# An introduction to fractional calculus

## Fundamental ideas and numerics

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**Jump length**

$\lambda(x)\mathrm{d}x$ produces the probability for a jump length in the interval $(x, x + \mathrm{d}x)$.

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**Waiting time**

$w(t)\mathrm{d}t$ produces the probability for a waiting time in the interval $(t, t + \mathrm{d}t)$.

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- $w(t) = \int_{-\infty}^{+\infty} \psi(x, t) \, \mathrm{d}x$, *waiting time*,
- If the jump length and waiting time are **independent random variables** then:

$$\psi(x, t) = w(t)\lambda(x).$$

# Characterization of CTRW

To categorise different CTRW one can look at the quantities

$$T = \int_0^{+\infty} t w(t)\,\mathrm{d}t, \text{ (Characteristic waiting time)},$$

and

$$\Sigma^2 = \int_{-\infty}^{+\infty} x^2 \lambda(x)\,\mathrm{d}x \text{ (Jump length variance)},$$

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The master (Langevin) equation for this process is then given by

$$\eta(x,t) = \int_{-\infty}^{+\infty} \mathrm{d}x' \int_0^{+\infty} \mathrm{d}t'\, \eta(x',t')\psi(x-x',t-t') + \delta(x)\delta(t),$$

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Pdf of having arrived at position $x$ at time $t$ – $\eta(x,t)$ – having just arrived at $x'$ at time $t'$ – $\eta(x',t')$ – with initial condition $\delta(x)$.

# Characterization of CTRW

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we can write the pdf of being in $x$ at time $t$ as

$$W(x,t) = \int_0^t \eta(x,t')\Psi(t-t'), \mathrm{d}t, \qquad \Psi(t) = 1 - \int_0^t w(t')\,\mathrm{d}t',$$

where the latter is the cumulative probability assigned to the probability of no jump event during the time interval $t - t'$.

## Fact I - Ordinary Diffusion

If both $T$ and $\Sigma^2$ are finite the long-time limit corresponds to Brownian motion, e.g., $w(t) = \tau^{-1} exp(-{}^{t}/_{\tau})$, $T = \tau$, $\lambda(x) = (4\pi\sigma^2)^{-1/2} \exp(-{}^{x^2}/_{4\sigma^2})$, $\Sigma^2 = 2\sigma^2$, we recover the standard diffusion equation.

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## Fact II - Subdifussion

The **characteristic waiting time** $T = \int_0^{+\infty} tw(t) \, \mathrm{d}t$ **diverges**, but the jump length variance $\Sigma^2 = \int_{-\infty}^{+\infty} x^2\lambda(x) \, \mathrm{d}x$ is finite, we obtain a **subdiffusive process**. Particles make long rests.

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**Asymptotic**

For $|x| \gg \sigma$, $1 < \mu < 2 \Rightarrow \lambda(x) \sim A_{\mu}\sigma^{-\mu}|x|^{-1-\mu}$.

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- then after a (double) inversion

$$\frac{\partial W}{\partial t} = K^{\mu} \cdot \frac{1}{\Gamma(1-\mu)} \frac{\mathrm{d}}{\mathrm{d}x} \int_{-\infty}^{x} W(\xi, t)(x-\xi)^{\alpha}\, \mathrm{d}\xi, \quad K = \frac{\sigma^{\mu}}{\tau}$$

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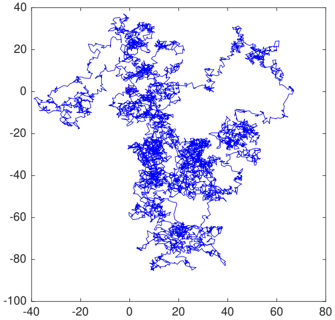
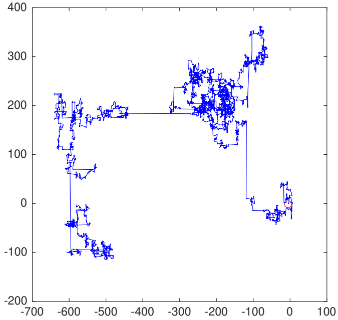
# Brownian jumps vs Lévy Flights




```
%% Brownian motion
N = 7000;
x = cumsum(randn(N,1));
y = cumsum(randn(N,1));
```

```
%% Levy distribution
N = 7000;
pd_levy = makedist('Stable','alpha',1.5,
↪  'beta',0,'gam',1, 'delta',0);
xl = cumsum(random(pd_levy,N,1));
yl = cumsum(random(pd_levy,N,1));
```

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$$\begin{cases} \frac{\partial W}{\partial t} = \theta \, {}^{RL}D^{\alpha}_{[0,x]} W(x,t) + (1-\theta) \, {}^{RL}D^{\alpha}_{[x,1]} W(x,t), & \theta \in [0,1], \\ W(0,t) = W(1,t) = 0, \\ W(x,t) = W_0(x). \end{cases} \tag{FDE$_1$}$$

# Finite Difference Approaches to Riemann–Liouville

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$$\frac{\mathrm{d}^n f}{\mathrm{d}x^n} = \lim_{h\to 0} \frac{\Delta^n f(x)}{h}, \quad \Delta^n f(x) = \sum_{j=0}^{n} \binom{n}{j} (-1)^j f(x - jh).$$

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Let's use again our favourite trick and replace $n \in \mathbb{N}$ with $\alpha \in \mathbb{R}$!

