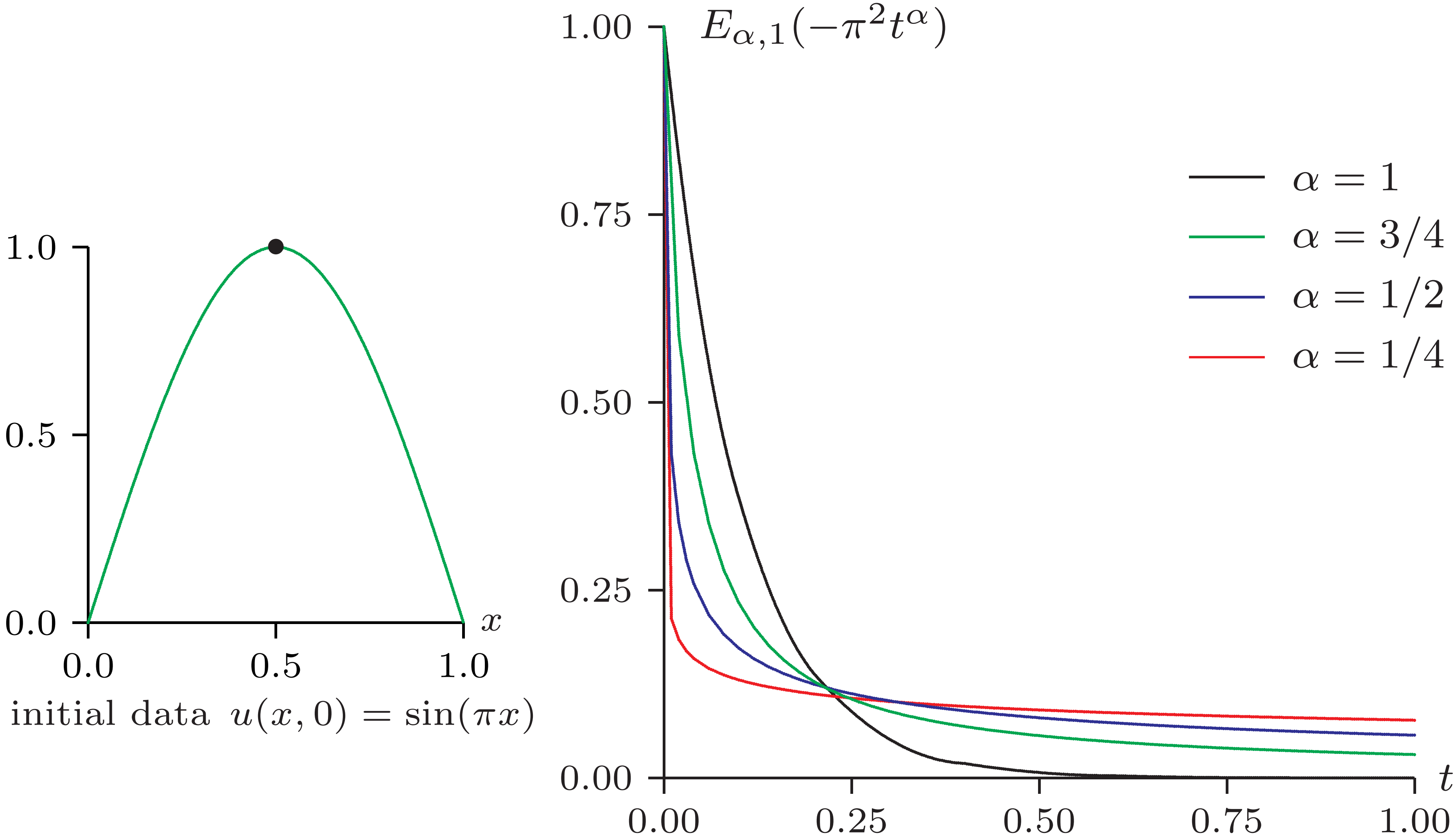
Everything is dominated by the weakly singular non-local operator.

- “Local arguments” don’t work (think strong Maximum Principle, pointwise estimates).
- The fractional pde has limited smoothing properties; lack of regularity affects typical “pde results”.
- There is no sequel to Crank-Nicolson from the parabolic case and the storage apart, the typical time-stepping methods are first order, or at best $1 + \alpha$ order, accurate.
- The entire history of the spatial solution must be maintained at each time step - this can be computationally significant in $\mathbb{R}^3$ situations

Subdiffusion is no longer a Markov process.



