A widespread deficiency in current rigorous analyses of time-fractional initial-boundary value problems

Martin Stynes

Beijing Computational Science Research Center

3rd Fractional Calculus Meeting
IUMA, Universidad de Zaragoza, Spain

25–27 September 2019

北京计算科学研究中心
BEIJING COMPUTATIONAL SCIENCE RESEARCH CENTER

Football

"Football is a game of two halves"

A famous example: Champions League Final 2005

Half-time: A.C.Milan 3 – 0 Liverpool
Full-time: A.C.Milan 3 – 3 Liverpool
— then Liverpool won on penalties

Spanish connections
Liverpool manager: Rafael Benítez
Their 3rd goal: Xabi Alonso

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Talk overview

Riemann-Liouville and Caputo fractional-order derivatives

A fractional initial-value problem (IVP)

Fractional-derivative initial-boundary value problem

Numerical methods with α-nonrobust error bounds

α-robust error bounds

Improved analyses of α-nonrobust error bounds

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

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

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 $0 < x \leq 1$ and all functions g such that $D^\alpha g(x)$ exists. Here $[\ldots]$ is the Riemann-Liouville fractional integral $J^{m-\alpha}$

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

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 $x \in (0,1]$,

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

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
3. Chain Rule impossibly complicated (so changes of independent variable are unhelpful)

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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 $0<x\leq 1$ 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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Caputo derivative: good and bad

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

Good properties:

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

$$\lim_{\alpha \to m^-} D_C^\alpha g(x) = \frac{d^m g}{dx^m}(x).$$

2. $D_C^\alpha(x^\beta) = 0$ for $\beta = 0,1,2,\ldots,m-1$, just like classical derivatives [good for solving ODES...]

Bad properties:

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

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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

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

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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Joint work with

Hu Chen, Beijing CSRC

Research supported in part by the National Natural Science Foundation of China under grant NSAF U1530401

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Fractional-derivative initial-boundary value problem (IBVP)

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

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

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

where $\alpha \in (0,1)$ is fixed, p is a positive constant,
$c \in C[0,l]$ with $c \geq 0$,
$f \in C(\bar{Q})$ where $\bar{Q} := [0,l] \times [0,T]$, and $\phi \in C[0,l]$.

Caputo fractional derivative D_t^α is defined by

$$D_t^\alpha g(x,t) := \frac{1}{\Gamma(1-\alpha)} \int_{s=0}^{t} (t-s)^{-\alpha} \frac{\partial g(x,s)}{\partial s}\, ds \quad \text{for } (x,t) \in Q$$
$$\equiv \left(J^{1-\alpha} \frac{\partial g(x,t)}{\partial t} \right)(t)$$

Behaviour of solution to IBVP

Existence, uniqueness, regularity:

Sakamoto & Yamamoto, J. Math. Anal. Appl. 2011

Stynes, O'Riordan & Gracia, SIAM J. Numer. Anal. 2017

Key feature of solution:

even when the data of the problem are smooth and compatible, typical solutions exhibit a weak singularity at the initial time $t = 0$. That is, for each fixed x, the solution behaves like a multiple of t^α as $t \to 0^+$, and one has:

$$\left|\frac{\partial^k u}{\partial x^k}(x,t)\right| \le C \quad \text{for } k = 0,1,2,3,4,$$

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

for all $(x,t) \in [0,l] \times (0,T]$.

Rigorous convergence analyses of numerical methods

In this talk we consider only those analyses that take into account this weak singularity of typical solutions of the IBVP.

(Many published papers fail to take this into account)

Reformulation of IBVP as $\alpha \to 1^-$

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

Fact: if w is absolutely continuous on $[0,T]$ with $w' \in C(0,T]$, then

$$\lim_{\alpha \to 1^-} [D_t^\alpha w(t)] = w'(t) \quad \text{for each } t \in (0,T].$$

Thus if (formally) we allow $\alpha \to 1^-$ in our IBVP, we get a classical parabolic IBVP

$$\frac{\partial v}{\partial t} - p\,\frac{\partial^2 v}{\partial x^2} + c(x)v = f(x,t)$$

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

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

Behaviour of IBVP solution as $\alpha \to 1^-$

$u(x,t)$ is the solution of our fractional IBVP with $0 < \alpha < 1$.

$v(x,t)$ is the solution of the classical parabolic IBVP with $\alpha = 1$.