# The Grünwald–Letnikov Fractional Derivative

**The Grünwald–Letnikov Fractional Derivative (Grünwald 1867; Letnikov 1868)**

Given $\mathbb{R} \ni \alpha > 0$ define the Grünwald–Letnikov fractional derivative of a function $f(x)$ as

$$ {}^{GL}D^{\alpha} f = \lim_{h \to 0} \frac{\Delta^{\alpha} f(x)}{h}, \quad \Delta^{\alpha} f(x) = \sum_{j=0}^{+\infty} \binom{\alpha}{j} (-1)^j f(x - jh), \quad \binom{\alpha}{j} = \frac{\Gamma(\alpha+1)}{j!\,\Gamma(\alpha - j + 1)}. $$

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- For what functions $f$ does it make sense?
- How is it related to the Riemann-Liouville (and henceforth to the Caputo) fractional derivative?
- If we can find an easy relation with the Riemann-Liouville derivative we can **use it to discretize** by truncating $\Delta^{\alpha}$ to a given $N$.

# The Grünwald–Letnikov Fractional Derivative

Let us collect the ingredients we need.

- The binomial series
$$(1+z)^{\alpha} = \sum_{j=0}^{+\infty} \binom{\alpha}{j} z^j,$$
converges for any $z \in \mathbb{C}$ with $|z| \leq 1$ and any $\alpha > 0$,
- The series
$$\sum_{j=0}^{+\infty} \left| \binom{\alpha}{j} (-1)^j \right| < +\infty,$$
converges, since $(1+(-1))^{\alpha} = 0$.

$\Rightarrow$ If we take $f$ to be bounded then ${}^{GL}D^{\alpha} f$ exists.

# The Grünwald–Letnikov Fractional Derivative

Let us take the Fourier transform of $\Delta^\alpha f(x)$

$$
\begin{aligned}
\int e^{-ikx} \sum_{j=0}^{+\infty} \binom{\alpha}{j} (-1)^j f(x - jh)\, \mathrm{d}x = & \sum_{j=0}^{+\infty} \binom{\alpha}{j} (-1)^j \int e^{-ikx} f(x - jh)\, \mathrm{d}x \\
= & \sum_{j=0}^{\infty} \binom{\alpha}{j} (-1)^j e^{-ikjh} \hat{f}(k) \\
= & (1 - e^{-ikh})^\alpha \hat{f}(k).
\end{aligned}
$$

- We are using the **uniform convergence** of the series $\Delta^\alpha f(x)$,
- furthermore we are **requiring** that each term is integrable.

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If $k \neq 0$ then the Fourier transform of the GL derivative operator is given by

$$h^{-\alpha} (ikh)^{\alpha} \left( \frac{1 - e^{-ikh}}{ikh} \right) \hat{f}(k) \to (ik)^{\alpha} \hat{f}(k), \text{ for } h \to 0.$$

The same holds by direct computation for $k = 0$.

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$\Rightarrow$ The Fourier transform **converges pointwise** to the same **Fourier transform** of the **Riemann-Liouville** derivative (we are also using the continuity Theorem of Fourier transform.)

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1. Let us look better into the *weights*

$$
\begin{aligned}
g_j^{(\alpha)} \triangleq (-1)^j \binom{\alpha}{j} &= \frac{(-1)^j \Gamma(\alpha+1)}{\Gamma(j+1)\Gamma(\alpha-j+1)} = \\
&= \frac{(-1)^j \alpha(\alpha-1)\cdots(\alpha-j+1)}{\Gamma(j+1)} \\
\text{Distribute } (-1)^j \rightarrow &= \frac{(-\alpha)(1-\alpha)\cdot(j-1-\alpha)}{\Gamma(j+1)} \\
&= \frac{-\alpha\Gamma(j-\alpha)}{\Gamma(j+1)\Gamma(1-\alpha)}
\end{aligned}
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$$g_j^{(\alpha)} \triangleq (-1)^j \binom{\alpha}{j} = \frac{-\alpha\Gamma(j-\alpha)}{\Gamma(j+1)\Gamma(1-\alpha)}$$

2. Using $\Gamma(x+1) = x\Gamma(x)$ and $\Gamma(x+1) \sim \sqrt{2\pi x}x^x e^{-x}$ for $x \to +\infty$

$$\begin{aligned} g_j^{(\alpha)} \sim & \frac{-\alpha}{\Gamma(1-\alpha)} \frac{\sqrt{2\pi(j-\alpha-1)}(j-\alpha-1)^{j-\alpha-1}e^{-(j-\alpha-1)}}{\sqrt{2\pi j}j^j e^{-j}} \\ = & \frac{-\alpha}{\Gamma(1-\alpha)} \underbrace{\sqrt{\frac{j-\alpha-1}{j}}}_{\to 1} \underbrace{\left(\frac{j-\alpha-1}{j}\right)^{j-\alpha-1}}_{\to e^{-(\alpha+1)}} j^{-\alpha-1} e^{\alpha+1} j^{-\alpha-1} \qquad j \to +\infty. \end{aligned}$$

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$$g_j^{(\alpha)} \triangleq (-1)^j \binom{\alpha}{j} = \frac{-\alpha\Gamma(j-\alpha)}{\Gamma(j+1)\Gamma(1-\alpha)}$$

2. Using $\Gamma(x+1) = x\Gamma(x)$ and $\Gamma(x+1) \sim \sqrt{2\pi x}x^x e^{-x}$ for $x \to +\infty$

$$g_j^{(\alpha)} \sim \frac{-\alpha}{\Gamma(1-\alpha)} j^{-\alpha-1} \qquad j \to +\infty.$$

3. Since $g_0^{(\alpha)} = 1$ we write the quotient

$$\frac{\Delta^\alpha f(x)}{\Delta x^\alpha} = (\Delta x)^{-\alpha} \left[ f(x) + \sum_{j=1}^{+\infty} g_j^{(\alpha)} f(x - j\Delta x) \right]$$

# The Grünwald–Letnikov Fractional Derivative

What is the connection then?

