Error analysis of a finite difference method on graded meshes for a time-fractional diffusion equation

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Joint work with

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Talk overview

The PDE and the behaviour of its solution

Finite difference method on a uniform mesh

Finite difference method on a graded mesh

Outline

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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 $\phi \in C[0,l]$.

The fractional derivative

D_t^α denotes the *Caputo fractional derivative* defined by

$$D_t^\alpha g(x,t) := \frac{1}{\Gamma(1-\alpha)} \int_{s=0}^{t} (t-s)^{-\alpha} \left(\frac{\partial g}{\partial t}\right)(x,s)\, ds$$

for $(x,t) \in Q$.

The derivative definition is *not* local (unlike classical derivatives).

Fact: if $g \in C^1(\bar{Q})$, then

$$\lim_{\alpha \to 1^-} [D_t^\alpha g(x,t)] = g_t(x,t) \quad \text{for each } (x,t) \in Q.$$

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*

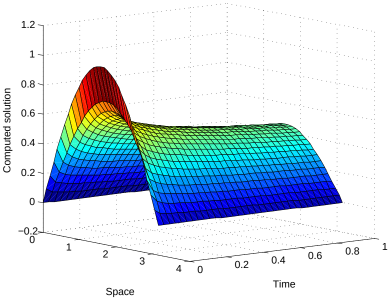
$$E_\alpha(z) := \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)}.$$

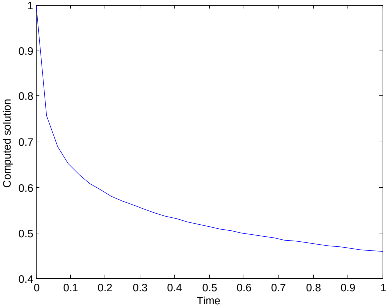
M-L function is fractional analogue of the exponential function:

$$D_t^\alpha E_\alpha(\lambda t^\alpha) = \lambda E_\alpha(t^\alpha).$$

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.





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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

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

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 is examined in K.Sakamoto and M.Yamamoto, J. Math. Anal. Appl., 382 (2011), 426–447.

Y.Luchko, Fract. Calc. Appl. Anal., 15 (2012) 141–160.

— uses separation of variables to prove existence and uniqueness of a classical solution to this problem

— i.e., a function u whose derivatives exist and satisfy the PDE and the initial-boundary conditions pointwise

— under some extra hypotheses on the data

Regularity of the solution u (part 2)

Can extend results of those papers to show that

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

and

$$\left| \frac{\partial^j u(x,t)}{\partial t^j} \right| \le C t^{\alpha - j} \text{ for } j = 1,2 \text{ and all } (x,t) \in Q$$

Here and subsequently, C denotes a generic constant that depends only on the data $\alpha, p, r, f, \phi, l, T$.

These bounds are sharp: they agree with the behaviour of our earlier example

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

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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

one must have $v \equiv 0$.

M.Stynes, *Too much regularity may force too much uniqueness*, Fract. Calc. Appl. Anal. 19 (2016), no. 6, 1554–1562.

Y.Lin and C.Xu, *Finite difference/spectral approximations for the time-fractional diffusion equation*, J. Comput. Phys., 225 (2007), 1533–1552. MathSciNet references: 207

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Consider the time-fractional heat equation

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Uniform mesh, spatial discretisation

Let M and N be positive integers. Set

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

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

u_{xx} is discretised using a standard approximation:

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

Discretisation in time

The Caputo fractional derivative

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

is approximated by the so-called L1 approximation

$$D_M^{\alpha} u_n^m := \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{m-1} \frac{u_n^{k+1} - u_n^k}{\tau} \int_{s=t_k}^{t_{k+1}} (t_m - s)^{-\alpha} \, ds$$

$$= \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \left[d_1 u_n^m - d_m u_n^0 + \sum_{k=1}^{m-1} (d_{k+1} - d_k) u_n^{m-k} \right] ,$$

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

The scheme

Thus we approximate the IBVP by the discrete problem

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

This discretisation is standard; it is considered for example in F.Liu, P.Zhuang & K.Burrage, *Numerical methods and analysis for a class of fractional advection-dispersion models*, Comput. Math. Appl., 64 (2012), 2990–3007.