Theorem

One has

$$\lim_{\alpha \to 1^-} \left[\max_{(x,t)\in\bar{Q}} |u(x,t) - v(x,t)| \right] = 0.$$

As $\alpha \to 1^-$, nothing bad happens

Topic of this half of the talk:

Despite this theorem, many convergence results for numerical methods (e.g., $\|\text{error}\| \le C(\tau^\alpha + h^2)$) have constants C that blow up as $\alpha \to 1^-$.

Note: This is a flaw only in the theoretical analysis — numerically, all methods tested perform nicely as $\alpha \to 1^-$

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Terminology

Given a numerical method for solving our IBVP with $0 < \alpha < 1$, we say that an error bound for this method that blows up as $\alpha \to 1^-$ is α-nonrobust.

If the error bound does not blow up as $\alpha \to 1^-$, then it is α-robust.

Outline

An error bound for the L1 scheme

Stynes, O'Riordan & Gracia, SIAM J. Numer. Anal. 2017

Finite difference method on a mesh $\{(x_m, t_n)\}$ that is uniform in space (with M mesh intervals) and graded in time (with N mesh intervals), so that mesh points are clustered near $t = 0$.
Standard classical finite difference method is used in space;
the L1 scheme is used for the time discretisation of D_t^α.
Write $\|w^n\|_\infty$ for the maximum of each mesh function $\{w_m^n\}$ at each time level t_n, i.e., $\|w^n\|_\infty := \max_{m=0,1,\ldots,M} |w_m^n|$.

Lemma

The solution of the general discrete problem $L_{M,N} v_m^n = g_m^n$ *satisfies*

$$\|v^n\|_\infty \leq \|v^0\|_\infty + \tau_n^\alpha \Gamma(2-\alpha) \sum_{j=1}^{n} \theta_{n,j} \|g^j\|_\infty$$

for $n = 1, 2, \ldots, N$, *where* $\tau_n = t_n - t_{n-1}$ *and the* $\theta_{n,j}$ *are certain positive stability multipliers.*

Stynes, O'Riordan & Gracia, SINUM 2017

Previous lemma is useful only if one has some bound on the $\theta_{n,j}$.

Lemma

Let the parameter β satisfy $\beta \le r\alpha$, where $r \ge 1$ is the user-chosen mesh grading parameter. Then for $n = 1, 2, \ldots, N$, one has

$$\tau_n^\alpha \sum_{j=1}^{n} j^{-\beta}\theta_{n,j} \le \frac{T^\alpha N^{-\beta}}{1-\alpha} = CN^{-\beta}.$$

Hence the main convergence result of this paper is α-nonrobust.

Kopteva, Math. Comp. 2019

This paper gives a simpler proof of the convergence result from Stynes, O'Riordan & Gracia, SINUM 2017

Proof of Lemma 2.1 relies on the inequality

$$\kappa_{n,1} \geq \frac{t_n^{-\alpha}}{\Gamma(1-\alpha)}$$

L1 scheme on uniform mesh, convergence away from $t = 0$

Gracia, O'Riordan & Stynes, Comput. Methods Appl. Math. 2018

When one uses a uniform temporal mesh, this papers demonstrates that one obtains a higher order of accuracy away from the initial time $t = 0$ than is predicted by the global convergence result of Stynes, O'Riordan & Gracia, SINUM 2017.

(Kopteva, Math Comp 2019, also proves this)

But the bound of Lemma 3 in this CMAM paper contains a factor $\Gamma(1 - \alpha)$ hidden in the constant multiplier, so the result is α-nonrobust.

Jin, Li & Zhou, Math. Comp. 2019

B. Jin, B. Li & Z. Zhou, *Subdiffusion with a time-dependent coefficient: analysis and numerical solution*, Math. Comp. 2019

Section 4, Time Discretization, uses backward Euler convolution quadrature on a uniform temporal grid.

"Remark 4.3: We briefly comment on the dependence of the constant C in error estimates on the fractional order α. At a few occasions, it can blow up as $\alpha \to 1^-$. . . This phenomenon does not fully agree with the results for the continuous model. . . . it is of interest to further refine the estimates to fill in the gap."

