Analytical and numerical methods for the time-fractional nonlinear diffusion

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Introduction
This talk is about a 1-D diffusion of moisture in building materials (such as siliceous brick).

- By $u(x, t)$ we denote the moisture concentration at $x$ at time $t$.
- We consider the following initial-boundary conditions:
  \[ u(0, t) = C, \quad u(x, 0) = 0. \]
- **Self-similarity** - a characteristic feature of diffusion in our experiment. Moisture concentration $u(x, t)$ can be drawn on a single curve [1]:
  \[ u(x, t) = U(\eta), \quad \eta = x/\sqrt{t}, \]
  for $U(0) = C$ i.e $U(\infty) = 0$. 

![Graph showing moisture content vs. x*t^(-1/2)]
Nature is tricky (and thus very interesting)!

- As it turns out, the diffusion not always behaves as we are used to.
- In a number of experiments (ex. [2-4]) the so-called Boltzmann scaling $\eta = x/t^{1/2}$ is not observed.
- A more appropriate and accurate is the anomalous diffusion scaling (Figure from [2])

$$u(x, t) = U(\eta), \quad \eta = x/t^{\alpha/2}, \quad 0 < \alpha < 2.$$
How to describe this mathematically?

- The classical diffusion equation does not work: for our initial-boundary conditions it possesses the $x/\sqrt{t}$ scaling.

- In [2,4] the following modification of the constitutive equation has been proposed

$$q = -D(u) \left( \frac{\partial u}{\partial x} \right)^{\frac{1}{\alpha} - 1}.$$ 

Result: very complicated equations (doubly degenerate PME) and average fitting accuracy.

- As it turned out, a more appropriate is to model this phenomenon by an equation with fractional derivative (see [5-7])

$$\frac{\partial^{\alpha} u}{\partial t^{\alpha}} = \frac{\partial}{\partial x} \left( D(u) \frac{\partial u}{\partial x} \right).$$

We obtain the sought scaling $x/t^{\alpha/2}$ with very small fitting errors.
Model

- We consider a 1D time-fractional porous medium equation

\[
\frac{\partial^\alpha u}{\partial t^\alpha} = \frac{\partial}{\partial x} \left( u^m \frac{\partial u}{\partial x} \right), \quad 0 < \alpha < 1, \quad m \geq 1,
\]

with initial-boundary conditions \( u(0, t) = 1, \ u(x, 0) = 0 \).

- We seek for a self-similar solution \( u(x, t) = U(\eta) \), where \( \eta = x/t^{\alpha/2} \). We obtain an ordinary integro-differential equation

\[
(U^m U')' = \left[ (1 - \alpha) - \alpha \frac{d}{d\eta} \right] F_\alpha U, \quad F_\alpha := I^{0,1-\alpha}_{-\frac{2}{\alpha}}, \quad m \geq 1,
\]

with \( U(0) = 1 \) and \( U(\infty) = 0 \), where the integral operator is of the Erdelyi-Kober type

\[
I^{a,b}_c U(\eta) := \frac{1}{\Gamma(b)} \int_0^1 (1 - z)^{b-1} z^a U(\eta z^{\frac{1}{c}}) dz.
\]
Physical derivation

- **Time-fractional porous medium equation is not** an ad-hoc choice.
- **We assume**
  - Water can be trapped in some regions of porous medium for prolonged periods of time \(\rightarrow\) **non-local** conservation law.
  - Constitutive relation \(\rightarrow\) **Darcy’s Law**.
  - Waiting times have a power-type weight \(\rightarrow\) emergence of **Caputo fractional derivative**.
  - **Zero** initial condition \(\rightarrow\) **equivalence** of Riemann-Liouville and Caputo derivatives.

- **The relevant paper with full derivation:**

Existence and uniqueness

First, we will show that the equation

\[(U^m U')' = \left[(1 - \alpha) - \frac{\alpha}{2} \eta \frac{d}{d\eta}\right] F_\alpha U, \quad m \geq 1,\]

with \(U(0) = 1\) and \(U(\infty) = 0\) possesses a unique compactly-supported solution.

This is a free-boundary problem.

The relevant paper:

Ł. Płociniczak, M. Świtała, *Existence and uniqueness results for a time-fractional nonlinear diffusion equation*, under review.
Existence and uniqueness

- We assume the compact support, i.e. there exists some $\eta^*$ such that $U(\eta) = 0$ for $\eta \geq \eta^*$ (physically motivated).
- The key-idea is to use the transformation (borrowed from the works of Okrasiński [9])

$$U(\eta) = \left( m(\eta^*)^2 \right)^\frac{1}{m} y(z), \quad z = 1 - \frac{\eta}{\eta^*},$$

which turns our free-boundary problem into an initial-value one

$$m(y^m y')' = \left[ (1 - \alpha) + \frac{\alpha}{2} (1 - z) \frac{d}{dz} \right] G_\alpha y, \quad 0 < \alpha < 1, \quad 0 \leq z \leq 1,$$

which $y(0) = 0$ ($G_\alpha$ is related to $F_\alpha$). What about the second condition?

- **Theorem**

The solution $y = y(z)$ of the above problem has to satisfy

$$y(z) \sim \left( \frac{\alpha}{2} \right)^{2-\alpha} \frac{\Gamma \left( \frac{2-\alpha}{m} \right)}{\Gamma \left( 1 - \alpha + \frac{2-\alpha}{m} \right)} \frac{z^{\frac{2-\alpha}{m}}}{(2 - \alpha) \left( 1 + \frac{1}{m} \right) - 1} \quad \text{for } z \to 0^+.$$
Existence and uniqueness

- Next, transform the problem into an equivalent integral equation

\[ y(z) = \left( \int_0^z G(z, t)F_\alpha y(t)dt \right)^{\frac{1}{m+1}} =: T(y)(z), \]

for some kernel \( G \).

