The numerical solution of time-fractional initial-boundary value problems

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Talk overview

Riemann-Liouville and Caputo fractional-order derivatives

A surprising (?) property of the Caputo derivative

A fractional initial-value problem (IVP)

A time-fractional initial-boundary value problem (IBVP)

Outline

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Motivation (integer-order derivatives)

Let $g \in C[0,1]$. Set $(Jg)(x) = \int_0^x g(t)\,dt$ for $0 \le x \le 1$.
Then $(Jg)'(x) = g(x)$ for $0 < x < 1$. Write as $\boxed{DJg = g}$.
Consider

$$(J^2 g)(x) = J(Jg)(x) = \int_{s=0}^{x} \left(\int_{t=0}^{s} g(t)\,dt \right) ds$$

$$= \int_{t=0}^{x} \int_{s=t}^{x} g(t)\,ds\,dt = \int_{t=0}^{x} (x-t) g(t)\,dt.$$

For $n = 1, 2 \ldots,$ get

$$(J^n g)(x) = \frac{1}{(n-1)!} \int_{t=0}^{x} (x-t)^{n-1} g(t) dt = \frac{1}{\Gamma(n)} \int_{t=0}^{x} (x-t)^{n-1} g(t) dt$$

Observe that for any nonnegative integers k and n one has

$$D^{n+k} J^n = D^{n+k-1}(DJ)J^{n-1} = D^{n+k-1} J^{n-1} = \cdots = D^k$$

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Defining a fractional derivative

“fractional” means “not an integer”

Let $\alpha \in \mathbb{R}$ satisfy $m - 1 < \alpha < m$ for some positive integer m.
We want to define the fractional derivative D^α.

Ideas:

- Generalise formula $D^k = D^{n+k} J^n$
- Exploit fact that integral operator J^n is defined for any positive real number n

Define

$$D^\alpha = D^m J^{m-\alpha}.$$

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Riemann-Liouville fractional derivative D^α

Let $\alpha \in \mathbb{R}$ satisfy $m-1 < \alpha < m$ for some positive integer m. The Riemann-Liouville fractional derivative D^α is defined by

$$D^\alpha g(x) = \left(\frac{d}{dx}\right)^m \left[\frac{1}{\Gamma(m-\alpha)} \int_{t=0}^{x} (x-t)^{m-\alpha-1} g(t)\, dt\right]$$

for $0 < x \le 1$ and all functions g such that $D^\alpha g(x)$ exists.

For example, if $g \in C^{m-1}[0,1]$ and $g^{(m-1)}$ is absolutely continuous on $[0,1]$, then $D^\alpha g$ exists.

[Necessary & sufficient conditions for existence of $D^\alpha g \in C[0,1]$: G.Vainikko, *Which functions are fractionally differentiable?*, Z.Anal.Anwend., 2016]

The definition of $D^\alpha g(x)$ is not local (unlike classical derivatives).

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R-L derivative: good and bad

$D^\alpha g$ where $m-1 < \alpha < m$ for some positive integer m.

Good property: let $g \in C^m[0,1]$. Then for each $x \in (0,1]$,

$$\lim_{\alpha \to (m-1)^+} D^\alpha g(x) = \frac{d^{m-1}g}{dx^{m-1}}(x), \quad \lim_{\alpha \to m^-} D^\alpha g(x) = \frac{d^m g}{dx^m}(x).$$

Bad properties:

1. $D^\alpha(1) \neq 0$; in fact $D^\alpha(x^\beta) = 0$ for $\beta = \alpha-1, \alpha-2, \ldots, \alpha-m$ [implications for solving ODES...]
2. Product Rule very complicated except in special cases
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Caputo fractional derivative D_C^α

Suppose $m-1 < \alpha < m$ for some positive integer m.
Define the Caputo fractional derivative D_C^α by

$$D_C^\alpha g(x) = D^\alpha \left[g(x) - T_{m-1}[g;0](x) \right],$$

where $T_{m-1}[g;0](x)$ denotes the Taylor polynomial of degree $m-1$ of the function g expanded around $x=0$.

