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

Martin Stynes

Beijing Computational Science Research Center, China

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Joint work with

José Luis Gracia, University of Zaragoza, Spain
Eugene O’Riordan, Dublin City University, Ireland

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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

The PDE and the behaviour of its solution

Finite difference method on a uniform mesh

Finite difference method on a graded mesh
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

\[
\begin{align*}
    u(0, t) &= u(l, t) = 0 \text{ for } t \in (0, T], \\
    u(x, 0) &= \phi(x) \text{ for } x \in [0, l],
\end{align*}
\]

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

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

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

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

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

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

$$D_t^\alpha E_\alpha(\lambda t^\alpha) = \lambda E_\alpha(t^\alpha).$$
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.
In this Example, one has \( \text{[recall that } 0 < \alpha < 1] \)

\[
\begin{align*}
 v_t(x, t) &\approx Ct^{\alpha - 1} \sin x \text{ as } t \to 0^+, \\
v_{tt}(x, t) &\approx Ct^{\alpha - 2} \sin x \text{ as } t \to 0^+,
\end{align*}
\]

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

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

— 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

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

and

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

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

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


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Outline

The PDE and the behaviour of its solution

Finite difference method on a uniform mesh

Finite difference method on a graded mesh
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 $u^m_n$.

$u_{xx}$ is discretised using a standard approximation:

\[ \frac{\partial^2 u}{\partial x^2}(x_n, t_m) \approx \delta_x^2 u^m_n := \frac{u^m_{n+1} - 2u^m_n + u^m_{n-1}}{h^2}. \]
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

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

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

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

\[ L_{N,M}u^m_n := D^\alpha_M u^m_n - p \delta_x^2 u^m_n + r(x_n)u^m_n = f(x_n, t_m) \]

for \(1 \leq n \leq N - 1, 1 \leq m \leq M;\)

\[ u^m_0 = 0, \quad u^m_N = 0 \quad \text{for } 0 < m \leq M, \]

\[ u^n_0 = \phi(x_n) \quad \text{for } 0 \leq n \leq N. \]

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 $L^\infty$ 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

$$\left| \frac{\partial^{\ell} u}{\partial t^\ell} (x, t) \right| \leq C(1 + t^{\alpha-\ell}) \quad \text{for } \ell = 0, 1, 2.$$
Previous numerical analysis: a criticism

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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

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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

\[ |D_M^\alpha u(x_n, t_m) - D_t^\alpha u(x_n, t_m)| \leq Cm^{-\alpha}. \]

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

**Theorem**

*For \( m = 1, 2, \ldots, M \) the solution \( u^m_n \) of the scheme satisfies*

\[ \max_{(x_n, t_m) \in \bar{Q}} |u(x_n, t_m) - u^m_n| \leq C(h^2 + \tau^\alpha). \]

Numerical experiments show that this bound is sharp.
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Let $M$ and $N$ be positive integers. Set

$$
x_n := nh \quad \text{for} \quad n = 0, 1, \ldots, N \quad \text{with} \quad h := l/N,
$$

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

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 $u^m_n$.

$u_{xx}$ is discretised as before.
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)

\[ D_M^\alpha u^m_n := \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{m-1} \frac{u_{n}^{k+1} - u_{n}^{k}}{\tau_{k+1}} \int_{s=t_k}^{t_{k+1}} (t_m - s)^{-\alpha} \, ds \]

\[ = \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{m-1} \frac{u_{n}^{k+1} - u_{n}^{k}}{\tau_{k+1}} \left[(t_m - t_k)^{1-\alpha} - (t_m - t_{k+1})^{1-\alpha}\right] \]
Lemma (temporal truncation error)

There exists a constant $C$ such that for all $(\mathbf{x}_m, t_n) \in Q$ one has

$$|D_N^\alpha u(\mathbf{x}_m, t_n) - D_t^\alpha u(\mathbf{x}_m, t_n)| \leq Cn^{-\min\{2-\alpha, r\alpha\}}.$$ 

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

Lemma (stability of L1 scheme)

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

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

where $\theta_{n,n} = 1$ 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 $j = 1, 2, \ldots, n - 1.$
Convergence on graded meshes

Theorem

The solution \( u_m^n \) of the scheme satisfies

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

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

Numerical experiments show our theorem is sharp.
Reference

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 😊


Mini-symposium on

Numerical methods
for fractional-derivative problems and applications

organised by Anatoly Alikhanov, Raytcho Lazarov & Martin Stynes