A Numerical Linear Algebra Perspective on Fractional Differential Equations

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2018

A Brief Introduction to Fractional Calculus

Newton, Leibniz and the Derivatives of Integer Order

In Newton's definition and notation we discover

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And notation is often a pathway to unforeseen generalization. . .

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But why *n* should be an integer?

In a letter by Leibniz to de L'Hospital[a],

> *"John Bernoulli seems to have told you of my having mentioned to him a marvelous analogy which makes it possible to say in a way that successive differentials are in geometric progression. One can ask what would be a differential having as its exponent a fraction. You see that the result can be expressed by an infinite series. Although this seems removed from Geometry, which does not yet know of such fractional exponents, it appears that one day these paradoxes will yield useful consequences, since there is hardly a paradox without utility. Thoughts that mattered little in themselves may give occasion to more beautiful ones."*

[a] September 30, 1695, Leibniz 1849-, II, XXIV, 197ff.

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Given a suitable function $f \in \mathcal{C}^0[c,b]$ how can we compute

$$ {}_cD_x^{-n} f(x) = \int_c^x dx_1 \int_c^{x_1} dx_2 \int_c^{x_2} dx_3 \cdots \int_c^{x_{n-1}} f(t)dt, \quad x < b? $$

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- If $G(x,t)$ is jointly continuous on $[c,b] \times [c,b]$:

$$ \int_c^x dx_1 \int_c^{x_1} G(x_1,t)dt = \int_c^x dt \int_t^x G(x_1,t)dx_1, $$

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- we start from the case $n = 2$ with $G(x_1, t) \equiv f(t)$:

$$ {}_cD_x^{-2} f(x) = \int_c^x dx_1 \int_c^{x_1} f(t)dt = \int_c^x f(t)\,dt \int_t^x dx_1 = $$
$$ = \int_c^x (x-t) f(t)dt $$

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- Then for $n = 3$

$$ \begin{aligned} {}_cD_x^{-3} f(x) &= \int_c^x dx_1 \int_c^{x_1} dx_2 \int_c^{x_2} f(t) dt \\ &= \int_c^x dx_1 \left[\int_c^{x_1} dx_2 \int_c^{x_2} f(t) dt \right] \\ &= \int_c^x dx_1 \int_c^{x_1} (x_1 - t) f(t) dt \\ &= \int_c^x f(t)\, dt \int_t^x (x_1 - t) dx_1 = \int_c^x f(t) \frac{(x-t)^2}{2} dt \end{aligned} $$

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- Then for a generic n by induction one gets:

$$ {}_cD_x^{-n} f(x) = \frac{1}{(n-1)!} \int_c^x (x-t)^{n-1} f(t)dt, $$

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... but we are still dealing with an integer number n of repetitions!

We can rewrite our expression for the n–fold integral

$$ {}_cD_x^{-n} f(x) = \frac{1}{(n-1)!} \int_c^x (x-t)^{n-1} f(t) dt, $$

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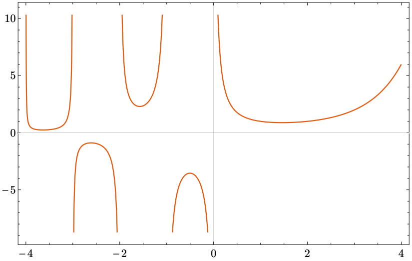
Enters the $\Gamma(\cdot)$ function

We can rewrite our expression for the n–fold integral

$$ {}_cD_x^{-n}f(x) = \frac{1}{\Gamma(n)} \int_c^x (x-t)^{n-1} f(t)dt, $$

$\Gamma(\cdot)$ is the **Euler Gamma**, i.e., the analytic continuation to all complex numbers (except the non–positive integers) of the convergent improper integral function

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



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Enters the $\Gamma(\cdot)$ function

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Remark: from Wielandt's Theorem we know that the Gamma function Γ is the only holomorphic function in the right half plane such that $\Gamma(z+1) = z\Gamma(z)$ and that is bounded in the strip $S = \{z \in \mathbb{C} : \Re z \in [1,2)\}$.

It represents a natural extension to the factorial!

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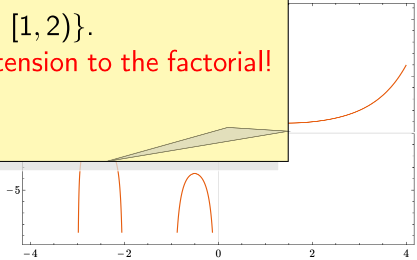

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$$ {}_cD_x^{-n}f(x) = \frac{1}{\Gamma(n)} \int_c^x (x-t)^{n-1} f(t)dt, $$

Riemann–Liouville Fractional Integral

Let $\Re\alpha > 0$, and let f be piecewise continuous on $J' = (0, +\infty)$ and integrable on any finite subinterval of $J = [0, +\infty)$.
Then for $t > 0$ we call

$$ {}_0D_t^{-\alpha}f(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-\xi)^{\alpha-1} f(\xi)\, d\xi. $$

the Riemann–Liouville fractional integral of f of order α.

Let's look to an example of Riemann–Liouville fractional integral, we wish to integrate the function $f(t) = t^{\mu}$ with $\mu > -1$ and $t > 0$

$$ {}_0D_t^{-\alpha} t^{\mu} = \frac{1}{\Gamma(\alpha)} \int_0^t (t-\xi)^{\alpha-1} \xi^{\mu} \, d\xi, $$

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$$ B(x,y) \triangleq \int_0^1 u^{x-1}(1-u)^{y-1} \, du = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)} \quad \Re x > 0, \Re y > 0. $$

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We do the substitution $u = \xi/t$, then

$$ {}_0D_t^{-\alpha} t^{\mu} = \frac{t^{\alpha+\mu}}{\Gamma(\alpha)} \int_0^1 u^{\mu}(1-u)^{\alpha-1} \, du = \frac{t^{\alpha+\mu}}{\Gamma(\alpha)} \frac{\Gamma(\mu+1)\Gamma(\alpha)}{\Gamma(\alpha+\mu+1)}. $$

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that shou … using the Euler …

$B(x, y)$ … $\Re y > 0$.

We do t…

We do not attempt the computation of fractional integrals of elementary functions as exponentials, sines and cosines, since they lead to the definition of higher transcendental functions. Numerical methods are strictly necessary.

$$ {}_0D_t^{-\alpha} t^\mu = \frac{t^{\alpha+\mu}}{\Gamma(\alpha)} \int_0^1 u^\mu (1-u)^{\alpha-1} \, du = . $$

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Exercise I

1. Compute the fractional integral of constant function $f(t) = K$ for a fixed constant K.
2. There exists several formulas for computing the values of the Gamma function, e.g., the Spouge's approximation

$$\begin{cases} \Gamma(z+1) = (z+a)^{z+1/2} e^{-z-a} \left(c_0 + \sum_{k=1}^{a-1} \frac{c_k}{z+k} + \varepsilon_a(z) \right), \\ c_0 = \sqrt{2\pi}, \\ c_k = \frac{(-1)^{k-1}}{(k-1)!} (-k+a)^{k-1/2} e^{-k+a}, \qquad k \in \{1, 2, \ldots, a-1\}. \end{cases}$$

   With $\varepsilon = \frac{|\Gamma(z-1)-\varepsilon_a(z)|}{\Gamma(z-1)} < a^{-1/2}(2\pi)^{-a-1/2}$, if $\Re z > 0$ and $a > 2$. For what value of a we obtain m significant digits? Can the formula be implemented as such? Is the theoretical bound sharp from the application point of view? Try to implement the procedure.

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- We propose the following Definition:

$$ \begin{aligned} {}_cD_t^{\alpha} f(t) =& D^n \, {}_cD_t^{-(n-\alpha)} f(t) \\ =& \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dt^n} \int_c^t (t-\xi)^{n-\alpha-1} f(\xi)\, d\xi \end{aligned} $$

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- A class of functions for which this exists is indeed the class of functions f for which the Riemann–Liouville fractional integral exists.

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Can we recover something similar? Is it linked to our integral definition?

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$$\frac{d^2 f}{dt^2} = \lim_{h \to 0} \frac{f'(t) - f'(t-h)}{h}$$

$$= \lim_{h \to 0} \frac{1}{h} \left(\frac{f(t) - f(t-h)}{h} - \frac{f(t-h) - f(t-2h)}{h} \right)$$

$$= \lim_{h \to 0} \frac{f(t) - 2f(t-h) + f(t-2h)}{h^2}$$

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$$\begin{aligned}\frac{d^3 f}{dt^3} &= \lim_{h\to 0} \frac{f''(t) - f''(t-h)}{h} \\ &= \lim_{h\to 0} \frac{f(t) - 3f(t-h) + 3f(t-2h) - f(t-3h)}{h^3}\end{aligned}$$

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n is still an integer…we replace it with $-p$ ($p < n$) in the binomial, then:

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n is still an integer... we replace it with $-p$ ($p < n$) in the binomial, then:

$$f_h^{(p)} \triangleq \frac{1}{h^{-p}} \sum_{r=0}^{n} \begin{bmatrix} p \\ r \end{bmatrix} f(t - rh).$$

A Brief Introduction to Fractional Calculus

But it doesn't look like a derivative at all...

> "The derivative of a function is the limit of the ratio of the increment of the function to the increment of the independent variable, when the latter increment varies and approaches the limit zero."

We have done repeated integrals, let us do repeated derivatives:

Question: for n fixed, what is the result of the limit

$$\lim_{h \to 0} f_h^{(p)} = ?$$

$$\frac{d^n f}{dt^n} = \dots \text{duction.}$$

n is still an int... in the binomial, then:

$$f_h^{(p)} \triangleq \frac{1}{h^{-p}} \sum_{r=0}^{n} \begin{bmatrix} p \\ r \end{bmatrix} f(t - rh).$$

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To find something more interesting than 0 let us choose n such that $h = {}^{t-c}/_{n}$, so that $n \to +\infty$ as $h \to 0$

A Brief Introduction to Fractional Calculus

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$p = 1$: for $t - nh = c$ and $f(t)$ continuous we have

$$\lim_{\substack{h \to 0 \\ nh = t-c}} f_h^{(-1)}(t) = \lim_{\substack{h \to 0 \\ nh = t-c}} h \sum_{r=0}^{n} f(t - rh)$$
$$= \int_0^{t-c} f(t-z)dz = \int_c^t f(\xi)d\xi.$$

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$$\lim_{\substack{h \to 0 \\ nh = t-c}} f_h^{(-1)}(t) = \int_c^t f(\xi) d\xi.$$

$p = 2$: since $\begin{bmatrix} 2 \\ r \end{bmatrix} = {}^{2 \cdot 3 \cdot \ldots \cdot (2+r-1)}/_{r!} = r + 1$ we find

$$\lim_{\substack{h \to 0 \\ nh = t-c}} f_h^{(-2)}(t) = \lim_{\substack{h \to 0 \\ nh = t-c}} h \sum_{r=0}^{n} (rh) f(t - rh)$$

$$= \int_0^{t-c} z f(t - z) dz = \int_c^t (t - \xi) f(\xi) d\xi.$$

A Brief Introduction to Fractional Calculus

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$$\lim_{\substack{h\to 0\\ nh=t-c}} f_h^{(-2)}(t) = \int_c^t (t-\xi)f(\xi)d\xi.$$

$p < n$ then by induction we conclude (again)

$$\lim_{\substack{h\to 0\\ nh=t-c}} f_h^{(-p)}(t) = \frac{1}{(p-1)!}\int_c^t (t-\xi)^{p-1}f(\xi)d\xi = {}_cD_t^{-p}f(t).$$

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We have proved the equality with the n–fold integrals, even if under stricter hypothesis. What about the generalization to an arbitrary positive $p \in \mathbb{R}$?