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4. $\sum_{j=0}^{+\infty} w_j = 0$. Then $g_j^{(\alpha)} < 0$ for all $j \geq 1$ and thus $\sum_{j=1}^{+\infty} g_j^{(\alpha)} = -1$. We **define** $b_j^{(\alpha)} = -w_j^{(\alpha)}$ for $j \geq 1$, so that

$$b_j \sim \frac{\alpha}{\Gamma(1-\alpha)} j^{-\alpha-1} \text{ for } j \to +\infty, \qquad \sum_{j=1}^{+\infty} b_j = 1.$$

# The Grünwald–Letnikov Fractional Derivative

Then we take $0 < \alpha < 1$

$$
\begin{aligned}
\frac{\Delta^\alpha f(x)}{\Delta x^\alpha} =& (\Delta x)^{-\alpha} \sum_{j=1}^{+\infty} [f(x) - f(x - j\Delta x)] b_j \\
\approx& \sum_{j=1}^{+\infty} [f(x) - f(x - j\Delta x)] \frac{\alpha}{\Gamma(1-\alpha)} (j\Delta x)^{-\alpha-1} \Delta x \\
\approx& \int_0^{+\infty} [f(x) - f(x - y)] \frac{\alpha}{\Gamma(1-\alpha)} y^{-\alpha-1} \,\mathrm{d}y
\end{aligned}
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\frac{\Delta^{\alpha} f(x)}{\Delta x^{\alpha}} &= (\Delta x)^{-\alpha} \sum_{j=1}^{+\infty} [f(x) - f(x - j\Delta x)] b_j \\
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&\approx \int_0^{+\infty} [f(x) - f(x-y)] \frac{\alpha}{\Gamma(1-\alpha)} y^{-\alpha-1} \, \mathrm{d}y
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$$

- Integrate by parts with $u = f(x) - f(x-y)$

$$
\frac{1}{\Gamma(1-\alpha)} \int_0^{+\infty} f'(x-y) y^{-\alpha} \, \mathrm{d}y = \frac{1}{\Gamma(1-\alpha)} \int_0^{+\infty} \frac{\mathrm{d}}{\mathrm{d}x} f(x-y) y^{-\alpha} \, \mathrm{d}y
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$$
{}^{CA}D^{\alpha}_{[0,+\infty]} f(x) = \frac{1}{\Gamma(1-\alpha)} \int_0^{+\infty} f'(x-y) y^{-\alpha} \, \mathrm{d}y = \frac{1}{\Gamma(1-\alpha)} \int_0^{+\infty} \frac{\mathrm{d}}{\mathrm{d}x} f(x-y) y^{-\alpha} \, \mathrm{d}y
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$$

- Integrate by parts with $u = f(x) - f(x-y)\ldots$ and when you swap the integral and the derivative

$$
{}^{RL}D^{\alpha}_{[0,+\infty]} = \frac{1}{\Gamma(1-\alpha)} \frac{\mathrm{d}}{\mathrm{d}x} \int_0^{+\infty} f(x-y) y^{-\alpha} \, \mathrm{d}y.
$$

# The Grünwald–Letnikov Fractional Derivative

Let us move everything to a fixed interval $[a, b]$.

**Grünwald–Letnikov *revisited***

Let $\alpha > 0$, $f \in \mathcal{C}^{\lceil \alpha \rceil}([a, b])$, $a < x \leq b$, then

$$ {}^{GL}D_{[a,x]} f(x) = \lim_{N \to +\infty} \frac{\Delta^{\alpha}_{h_N} f(x)}{h_N^{\alpha}} = \lim_{N \to +\infty} \frac{1}{h_N^{\alpha}} \sum_{k=0}^{N} (-1)^k \binom{\alpha}{k} f(x - k h_N), $$

with $h_N = (x - a)/N$.

In the definition we have implicitly extended $f$ (with an abuse of notation) in such a way that

$$ f : (-\infty, b] \to \mathbb{R}, \qquad x \mapsto \begin{cases} f(x), & \text{if } x \in [a, b], \\ 0, & \text{if } x \in (-\infty, a). \end{cases} $$

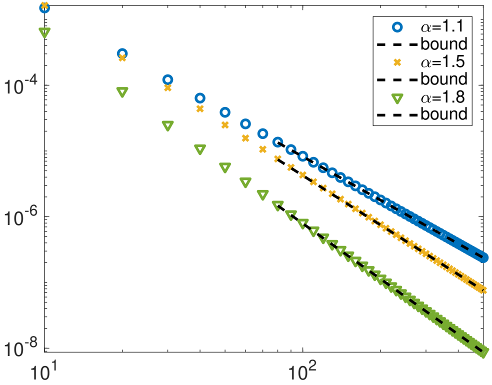
# Computing the coefficients

We can compute $N+1$ $g_j^{(\alpha)}$ coefficients in $3N+1$ flops by using the recurrence relation

$$g_j^{(\alpha)} = \left(1 - \frac{\alpha+1}{j}\right) g_{j-1}^{\alpha}, \quad g_0 = 1.$$

In a line of code

```
function [g] = gl(n,alpha)
%GL Produces the N+1 Grunwald-Letnikov
↪  coefficients for a given alpha
g = cumprod([1, 1 - ((alpha+1) ./
↪  (1:n))]);
end
```



# A finite difference discretization

Before going to the two-sided case in (FDE$_1$), let us start with the simpler case

$$\frac{\partial w}{\partial t} = -v(x)\frac{\partial w}{\partial x} + d(x)\,{}^{RL}D^{\alpha}_{[0,x]} w + f(x,t), \qquad 1 < \alpha \leq 2,\ v(x), d(x) \geq 0.$$

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1. Substitute the Riemann-Liouville derivative with the Grünwald–Letnikov one,

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2. Choose $N \in \mathbb{N}$ at which to truncate the series expansions
$$\frac{\partial w_i}{\partial t} = -v_i\frac{w_i - w_{i-1}}{h_N} + \frac{d_i}{h_N^{\alpha}}\sum_{k=0}^{i}(-1)^k\binom{\alpha}{k}w_{i-k} + f_i,$$

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3. Now we need to select a scheme for discretizing it in time: *explicit*? *implicit*?