Time evolution of $u_t - u_{xx} = 0$ at $x = \frac{1}{2}$, $u(x,0) = \sin(\pi x)$



Time evolution of $\partial_t^\alpha - u_{xx} = 0$, at $x = \frac{1}{2}$, $u(x,0) = \sin(\pi x)$

Inverse Problems

An unlimited number of questions; we will merely (and very briefly look at)

Inverse Problems

An unlimited number of questions; we will merely (and very briefly look at)

- How do we determine the fractional exponent?
- The backwards diffusion problem
- An unknown source of the form $F = \chi(D)$ and overposed flux data

As a teaser to many in the audience:

$\diamondsuit$ Regularization methods based on fractional operators.

For the single exponent α it is usually straightforward to determine this - usually in addition to the main purpose of computing a coefficient.

The main idea is based on the solution being analytic in α. From, say, a flux measurement $g(t)$ on $\partial\Omega$, the limiting behaviour as $t \to 0$ reveals α. Alternatively, one can take the Laplace transform.

For the single exponent α it is usually straightforward to determine this - usually in addition to the main purpose of computing a coefficient.

The main idea is based on the solution being analytic in α. From, say, a flux measurement $g(t)$ on $\partial\Omega$, the limiting behaviour as $t \to 0$ reveals α. Alternatively, one can take the Laplace transform.

For the multi-α situation analyticity again plays the crucial role.

Taking the Laplace transform $t \to s$, we obtain a rational function in s with coefficients depending on q_j and α_j. These may be backed out in sequence using analytic continuation in s. Extremely ill-posed. [Li, Yamamoto: 2014]

For the single exponent α it is usually straightforward to determine this - usually in addition to the main purpose of computing a coefficient.

The main idea is based on the solution being analytic in α. From, say, a flux measurement $g(t)$ on $\partial\Omega$, the limiting behaviour as $t \to 0$ reveals α. Alternatively, one can take the Laplace transform.

For the multi-α situation analyticity again plays the crucial role.

Taking the Laplace transform $t \to s$, we obtain a rational function in s with coefficients depending on q_j and α_j. These may be backed out in sequence using analytic continuation in s. Extremely ill-posed. [Li, Yamamoto: 2014]

The distributed situation is more complex as the function $\mu(\alpha)$ need not only be continuous. A representation theorem involving $\mu(\alpha)$ and kernel M is obtained and showing that M can be expanded in powers of α and that these are sufficiently dense so that the Müntz-Szász Theorem applies. [R, Zhang].

The Backwards Diffusion Problem

Given

$$u_t = u_{xx} \qquad 0 < x < 1, \quad 0 < t < T$$

$$u(0,t) = u(1,t) = 0 \qquad u(x,0) = u_0(x)$$

We measure $u(x,T)$ and wish to recover the initial value $u_0(x)$.

Given

$$u_t = u_{xx} \qquad 0 < x < 1, \quad 0 < t < T$$

$$u(0,t) = u(1,t) = 0 \qquad u(x,0) = u_0(x)$$

We measure $u(x,T)$ and wish to recover the initial value $u_0(x)$.

$\phi_n(x) = \sqrt{2}\sin n\pi x$, $c_n = \langle u_0, \phi_n \rangle$, $d_n = \langle u(\cdot,T), \phi_n \rangle$, $\lambda_n = n^2\pi^2$.

Given

$$u_t = u_{xx} \qquad 0 < x < 1, \quad 0 < t < T$$

$$u(0,t) = u(1,t) = 0 \qquad u(x,0) = u_0(x)$$

We measure $u(x,T)$ and wish to recover the initial value $u_0(x)$.

$\phi_n(x) = \sqrt{2}\sin n\pi x$, $c_n = \langle u_0, \phi_n \rangle$, $d_n = \langle u(\cdot, T), \phi_n \rangle$, $\lambda_n = n^2\pi^2$.

$$u_t = u_{xx}$$

$$u(x,t) = \sum c_n e^{-\lambda_n t}\phi_n(x)$$

$$u_0(x) = \sum d_n e^{\lambda_n T}\phi_n(x)$$

Recover $\{c_n\}$: $c_n = e^{n^2\pi^2 T} d_n$

Amazingly ill-posed

Given

$$u_t = u_{xx} \qquad 0 < x < 1, \quad 0 < t < T$$

$$u(0,t) = u(1,t) = 0 \qquad u(x,0) = u_0(x)$$

We measure $u(x,T)$ and wish to recover the initial value $u_0(x)$.