Properties of discrete system

At each time level,

- Must solve a tridiagonal linear system; matrix is an M-matrix so scheme satisfies a discrete maximum principle.
- Have to use computed solutions at *all* previous time levels

Previous numerical analysis: a criticism

—In our discussion of convergence,
we consider only the discrete L^∞ norm—

There exist papers (e.g., Liu, Zhang & Burrage 2012) that consider problems and discretisations like ours, and prove $O(h^2 + \tau^{2-\alpha})$ convergence of the numerical method, under the hypothesis that the solution u of the original problem is in $C^{4,2}(\bar{Q})$ —which is satisfied only for very special data!

We are interested in proving a convergence result under the realistic hypothesis that $u \in C^{4,0}(\bar{Q})$ with

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

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Numerical evidence

Numerical experiments with our simple but typical first Example

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

show that for our numerical method one obtains $O(h^2+\tau^\alpha)$ convergence, not the $O(h^2+\tau^{2-\alpha})$ that occurs only for unrealistically smooth solutions.

Truncation error; convergence of scheme

Temporal truncation error: one can show (a bit long and messy) that

$$|D_M^\alpha u(x_n, t_m) - D_t^\alpha u(x_n, t_m)| \le Cm^{-\alpha}.$$

Also need to sharpen stability estimate of Liu, Zhang & Burrage 2012.

Theorem

For $m = 1, 2, \ldots, M$ the solution u_n^m of the scheme satisfies

$$\max_{(x_n, t_m)\in\bar{Q}} |u(x_n, t_m) - u_n^m| \le C(h^2 + \tau^\alpha).$$

Numerical experiments show that this bound is sharp.

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Mesh 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.

Set $\tau_m = t_m - t_{m-1}$ for $m = 1, 2, \ldots, M$.

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

u_{xx} is discretised as before

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Discretisation in time

The Caputo fractional derivative

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

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

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

Truncation error and stability on graded meshes

Lemma (temporal truncation error)

There exists a constant C such that for all $(x_m, t_n) \in Q$ one has

$$|D_N^\alpha u(x_m, t_n) - D_t^\alpha u(x_m, t_n)| \le C n^{-\min\{2-\alpha,\, r\alpha\}}.$$

Also need to prove new discrete stability result (delicate).

Lemma (stability of L1 scheme)

For $n = 1, 2, \ldots, N$ one has

$$\|u^n\|_\infty \le \|u^0\|_\infty + \tau_n^\delta \Gamma(2-\delta) \sum_{j=1}^{n} \theta_{n,j} \|f^j\|_\infty$$

$$\text{where} \quad \theta_{n,n} = 1 \text{ and } \theta_{n,j} = \sum_{k=1}^{n-j} \tau_{n-k}^\delta (d_{n,k} - d_{n,k+1}) \theta_{n-k,j}$$

for $n = 1, 2 \ldots, N$ and $j = 1, 2, \ldots, n-1$.

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Convergence on graded meshes

Theorem

The solution u_m^n of the scheme satisfies

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

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

Numerical experiments show our theorem is sharp.

Reference

Martin Stynes, Eugene O'Riordan and José Luis Gracia,
Error analysis of a finite difference method on graded meshes for a time-fractional diffusion equation,
SIAM J. Numer. Anal. 55 (2017), 1057–1079.

Future work

- Alternative discretizations of the fractional derivative?
- Some alternative way of dealing with the weak singularity at $t = 0$?
- Two spatial dimensions?
- etc. etc.

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

7th Conference on Finite Difference Methods: Theory and Applications, 11–16 June 2018 in Lozenetz, Bulgaria

Mini-symposium on

Numerical methods
for fractional-derivative problems and applications

organised by Anatoly Alikhanov, Raytcho Lazarov & Martin Stynes