# A finite difference discretization: explicit Euler

Let us select **explicit Euler**

$$\frac{w_i^{n+1} - w_i^n}{\Delta t} = -v_i \frac{w_i^n - w_{i-1}^n}{h_N} + \frac{d_i}{h_N^\alpha} \sum_{k=0}^{i} (-1)^k \binom{\alpha}{k} w_{i-k}^n + f_i^n,$$

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- For convenience we call $g_k = (-1)^k \binom{\alpha}{k}$,

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Let us select **explicit Euler**

$$w_i^{n+1} = w_i^n - \Delta t\, v_i \frac{w_i^n - w_{i-1}^n}{h_N} + \Delta t\, \frac{d_i}{h_N^\alpha} \sum_{k=0}^{i} g_k w_{i-k}^n + f_i^n,$$

- For convenience we call $g_k = (-1)^k \binom{\alpha}{k}$,
- Rearrange everything to compute $w_i^{n+1}$

# A finite difference discretization: explicit Euler

Let us select **explicit Euler**

$$w_i^{n+1} = \left(1 - \frac{\Delta t}{h_N} v_i + \frac{\Delta t}{h_N^\alpha} d_i\right) w_i^n + \left(\frac{v_i}{h_N} - \frac{\alpha}{h_N^\alpha} d_i\right) \Delta t w_{i-1}^n + \frac{d_i \Delta t}{h_N^\alpha} \sum_{k=2}^{i} g_k w_{i-k}^n + f_i^n \Delta t,$$

- For convenience we call $g_k = (-1)^k \binom{\alpha}{k}$,
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- Rearrange everything to compute $w_i^{n+1}$, and using that $g_0 = 1$, $g_1 = -\alpha$
- Is this *stable*? Do we have to put a restriction on the choice of $h_N$ and $\Delta t$?

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- Suppose that $w_i^0$ is affected by an error, i.e., $\hat{w}_i^0 = w_i^0 + \epsilon_i^0$, we can then look at the **propagation of the error**,

# A finite difference discretization: explicit Euler

Let us select **explicit Euler**

$$\hat{w}_i^1 = \left(1 - \frac{\Delta t}{h_N} v_i + \frac{\Delta t}{h_N^\alpha} d_i\right) \hat{w}_i^0 + \left(\frac{v_i}{h_N} - \frac{\alpha}{h_N^\alpha} d_i\right) \Delta t w_{i-1}^n + \frac{d_i \Delta t}{h_N^\alpha} \sum_{k=2}^{i} g_k w_{i-k}^n + f_i^n \Delta t,$$

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- We call $\mu_i = 1 - {}^{\Delta t}/_{h_N} v_i + {}^{\Delta t}/_{h_N^\alpha} d_i$

# A finite difference discretization: explicit Euler

Let us select **explicit Euler**

$$\hat{w}_i^1 = \mu_i \hat{w}_i^0 + \left( \frac{v_i}{h_N} - \frac{\alpha}{h_N^\alpha} d_i \right) \Delta t w_{i-1}^n + \frac{d_i \Delta t}{h_N^\alpha} \sum_{k=2}^{i} g_k w_{i-k}^n + f_i^n \Delta t,$$

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- By iterating the argument we found that the error at step $n$ is amplified by the factor $\mu_i$, that is

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- By iterating the argument we found that the error at step $n$ is amplified by the factor $\mu_i$, that is
$$\epsilon_i^n = \mu_i^n \epsilon_i^0.$$
- To have stability we need to require that exist $h_N$ such that $|\mu_i| < 1$ for all $h < h_N$.

# A finite difference discretization: explicit Euler

$$\mu_i \equiv 1 - \frac{\Delta t}{h_N} v_i + \frac{\Delta t}{h_N^\alpha} d_i < 1 \;\Leftrightarrow\; h_N > \left(\frac{d_i}{v_i}\right)^{1/\alpha - 1}$$

⚠ The method is not stable as $h$ is refined!

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**Theorem (Meerschaert and Tadjeran 2004)**

The **explicit** Euler solution method based on the Grünwald–Letnikov approximation of the Riemann-Liouville fractional derivative is unstable.

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# A finite difference discretization: ex/implicit Euler

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And now what? How do we fix it?

# The Shifted Grünwald–Letnikov Fractional Derivative

## Shifted Grünwald–Letnikov Fractional Derivative

Let $\alpha > 0$, $f \in \mathcal{C}^{\lceil\alpha\rceil}([a,b])$, $a < x \leq b$, $\mathbb{N} \ni p > 0$ then

$$ {}^{GL}D_{[a,x]} f(x) = \lim_{N \to +\infty} \frac{\Delta^{\alpha}_{h_N} f(x)}{h_N^{\alpha}} = \lim_{N \to +\infty} \frac{1}{h_N^{\alpha}} \sum_{k=0}^{N} (-1)^k \binom{\alpha}{k} f(x - (k-p)h_N), $$

with $h_N = (x-a)/N$.

If we **repeat the argument with the Fourier transform**, we discover

$$ \mathfrak{F}\{{}^{GL}D_{[a,x]} f(x)\}(k) = (-ik)^{\alpha} \omega(-ikh) \hat{f}(k), $$

with

$$ \omega(z) = \left( \frac{1 - e^{-z}}{z} \right)^{\alpha} e^{zp} = 1 - \left( p - \frac{\alpha}{2} \right) z + O(|z|^2). $$

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$$

with $h_N = (x - a)/N$.