If $g \in C^{m-1}[0,1]$ and $g^{(m-1)}$ is absolutely continuous on $[0,1]$, then for $0 < x \le 1$ one also has the equivalent formulation

$$D_C^\alpha g(x) := \frac{1}{\Gamma(m-\alpha)} \int_{t=0}^{x} (x-t)^{m-\alpha-1} g^{(m)}(t)\, dt.$$

Could get this from identity $D^\alpha u = J^{m-\alpha} D^m u$, which is valid for integer m, α with $m > \alpha$ if $0 = u(0) = u'(0) = \cdots = u^{(m-1)}(0)$.

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Bad properties:

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$$\lim_{\alpha \to (m-1)^+} D_C^\alpha g(x) \neq \frac{d^{m-1} g}{dx^{m-1}}(x) \quad \text{in general.}$$

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Outline

If g is smooth, then...

Lemma

Suppose $m-1<\alpha<m$ for some positive integer m and $g \in C^m[0,1]$. Then $\lim_{x\to 0^+} D_C^\alpha g(x) = 0$.

Proof.

Because $g \in C^m[0,1]$, there is a constant C such that $|g^{(m)}(t)| \le C$ for $0 \le t \le 1$. Hence for $0 < x \le 1$ one has

$$
\begin{aligned}
|D_C^\alpha g(x)| &= \left| \frac{1}{\Gamma(m-\alpha)} \int_{t=0}^{x} (x-t)^{m-\alpha-1} g^{(m)}(t)\, dt \right| \\
&\le \frac{C}{\Gamma(m-\alpha)} \int_{t=0}^{x} (x-t)^{m-\alpha-1}\, dt \\
&= \frac{C}{(m-\alpha)\Gamma(m-\alpha)} x^{m-\alpha}.
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Thus $\lim_{x\to 0^+} D_C^\alpha g(x) = 0$ since $m > \alpha$. □

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Thus $\lim_{x\to 0^+} D_C^\alpha g(x) = 0$ since $m > \alpha$. □

Heuristic explanation

Recall that when $m-1<\alpha<m$, then

$$D_C^\alpha g(x) = D^\alpha\left[g(x) - T_{m-1}[g;0](x)\right].$$

Since $g \in C^m[0,1]$, one has (roughly)

$$g(x) - T_{m-1}[g;0](x) \sim C_1 x^m \quad \text{near} \quad x=0$$

and consequently

$$D_C^\alpha g(x) \sim D^\alpha(C_1 x^m) = C_2 x^{m-\alpha} \to 0 \quad \text{as } x \to 0^+.$$

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The fractional-derivative IVP

Consider the fractional-derivative initial-value problem

$$D_t^\alpha w(t) = g(t) \text{ for } t \in (0, T], \quad w(0) = w_0,$$

where g is a given smooth function,
and $D_t^\alpha w$ is a Caputo fractional derivative of order $\alpha \in (0, 1)$.

Behaviour of solution to IVP

Take the simplest problem where $g(t) \equiv 1$:

$$D_t^\alpha w(t) = 1 \text{ for } t \in (0, T], \quad w(0) = w_0.$$

Then

$$w(t) = w_0 + \frac{t^\alpha}{\Gamma(\alpha+1)} \text{ for } 0 \le t \le T.$$

Observe that $w \in C[0, T]$ but, since $0 < \alpha < 1$,

$$w'(t) = \frac{\alpha t^{\alpha-1}}{\Gamma(\alpha+1)} \text{ blows up as } t \to 0^+.$$

Of course higher-order derivatives of w also blow up at $t = 0$.
Very different from the classical integer-derivative situation!

Any good numerical method for this class of problems has to handle this weak singularity in typical solutions.

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Huge growth in research activity

MathSciNet data: papers published with anywhere "fractional derivative" and "MSC primary classification 65" (i.e., numerical methods/analysis)

1990–1999: 24 papers
2000–2009: 113 papers
2010–2019: 1284 papers
Why such a large increase?

Two reasons:
(i) More applications found where fractional derivatives offer good approximations
(ii) Not very difficult to write papers in this area if you make strong assumptions! Solutions to fractional-derivative differential equations typically have weak singularities, but $>$ 80% of papers assume that solutions are smooth [i.e., no singularities].