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We have proved the equality with the n–fold integrals, even if under stricter hypothesis. What about the generalization to an arbitrary positive $p \in \mathbb{R}$?

It can be done, but requires a technical Lemma by Letnikov 1868. We focus instead on the derivative of arbitrary order.

$p < n$ then by induction we conclude (again)

$$\lim_{\substack{h \to 0 \\ nh = t-c}} f_h^{(-p)}(t) = \frac{1}{(p-1)!} \int_c^t (t-\xi)^{p-1} f(\xi) d\xi = {}_c D_t^{-p} f(t).$$

We need to compute the limit for $\Re p > 0$:

$$\lim_{\substack{h\to 0\\ nh=t-c}} \frac{1}{h^p}\sum_{r=0}^{n}(-1)^r\binom{p}{r}f(t-rh) \equiv \lim_{\substack{h\to 0\\ nh=t-c}} f_h^{(p)}(t).$$

It is easy to prove that

$$\binom{p}{r} = \binom{p-1}{r} + \binom{p-1}{r-1},$$

thus

$$\begin{aligned} f_h^{(p)}(t) =& \frac{1}{h^p}\sum_{r=0}^{n}(-1)^r\binom{p-1}{r}f(t-rh) \\ &+ \frac{1}{h^p}\sum_{r=0}^{n}(-1)^r\binom{p-1}{r-1}f(t-rh) \end{aligned}$$

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It is easy to prove that

$$\binom{p}{r} = \binom{p-1}{r} + \binom{p-1}{r-1},$$

thus

$$\begin{aligned} f_h^{(p)}(t) =& (-1)^n\binom{p-1}{n}h^{-p}f(c) \\ &+ \frac{1}{h^p}\sum_{r=0}^{n-1}\binom{p-1}{r}\left[f(t-rh) - f(t-(r+1)h)\right] \end{aligned}$$

We need to compute the limit for $\Re p > 0$:

$$\lim_{h \to 0} \frac{1}{h^p} \sum^{n} (-1)^r \binom{p}{r} f(t - rh) \equiv \lim_{h \to 0} f_h^{(p)}(t).$$

It is easy

Remark: the quantity

$$\Delta^1 f(t - rh) \triangleq [f(t - rh) - f(t - (r+1)h)]$$

is the first–order backward difference of f at the point $\xi = t - rh$.

thus

$f_h^{(p)}$

$$+ \frac{1}{h^p} \sum_{r=0}^{n-1} \binom{p-1}{r} [f(t - rh) - f(t - (r+1)h)]$$

We can now iterate the binomial identity m–times to obtain:

$$f_h^{(p)}(t) = \sum_{k=0}^{m} (-1)^{n-k} \binom{p-k-1}{n-k} \frac{1}{h^p} \Delta^k f(c+kh) + \frac{1}{h^p} \sum_{r=0}^{n-m-1} (-1)^r \binom{p-m-1}{r} \Delta^{m+1} f(t-rh).$$

We can now iterate the binomial identity m–times to obtain:

$$\lim_{\substack{h\to 0\\ nh=t-c}} f_h^{(p)}(t) = \lim_{\substack{h\to 0\\ nh=t-c}} \sum_{k=0}^{m} (-1)^{n-k} \binom{p-k-1}{n-k} \frac{1}{h^p} \Delta^k f(c+kh)$$

$$+ \frac{1}{h^p} \sum_{r=0}^{n-m-1} (-1)^r \binom{p-m-1}{r} \Delta^{m+1} f(t-rh).$$

We compute now the limit part–by–part, starting from

$$\lim_{\substack{h\to 0\\ nh=t-c}} (-1)^{n-k} \binom{p-k-1}{n-k} \frac{1}{h^p} \Delta^k f(c+kh)$$

$$= \lim_{\substack{h\to 0\\ nh=t-c}} (-1)^{n-k} \binom{p-k-1}{n-k} (n-k)^{p-k} \left(\frac{n}{n-k}\right)^{p-k} \cdot$$

$$\cdot (nh)^{k-p} \frac{\Delta^k f(c+kh)}{h^k}$$

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And now:

$$\lim_{\substack{h\to 0\\ nh=t-c}} (nh)^{k-p} = (t-c)^{-p+k},$$

$$= \lim_{\substack{h\to 0\\ nh=t-c}} (-1)^{n-k}\binom{p-k-1}{n-k}(n-k)^{p-k}\left(\frac{n}{n-k}\right)^{p-k}\cdot$$

$$\cdot (nh)^{k-p}\frac{\Delta^k f(c+kh)}{h^k}$$

And now:

$$\lim_{\substack{h\to 0\\ nh=t-c}} (nh)^{k-p} = (t-c)^{-p+k},$$

$$\lim_{\substack{h\to 0\\ nh=t-c}} (-1)^{n-k}\binom{p-k-1}{n-k}(n-k)^{p-k}$$

$$= \lim_{n\to+\infty} \frac{(-p+k+1)(-p+k+2)\dots(-p+n)}{(n-k)^{-p+k}(n-k)!}$$

$$= \frac{1}{\Gamma(-p+k+1)} \quad (\text{since } \Gamma(z) = \lim_{n\to+\infty} \frac{n!n^z}{z(z+1)\cdot\ldots\cdot(z+n)})$$

$$= \lim_{\substack{h\to 0\\ nh=t-c}} (-1)^{n-k}\binom{p-k-1}{n-k}(n-k)^{p-k}\left(\frac{n}{n-k}\right)^{p-k}\cdot$$

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$$\lim_{n\to+\infty} (-1)^{n-k}\binom{p-k-1}{n-k}(n-k)^{p-k} = \frac{1}{\Gamma(-p+k+1)},$$

$$\lim_{n\to+\infty} \left(\frac{n}{n-k}\right)^{p-k} = 1,$$

We

$$= \lim_{\substack{h\to 0\\ nh=t-c}} (-1)^{n-k}\binom{p-k-1}{n-k}(n-k)^{p-k} \left(\frac{n}{n-k}\right)^{p-k} \cdot$$

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$$\lim_{n\to+\infty} \left(\frac{n}{n-k}\right)^{p-k} = 1,$$

$$\lim_{h\to 0} \frac{\Delta^k f(c+kh)}{h^k} = f^{(k)}(c).$$

$$= \lim_{\substack{h\to 0\\ nh=t-c}} (-1)^{n-k}\binom{p-k-1}{n-k}(n-k)^{p-k}\left(\frac{n}{n-k}\right)^{p-k} \cdot$$

$$\cdot (nh)^{k-p}\frac{\Delta^k f(c+kh)}{h^k}$$

We can now iterate the binomial identity m–times to obtain:

$$\lim_{\substack{h\to 0\\ nh=t-c}} f_h^{(p)}(t) = \lim_{\substack{h\to 0\\ nh=t-c}} \sum_{k=0}^{m} \frac{f^{(k)}(c)(t-c)^{-p+k}}{\Gamma(-p+k+1)} + \frac{1}{h^p}\sum_{r=0}^{n-m-1}(-1)^r \binom{p-m-1}{r} \Delta^{m+1} f(t-rh).$$

We compute now the limit part–by–part, then for the second part we need again the Letnikov's Lemma, to obtain

$$\lim_{\substack{h\to 0\\ nh=t-c}} \frac{1}{h^p}\sum_{r=0}^{n-m-1}(-1)^r \binom{p-m-1}{r} \Delta^{m+1} f(t-rh) = \frac{1}{\Gamma(-p+m+1)} \int_c^t (t-\xi)^{m-p} f^{(m+1)}(\xi)d\xi.$$

We can now iterate the binomial identity m–times to obtain:

$$\lim_{\substack{h\to 0\\ nh=t-c}} f_h^{(p)}(t) = \sum_{k=0}^{m} \frac{f^{(k)}(c)(t-c)^{-p+k}}{\Gamma(-p+k+1)} + \frac{1}{\Gamma(-p+m+1)} \int_c^t (t-\xi)^{m-p} f^{(m+1)}(\xi)d\xi.$$

The assumptions we have used to derive this formula are

- $f^{(k)}(t)$, $k = 1, 2, \ldots, m+1$, continuous in $[c, t]$,
- $m \in \mathbb{N}$ such that $p - 1 < m < p < m + 1$.

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- $f^{(k)}(t)$, $k = 1, 2, \ldots, m+1$, continuous in $[c, t]$,
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What is the link between the Riemann–Liouville Integral Definition and the Grünwald–Letnikov Limit Definition?

A Brief Introduction to Fractional Calculus

Three derivatives board a lecture...

- Derivative of Integer Order $n \in \mathbb{N}$

$$\frac{d^n f(t)}{dt^n} = \lim_{h \to 0} \frac{f^{(n-1)}(t) - f^{(n-1)}(t-h)}{h},$$

- Riemann–Liouville derivative of order α, $\Re\alpha > 0$, $n = \lceil \alpha \rceil$

$${}^{RL}_{c}D_t^{\alpha} f(t) = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dt^n} \int_c^t (t-\xi)^{n-\alpha-1} f(\xi)\, d\xi$$

- Grünwald–Letnikov Derivative of order α, $\Re\alpha > 0$, $n = \lceil \alpha \rceil$

$${}^{GL}_{c}D_t^{\alpha} f(t) = \sum_{k=0}^{n-1} \frac{f^{(k)}(c)(t-c)^{-\alpha+k}}{\Gamma(-\alpha+k+1)} + \frac{1}{\Gamma(n-\alpha)} \int_c^t (t-\xi)^{n-\alpha-1} f^{(n)}(\xi) d\xi$$

Observe that:

$$\sum_{k=0}^{n-1} \frac{f^{(k)}(c)(t-c)^{-\alpha+k}}{\Gamma(-\alpha+k+1)} + \frac{1}{\Gamma(n-\alpha)} \int_c^t (t-\xi)^{n-\alpha-1} f^{(n)}(\xi) d\xi$$

can be written as

$$\frac{d^n}{dt^n} \left(\sum_{k=0}^{n-1} \frac{f^{(k)}(c)(t-c)^{n+k-\alpha}}{\Gamma(1+n+k-\alpha)} + \frac{1}{\Gamma(2n-\alpha)} \int_c^t (t-\xi)^{2n-\alpha-1} f^{(n)}(\xi)\, d\xi \right)$$

Observe that:

$$\sum_{k=0}^{n-1} \frac{f^{(k)}(c)(t-c)^{-\alpha+k}}{\Gamma(-\alpha+k+1)} + \frac{1}{\Gamma(n-\alpha)} \int_c^t (t-\xi)^{n-\alpha-1} f^{(n)}(\xi) d\xi$$

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If we integrate n times by parts we find

$$\begin{aligned} &\frac{1}{\Gamma(2n-\alpha)} \int_c^t (t-\xi)^{2n-\alpha-1} f^{(n)}(\xi)\, d\xi \\ &= \frac{1}{\Gamma(2n-\alpha)} \left((t-\xi)^{2n-\alpha-1} f^{(n-1)}(\xi) \Big|_c^t \right. \\ &\left. +(2n-\alpha-1) \int_c^t (t-\xi)^{2n-\alpha-2} f^{(n-1)}(\xi)\, d\xi \right) \end{aligned}$$

Observe that:

$$\sum_{k=0}^{n-1} \frac{f^{(k)}(c)(t-c)^{-\alpha+k}}{\Gamma(-\alpha+k+1)} + \frac{1}{\Gamma(n-\alpha)} \int_c^t (t-\xi)^{n-\alpha-1} f^{(n)}(\xi) d\xi$$

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If we integrate n times by parts we find

$$\frac{1}{\Gamma(2n-\alpha)} \int_c^t (t-\xi)^{2n-\alpha-1} f^{(n)}(\xi)\, d\xi$$

$$= -\frac{(t-c)^{2n-\alpha-1} f^{(n-1)}(c)}{\Gamma(2n-\alpha)} + \frac{1}{\Gamma(2n-\alpha-1)} \int_c^t (t-\xi)^{2n-\alpha-2} f^{(n-1)}(\xi)\, d\xi$$

A Brief Introduction to Fractional Calculus

Three derivatives board a lecture...