If we **repeat the argument with the Fourier transform**, we discover

$$
\mathfrak{F}\{{}^{GL}D_{[a,x]} f(x)\}(k) = (-ik)^{\alpha} \hat{f}(k) + (ik)^{\alpha} (\omega(-ikh) - 1) \hat{f}(k)
$$

with

$$
\omega(z) = \left( \frac{1 - e^{-z}}{z} \right)^{\alpha} e^{zp} = 1 - \left( p - \frac{\alpha}{2} \right) z + O(|z|^2) \Rightarrow |\omega(-ix) - 1| \leq Cx \, \forall \, x \in \mathbb{R}.
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with

$$|\phi(k,h)| \leq |k|^{\alpha} C |hk| |\hat{f}(k)| \Rightarrow |\phi(h,x)| < ICh, \quad I = \int_{-\infty}^{+\infty} (1 + |k|)^{\alpha+1} |\hat{f}(k)| \,\mathrm{d}k < +\infty.$$

# The Shifted Grünwald–Letnikov Fractional Derivative

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Let $\alpha > 0$, $f \in \mathcal{C}^{\lceil \alpha \rceil}([a, b])$, $a < x \leq b$, $\mathbb{N} \ni p > 0$ then

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with $h_N = (x - a)/N$.

- They give the same operator uniformly in $x$ as $h \to 0$, therefore we can use the shifted version with *any* shift to approximate the Riemann-Liouville derivative,

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? Let us see if using the *shifted version* with $p = 1$ solves our **stability problem**.

# Back to finite differences: implicit Euler

We use the **shifted Grünwald–Letnikov** and the **implicit Euler** method

$$\frac{w_i^{n+1} - w_i^n}{\Delta t} = -v_i \frac{w_i^{n+1} - w_{i-1}^{n+1}}{h_N} + \frac{d_i}{h_N^\alpha} \sum_{k=0}^{i+1} g_k w_{i-k+1}^{n+1} + f_i^{n+1}.$$

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$$w_i^{n+1} - w_i^n = -E_i(w_i^{n+1} - w_{i-1}^{n+1}) + B_i \sum_{k=0}^{i+1} g_k w_{i-k+1}^{n+1} + \Delta t f_i^{n+1}.$$

- Set $E_i = {}^{v_i \Delta t}/_{h_N}$,
  $B_i = {}^{d_i \Delta t}/_{h_N^{\alpha}}$,

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$$-g_0 B_i w_{i+1}^{n+1} + (1 + E_i - g_i B_i) w_i^{n+1} - (E_i + g_2 B_i) w_{i-1}^{n+1} - B_i \sum_{k=3}^{i+1} g_k w_{i-k+1}^{n+1} = c_i^n + \Delta t\, f_i^{n+1}.$$

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- and obtain

$$A_N \mathbf{w}^{n+1} = \mathbf{w}^n + \Delta t\, \mathbf{f}^{n+1}.\quad \begin{bmatrix} 1 & 0 & 0 & \cdots & \cdots & 0 \\ -E_1 - g_2 B_1 & 1 + E_1 - g_1 B_1 & -g_0 B_1 & \ddots & & \\ -g_3 B_2 & -E_2 - g_2 B_2 & 1 + E_2 - g_1 B_2 & -g_0 B_2 & \ddots & \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ -g_N B_{N-1} & \cdots & \cdots & \cdots & \cdots & -g_0 B_{N-1} \\ 0 & \cdots & \cdots & \cdots & \cdots & 1 \end{bmatrix}$$

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$$\begin{aligned} \mathbf{w}^{n+1} &= [w_0^{n+1}, w_1^{n+1}, \ldots, w_N^{n+1}]^T, \\ \mathbf{w}^n &= [w_0^n, w_1^n, \ldots, w_N^n]^T, \\ \mathbf{f}^{n+1} &= \Delta t [0, f_1^n, \ldots, f_{N-1}^n, 0]^T. \end{aligned}$$

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$$\begin{aligned} \mathbf{w}^{n+1} =& [w_0^{n+1}, w_1^{n+1}, \ldots, w_N^{n+1}]^T, \\ \mathbf{w}^{n} =& [w_0^{n}, w_1^{n}, \ldots, w_N^{n}]^T, \\ \mathbf{f}^{n+1} =& \Delta t [0, f_1^n, \ldots, f_{N-1}^n, 0]^T. \end{aligned}$$

To prove **stability** we need to have $\rho(A_N^{-1}) \leq 1$:

$$\epsilon^1 = A_N^{-1} \epsilon^0.$$

# Back to finite differences: implicit Euler

Let $(\lambda, \mathbf{x})$ be an eigencouple of $A_N$, i.e., $A_N\mathbf{x} = \lambda\mathbf{x}$, $\mathbf{x} \neq \mathbf{0}$.