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The mesh

IVP is: with $0 < \alpha < 1$,

$$D_t^\alpha u(t) = g(t) \text{ for } t \in (0, T], \quad u(0) = u_0.$$

Let M be a positive integer. Set

$$t_m := m\tau \quad \text{for } m = 0, 1, \ldots, M \text{ with } \tau := T/M.$$

Computed approximation to the solution at each mesh point t_m is denoted by u^m.

The Caputo fractional derivative

$$\begin{aligned} D_t^\alpha u(t_m) &= \frac{1}{\Gamma(1-\alpha)} \int_{s=0}^{t_m} (t_m - s)^{-\alpha} u'(s)\, ds \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{m-1} \int_{s=t_k}^{t_{k+1}} (t_m - s)^{-\alpha} u'(s)\, ds \end{aligned}$$

The L1 discretisation

$$D_t^{\alpha} u(t_m) = \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{m-1} \int_{s=t_k}^{t_{k+1}} (t_m - s)^{-\alpha} u'(s)\, ds$$

is approximated by the so-called L1 approximation

$$\begin{aligned} D_M^{\alpha} u^m &:= \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{m-1} \frac{u^{k+1} - u^k}{\tau} \int_{s=t_k}^{t_{k+1}} (t_m - s)^{-\alpha}\, ds \\ &= \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \left[d_1 u^m - d_m u^0 + \sum_{k=1}^{m-1} (d_{k+1} - d_k) u^{m-k} \right], \end{aligned}$$

with $d_k := k^{1-\alpha} - (k-1)^{1-\alpha}$ for $k \geq 1$.
Here $d_1 = 1$ and $d_k > d_{k+1} > 0$.

The finite difference method

Solve the linear system

$$D_M^\alpha u^m = g(t_m) \ \text{ for } m = 1, 2, \ldots, M, \quad u^0 = u(0).$$

M-matrix, but not sparse — lower Hessenberg matrix.
Can prove (under realistic regularity hypotheses) that

$$\max_m |u(t_m) - u^m| \leq CM^{-\alpha}$$

for some fixed constant C, and this result is sharp.

Method is convergent — but order of convergence α is low.
Can it be improved?

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Graded mesh

Let M be a positive integer. Set

$$t_m := T(m/M)^r \text{ for } m = 0, 1, \ldots, M$$

with mesh grading $r \geq 1$ chosen by the user.

If $r = 1$, then mesh is uniform.
When $r > 1$, then mesh points are clustered near $t = 0$.

Discretisation of Caputo derivative

The Caputo fractional derivative

$$D_t^{\alpha} u(t_m) = \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{m-1} \int_{s=t_k}^{t_{k+1}} (t_m - s)^{-\alpha} u'(s)\, ds$$

is again approximated by the L1 approximation (but now the mesh is nonuniform in time)

$$\begin{aligned} D_M^{\alpha} u^m &:= \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{m-1} \frac{u^{k+1} - u^k}{t_{k+1} - t_k} \int_{s=t_k}^{t_{k+1}} (t_m - s)^{-\alpha}\, ds \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{m-1} \frac{u^{k+1} - u^k}{t_{k+1} - t_k} \left[(t_m - t_k)^{1-\alpha} - (t_m - t_{k+1})^{1-\alpha} \right] \end{aligned}$$

Convergence on graded mesh

Theorem

The computed solution u^m satisfies

$$\max_m |u(t_m) - u^m| \leq CM^{-\min\{2-\alpha, r\alpha\}}$$

Hence: for $r \geq (2-\alpha)/\alpha$,
the rate of convergence is $O\left(M^{-(2-\alpha)}\right)$.

Numerical experiments show our theorem is sharp.