Some other papers containing α-nonrobust error estimates

Mustapha & Schötzau, IMAJNA 2014

Le, McLean & Mustapha, SIAM J. Numer. Anal. 2016

Jin, Li & Zhou, SIAM J. Numer. Anal. 2018

Karaa, SIAM J. Numer. Anal. 2018

Karaa, Mustapha & Pani, J. Sci. Comput. 2018

Liao, Li & Zhang, SIAM J. Numer. Anal. 2018

Chen & Stynes, J. Sci. Comput. 2019

etc. etc.

Lemma (Mustapha & Schötzau, IMAJNA 2014)

Let $v \in C[0,T]$. Then for $t \in [0,T]$ one has

$$\int_{t=0}^{t} (vJ^{\alpha}v)(s)\,ds \geq \cos\left(\frac{\alpha\pi}{2}\right) \int_{t=0}^{t} \left(J^{\alpha/2}v(s)\right)^2 ds$$

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Outline

α-robust error bounds for temporal discretisation

[* $\equiv$ Laplace transform argument]

1. Cuesta, Lubich & Palencia: Math. Comp. 2006*
2. McLean & Mustapha: Numer. Alg. 2009, Numer. Alg. 2011, IMAJNA 2012, SIAM J. Numer. Anal. 2013
3. Jin, Lazarov & Zhou: SIAM J. Sci. Comput. 2016*
   Jin, Li & Zhou: SIAM J. Sci. Comput. 2017*, IMAJNA 2018*
4. Huang, Le & Stynes, IMAJNA (to appear, doi:10.1093/imanum/drz006) — analysis based on

Lemma

Let α satisfy $1/2 < \alpha < 1$. Assume that $v \in L^2(0,T)$. Then for $t \in [0,T]$ one has

$$\int_0^t (vJ^\alpha v)(s)\,ds \geq \frac{1}{2} J^{1-\alpha}\left(J^\alpha v(t)\right)^2$$

α-robust error bounds for temporal discretisation

[* $\equiv$ Laplace transform argument]

1. Cuesta, Lubich & Palencia: Math. Comp. 2006*
2. McLean & Mustapha: Numer. Alg. 2009, Numer. Alg. 2011, IMAJNA 2012, SIAM J. Numer. Anal. 2013
3. Jin, Lazarov & Zhou: SIAM J. Sci. Comput. 2016*
   Jin, Li & Zhou: SIAM J. Sci. Comput. 2017*, IMAJNA 2018*
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Outline

Stynes, O'Riordan & Gracia, SIAM J. Numer. Anal. 2017

Lemma

[Old version] Let the parameter β satisfy $\beta \le r\alpha$, where $r \ge 1$ is the user-chosen mesh grading parameter. Then for $n = 1, 2, \dots, N$, one has

$$\tau_n^{\alpha} \sum_{j=1}^{n} j^{-\beta} \theta_{n,j} \le \frac{T^{\alpha} N^{-\beta}}{1-\alpha}.$$

Only values used are $\beta = 0$ and $\beta = \min\{2-\alpha, r\alpha\}$.

[New version] Let $\gamma \in (0,1)$ be a constant. Then for $n = 1, 2, \dots, N$, one has

$$\tau_n^{\alpha} \sum_{j=1}^{n} j^{r(\gamma-\alpha)} \theta_{n,j} \le \frac{\Gamma(1+\gamma-\alpha)}{\Gamma(1+\gamma)\Gamma(2-\alpha)} T^{\alpha} \left(\frac{t_n}{T}\right)^{\gamma} N^{r(\gamma-\alpha)}.$$

Idea: use Chebshev's sorting inequality as in papers of Liao et al.

Stynes, O'Riordan & Gracia, SIAM J. Numer. Anal. 2017

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Other papers whose error bounds we can make α-robust

Gracia, O'Riordan & Stynes, Comput. Methods Appl. Math. 2018

Liao, McLean & Zhang (analysis of Alikhanov scheme), ArXiv preprint 2018

Chen, Holland & Stynes (analysis of Grünwald-Letnikov scheme for IVP), Appl. Numer. Math. 2019

Open Problem: there are several α-nonrobust papers where it's not clear whether one can improve the analysis to make the results α-robust

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The last slide

Hu Chen & Martin Stynes, *Blow-up of error estimates in time-fractional initial-boundary value problems*
—preprint on Researchgate

Thank you for your attention $\ddot{\smile}$ $\bigtriangledown$

My ORCID QR code:

https://www.researchgate.net/profile/Martin_Stynes