Observe that:

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If we integrate n times by parts and sum

$$\frac{d^n}{dt^n} \left(\frac{1}{\Gamma(n-\alpha)} \int_c^t (t-\xi)^{n-\alpha-1} f(\xi)\, d\xi \right)$$

$$\Rightarrow {}^{GL}_{c}D^{\alpha}_{t} f(t) \equiv {}^{RL}_{c}D^{\alpha}_{t} f(t)$$

A Brief Introduction to Fractional Calculus

Three derivatives board a lecture...

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$$\Rightarrow {}_c^{GL}D_t^{\alpha} f(t) \equiv {}_c^{RL}D_t^{\alpha} f(t)$$

If $f(t)$ is $(n-1)$–times continuously differentiable in $[c, t]$ and $f^{(n)}(t)$ is integrable in $[c, t]$.

The equivalence (even if under somewhat restrictive assumptions) between the Riemann–Liouville and the Grünwald–Letnikov derivatives is very important for us, since we can use it to discretize the first one on the interval $[c, T]$ with stepsize $h = \frac{T-c}{M}$, $M \in \mathbb{N}$ in $t_m = c + mh$:

A Brief Introduction to Fractional Calculus

Three derivatives board a lecture. . . and a numerical method comes out!

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$$
\begin{aligned}
{}^{RL}_{c}D^{\alpha}_{t} f(t)\Big|_{t=t_n} &= \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dt^n} \int_c^t (t-\xi)^{n-\alpha-1} f(\xi)\, d\xi \Big|_{t=t_m} \\
&= \lim_{\substack{h \to 0 \\ Mh = T-c}} \frac{1}{h^{\alpha}} \sum_{r=0}^{M} (-1)^r \binom{\alpha}{r} f(t - rh) \Big|_{t=t_m} \\
&\approx \frac{1}{h^{\alpha}} \sum_{r=0}^{m} (-1)^r \binom{\alpha}{r} f(t_{m-r}).
\end{aligned}
$$

A Brief Introduction to Fractional Calculus

A matter of Left– and Right–side

Histoire socialiste de la France contemporaine (tome I)

Until now we have used

- integration on the interval $[c, t]$ with fixed c and moving $t > c$,
- backward differences,

nobody stops us from using instead

- integration on the interval $[t, T]$ with fixed c and moving $t < T$,
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It should not be too surprising that everything could be restated this way. . .

A Brief Introduction to Fractional Calculus

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$$ {}^{RL}_{\ t}D^{\alpha}_{c} f(t) = \frac{(-1)^n}{\Gamma(n-\alpha)} \frac{d^n}{dt^n} \int_t^c (\xi - t)^{n-\alpha-1} f(\xi)\, d\xi $$

A Brief Introduction to Fractional Calculus

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- Grünwald–Letnikov Derivative of order α, $\Re\alpha > 0$, $n = \lceil\alpha\rceil$

$$ {}_{c}^{GL}D_t^{\alpha} f(t) = \lim_{\substack{h \to 0 \\ Mh = c - T}} \frac{1}{h^{\alpha}} \sum_{r=0}^{M} (-1)^r \binom{\alpha}{r} f(t + rh) $$

1. Compute

$$ {}^{RL}_{\;0}D_t^{\alpha} t^{\mu}, \quad \mu \in \mathbb{R}, \quad \mu > 0. $$

2. Let $\omega_k^{(\alpha)}$ be the coefficients $\omega_k^{(\alpha)} = (-1)^k \binom{\alpha}{k}$, prove that they can be computed recursively as

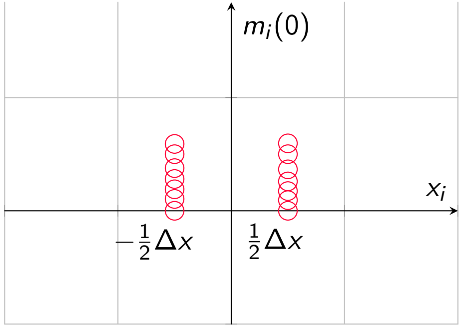
$$ \begin{cases} \omega_0^{(\alpha)} = 1, & k = 0, \\ \omega_k^{(\alpha)} = \left(1 - \frac{1+\alpha}{k}\right) \omega_{k-1}^{(\alpha)}, & k \geq 1. \end{cases} $$

Fractional Diffusion Equations

Back to the basics

Before starting with fractional diffusion let us revise ordinary diffusion equations

- Consider two heaps of N particles sitting on the axis at the position $x = \pm{}^1\!/_2\Delta x$,



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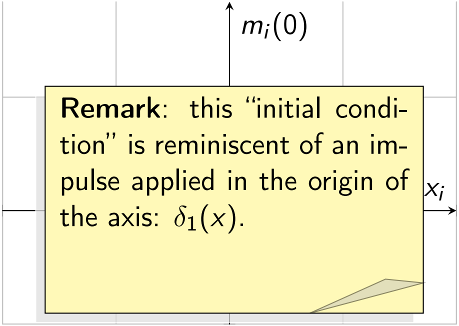
- Consider two heaps of N particles sitting on the axis at the position $x = \pm{}^1\!/_2\Delta x$,



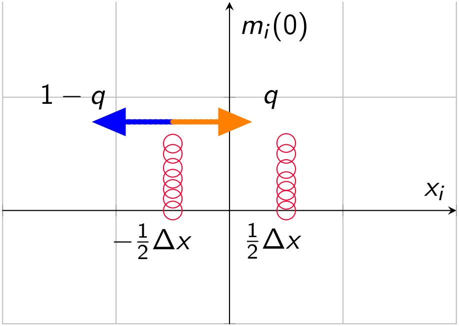
Remark: this "initial condition" is reminiscent of an impulse applied in the origin of the axis: $\delta_1(x)$.

Fractional Diffusion Equations

Back to the basics

Before starting with fractional diffusion let us revise ordinary diffusion equations

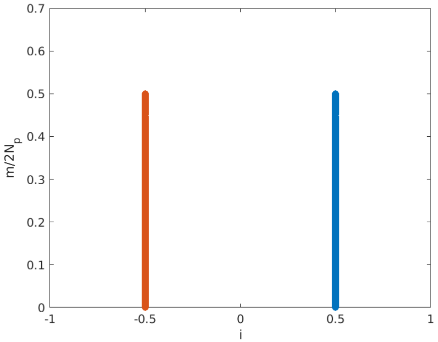
- We start a clock, then at each time–step Δt every particles make a random choiche with probability q of going to the right (or $1 - q$ of going to the left),



Fractional Diffusion Equations

Back to the basics

- After n_T steps each particles attains the position $x_i = (i - 1/2)\Delta x$ for $i \in \mathbb{Z}$ and we call $m_i(n)$ the number of particles in each position



- Since particles do not disappear, we have a *conservation of mass*, i.e.,

$$\sum_{i=-n}^{n+1} m_i(k) = 2N, \qquad \forall\, n \in \mathbb{N}, \forall\, k = 0, \ldots, n,$$

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- thus the density distribution of the particles is defined as

$$p_i(n) \triangleq \frac{1}{2N} m_i(n), \qquad \forall i = -n, \ldots, n+1, \qquad \sum_{i=-n}^{n+1} p_i(n) = 1,$$

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- to reach our diffusion equation we need only to define now the expected particle position (at step n)

$$\bar{x}(n) \triangleq \sum_{i=-n}^{n+1} x_i p_i(n),$$

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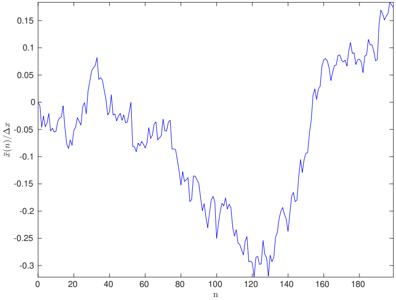
- to reach our diffusion equation we need only to define now the expected particle position (at step n) $\bar{x}(n)$ and the variance:

$$s^2(n) \triangleq \sum_{i=-n}^{n+1} (x_i - \bar{x}(n))^2 p_i(n) = -\bar{x}^2(n) + \sum_{i=-n}^{n+1} x_i^2 p_i(n).$$

Fractional Diffusion Equations

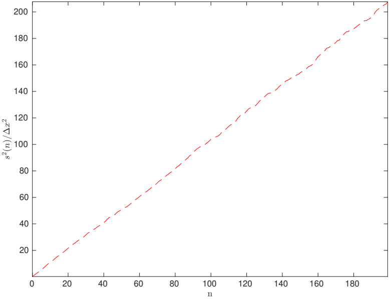
Back to the basics

The mean position moves from zero, but remains small



$$\frac{\bar{x}}{\Delta x} \propto c\Delta x, \quad c < 1.$$

The scaled variance grows (almost) at a constant rate!



$$\frac{ds^2}{dn}\frac{1}{\Delta x^2} \approx 1 \overset{t=n\Delta t}{\Rightarrow} \frac{ds^2}{dt} \approx \frac{\Delta x^2}{\Delta t}.$$

Fractional Diffusion Equations

Back to the basics

The (linear) growth of the variaton is explained in terms of the unsteady diffusion equation:

$$\begin{cases} \dfrac{\partial u}{\partial t} = \kappa \dfrac{\partial^2 u}{\partial x^2}, \\ u(x,0) = \delta_1(x). \end{cases}$$

By definition the solution of this equation is the Green's function

$$u(x,t) \equiv \mathcal{G}(x,t) \triangleq \frac{1}{\sqrt{4\kappa\pi t}} \exp\left(-\frac{x^2}{4\kappa t}\right), \qquad t > 0,$$

and it is easy to prove that

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Fractional Diffusion Equations

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Remark: the quantity

$$\kappa = \frac{1}{2}\frac{\Delta x^2}{\Delta t}$$

is called *Einstein diffusivity*, by it $\mathcal{G}(x,t)$ is in perfect agreement with the results of the discrete simulation.

By definition th ... en's function

$u(x,t) \equiv$ ... $t > 0,$

and it is easy t

$$\sigma^2(t) \equiv \int_{-\infty}^{+\infty} x^2 \mathcal{G}(x,t)dx = 2\kappa t.$$

Fractional Diffusion Equations

Anomalous Diffusion

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Fractional Diffusion Equations

Anomalous Diffusion

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- In our particle model, this means having a significant fraction of particles that are able to perform long jumps $\Rightarrow$ no more Brownian walkers!
- Discrete probability distributions that produce this phenomenon are model by finite characteristic waiting time and diverging jump length variance.
- By the same Einstein–like procedure, we can extract several type of "Fractional Diffusion Equation", in which we replace the ordinary second order derivative with a combination of Riemann–Liouville fractional derivatives.

R. Metzler and J. Klafter, The random walk's guide to anomalous diffusion: a fractional dynamics approach, Phys. Rep. **339** (2000), no. 1, 77 pp.