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2. Then $\sum_{j=0}^{N} (A_N)_{i,j} x_j = x_i$, and thus

$$\lambda = A_{i,i} + \sum_{\substack{j=0 \\ j \neq i}}^{N} (A_N)_{i,j} \frac{x_j}{x_i},$$

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3. If $i = 0$ or $i = N$ then $\lambda = 1$, otherwise

$$\lambda = 1 + E_i - g_1 B_1 - g_0 B_i \frac{x_{i+1}}{x_i} (E_i + g_2 B_i) \frac{x_{i-1}}{x_i} - B_i \sum_{j=0}^{i-2} h_{i-j+1} \frac{x_j}{x_i}$$

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$$\lambda = 1 + E_i(1 - {}^{x_{i-1}}/_{x_i}) - B_i \left[ g_1 + \sum_{\substack{j=0 \\ j\neq i}}^{i+1} g_{i-j+1} \frac{x_j}{x_i} \right]$$

# Back to finite differences: implicit Euler

4. We have $\sum_{k\geq 0} g_k = 0$, $\alpha \in (1,2]$ and thus $g_1 = -\alpha$ and $g_k \geq 0$ for $k \neq 1$, thus

$$-g_1 \geq \sum_{\substack{k=0\\k\neq 1}}^{j} g_k \qquad \forall j = 0,1,2,\ldots$$

furthermore $|x_j/x_i| < 1$, and thus

$$\sum_{\substack{j=0\\j\neq i}}^{i+1} g_{i-j+1}\left|\frac{x_j}{x_i}\right| \leq \sum_{\substack{j=0\\j\neq i}}^{i+1} g_{i-j+1} \leq -g_1.$$

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3. If $i = 0$ or $i = N$ then $\lambda = 1$, otherwise

$$|\lambda| \geq 1 + \underbrace{E_i}_{\geq 0}(1 - \underbrace{{}^{x_{i-1}}/_{x_i}}_{\leq 1}) + \underbrace{B_i}_{\geq 0}\left[g_1 + \sum_{\substack{j=0 \\ j\neq i}}^{i+1} g_{i-j+1} \left|\frac{x_j}{x_i}\right|\right] \geq 1.$$

# Back to finite differences: implicit Euler

**Theorem (Meerschaert and Tadjeran 2004)**

The implicit Euler method solution to

$$\frac{\partial w}{\partial t} = -v(x)\frac{\partial w}{\partial x} + d(x)\,{}^{RL}D^{\alpha}_{[0,x]} w + f(x,t), \qquad 1 < \alpha \leq 2,\ v(x), d(x) \geq 0.$$

with boundary conditions $w(0,t) = 0$, $w(1,t) = 0$ for all $t \geq 0$, based on the shifted Grünwald–Letnikov approximation with $h_N = 1/N$, is consistent of order $O(h + \Delta t)$ and *unconditionally stable*.

- We have only a left-sided fractional derivative, we could put a non-homogeneous condition on the right-hand side,
- We can now start **looking into the matrices** to devise solution strategies for the *sequence of linear systems*

$$A_N \mathbf{w}^{n+1} = \mathbf{w}^n + \Delta t\, \mathbf{f}^{n+1}.$$

# Grünwald–Letnikov matrices

To look at the matrices we go back to the first form of the diffusion equation ($\text{FDE}_1$)

$$\begin{cases} \frac{\partial W}{\partial t} = \theta\, {}^{RL}D^{\alpha}_{[0,x]} W(x,t) + (1-\theta)\, {}^{RL}D^{\alpha}_{[x,1]} W(x,t), & \theta \in [0,1], \\ W(0,t) = W(1,t) = 0, \\ W(x,t) = W_0(x). \end{cases}$$

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1. Substitute the Riemann-Liouville derivative with the Grünwald–Letnikov one,
2. Choose $N \in \mathbb{N}$ at which to truncate the *shifted* series expansions

$$h_N^{\alpha} \frac{\partial W_i}{\partial t} = \theta \sum_{k=0}^{i+1} (-1)^k \binom{\alpha}{k} W_{i-k+1} + (1-\theta) \sum_{k=0}^{N-i+2} (-1)^k \binom{\alpha}{k} W_{i+k-1}, \; i = 0, \ldots, N.$$

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1. Substitute the Riemann-Liouville derivative with the Grünwald–Letnikov one,
2. Choose $N \in \mathbb{N}$ at which to truncate the *shifted* series expansions
3. Apply, e.g., *backward Euler* to discretize the derivative w.r.t. time

$$\frac{h_N^{\alpha}}{\Delta t}(W_i^{j+1} - W_i^{j}) = \theta \sum_{k=0}^{i-k+1} (-1)^k \binom{\alpha}{k} W^j_{i-k+1} + (1-\theta) \sum_{k=0}^{N+i-2} (-1)^k \binom{\alpha}{k} W^j_{i+k-1}, \quad \begin{array}{l} i = 0, \ldots, N, \\ j = 0, \ldots, M-1. \end{array}$$

# The matrix formulation

We call again $\mathbf{w}^j$, $\mathbf{w}^{j+1}$ the vectors containing the solution **on inner grid points**, then we can rewrite the set of linear equations as

$$\left( I_N - \frac{\Delta t}{h_N^\alpha} \left[ \theta G_N + (1-\theta) G_N^T \right] \right) \mathbf{w}^{n+1} = \mathbf{w}^n$$

where

$$G_N = \begin{bmatrix} 1 & 0 & \cdots & \cdots & 0 \\ g_2 & g_1 & g_0 & & \\ \vdots & \ddots & \ddots & \ddots & \\ \vdots & & \ddots & \ddots & g_0 \\ g_{N-1} & \cdots & g_3 & g_2 & g_1 \\ 0 & \cdots & \cdots & 0 & 1 \end{bmatrix}$$

```
function G = glmatrix(N,alpha)
%%GLMATRIX produces the GL discretization of
% the Riemann-Liouville derivative
g = gl(N,alpha);
c = zeros(N,1); r = zeros(1,N);
r(1:2) = g(2:-1:1);
c(1:N) = g(2:end);
G = toeplitz(c,r);
end
```

# The matrix formulation

To obtain a simple code for the complete problem

```
%% Discretization data
hN = 1/(N-1); x = 0:hN:1;
dt = hN; t = 0:dt:1;
%% Discretize
G = glmatrix(N,alpha); Gt =
↪  glmatrix(N,alpha).';
I = eye(N,N);
% apply B.C.
G(1,:) = -I(1,:); G(N,:) = -I(N,:);
Gt(1,:) = -I(1,:); Gt(N,:) = -I(N,:);
% Left-hand side
A = I - dt/hN^alpha*(theta*G + (1-theta)*Gt);
% Right-hand side
w = w0(x).';
```

- Select $\theta = 1/2$, $\alpha = 3/2$, and $W_0(x) = 5x(1-x)$,
- Discretize the interval $[0,1]$ on $N$ points,
- Build the $I$ and $G_N$ matrices,
- Apply the Dirichlet b.c.s,
- Assemble $A$ and $\mathbf{w}^0$.