$\phi_n(x) = \sqrt{2}\sin n\pi x$, $c_n = \langle u_0, \phi_n\rangle$, $d_n = \langle u(\cdot,T), \phi_n\rangle$, $\lambda_n = n^2\pi^2$.

$$u_t = u_{xx}$$

$$u(x,t) = \sum c_n e^{-\lambda_n t}\phi_n(x)$$

$$u_0(x) = \sum d_n e^{\lambda_n T}\phi_n(x)$$

Recover $\{c_n\}$: $c_n = e^{n^2\pi^2 T} d_n$

Amazingly ill-posed

$$D_t^\alpha u = u_{xx}$$

$$u(x,t) = \sum c_n E_{\alpha,1}(-\lambda_n t^\alpha)\phi_n(x)$$

$$u_0(x) = \sum d_n [E_{\alpha,1}(-\lambda_n T^\alpha)]^{-1}\phi_n(x)$$

Recover $\{c_n\}$: $c_n = \frac{1}{E_{\alpha,1}(-\lambda_n T^\alpha)} d_n$

How ill-posed?

Look at the asymptotic: if $\lambda_n T >> 1$, $E_{\alpha,1}(-\lambda_n T^\alpha) \approx C\lambda_n T^\alpha$.

The n^{th} Fourier mode of u_0 equals that of g multiplied by $\lambda_n \approx n^2\pi^2$

– a two derivative loss in Fourier space

– control of $u(:,T)$ in $\dot{H}^2(\Omega)$ controls u_0 in L^2.

Look at the asymptotic: if $\lambda_n T >> 1$, $E_{\alpha,1}(-\lambda_n T^\alpha) \approx C\lambda_n T^\alpha$.

The n^{th} Fourier mode of u_0 equals that of g multiplied by $\lambda_n \approx n^2\pi^2$

– a two derivative loss in Fourier space

– control of $u(:,T)$ in $\dot{H}^2(\Omega)$ controls u_0 in L^2.

Stability estimate $c\|u(T)\|_{\dot{H}^2(\Omega)} \leq \|u(0)\|_{L^2} \leq C\|u(T)\|_{\dot{H}^2(\Omega)}$

[Liu, Yamamoto: 2010]

Look at the asymptotic: if $\lambda_n T >> 1$, $E_{\alpha,1}(-\lambda_n T^\alpha) \approx C\lambda_n T^\alpha$.

The n^{th} Fourier mode of u_0 equals that of g multiplied by $\lambda_n \approx n^2\pi^2$

– a two derivative loss in Fourier space

– control of $u(:,T)$ in $\dot{H}^2(\Omega)$ controls u_0 in L^2.

Stability estimate $\quad c\|u(T)\|_{\dot{H}^2(\Omega)} \leq \|u(0)\|_{L^2} \leq C\|u(T)\|_{\dot{H}^2(\Omega)}$

[Liu, Yamamoto: 2010]

The backwards fractional derivative problem is only mildly ill-conditioned

Look at the asymptotic: if $\lambda_n T >> 1$, $E_{\alpha,1}(-\lambda_n T^\alpha) \approx C\lambda_n T^\alpha$.

The n^{th} Fourier mode of u_0 equals that of g multiplied by $\lambda_n \approx n^2\pi^2$

– a two derivative loss in Fourier space

– control of $u(:,T)$ in $\dot{H}^2(\Omega)$ controls u_0 in L^2.

Stability estimate $c\|u(T)\|_{\dot{H}^2(\Omega)} \leq \|u(0)\|_{L^2} \leq C\|u(T)\|_{\dot{H}^2(\Omega)}$

[Liu, Yamamoto: 2010]

The backwards fractional derivative problem is only mildly ill-conditioned

Fractional diffusion completely changes the paradigm here

Look at the asymptotic: if $\lambda_n T >> 1, \; E_{\alpha,1}(-\lambda_n T^\alpha) \approx C\lambda_n T^\alpha$.

The n^{th} Fourier mode of u_0 equals that of g multiplied by $\lambda_n \approx n^2\pi^2$

– a two derivative loss in Fourier space

– control of $u(:,T)$ in $\dot{H}^2(\Omega)$ controls u_0 in L^2.

Stability estimate $c\|u(T)\|_{\dot{H}^2(\Omega)} \le \|u(0)\|_{L^2} \le C\|u(T)\|_{\dot{H}^2(\Omega)}$

[Liu, Yamamoto: 2010]

The backwards fractional derivative problem is only mildly ill-conditioned

Fractional diffusion completely changes the paradigm here

But do we have the complete story?

Look at the asymptotic: if $\lambda_n T >> 1$, $E_{\alpha,1}(-\lambda_n T^\alpha) \approx C\lambda_n T^\alpha$.

The n^{th} Fourier mode of u_0 equals that of g multiplied by $\lambda_n \approx n^2\pi^2$

– a two derivative loss in Fourier space

– control of $u(:,T)$ in $\dot{H}^2(\Omega)$ controls u_0 in L^2.