Fractional Diffusion Equations

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There are more distributions in heaven and earth... we can consider also Continuous Time Random Walk (CTRW) with anomalous properties, these produces Fractional Differential Equation with Fractional Derivatives in time, but we are excluding them from our presentation.

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Fractional Diffusion Equations

One-Sided Space-Fractional Diffusion Equation

We consider the following space–fractional diffusion equation with Dirichlet boundary conditions

$$\begin{cases} \dfrac{\partial u}{\partial t} = d(x)\, {}^{RL}_{\ a}D^{\alpha}_{t} u + g(x,t), & (x,t) \in (a,b) \times (0,T], \\ u(x,0) = u_0(x), & x \in (a,b), \\ u(a,t) = u_a(t),\ u(b,t) = u_b(t), & t \in (0,T]. \end{cases}$$

where $\alpha \in (1,2]$ and $d(x) > 0$.

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Fractional Diffusion Equations

One-Sided Space-Fractional Diffusion Equation – Building the Discretization

- The time domain is $[0, T]$, then Δt is the time step size and $\Delta t = {}^{T}/_{n_T}$, i.e., $\{t_n = n\Delta\}_{n=0}^{n_T}$,
- The space domain is $I = (a, b)$, then the space step size is $\Delta\, x = {}^{(b-a)}/_{N}$ for N a positive integer, i.e., $\{x_i = a + i\Delta x\}_{i=0}^{N}$,
- We approximate the function values with $u_i^{(n)} = u(x_i, t_n)$, and $g_i^{(n)} = g(x_i, t_n)$ or, in vector form, as $\mathbf{u}^{(n)} = (u_0^{(n)}, \ldots, u_N^{(n)})^T$ and $\mathbf{g}^{(n)} = (g_0^{(n)}, \ldots, g_N^{(n)})^T$, $d_i = d(x_i)$,

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- If we choose Explicit Euler method as time integrator we find

$$\frac{u_i^{(n+1)} - u_i^{(n)}}{\Delta t} = \frac{d_i}{\Delta x^\alpha} \sum_{j=0}^{i} \omega_j^{(\alpha)} u_{i-j}^{(n)} + g_i^{(n)}, \quad i = 1, 2, \ldots, N-1,$$

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Fractional Diffusion Equations

One-Sided Space-Fractional Diffusion Equation – Stability

Before thinking of solving the discrete equation given by the two methods we need to inquire about their numerical stability, Before thinking of solving the discrete equation given by the two methods we need to inquire about their numerical stability,

Numerical Stability: "the method is stable if the total variation of the numerical solution at a fixed time remains bounded as the step size goes to zero."

Fractional Diffusion Equations

One-Sided Space-Fractional Diffusion Equation – Stability

Before thinking of solving the discrete equation given by the two methods we need to inquire about their numerical stability, therefore, we start from the Explicit Euler and assume that

- $u_i^{(0)}$ is perturbed by an error $\varepsilon_i^{(0)}$, then we are working instead with $\underline{u}_i^{(0)} = u_i^{(0)} + \varepsilon_i^{(0)}$
- now we propagate the perturbation by letting the method march in time $\Rightarrow \underline{u}_i^{(1)} = u_i^{(1)} + \varepsilon_i^{(1)}$

$$\begin{aligned}\underline{u}_i^{(1)} =& \mu_i \underline{u}_i^{(0)} + \frac{\Delta t}{\Delta x^\alpha} d_i \sum_{j=1}^{i} \omega_j^{(\alpha)} u_{i-j}^0 + \Delta t g_i^{(0)} \\ =& \mu_i \varepsilon_i^0 + u_i^1, \qquad \mu_i = 1 + \frac{\Delta\, t}{\Delta x^\alpha} d_i\end{aligned}$$

- By linearity, after n iterations, $\varepsilon_i^{(n)} = \mu_i^{(n)} \varepsilon_i^{(0)}$.

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$$\underline{u}_i^{(1)} \quad \ldots \quad \varepsilon_i^{(0)}$$

$$|\mu_i| > 1, \quad \forall \Delta x \text{ suff.ly small}$$

The method is not stable!

- By linearity, after n iterations, $\varepsilon_i^{(n)} = \mu_i^{(n)} \varepsilon_i^{(0)}$.

Similarly for the Implicit Euler

- we can compute the solution as

$$\left(1 - \frac{d_i \Delta t}{\Delta x^\alpha}\right) u_i^{(n+1)} = u_i^{(n)} + \frac{d_i \Delta t}{\Delta x^\alpha} \sum_{j=1}^{i} \omega_j^{(\alpha)} u_{i-j}^{(n+1)} + \Delta t \, g_i^{(n+1)}$$

- then, assuming again that $u_i^{(0)}$ is perturbed by an error $\varepsilon_i^{(0)}$, we find

$$u_i^{(n+1)} = \mu_i u_i^{(n)} + \mu_i \left(\frac{d_i}{\Delta x^\alpha} \sum_{j=1}^{i} \omega_j^{(\alpha)} u_{i-j}^{(n+1)} + g_i^{(n+1)} \right) \Delta t$$

  where $\mu_i = (1 - {}^{d_i \Delta t}/_{\Delta x^\alpha})^{-1}$,
- By linearity, after n iterations, $\varepsilon_i^{(n)} = \mu_i^{(n)}$, we find $\varepsilon_i^{(n)} = \mu_i^n \varepsilon_i^{(0)}$.

Fractional Diffusion Equations

One-Sided Space-Fractional Diffusion Equation – Stability

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Fractional Diffusion Equations

One-Sided Space-Fractional Diffusion Equation – Stability & Convergence

To remedy to this uncomfortable situation, we introduce a simple variant of the Grünwald–Letnikov approximation: we simply shift the function evaluations to the right!

$$ {}^{RL}_{\ a}D^{\alpha}_{x} u(x,t)\Big|_{x=x_i} \approx \frac{1}{\Delta x^{\alpha}} \sum_{j=0}^{i+p} \omega_j^{(\alpha)} u(x_{i-j} + p\Delta x, t) $$

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- For an opportune value p we can prove that this modification makes the two methods consistent and (conditionally/unconditionally) stable
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How do we select the value of p?

Fractional Diffusion Equations

One-Sided Space-Fractional Diffusion Equation – Consistency

We assume working with $u \in \mathbb{L}^1(\mathbb{R}) \cap \mathcal{C}^{1+\alpha}(\mathbb{R})$

- Let $\mathcal{F}[u](k) = \hat{u}(k) = \int e^{i\,k\,x} u(x) dx$ be the Fourier transform of u,
- We compute the Fourier Transform of our shifted approximation

$$\begin{aligned}
\mathcal{F}&\left[\frac{1}{\Delta x^\alpha}\sum_{j=0}^{+\infty}(-1)^j\binom{\alpha}{j}u(x_{i-j+p},t)\right](k) \\
&= \frac{1}{\Delta x^\alpha}\sum_{j=0}^{+\infty}(-1)^j\binom{\alpha}{j}e^{ik(j-p)\Delta x}\,\hat{u}(k) \\
&= \frac{1}{\Delta x^\alpha}e^{-ik\Delta x\,p}\left(1-e^{ik\Delta\,x}\right)^\alpha\hat{u}(k) \\
&= \frac{1}{\Delta x^\alpha}(-ik\Delta x)^\alpha\left(\frac{1-e^{ik\Delta x}}{-ik\Delta x}\right)^\alpha e^{-ik\Delta x\,p}\hat{u}(k) \\
&= (-ik)^\alpha\omega(-ik\Delta x)\hat{u}(k),
\end{aligned}$$

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$$\mathcal{F}\left[\frac{1}{\Delta x^{\alpha}} \sum_{j=0}^{+\infty} (-1)^j \binom{\alpha}{j} u(x_{i-j+p}, t)\right](k)$$
$$= (-ik)^{\alpha} \omega(-ik\Delta x) \hat{u}(k),$$

- where $(ik)^{\alpha} = \operatorname{sign}(u)|u|^{\alpha} \exp({}^{i\pi\alpha}/_{2})$ and

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

We can then express

$$
\begin{aligned}
(-ik)^{\alpha}\omega(-ik\Delta x)\hat{f}(k) =& (-ik)^{\alpha}\hat{u}(k) + (-ik)^{\alpha}(\omega(-ik\Delta x) - 1)\hat{u}(k) \\
=& \mathcal{F}[D^{\alpha}u](k) + \hat{\varphi}(\Delta x, k),
\end{aligned}
$$

where

- $\mathcal{F}[D^{\alpha}u](k)$ is the Fourier transform of the RL Derivative of order α,
- $\varphi(\Delta x, x) = \frac{1}{2\pi i}\int_{-\infty}^{+\infty} e^{-ikx}\hat{\varphi}(\Delta x, k)dk,$
- $|\hat{\varphi}(\Delta x, x)| \leq |k|^{\alpha} C|hk||\hat{u}(k)|.$

Then

$$
|\varphi(\Delta x, x)| \leq \int_{-\infty}^{+\infty} \left| e^{-ikx}(-ik)^{\alpha}(\omega(-ik\Delta x) - 1)\hat{u}(k) \right| dk
$$

Fractional Diffusion Equations

One-Sided Space-Fractional Diffusion Equation – Consistency

We can then express

$(-ik)$ … $)\hat{u}(k)$

- $|\omega(-ik\Delta x) - 1| \leq C|k\Delta x|$, with $C = |p - \alpha/2|$

where

- … of
  o…
- …
- …

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- $|(-ik)^{\alpha}| \le |k|^{\alpha}\,|\exp({}^{i\pi\alpha}/_{2})|$

$(-ik)$ … $)\hat{u}(k)$

where

- $\mathcal{F}$ … of
  o
- φ
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Then

$$|\varphi(\Delta x, x)| \le \int_{-\infty}^{+\infty} \left| e^{-ikx} (-ik)^{\alpha} (\omega(-ik\Delta x) - 1)\hat{u}(k) \right| dk$$

Fractional Diffusion Equations

One-Sided Space-Fractional Diffusion Equation – Consistency

We can then express

- $|\omega(-ik\Delta x) - 1| \le C|k\Delta x|$, with $C = |p - \alpha/2|$
- $|(-ik)^\alpha| \le |k|^\alpha |\exp(i\pi\alpha/2)|$
- $I = \int_{-\infty}^{+\infty} (1 + |k|)^{\alpha+1} |\hat{u}(k)| < \infty$

  $u \in \mathbb{L}^1(\mathbb{R}) \cap \mathcal{C}^{1+\alpha}(\mathbb{R})$

where

Then

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Fractional Diffusion Equations

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- $|(-ik)^\alpha| \leq |k|^\alpha |\exp(i\pi\alpha/2)|$
- $I = \displaystyle\int_{-\infty}^{+\infty} (1 + |k|)^{\alpha+1} |\hat{u}(k)| < \infty$
  $u \in \mathbb{L}^1(\mathbb{R}) \cap \mathcal{C}^{1+\alpha}(\mathbb{R})$
- We have obtained order 1 consistency!

Then

$$|\varphi(\Delta x, x)| \leq \int_{-\infty}^{+\infty} \left| e^{-ikx}(-ik)^\alpha(\omega(-ik\Delta x) - 1)\hat{u}(k) \right| dk$$

$$\leq IC\Delta x = I|p - \alpha/2|\Delta x$$

We can then express

$(-ik)$ … $)\hat{u}(k)$

where

- $\mathcal{F}$ … of o…
- φ …
- $|\varphi$ …

- $|\omega(-ik\Delta x) - 1| \leq C|k\Delta x|$, with $C = |p - \alpha/2|$
- $|(-ik)^{\alpha}| \leq |k|^{\alpha} |\exp(i\pi\alpha/2)|$
- $I = \int_{-\infty}^{+\infty} (1 + |k|)^{\alpha+1} |\hat{u}(k)| < \infty$
  $u \in \mathbb{L}^1(\mathbb{R}) \cap \mathcal{C}^{1+\alpha}(\mathbb{R})$
- We have obtained order 1 consistency!
- **Question:** for what p we obtain the best constant ($\alpha \in (1,2)$)?