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A surprising (?) property of the Caputo derivative

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Fractional-derivative PDE (initial-boundary value problem)

$$Lu := D_t^\alpha u - p\frac{\partial^2 u}{\partial x^2} + r(x)u = f(x,t)$$

for $(x,t) \in Q := (0,l) \times (0,T]$, with

$$u(0,t) = u(l,t) = 0 \text{ for } t \in (0,T],$$
$$u(x,0) = \phi(x) \text{ for } x \in [0,l],$$

where $D_t^\alpha u$ is a Caputo fractional derivative of order $\alpha \in (0,1)$,
p is a positive constant,
the functions r, f are continuous on $\bar{Q} := [0,l] \times [0,T]$
with $r(x) \geq 0$ for all x,
and $\phi \in C[0,l]$.

Example (part 1)

Example. Consider the fractional heat equation

$$D_t^\alpha v - \frac{\partial^2 v}{\partial x^2} = 0 \quad \text{on } (0, \pi) \times (0, T]$$

with initial condition $v(x, 0) = \sin x$
and boundary conditions $v(0, t) = v(\pi, t) = 0.$
Its solution is

$$v(x, t) = E_\alpha(-t^\alpha) \sin x \quad \text{for } (x, t) \in [0, \pi] \times [0, 1],$$

where the *Mittag-Leffler function*

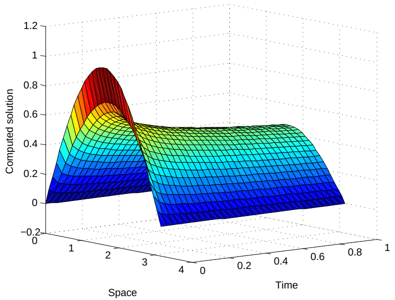
$$E_\alpha(z) := \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)} .$$

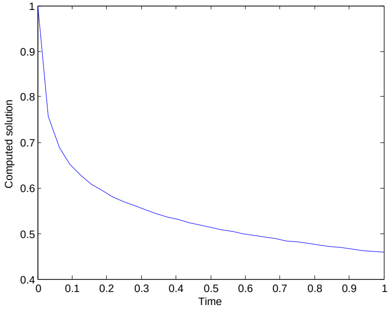
M-L function is fractional analogue of the exponential function:

$$D_t^\alpha E_\alpha(\lambda t^\alpha) = \lambda E_\alpha(\lambda t^\alpha) \ \forall \lambda \in \mathbb{R}.$$

Graph of solution to Example

Plot of surface $v(x,t)$ and its cross-section at $x = \pi/2$ when $\alpha = 0.3$. An initial layer in v at $t = 0$ is evident.
Near $t = 0$ one has $v(x,t) \approx \sin x + w(x)t^{\alpha}$, some function w





Example (part 2)

In this Example, one has [recall that $0 < \alpha < 1$]

$$v_t(x,t) \approx Ct^{\alpha-1} \sin x \text{ as } t \to 0^+,$$
$$v_{tt}(x,t) \approx Ct^{\alpha-2} \sin x \text{ as } t \to 0^+,$$

while

$$\left| \frac{\partial^i v(x,t)}{\partial x^i} \right| \leq C \text{ for } i = 0, 1, 2, 3, 4 \text{ and all } (x,t) \in \bar{Q}.$$

Regularity of the solution u (part 1)

Return to our problem

$$Lu := D_t^\alpha u - p\,\frac{\partial^2 u}{\partial x^2} + r(x)u = f(x,t).$$

Existence/uniqueness/regularity of the solution
can be shown by a separation of variables argument under some extra hypotheses on the data.
Bounds on derivatives of the solutions are similar to those in our earlier example.

K.Sakamoto and M.Yamamoto, *Initial value/boundary value problems for fractional diffusion-wave equations and applications to some inverse problems*, J.Math.Anal.Appl., 2011.

Y.Luchko, *Initial-boundary-value problems for the one-dimensional time-fractional diffusion equation*, Fract.Calc.Appl.Anal., 2012.

You can't assume too much regularity!

Consider the time-fractional heat equation

$$D_t^\alpha v - \frac{\partial^2 v}{\partial x^2} = 0 \quad \text{on } (0,\pi) \times (0,T]$$

with initial condition $v(x,0) = \phi(x) \in C^2[0,1]$
satisfying $\phi(0) = \phi(\pi) = 0$ and $v(0,t) = v(\pi,t) = 0$.
If one assumes that $v_t(x,t)$ is continuous on $[0,\pi] \times [0,T]$, then for fixed x, by our earlier lemma one has $\lim_{t\to 0} D_t^\alpha v(x,t) = 0$.
Now consider $\lim_{t\to 0}$ of the PDE: get $0 - \phi''(x) = 0 \, \forall x \in (0,\pi)$.
But we know that $\phi(0) = \phi(\pi) = 0$; hence $\phi \equiv 0$. Consequently

one must have $v \equiv 0$.