Stability estimate $c\|u(T)\|_{\dot{H}^2(\Omega)} \leq \|u(0)\|_{L^2} \leq C\|u(T)\|_{\dot{H}^2(\Omega)}$

[Liu, Yamamoto: 2010]

The backwards fractional derivative problem is only mildly ill-conditioned

Fractional diffusion completely changes the paradigm here

But do we have the complete story?

Conjecture:

Reconstructing u_0 from $u(x,T)$ is always easier in the fractional case

Look at the asymptotic: if $\lambda_n T >> 1$, $E_{\alpha,1}(-\lambda_n T^\alpha) \approx C\lambda_n T^\alpha$.

The n^{th} Fourier mode of u_0 equals that of g multiplied by $\lambda_n \approx n^2\pi^2$

– a two derivative loss in Fourier space

– control of $u(:,T)$ in $\dot{H}^2(\Omega)$ controls u_0 in L^2.

Stability estimate $c\|u(T)\|_{\dot{H}^2(\Omega)} \leq \|u(0)\|_{L^2} \leq C\|u(T)\|_{\dot{H}^2(\Omega)}$

[Liu, Yamamoto: 2010]

The backwards fractional derivative problem is only mildly ill-conditioned

Fractional diffusion completely changes the paradigm here

But do we have the complete story?

Conjecture:

Reconstructing u_0 from $u(x,T)$ is always easier in the fractional case

The answer is no, and the difference can be substantial.

A is a strongly elliptic pdo in Ω with eigenfunction/eigenvalues $\{\phi_n(x), \lambda_n\}$.

$$\begin{aligned} \partial_t^\alpha u(x,t) - Au(x,t) &= f(x) = \chi(D) \quad (x,t) \in \Omega \times (0,T], \\ u(x,t) &= 0 \quad (x,t) \in \partial\Omega \times (0,T], \\ u(x,0) &= u_0(x) \quad = 0 \quad x \in \Omega \end{aligned}$$

We wish to recover the (starlike) subdomain $D \subset \Omega$ from data

$$g_i(t) := \frac{\partial u}{\partial \nu}\bigg|_P, \quad P = \{x_i\} \in \partial\Omega$$

where P is a (small) number of discrete points on the boundary $\partial\Omega$.

Let $F = F_i = F(D)$ be the map from D to $\{g_i\}$.

A is a strongly elliptic pdo in Ω with eigenfunction/eigenvalues $\{\phi_n(x), \lambda_n\}$.

$$\partial_t^\alpha u(x,t) - Au(x,t) = f(x) = \chi(D) \quad (x,t) \in \Omega \times (0,T],$$
$$u(x,t) = 0 \quad (x,t) \in \partial\Omega \times (0,T],$$
$$u(x,0) = u_0(x) \quad = 0 \quad x \in \Omega$$

We wish to recover the (starlike) subdomain $D \subset \Omega$ from data

$$g_i(t) := \frac{\partial u}{\partial \nu}\bigg|_P, \quad P = \{x_i\} \in \partial\Omega$$

where P is a (small) number of discrete points on the boundary $\partial\Omega$.

Let $F = F_i = F(D)$ be the map from D to $\{g_i\}$.

Theorem. $\exists$ $P = \{x_1, x_2\}$ *such that the linearized map* F' *is injective.*

Case $\alpha = 1$, [Hettlich, R]. Case $\alpha < 1$, [R, Zhang].

A is a strongly elliptic pdo in Ω with eigenfunction/eigenvalues $\{\phi_n(x), \lambda_n\}$.

$$\partial_t^\alpha u(x,t) - Au(x,t) = f(x) = \chi(D) \quad (x,t) \in \Omega \times (0,T],$$
$$u(x,t) = 0 \quad (x,t) \in \partial\Omega \times (0,T],$$
$$u(x,0) = u_0(x) \quad = 0 \quad x \in \Omega$$

We wish to recover the (starlike) subdomain $D \subset \Omega$ from data

$$g_i(t) := \frac{\partial u}{\partial \nu}\Big|_P, \quad P = \{x_i\} \in \partial\Omega$$

where P is a (small) number of discrete points on the boundary $\partial\Omega$.

Let $F = F_i = F(D)$ be the map from D to $\{g_i\}$.

Theorem. $\exists$ $P = \{x_1, x_2\}$ *such that the linearized map* F' *is injective.*

Case $\alpha = 1$, [Hettlich, R]. Case $\alpha < 1$, [R, Zhang].

Very ill-conditioned! How does this depend on α?