Then

$$|\varphi(\Delta x, x)| \leq \int_{-\infty}^{+\infty} \left| e^{-ikx}(-ik)^{\alpha}(\omega(-ik\Delta x) - 1)\hat{u}(k) \right| dk$$

$$\leq IC\Delta x = I|p - \alpha/2|\Delta x$$

We investigate again the stability with the $p = 1$ shifted formula!

- Explicit Euler Method:

$$\frac{u_i^{(n+1)} - u_i^{(n)}}{\Delta t} = \frac{d_i}{\Delta x^\alpha} \sum_{j=0}^{i+1} \omega_j^{(\alpha)} u_{i+1-j}^{(n)} + g_i^{(n)}, \quad i = 1, 2, \ldots, N-1,$$

that in matrix form reads as

$$\mathbf{u}^{(n+1)} = \left(I + \frac{\Delta t}{\Delta x^\alpha} DS \right) \mathbf{u}^{(n)} + \Delta t \mathbf{g}^{(n)} + \frac{\Delta t}{\Delta x^\alpha} \left(\mathbf{b}_l^{(\alpha)} u_0^{(n)} + \mathbf{b}_r^{(\alpha)} \mathbf{u}_N^{(n)} \right)$$

where:

$$S = \begin{bmatrix} \omega_1^{(\alpha)} & \omega_0^{(\alpha)} & 0 & \cdots & 0 \\ \omega_2^{(\alpha)} & \omega_1^{(\alpha)} & \omega_0^{(\alpha)} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \omega_{N-2}^{(\alpha)} & \omega_{N-3}^{(\alpha)} & \omega_{N-4}^{(\alpha)} & \cdots & \omega_0^{(\alpha)} \\ \omega_{N-1}^{(\alpha)} & \omega_{N-2}^{(\alpha)} & \omega_{N-3}^{(\alpha)} & \cdots & \omega_1^{(\alpha)} \end{bmatrix}, \qquad D = \begin{bmatrix} d_1 & & & \\ & d_2 & & \\ & & \ddots & \\ & & & d_{N-1} \end{bmatrix}.$$

Fractional Diffusion Equations

One-Sided Space-Fractional Diffusion Equation – Back to Stability

We investigate again the stability with the $p = 1$ shifted formula!

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where:

$$I = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix}, \qquad \mathbf{b}_l^{(\alpha)} = \begin{bmatrix} d_2 \omega_2^{(\alpha)} \\ d_3 \omega_3^{(\alpha)} \\ \vdots \\ d_{N-1} \omega_{N-1}^{(\alpha)} \\ d_N \omega_N^{(\alpha)} \end{bmatrix}, \qquad \mathbf{b}_r^{(\alpha)} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ d_0 \omega_0^{(\alpha)} \end{bmatrix}.$$

Fractional Diffusion Equations

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- Implicit Euler Method:

$$\left(I - \frac{\Delta t}{\Delta x^{\alpha}} DS \right) \mathbf{u}^{(n+1)} = \mathbf{u}^{(n)} + \Delta t \mathbf{g}^{(n+1)} + \frac{\Delta t}{\Delta x^{\alpha}} \left(\mathbf{b}_l^{(\alpha)} u_0^{(n+1)} + \mathbf{b}_r^{(\alpha)} \mathbf{u}_N^{(n+1)} \right)$$

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Then stability is equivalent to having the eigenvalues of the time propagators $\left(I + \frac{\Delta t}{\Delta x^{\alpha}} DS\right)$ and $\left(I - \frac{\Delta t}{\Delta x^{\alpha}} DS\right)^{-1}$ in the region of stability of the Explicit and Implicit Euler methods.

Fractional Diffusion Equations

One-Sided Space-Fractional Diffusion Equation – Back to Stability

We need to bound the Eigenvalues λ of the matrix $I + \frac{\Delta t}{\Delta x^\alpha} DS$, since this is a matrix polynomial in DS, we start working on it:

- From Gerschgorin first Theorem we have

$$|\lambda - d_i \omega_1^{(\alpha)}| \leq d_i \omega_0^{(\alpha)} + d_i \sum_{j=2}^{i} \omega_j^{(\alpha)} \leq -d_i \omega_1^{(\alpha)},$$

  thus

$$-2\alpha \max_{i=0,\ldots,N} d_i = 2 \max_{i=0,\ldots,N} d_i \omega_1^{(\alpha)} \leq 2 d_i \omega_1^{(\alpha)} \leq \lambda < 0,$$

  and then the Explicit Euler Method is stable if

$$1 - 2\frac{\Delta t}{\Delta x^\alpha} \alpha \max_{i=0,\ldots,N} d_i \geq -1 \Leftrightarrow \frac{\Delta t}{\Delta x^\alpha} \leq \frac{1}{\alpha \max_{i=0,\ldots,N} d_i}$$

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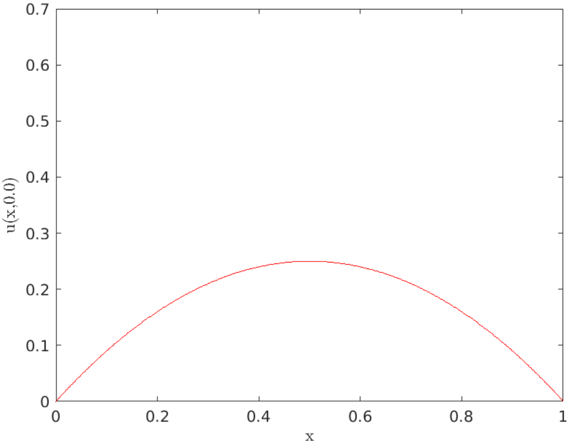
- on the other hand, since the eigenvalues of $I - \frac{\Delta t}{\Delta x^{\alpha}} DS$ are all equal or greater than 1, the Implicit Euler Method is unconditionally stable.

Fractional Diffusion Equations

An Example



Fractional Diffusion Equations

A more general case

Having discussed the one–sided equation then its simplest (and more natural) generalization is given by

$$\begin{cases} \dfrac{\partial u}{\partial t} = d_{+}(x,t)\, {}^{RL}_{\ a}D^{\alpha}_{t} u + d_{-}(x,t)\, {}^{RL}_{\ t}D^{\alpha}_{b} u + g(x,t), & (x,t) \in (a,b) \times (0,T], \\ u(x,0) = u_0(x), & x \in (a,b), \\ u(a,t) = u_a(t),\ u(b,t) = u_b(t), & t \in (0,T]. \end{cases}$$

where $\alpha \in (1,2]$ and $d_{+}(x,t), d_{-}(x,t) > 0$.

Exercise III

- The Crank–Nicolson method with $p = 1$ for the one–sided problem is given by

$$\frac{u_i^{(n+1)} - u_i^{(n)}}{\Delta t} = \frac{d_i}{2\Delta x^\alpha} \left[\sum_{j=0}^{i+1} \omega_j^{(\alpha)} u_{i+1-j}^{(n+1)} + g_i^{(n+1)} + \sum_{j=0}^{i+1} \omega_j^{(\alpha)} u_{i+1-j}^{(n)} + g_i^{(n)} \right]$$

  - Write the matrix form of the method,
  - Prove that the method is unconditionally stable.
- Write down the matrix sequence generated for the two–sided equation with $p = 1$ shifted Grünwald–Letnikov discretization and backward Euler method. Prove that the obtained discretization scheme is still convergent.

Matrix Sequences

From the discretization of the Fractional Diffusion Equation we have obtained several matrices, what we are going to do in this section is analyzing them to uncover their properties, if we assume that $d(x) \equiv 1$

Matrix Sequences

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- then the building block of the discretization is the matrix

$$\{S_N\}_N = \begin{bmatrix} \omega_1^{(\alpha)} & \omega_0^{(\alpha)} & 0 & \cdots & 0 \\ \omega_2^{(\alpha)} & \omega_1^{(\alpha)} & \omega_0^{(\alpha)} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \omega_{N-2}^{(\alpha)} & \omega_{N-3}^{(\alpha)} & \omega_{N-4}^{(\alpha)} & \cdots & \omega_0^{(\alpha)} \\ \omega_{N-1}^{(\alpha)} & \omega_{N-2}^{(\alpha)} & \omega_{N-3}^{(\alpha)} & \cdots & \omega_1^{(\alpha)} \end{bmatrix}_{(N-1)\times(N-1)}$$

  - This is a sequence of Toeplitz Matrices,
  - This is a lower Hessenberg Matrix,
  - The elements $\{\omega_j^{(\alpha)}\}_j$ decay away from the main diagonal,
  - It is a dense matrix.

Matrix Sequences

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- then ... rix

$\{$ ... $(N-1)$

Remark:

- the matrix being Toeplitz correspond to the operator being (almost) translation invariant,
- the matrix being Dense correspond to the operator being non–local.

For a reasonable discretization every matrix property should correspond to a property of the operator!

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Matrix Sequences

Toeplitz Structure

- A Toeplitz Matrix is a matrix with constant coefficients along the diagonals

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

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- A subset of this linear space of matrices is given by the matrices for which exists an $f \in \mathbb{L}^1([-\pi, \pi])$, such that

$$t_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\theta) e^{-ik\theta} d\theta, \;\; k = 0, \pm 1, \pm 2, \dots,$$

the t_k are the Fourier coefficients of f. In this case we write $T_n = T_n(f)$ where f is the *generating function* of the matrix $T_n(f)$.

Matrix Sequences

Toeplitz Structure

Our matrix sequence is exactly a sequence of this type!

- We can construct the generating function directly:

$$
\begin{aligned}
f_\alpha(\theta) =& \sum_{k=0}^{+\infty} \omega_k^{(\alpha)} e^{i(k-1)\theta} = \sum_{k=0}^{\infty} (-1)^k \binom{\alpha}{k} e^{i(k-1)\theta} \\
=& \sum_{k=0}^{+\infty} \binom{\alpha}{k} e^{i(k-1)\theta} e^{ik\pi} = e^{-i\theta} \sum_{k=0}^{+\infty} \binom{\alpha}{k} e^{k(\theta+k)} \\
=& e^{-i\theta} \left(1 + e^{i(\theta+\pi)}\right)^\alpha = e^{-i\theta} \left(1 - e^{i\theta}\right)^\alpha,
\end{aligned}
$$

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Asymptotic singular values distribution

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

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

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

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Asymptotic eigenvalue distribution

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

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

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- . . . and from that knowledge efficient preconditioners can be built.

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- And a lot more technical (at least to prove) that with these ingredient a generalization of the Toeplitz matrices for these cases can be built.

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- And a lot more technical (at least to prove) that with these ingredient a generalization of the Toeplitz matrices for these cases can be built.
- The very good news is that the machinery is quite easy to use!

Matrix Sequences

Generalized Locally Toeplitz Structure

GLT 1. If $\{A_n\}_n \sim_{\mathrm{GLT}} \kappa$ then $\{A_n\}_n \sim_\sigma \kappa$. If $\{A_n\}_n \sim_{\mathrm{GLT}} \kappa$ and the matrices A_n are Hermitian then $\{A_n\}_n \sim_\lambda \kappa$.