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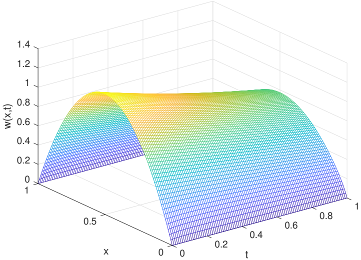
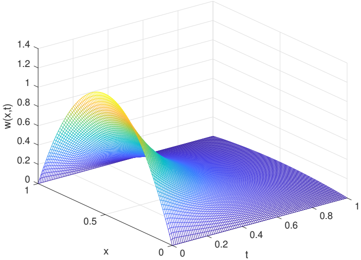
March the scheme in time:

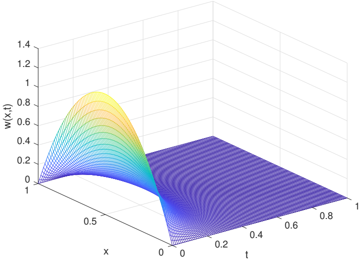
```
for i=2:N
  w = A\w;
end
```



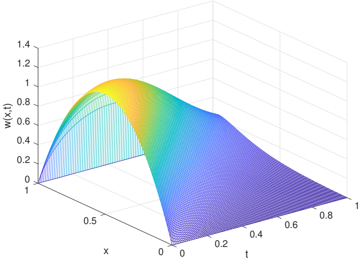

$\alpha = 1.1,\ \theta = 0.5$



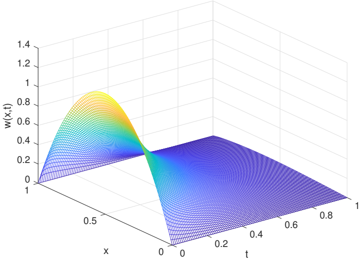

$\alpha = 1.5,\ \theta = 0.5$



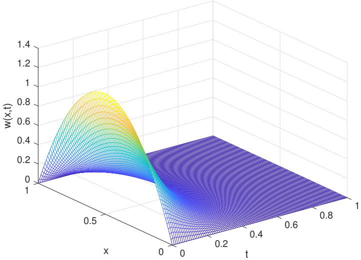

$\alpha = 2.0,\ \theta = 0.5$




$\alpha = 1.1,\ \theta = 0.1$




$\alpha = 1.5,\ \theta = 0.3$




$\alpha = 1.8,\ \theta = 0.9$

# The solution step

- How can we **efficiently solve** the linear systems

$$A\mathbf{w}^{n+1} = \mathbf{w}^{n},$$

  needed for the time-stepping?
- Can we find a reliable procedure working also for **multi-dimensional cases**?
- Is **dense linear algebra** a compulsory choice?

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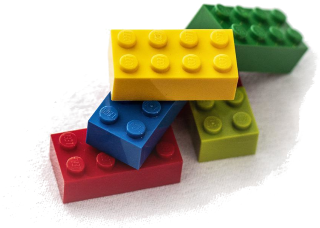
These matrices have structures we can **exploit**!



# Toeplitz matrices

## Toeplitz matrix

A **Toeplitz matrix** is a matrix whose entries are constant along the diagonals

$$T_n(f) = \begin{bmatrix} t_0 & t_{-1} & \dots & t_{2-n} & t_{1-n} \\ t_1 & t_0 & t_{-1} & \dots & t_{2-n} \\ \vdots & t_1 & t_0 & \ddots & \vdots \\ t_{n-2} & \dots & \ddots & \ddots & t_{-1} \\ t_{n-1} & t_{n-2} & \dots & t_1 & t_0 \end{bmatrix}.$$

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## Generating function

$$f(x) = \sum_{k=-\infty}^{+\infty} t_k e^{i\cdot kx}, \quad t_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(\theta) e^{-ik\theta} d\theta,\ k = 0, \pm1, \pm2, \dots$$

the $t_k$ are the Fourier coefficients is called a *generating function* of the matrix $T_n(f)$.

# Circulant matrices

## Circulant matrix

A **Circulant matrix** $C_n \in \mathbb{R}^{n\times n}$ is a Toeplitz matrix in which each row is a cyclic shift of the row above it, i.e., $(C_n)_{i,j} = c_{(j-i) \mod n}$:

$$C_n = \begin{bmatrix} c_0 & c_1 & c_2 & \cdots & \cdots & c_{n-1} \\ c_{n-1} & c_0 & c_1 & \ddots & & \vdots \\ c_{n-2} & c_{n-1} & c_0 & c_1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & c_2 \\ \vdots & & \ddots & \ddots & c_0 & c_1 \\ c_1 & \cdots & \cdots & c_{n-2} & c_{n-1} & c_0 \end{bmatrix}.$$