M.Stynes, *Too much regularity may force too much uniqueness*, Fract.Calc.Appl.Anal., 2016

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Discretisation: mesh uniform in space, graded in time

Let M and N be positive integers. Set

$$x_n := nh \quad \text{for } n = 0, 1, \ldots, N \text{ with } h := l/N,$$
$$t_m := T(m/M)^r \text{ for } m = 0, 1, \ldots, M$$

with mesh grading $r \geq 1$ chosen by the user.

Computed approximation to the solution at each mesh point (x_n, t_m) is denoted by u_n^m

Use L1 discretisation $D_M^\alpha u_n^m$ of Caputo derivative $D_t^\alpha u(x_n, t_m)$

and u_{xx} is discretised using a classical approximation:

$$\frac{\partial^2 u}{\partial x^2}(x_n, t_m) \approx \delta_x^2 u_n^m := \frac{u_{n+1}^m - 2u_n^m + u_{n-1}^m}{h^2}.$$

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The difference scheme

Thus we approximate the IBVP by the discrete problem

$$
\begin{aligned}
&D_M^\alpha u_n^m - p\,\delta_x^2 u_n^m + r(x_n) u_n^m = f(x_n, t_m) \\
&\qquad\qquad\qquad \text{for } 1 \le n \le N-1,\ 1 \le m \le M; \\
&u_0^m = 0, \quad u_N^m = 0 \ \text{ for } 0 < m \le M, \\
&u_n^0 = \phi(x_n) \ \text{ for } 0 \le n \le N.
\end{aligned}
$$

This discretisation has been used by several authors *but* their error analyses assume that u_t is continuous at $t = 0$
— so they used meshes that were uniform in time

Convergence on graded meshes

Theorem

Assume the realistic hypothesis that $u \in C^{4,0}(\bar{Q})$ *with*

$$\left| \frac{\partial^\ell u}{\partial t^\ell}(x,t) \right| \le C(1 + t^{\alpha-\ell}) \quad \text{for } \ell = 0,1,2.$$

Then the solution u_m^n *of the scheme satisfies*

$$\max_{(x_m,t_n)\in\bar{Q}} |u(x_m,t_n) - u_m^n| \le C\left(h^2 + M^{-\min\{2-\alpha,\, r\alpha\}}\right).$$

Hence: for $r \ge (2-\alpha)/\alpha$, rate of convergence $O\left(h^2 + M^{-(2-\alpha)}\right)$.

Numerical experiments show our theorem is sharp.

M.Stynes, E.O'Riordan and J.L.Gracia,
Error analysis of a finite difference method on graded meshes for a time-fractional diffusion equation, SIAM J. Numer. Anal., 2017.

(Respectable) other work on this problem

See papers of

(i) Bangti Jin, Raytcho Lazarov, Buyang Li, Zhi Zhou, et al.

(ii) Natalia Kopteva

(iii) Kim-Ngan Le, Bill McLean, Kassem Mustapha, et al.

(iv) Hong-lin Liao, Jiwei Zhang, et al.

and references appearing in these papers

Useful survey:

B.Jin, R.Lazarov & Z.Zhou, *Numerical methods for time-fractional evolution equations with nonsmooth data: a concise overview.* Comput. Methods Appl. Mech. Engrg. 346 (2019), 332–358.

General Reading

- K.Diethelm, *The analysis of fractional differential equations*, Springer-Verlag, Berlin, 2010.
- M.Stynes, *Singularities*, Handbook of fractional calculus with applications Vol. 3, pages 287–305, De Gruyter, Berlin, 2019.

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http://www.csrc.ac.cn/en/event/workshop/2020-01-10/103.html

Thank you for your attention ⌣̈

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