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GLT 2. If $\{A_n\}_n \sim_{\mathrm{GLT}} \kappa$ and $A_n = X_n + Y_n$, where

- every X_n is Hermitian,
- $\|X_n\|, \|Y_n\| \le C$ for some constant C independent of n,
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GLT 3. We have

- $\{T_n(f)\}_n \sim_{\mathrm{GLT}} \kappa(x,\theta) = f(\theta)$ if $f \in L^1([-\pi,\pi])$,
- $\{D_n(a)\}_n \sim_{\mathrm{GLT}} \kappa(x,\theta) = a(x)$ if $a : [0,1] \to \mathbb{C}$ is Riemann-integrable,
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- $\{\alpha A_n + \beta B_n\}_n \sim_{\mathrm{GLT}} \alpha\kappa + \beta\xi$ for all $\alpha, \beta \in \mathbb{C}$,
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GLT 5. If $\{A_n\}_n \sim_{\mathrm{GLT}} \kappa$ and $\kappa \ne 0$ a.e. then $\{A_n^\dagger\}_n \sim_{\mathrm{GLT}} \kappa^{-1}$.

Matrix Sequences

Generalized Locally Toeplitz Structure

With this machinery we can compute the symbol for the time–stepping operator of the two–sided fractional diffusion equation:

$$A_N \triangleq \nu I + D_N^+ S_N + D_N^- S_N^T, \qquad \nu = \frac{\Delta x^\alpha}{\Delta t}$$

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Matrix Sequences

Generalized Locally Toeplitz Structure

With this machinery we can compute the symbol for the time–stepping operator of the two–sided fractional diffusion equation:

$$A_N \triangleq \nu I + D_N^+ S_N + D_N^- S_N^T, \qquad \nu = \frac{\Delta x^\alpha}{\Delta t}$$

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- By **GLT2**, **GLT4**, and assuming that $\nu = o(1)$ we discover that $\{\nu I\}_N \sim_{\text{GLT}} 0$ and conclude that: $\{A_N\}_N \sim_{\text{GLT}} g_\alpha(\hat{x},\theta)$.

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With this machinery we can compute the symbol for the time–stepping operator of the two–sided fractional diffusion equation:

For general $d_{\pm}(x)$ this is sufficient only for obtaining singular value distribution via the first part of **GLT1**.
If $d_{+} \equiv d_{-} \triangleq d$, then $\{A_N\}_N \sim_{\text{GLT}} \{D_N^{-1} A_N D_N\} \sim_{\lambda} \hat{d}(\hat{x})(f_\alpha(\theta) + f_\alpha(-\theta))$, where we have used the Hermitian part of **GLT1**.

- By **GL**[...]) $\hat{x} \in [0,1]$
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  $D_N^{+} S_N + D_N^{-} S_N^{T} \sim_{\text{GLT}} g_\alpha(\hat{x},\theta) = \hat{d}_{+}(\hat{x}) f_\alpha(\theta) + \hat{d}_{-}(\hat{x}) f_\alpha(-\theta)$
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- This information can be exploited for building band–Toeplitz and Multigrid preconditioners.

M. Donatelli, M. Mazza and S. Serra-Capizzano, Spectral analysis and structure preserving preconditioners for fractional diffusion equations, J. Comput. Phys. **307** (2016), 262-279.

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Matrix Sequences

Decay Behavior

Let's change perspective! We have looked at the spectral properties of the matrix, let us look now at the magnitude of their elements. From the definition of the coefficients $\omega_\kappa^{(\alpha)} = (-1)^k \binom{\alpha}{k}$ the following properties (for $\alpha \in (1,2)$) are easily obtained

- $\omega_0^{(\alpha)} = 1$ and $\omega_1^{(\alpha)} = -\alpha$,
- $\sum_{k=0}^{+\infty} \omega_k^{(\alpha)} = 0$,
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- $\omega_0^{(\alpha)} > \omega_2^{(\alpha)} > \omega_3^{(\alpha)} > \ldots > 0$,

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This decay property is very useful! And more can be said about it:

$$|\omega_k^{(\alpha)}| = O(k^{-\alpha-1}), \quad \text{for } k \to +\infty.$$

That descend from the limit

$$\lim_{x \to +\infty} \frac{\Gamma(x+\alpha)}{x^\alpha \Gamma(x)} = 1, \ \ \forall \alpha \in \mathbb{R}.$$

Matrix Sequences

Decay Behavior is inherited from the "Short Memory Principle"

This **decaying property** of the entries of the discretization matrices is a **structural property** of the fractional differential operators.

- Let us fix a *memory length* $a \leq L < x$,
- Then ${}^{RL}_{a}D^{\alpha}_{x}u(x) \approx {}^{RL}_{a-L}D^{\alpha}_{x}u(x), \;\; x > a + L$,
- The approximation error for $a + L \leq x \leq b$ is given by:

$$E(x) = |\,{}^{RL}_{a}D^{\alpha}_{x}u(x) - {}^{RL}_{a-L}D^{\alpha}_{x}u(x)| \leq \frac{\sup_{x\in[a,b]} u(x)}{L^{\alpha}|\Gamma(1-\alpha)|},$$

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We have obtained these results for the time–propagator matrix, what about its inverse?
More generally, knowing a decay pattern in a sequence of matrices what can be said about the sequence of the inverses?

Matrix Sequences

Decay Behavior of the Sequence of the Inverses

Decay behavior of matrix sequences is a very studied topic and thus there are many results dealing with several cases

- banded matrices,
- inverses of matrices with polynomial/exponential decay,
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For the application we have in mind we are mostly interested in this case.

S. Jaffard, Propriétés des matrices “bien localisées” près de leur diagonale et quelques applications, Ann. Inst. H. Poincaré Anal. Non Linéaire **7** (1990), no. 5, 461-476.

Matrix Sequences

Polynomial and Exponential Decay

The sets of invertible matrix $(A)_{h,k} \in \mathcal{B}(\ell^2(\mathbb{K}))$, $\mathbb{K} = \mathbb{Z}, \mathbb{N}$, such that either

$$|a_{h,k}| \leq C(1 + |h-k|)^{-s},$$

or

$$|a_{h,k}| \leq C \exp(-\gamma |h-k|)$$

are two algebras, respectively, Q_s and $\mathcal{E}_\gamma$, i.e., their inverses have the same decay behavior.

- We have interpreted our matrices as elements of sequences of matrices with growing size, we can take the opposite point of view, i.e., our matrices are *section* of infinite operators.
- Thus the requirement $(A)_{h,k} \in \mathcal{B}(\ell^2(\mathbb{K}))$ is indeed a requirement on the underlying operator!

How can we discover if $(A)_{h,k} \in \mathcal{B}(\ell^2(\mathbb{K}))$?

Matrix Sequences

Polynomial and Exponential Decay

How can we discover if $(A)_{h,k} \in \mathcal{B}(\ell^2(\mathbb{K}))$?

- You (may) know that a linear and bounded operator A on a Banach space X is invertible in $\mathcal{B}(X)$ if (and only if) its kernel is $\{0\}$ and its range is all of X (usually known as Banach's Theorem), How can we discover if $(A)_{h,k} \in \mathcal{B}(\ell^2(\mathbb{K}))$?

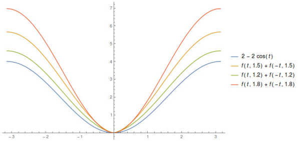
- You (may) know that a linear and bounded operator A on a Banach space X is invertible in $\mathcal{B}(X)$ if (and only if) its kernel is $\{0\}$ and its range is all of X (usually known as Banach's Theorem),
- For Toeplitz sequences this can be rewritten in a simple way:

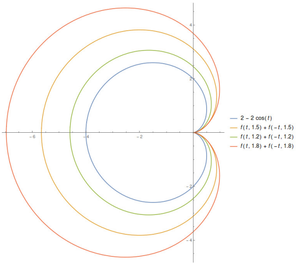
> Let $\mathbb{T} = [0, 2\pi]$, then if $f \in \mathcal{C}(\mathbb{T})$ the Toeplitz operator $T(f)$ is invertible on ℓ^2 if and only if $0 \notin f(\mathbb{T})$ and if the *winding number* of the curve $f(\mathbb{T})$ around the origin is exactly 0, i.e.,
>
> $$\nu(f, 0) = \oint_{f(\mathbb{T})} \frac{d\,z}{z} = 0.$$

Matrix Sequences

Polynomial and Exponential Decay

This is not a very good news...





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Matrix Sequences

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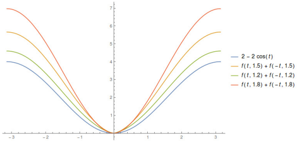

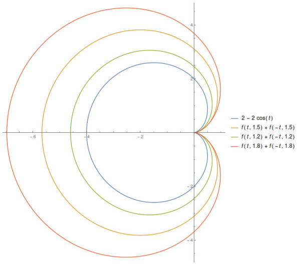

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- This is a characteristic of differential operators they are not bounded (classical example $f_n = \sin(nx)$, $\|f_n\|_\infty = 1$ for $n \geq 2$, but $(Df_n)(x) = n\cos(nx)$, and hence $\|Df_n\|_\infty = n$) and have non–zero kernel

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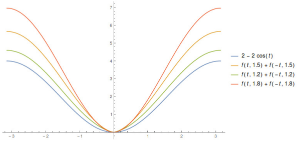

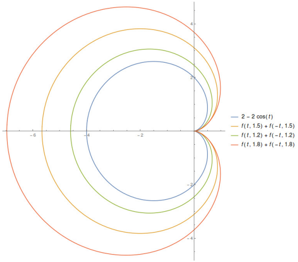

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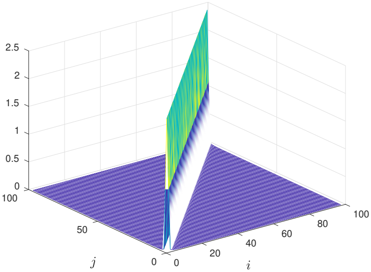
- Moreover, if you think at the Green functions as "inverses" of derivatives, they have usually support in all the domain.

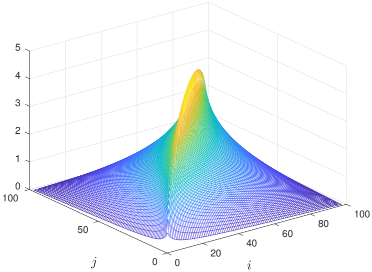
Matrix Sequences

Polynomial and Exponential Decay

But, on the other hand, numerical experiments do tell us something different:



$|S_{h,k}| = |(S_{100} + S_{100}^T)_{h,k}|$



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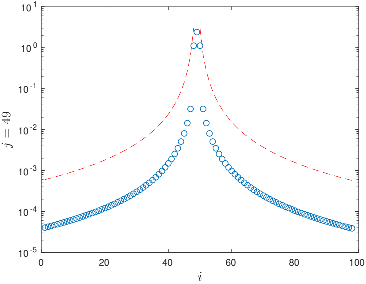

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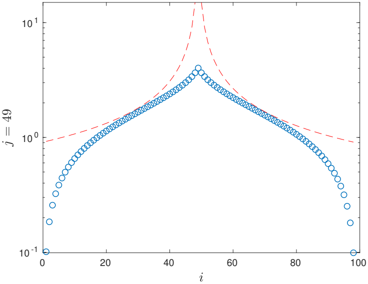

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These matrices do not form an algebra anymore, but polynomial decay is still there (even if with different order and a different constant).