# Toeplitz and Circulant matrices: some properties

## Properties

1. The operator $T_n : \mathbb{L}^1[-\pi, \pi] \to \mathbb{C}^{n\times n}$ defined by the Toeplitz matrix construction is linear and positive, i.e., if $f \geq 0$ then $T_n(f) = T_n(f)^H \; \forall\, n$ and $\mathbf{x}^H T_n(f)\mathbf{x} \geq 0$ $\forall\, \mathbf{x} \in \mathbb{C}^n$.
2. Given $f \in \mathbb{L}^1[-\pi, \pi]$ such that $m_f = \operatorname{ess\,inf}(f)$ and $M_f = \operatorname{ess\,sup}(f)$.
   If $m_f > -\infty$ then $m_f \leq \lambda_j(T_n(f)) \; \forall j = 1, \dots, n$;
   If $M_f < \infty$ then $M_f \geq \lambda_j(T_n(f)) \; \forall j = 1, \dots, n$.
   If $f$ is not identical to a real constant and both the inequalities hold,
   $$m_f < \lambda_j(T_n(f)) < M_f \;\; \forall j = 1, \dots, n.$$
3. Circulant matrices are simultaneously diagonalized by the unitary matrix $F_n$
   $$(F_n)_{j,k} = \frac{1}{\sqrt{n}} e^{\frac{-2\pi i\, j\, k}{n}}, \mathcal{C} = \left\{ C_n \in \mathbb{C}^{n\times n} \mid C_n = FDF^H \;:\; D = \operatorname{diag}(d_0, d_1, \dots, d_{n-1}) \right\}.$$

# Asymptotic distribution - I

## Asymptotic eigenvalue distribution

Given a sequence of matrices $\{X_n\}_n \in \mathbb{C}^{d_n \times d_n}$ with $d_n = \{\dim X_n\}_n \overset{n \to +\infty}{\longrightarrow} \infty$ monotonically and a $\mu$-measurable function $f : D \to \mathbb{R}$, with $\mu(D) \in (0, \infty)$, we say that the sequence $\{X\}_n$ is distributed in the sense of the eigenvalues as the function $f$ and write $\{X_n\}_n \sim_\lambda f$ if and only if,

$$\lim_{n \to \infty} \frac{1}{d_n} \sum_{j=0}^{d_n} F(\lambda_j(X_n)) = \frac{1}{\mu(D)} \int_D F(f(t))dt, \ \ \forall F \in \mathcal{C}_c(D),$$

where $\lambda_j(\cdot)$ indicates the $j$-th eigenvalue.

# Asymptotic distribution - II

## Asymptotic singular value distribution

Given a sequence of matrices $\{X_n\}_n \in \mathbb{C}^{d_n \times d_n}$ with $d_n = \{\dim X_n\}_n \xrightarrow{n\to+\infty} \infty$ monotonically and a $\mu$-measurable function $f : D \to \mathbb{R}$, with $\mu(D) \in (0,\infty)$, we say that the sequence $\{X\}_n$ is distributed in the sense of the singular values as the function $f$ and write $\{X_n\}_n \sim_\sigma f$ if and only if

$$\lim_{n\to\infty} \frac{1}{d_n} \sum_{j=0}^{d_n} F(\sigma_j(X_n)) = \frac{1}{\mu(D)} \int_D F(|f(t)|)dt, \quad \forall F \in \mathcal{C}_c(D),$$

where $\sigma_j(\cdot)$ is the $j$-th singular value.

# Asymptotic distribution - III

**Theorem (Asymptotic distribution of Toeplitz matrices)**

Given the generating function $f$, $T_n(f)$ is distributed in the sense of the eigenvalues as $f$, written also as $T_n(f) \sim_\lambda f$, if one of the following conditions hold:

1. (Grenander and Szegö 2001): $f$ is real valued and $f \in \mathbb{L}^\infty$,
2. (Tyrtyshnikov 1996): $f$ is real valued and $f \in \mathbb{L}^2$.

Moreover, $T_n(f)$ is distributed in the sense of the singular values as $f$, written also as $T_n(f) \sim_\sigma f$, if one of the following conditions hold:

1. (Avram 1988; Parter 1986): $f \in \mathbb{L}^\infty$,
2. (Tyrtyshnikov 1996): $f \in \mathbb{L}^2$.

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  - **Yes!** And we have already computed it several times! The coefficients $\{g_k^{(\alpha)}\}_k$ where given by the **binomial expansion** of $(1+z)^\alpha$, and thus

$$f(\theta) = e^{-i\theta} \left(1 + \exp(i(\theta + \pi))\right)^{\alpha}, \qquad \theta \in [0, 2\pi)$$

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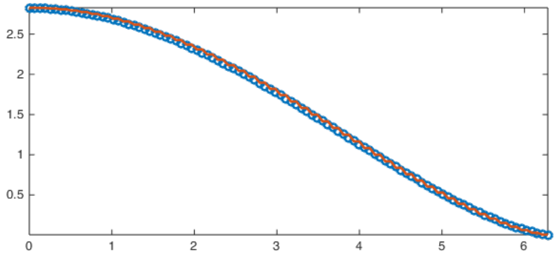
```
N = 100;
alpha = 1.5;
G = glmatrix(N,alpha);
s = @(t) exp(-1i*t).*(1 + ...
 exp(1i*(t+pi))).^alpha;
sv = svd(G);
th = linspace(0,2*pi,N);
plot(th,sv,'o',th,sort(abs(s(th)),...
 'descend'),'-','LineWidth',2);
```



# Conclusion and summary

- We introduced **p**artial **d**ifferential **e**quations with **f**ractional (FPDE) derivative with respect to the space variables,
- we connected *fractional diffusion* and continuous time random walk using *Lévy flights*,
- we introduced the Grünwald-Letnikov fractional derivative, highlighted the connection with the Riemann-Liouville derivative.
- We introduced a *stable discretization* of finite difference type,
- and we started investigating the structure of the underlying matrices.

Next up

- Investigating the structure of the underlying matrices for different FPDEs.
- Looking into some preconditioners and solution strategies based on structured matrices.

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