A is a strongly elliptic pdo in Ω with eigenfunction/eigenvalues $\{\phi_n(x), \lambda_n\}$.

$$\partial_t^\alpha u(x,t) - Au(x,t) = f(x) = \chi(D) \quad (x,t) \in \Omega \times (0,T],$$
$$u(x,t) = 0 \quad (x,t) \in \partial\Omega \times (0,T],$$
$$u(x,0) = u_0(x) \quad = 0 \quad x \in \Omega$$

We wish to recover the (starlike) subdomain $D \subset \Omega$ from data

$$g_i(t) := \frac{\partial u}{\partial \nu}\bigg|_P, \qquad P = \{x_i\} \in \partial\Omega$$

where P is a (small) number of discrete points on the boundary $\partial\Omega$.

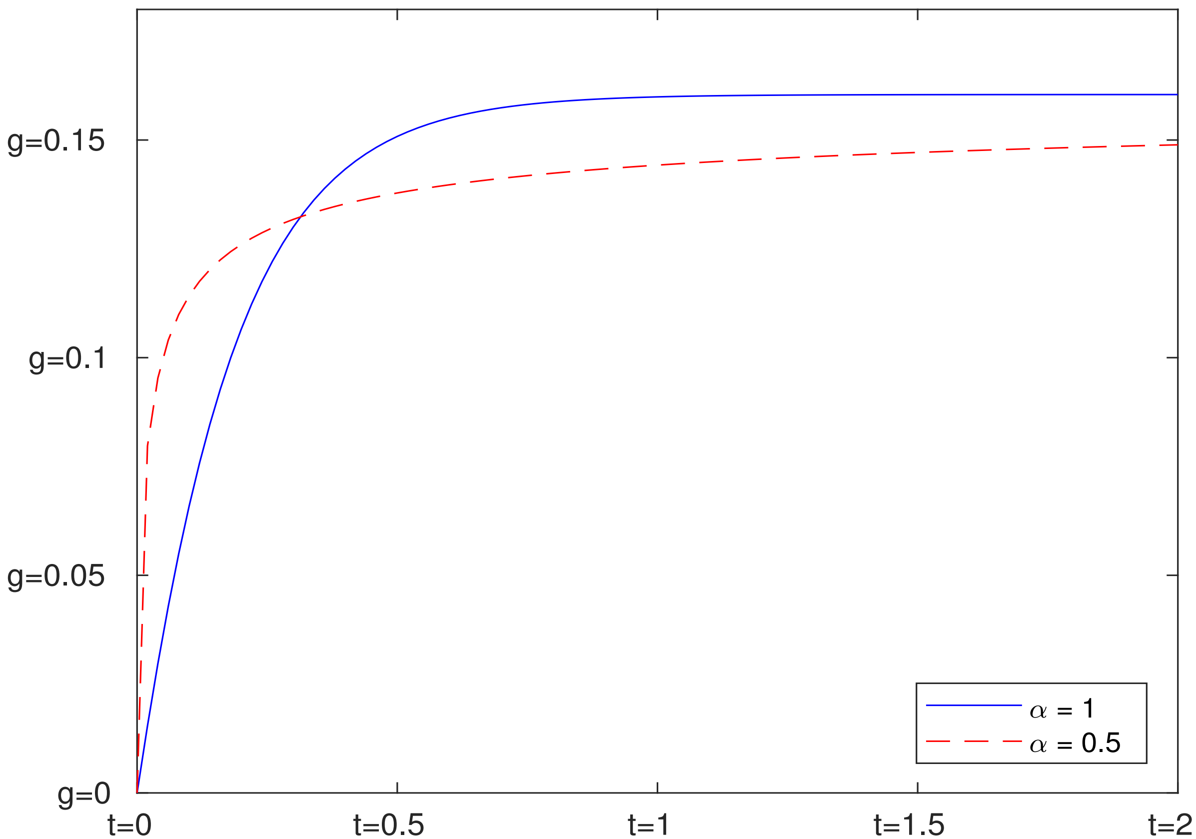
Let $F = F_i = F(D)$ be the map from D to $\{g_i\}$.

Theorem. $\exists \ P = \{x_1, x_2\}$ *such that the linearized map* F' *is injective.*

Case $\alpha = 1$, [Hettlich, R]. Case $\alpha < 1$, [R, Zhang].

Very ill-conditioned! How does this depend on α?

Depends on the selected **time** points, $\{t_k\}$, in measuring $g_i(t_k)$!



Profile of $g(t)$ for $\alpha = \frac{1}{2}$ and $\alpha = 1$ from a circle centre origin.

Obrigado