Matrix Sequences

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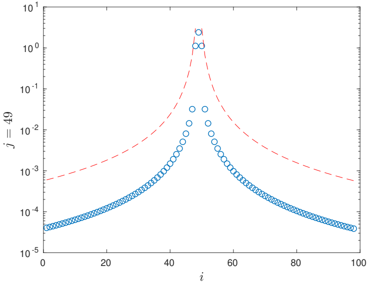

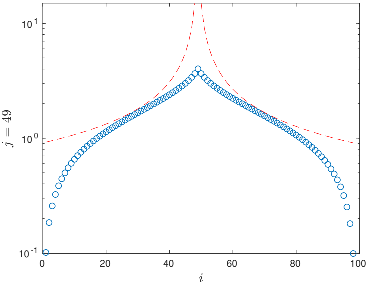

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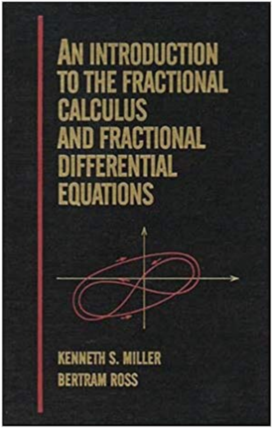
This information can be used to produce approximate sparse inverses for this matrix sequence!

Conclusions

We have

- introduced (some) concept(s) of Fractional Derivative,
- revised the classical diffusion equation,
- discussed the phenomenon of anomalous diffusion,
- introduced the fractional diffusion equation,
- produced discretizations and numerical schemes,
- discussed properties of the discrete problems.

Books



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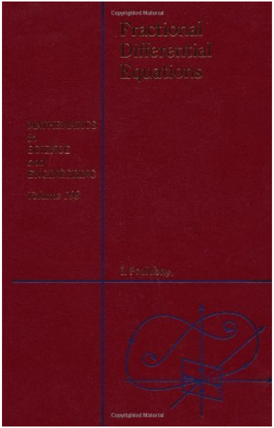

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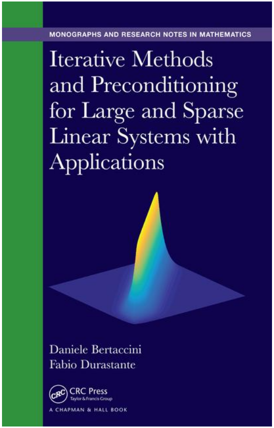

Bertaccini, D., and F. Durastante. Iterative Methods and Preconditioning for Large and Sparse Linear Systems with Applications. Chapman and Hall/CRC, 2018.

Useful Readings I

- Theory of Fractional Differential Equations

R. Metzler and J. Klafter, The random walk's guide to anomalous diffusion: a fractional dynamics approach, Phys. Rep. **339** (2000), no. 1, 77 pp.

- Discretizations and Numerical Methods

M. M. Meerschaert and C. Tadjeran, Finite difference approximations for fractional advection-dispersion flow equations, J. Comput. Appl. Math. **172** (2004), no. 1, 65-77.

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Useful Readings II

- Iterative Methods and Preconditioners

D. Bertaccini and F. Durastante, Solving mixed classical and fractional partial differential equations using short-memory principle and approximate inverses, Numer. Algorithms **74** (2017), no. 4, 1061-1082.

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M. Donatelli, M. Mazza and S. Serra-Capizzano, Spectral analysis and structure preserving preconditioners for fractional diffusion equations, J. Comput. Phys. **307** (2016), 262-279.

Useful Readings III

- H. Moghaderi et al., Spectral analysis and multigrid preconditioners for two-dimensional space-fractional diffusion equations, J. Comput. Phys. **350** (2017), 992-1011.

- Generalized Locally Toeplitz Theory

- C. Garoni and S. Serra-Capizzano, Generalized Locally Toeplitz Sequences: Theory and Applications, Volume 1. Springer, 2017.
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Solution of the Diffusion Equation by Finite Differences

The main idea of *Finite Difference* (FD) methods for solving PDEs is to replace spatial and time derivatives of the strong form of the differential equations by numerical approximation (evaluation) on a time and space grid.

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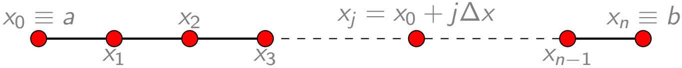

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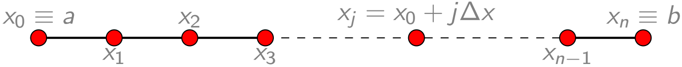

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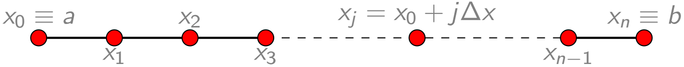

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- and consider the values $\{f_j\}_{j=0}^{n} = \{f(x_j)\}_{j=0}^{n}$
- Can we approximate the values of $f'(x_j)$, for $j = 1, \dots, n-1$, by using only the values of f at the knots $\{f_j\}_{j=0}^{n}$?

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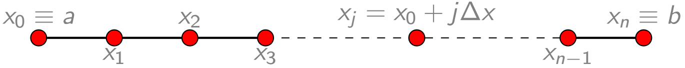
The main idea of *Finite Difference* (FD) methods for solving PDEs is to replace spatial and time derivatives of the strong form of the differential equations by numerical approximation (evaluation) on a time and space grid.

- Given a function $f : [a, b] \subset \mathbb{R} \to \mathbb{R}$ and an integer $n \in \mathbb{N}$ we can subdivide the interval $[a, b]$ into intervals of length $\Delta x = {}^{(b-a)}/_{n}$ with grid points $\{x_j\}_{j=0}^{n} = \{x_j = x_0 + j\Delta x\}_{j=0}^{n}$:



,

- and consider the values $\{f_j\}_{j=0}^{n} = \{f(x_j)\}_{j=0}^{n}$
- Can we approximate the values of $f'(x_j)$, for $j = 1, \ldots, n-1$, by using only the values of f at the knots $\{f_j\}_{j=0}^{n}$?

The answer is YES! But let's see how we can achieve it

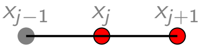
Solution of the Diffusion Equation by Finite Differences

Building the FD formulas

From the Definition we know that:

- The first derivative of f at $x = x_j$ can be expressed by using knots for $j' > j$

$$f'(x_j) \triangleq \lim_{\Delta x \to 0} \frac{f_{j+1} - f_j}{\Delta x} \approx \frac{f_{j+1} - f_j}{\Delta x} \triangleq D_+ f_j,$$



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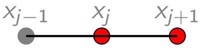
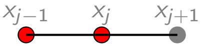


- or equivalently by using knots for $j' < j$

$$f'(x_j) \triangleq \lim_{\Delta x \to 0} \frac{f_j - f_{j-1}}{\Delta x} \approx \frac{f_j - f_{j-1}}{\Delta x} \triangleq D_- f_j,$$



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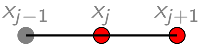

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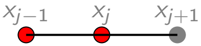
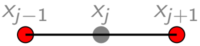


- at last we can consider the arithmetic mean of previous two:

$$f'(x_j) \approx D_0 f_j \triangleq \frac{1}{2}(D_- f_j + D_+ f_j) = \frac{f_{j+1} - f_{j-1}}{2\Delta x},$$



Solution of the Diffusion Equation by Finite Differences

Building the FD formulas

So what formula do we actually chose?

- We use Taylor Expansions to decide!

$$
\begin{aligned}
f_{j+1} =& f_j + \Delta x f_j' + \frac{1}{2}\Delta x^2 f_j'' + \frac{1}{3}\Delta x^3 f_j''' + O(\Delta x^4), \\
f_{j-1} =& f_j - \Delta x f_j' + \frac{1}{2}\Delta x^2 f_j'' - \frac{1}{3}\Delta x^3 f_j''' + O(\Delta x^4),
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$$

- from which it is easy to see that

$$
\begin{aligned}
D_+ f_j - f_j' =& \frac{1}{2}\Delta x f_j'' + \frac{1}{6}\Delta x^2 f_j''' + O(\Delta x^3) = O(\Delta x)\\
D_- f_j - f_j' =& -\frac{1}{2}\Delta x f_j'' + \frac{1}{6}\Delta x^2 f_j''' + O(\Delta x^3) = O(\Delta x)\\
D_0 f_j - f_j' =& \frac{1}{6}\Delta x^2 f_j''' + O(\Delta x^4) = O(\Delta x^2)
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So what formula do we actually chose?

- We use Taylor Expansions to decide!

We have discovered that

- D_- and D_+ produce *first order* approximations.
- D_0 produces *second order* approximation.

$$D_+f_j - f_j' = \frac{1}{2}\Delta x f_j'' + \frac{1}{6}\Delta x^2 f_j''' + O(\Delta x^3) = O(\Delta x)$$

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We have discovered that

- D_- and D_+ produce *first order* approximations.
- D_0 produces *second order* approximation.

Now, to obtain the discretization of our diffusion equation we need a FD formula for the second derivative of $f(x)$...

$$D_+ f_j - f_j' = \frac{1}{2}\Delta x f_j'' + \frac{1}{6}\Delta x^2 f_j''' + O(\Delta x^3) = O(\Delta x)$$

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Solution of the Diffusion Equation by Finite Differences

Building the FD formulas

There are several ways to obtain a formula for $f''(x_j)$, since $f''(x) = (f'(x))'$ an idea could be

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\begin{aligned}
D^2 f_j =& D_+ D_- f_j \\
=& \frac{1}{\Delta x}[D_- f_{j+1} - D_- f_j] = \frac{1}{\Delta x}\left[\frac{f_{j+1} - f_j}{\Delta x} - \frac{f_j - f_{j-1}}{\Delta x}\right] \\
=& \frac{f_{j-1} - 2f_j + f_{j+1}}{2\Delta x^2},
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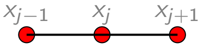

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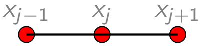

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- This is completely equivalent to $D^2 f_j = D_- D_+ f_j$ or to $D_0^{\Delta x/2} D_0^{\Delta x/2} f_j$, where $D_0^{\Delta x/2}$ is the centered difference on a grid of stepsize $\Delta x/2$,

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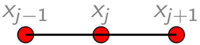

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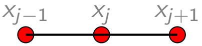

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- $f''_j = D^2 f_j + O(\Delta x^2)$,
- by this trick and the repeated derivative formula we have seen FD for higher order derivative can be readily obtained.

Solution of the Diffusion Equation by Finite Differences

Discretizing the Diffusion Equation

Let us start from the steady state diffusion equation, i.e.,

$$\text{given } f(x) \text{ find } u \text{ s.t. } \begin{cases} u''(x) = f(x), \quad x \in (0,1), \\ u(0) = \alpha, \\ u(1) = \beta, \end{cases}$$

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if we use the grid on $(0,1)$ with stepsize $\Delta x = {}^1/_{n+1}$, $n \in \mathbb{N}$ we can write the following discrete approximation

$$\text{find } u_1, \ldots, u_n \text{ s.t. } \begin{cases} \frac{1}{\Delta x}(u_{j-1} - 2u_j + u_{j+1}) = f_j, & j = 1, \ldots, n \\ u_0 = \alpha, \\ u_{n+1} = \beta, \end{cases}$$

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to find an approximation of the solution on the knots we need only to solve a set of n linear equations.

By collecting everything in a matrix form we find

$$A_n \mathbf{u}_n \equiv \frac{1}{\Delta x^2} \begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-1} \\ u_n \end{bmatrix} = \begin{bmatrix} f_1 - {}^{\alpha}\!/_{\Delta x^2} \\ f_2 \\ \vdots \\ f_{n-1} \\ f_n - {}^{\beta}\!/_{\Delta x^2} \end{bmatrix} \equiv \mathbf{f}_n$$

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"Solving a linear boundary value problem" $\approx$ "Solving a Linear System"

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"Solving a linear boundary value problem" $\approx$ "Solving a Linear System"

To be sure that what we have done is "reasonable" we need to have that the error between the values of the true solution $\hat{u}$ on the grid and the values $\{u_j\}_{j=1}^{n}$ goes to zero as $\Delta x \to 0$ ($n \to +\infty$).

Solution of the Diffusion Equation by Finite Differences

Local Truncation Error, Global Error, Stability, Consistency and Convergence

Let $\hat{\mathbf{u}}$ be the vector of the evaluations of the true solution on the grid $\{x_j\}$, we need to bound one norm of the vector $\mathbf{e}_n = \mathbf{u}_n - \hat{\mathbf{u}}_n$, e.g.,

$$\|\mathbf{e}_n\|_\infty, \qquad \|\mathbf{e}_n\|_{1,\Delta x} = \Delta x \sum_{j=1}^{n} |e_j|, \qquad \|\mathbf{e}_n\|_{2,\Delta x} = \left(\Delta x \sum_{j=1}^{n} |e_j|^2\right)^{1/2},$$

- if we call Local Truncation Error the vector

$$\boldsymbol{\tau}_n = A_n \hat{\mathbf{u}} - \mathbf{f}_n$$

- then the Global Error $\mathbf{e}$ satisfies the equation

$$A_n \mathbf{e}_n = -\boldsymbol{\tau}_n, \qquad e_0 = e_{n+1} = 0,$$

- therefore we can express the Global Error in terms of known quantities

$$\mathbf{e}_n = -A_n^{-1}\boldsymbol{\tau}_n \Rightarrow \|\mathbf{e}_n\| \leq \|A_n^{-1}\|\|\boldsymbol{\tau}_n\|$$

Solution of the Diffusion Equation by Finite Differences

Local Truncation Error, Global Error, Stability, Consistency and Convergence

Suppose an FD method for a linear BVP gives a sequence of matrix equations of the form $A_n \mathbf{u}_n = \mathbf{f}_n$, where the meshwidth is given by $\Delta x = o(1/n)$ for $n \to +\infty$. We say that the method is stable if A_n^{-1} exists for all Δx sufficiently small ($\Delta x < \bar{\Delta} x$), and if there exists a constant C independent from Δx, such that

$$\|A_n^{-1}\| \leq C, \qquad \forall\, \Delta x < \bar{\Delta} x.$$

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"consistency" + "stability" ⇒ "convergence"

$$\|\mathbf{e}_n\| \leq \|A_n^{-1}\|\|\boldsymbol{\tau}_n\| \leq C\|\boldsymbol{\tau}_n\| \to 0, \text{ as } \Delta x \to 0.$$

The Finite Difference method for the Steady State Diffusion Equation is

- stable in both norms $\|\cdot\|_{2,\Delta x}$ and $\|\cdot\|_{\infty}$,
- consistent in both norms $\|\cdot\|_{2,\Delta x}$ and $\|\cdot\|_{\infty}$ (straightforward from the computations for the order of convergence of the finite difference formulas),

therefore the method is convergent! If we refine the grid size Δx, i.e., if we increase the number of grid nodes n, the error between the approximated and true solution decreases as on $O(\Delta x^2)$.

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We consider now the time–marching case!

Solution of the Diffusion Equation by Finite Differences

Discretization in the time direction

We need to discretize now the equation:

$$\begin{cases} \dfrac{\partial u}{\partial t} = -\kappa \dfrac{\partial^2 u}{\partial x^2} + f(x,t), & (x,t) \in (0,1) \times (0,T] \\ u(x,0) = u_0(x), & x \in (0,1), \\ u(0,t) = \alpha(t), & t \in (0,T], \\ u(1,t) = \beta(t), & t \in (0,T]. \end{cases}$$

- We have just seen how to deal with the derivative in space: $\mathbf{u}_n'(t) = -\kappa A_n \mathbf{u}_n(t) + \mathbf{f}_n(t)$

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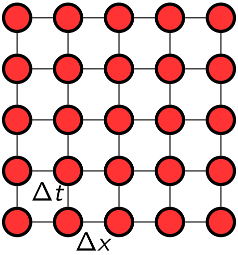
- We have just seen how to deal with the derivative in space: $\mathbf{u}_n'(t) = -\kappa A_n \mathbf{u}_n(t) + \mathbf{f}_n(t)$
- We put a grid of stepsize $\Delta t = T/(M+1)$ for $M \in \mathbb{N}$, on the time direction $\{t_m\}_{m=0}^{M+1} = \{m\Delta t\}_{m=0}^{M+1}$



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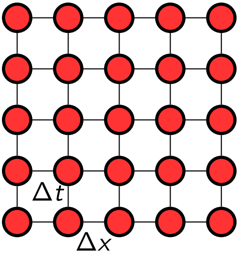
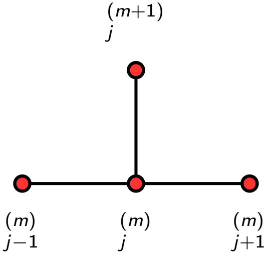


We can discretize $\dfrac{\partial u}{\partial t}$ by the 1D difference in time: $D_{\pm,t}$.

Solution of the Diffusion Equation by Finite Differences

Forward and Backward Euler

Forward (Explicit) Euler



$$D_{+,t}\mathbf{u}_n^{(m)} = -A_n\mathbf{u}_n^{(m)} + \mathbf{f}_n^{(m)}$$

$$\frac{u_n^{(m+1)} - u_n^{(m)}}{\Delta t} = -A_n\mathbf{u}_n^{(m)} + \mathbf{f}_n^{(m)}$$

$$\mathbf{u}_n^{m+1} = (I - \Delta t A_n)\mathbf{u}_n^{(m)} + \Delta t\mathbf{f}_n^{(m)}$$

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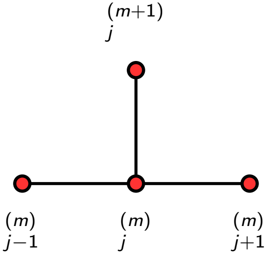

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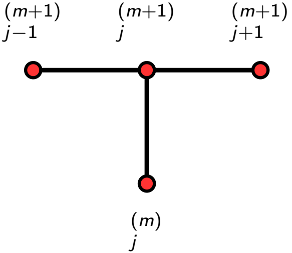
Backward (Implicit) Euler



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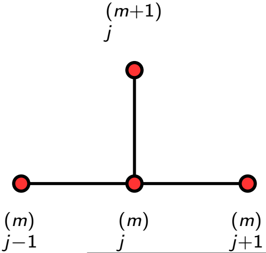
Solution of the Diffusion Equation by Finite Differences

Forward and Backward Euler

Forward (Explicit) Euler



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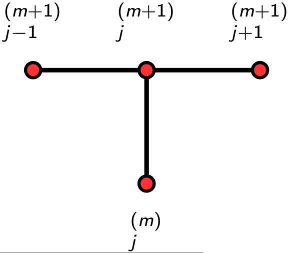


$D_{+,t}\mathbf{u}_n^{(m)}$ … $^{+1)} + \mathbf{f}_n^{(m+1)}$

$\frac{u_n^{(m+1)} - u_n^{(\dots}}{\Delta t}$ … $^{m+1)} + \mathbf{f}_n^{(m+1)}$

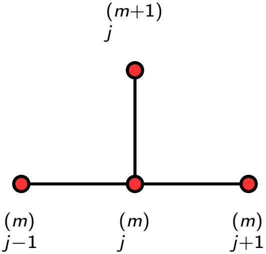
$\mathbf{u}_n^{m+1} = (I -$ … $^{+1)} + \Delta t \mathbf{f}_n^{(m+1)}$

By using again the vector $\hat{\mathbf{u}}_n^{(m)}$ of the evaluation of the true solution in t_m is possible to express again the error vector $\mathbf{e}^{(m)}$ for the two methods!

Solution of the Diffusion Equation by Finite Differences

Forward and Backward Euler

Forward (Explicit) Euler



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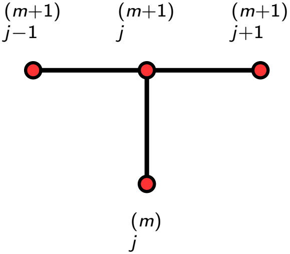

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Solution of the Diffusion Equation by Finite Differences

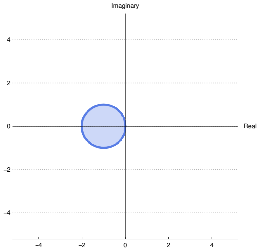
Stability and Convergence

- As it was for the BVP we need a suitable concept of stability, so let us consider the scalar test problem:

$$u'(t) = \lambda u(t), \qquad \lambda \in \mathbb{C},$$

if we apply Explicit Euler to this equation we obtain $u^{(n+1)} = (1 + \Delta t \lambda) u^{(n)}$, thus we define the region of absolute stability of this method as

$$\mathcal{R} = \{z \in \mathbb{C} \,:\, |1 + z| \leq 1\}, \qquad z = \Delta t \lambda.$$



$\mathcal{R}$ for Forward Euler Method

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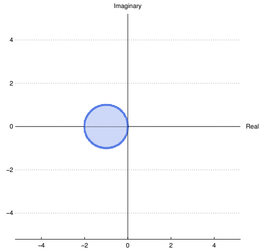

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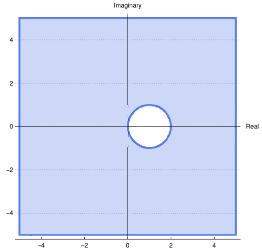

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Soluti

Stability

In practice what we are solving is a system of linear ODEs, for which the coefficient matrix is the space discretization of our liner PDE. Then the value λ represents an eigenvalue of such matrix.

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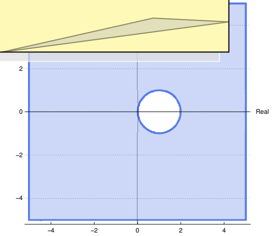

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- if we use Forward Euler method, we need to require that $|1 + \Delta t\lambda| \leq 1$ for λ any eigenvalue of $-\kappa A_n$, i.e,

$$\frac{\kappa \Delta t}{\Delta x^2} \leq \frac{1}{2},$$

in this case we say that the method is conditionally stable.

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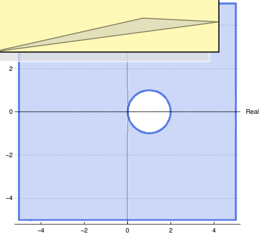

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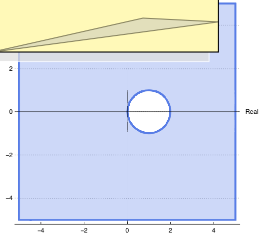

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The two method we have investigate have the form:

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for all $\Delta t > 0$ and integers m for which $\Delta t \cdot m \leq T$.

Solution of the Diffusion Equation by Finite Differences

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References

A very good introduction and a gateway to the wide literature on FD methods is represented by

R. J. LeVeque, *Finite difference methods for ordinary and partial differential equations*, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2007.

for the issues regarding time–marching schemes the classical reference is

J. D. Lambert, *Numerical methods for ordinary differential systems*, John Wiley & Sons, Ltd., Chichester, 1991.

Back to Fractional Diffusion Equation