- Nonlinear operator \( T \) is monotone and homogeneous of degree \( \frac{1}{m+1} \).

- **Theorem ([10], P.J. Bushell, 1976)**

  *Suppose that \( T : K \to K \) is a monotone increasing mapping which is homogeneous of degree \( p \) with \( 0 < p < 1 \). If there exists \( \varphi \in K_0 \) such that*

  \[ \gamma_1 \varphi \leq T(\varphi) \leq \gamma_2 \varphi, \]

  *for some positive constants \( \gamma_{1,2} \) then \( T \) has a unique fixed-point \( y \in K_0 \).*
Existence and uniqueness

**Theorem**

Let \( \varphi(z) := z^{\frac{2-\alpha}{m}} \), then

\[
\gamma_1 \varphi \leq T(\varphi) \leq \gamma_2 \varphi,
\]

with

\[
\gamma_1 = \left\{ \begin{array}{ll}
\left( \frac{\alpha}{2} \right)^{1-\alpha} \frac{\Gamma \left( \frac{2-\alpha}{m} \right)}{\Gamma \left( 2 - \alpha + \frac{2-\alpha}{m} \right)} \frac{1}{2 - \alpha + m(3 - \alpha)} \right)^{\frac{1}{m+1}}, & 0 < \alpha \leq 1 - \frac{1}{m+1}; \\
\left( \frac{\alpha}{2} \right)^{2-\alpha} \frac{\Gamma \left( 1 + \frac{2-\alpha}{m} \right)}{\Gamma \left( 2 - \alpha + \frac{2-\alpha}{m} \right)} \frac{1}{2 - \alpha} \right)^{\frac{1}{m+1}}, & 1 - \frac{1}{m+1} < \alpha \leq 1,
\end{array} \right.
\]

\[
\gamma_2 = \Gamma(3 - \alpha)^{-\frac{1}{m+1}}.
\]

Existence and uniqueness follows from Bushell’s Theorem.
Approximate solutions

- Now, we will find some approximate solutions of our problem.
- The strategy is to substitute the E-K operator (nonlocal) by some local approximation. This can be accurate for $\alpha \to 1^-$.
- The relevant papers:


Approximate solutions

■ Theorem

For analytic $U$ and $a > -1$, $b > 0$, $c > 0$ we have the following representation

$$I_c^{a,b} U(\eta) = \sum_{k=0}^{\infty} \lambda_k U^{(k)}(\eta) \frac{\eta^k}{k!},$$

where $\lambda_k = \sum_{j=0}^{k} \binom{k}{j} (-1)^{k-j} \frac{\Gamma\left(a+\frac{j}{c}+1\right)}{\Gamma\left(a+b+\frac{j}{c}+1\right)}$. Moreover, we have an asymptotic expansion when $k \to \infty$

$$\lambda_k \sim (-1)^k c \frac{\Gamma\left(c(a+1)\right)}{\Gamma(b)} \Gamma\left(c(a+1)\right) \left(\frac{1}{k}\right)^{c(a+1)}.$$

■ The series converges very fast, especially for $\eta$ close to 0. *We can use it* and obtain a series of useful approximations $U_i$. 

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Numerical results

Figure: On the left: front position $\eta^*(t)$ (solid line) and its approximation $\eta_3^*(t) = \eta_3^* t^{\alpha/2}$ (dashed line). On the right: cumulative moisture (solid line) and approximations $I_1$ (dashed line) i $I_2$ (dot-dashed line). Here, $\alpha = 0.95$ and $m = 2$. 
Numerical results

**Figure:** Fitting $U_3$ with experimental data from [2]. On the left: a self-similar profile; on the right: time evolution. Here $\alpha = 0.855$, $C = 0.71 \text{ m}^3/\text{m}^3$, $m = 6.98$, $D_0 = 5.36 \text{ mm/s}^{0.855}$. 
Inverse problems

- In applications it is possible to measure $U$, but how to infer about the material properties of the medium?
- The relevant quantity is the diffusivity $D(U)$.
- Our (inverse) problem is to find $D(U)$ provided we know $U$.
- The relevant paper:

Inverse Problems

- **Definition**
  A mathematical problem (for example a differential or algebraic equation) is called a **well-posed problem** if it has all of the following properties
  - it has a solution,
  - it has only one solution,
  - it is continuous with respect to the perturbations in the initial data (stability).

If a problem is not well-posed it is called **ill-posed**. Inverse problems usually belong to this class.
Diffusivity identification

- Existence and uniqueness (up to a constant $D_s$) - easy integration

\[
D(U(\eta)) = \frac{1}{U'(\eta)} \left[ D_s U'(0) + \left(1 - \frac{\alpha}{2}\right) \int_0^\eta F_\alpha U(z) dz - \frac{\alpha}{2} \eta F_\alpha U(\eta) \right].
\]

- What about stability and computational cost?
- For the latter we have an approximation (based on our previous results)

\[
\tilde{D}(U(\eta)) = \frac{1}{U'(\eta)} \left[ D_s U'(0)
+ \left(\frac{1}{\Gamma(1-\alpha)} + \frac{\alpha}{2\Gamma(2-\alpha)}\right) \int_0^\eta U(z) dz - \frac{\alpha}{2\Gamma(2-\alpha)} \eta U(\eta) \right].
\]

As we can see, this formula does not require double integration (much cheaper in applications).
Main results

Definition
For $\eta_0 > 0$ the \textbf{supremum norm} of a function $U : [0, \infty] \to \mathbb{R}$ is defined by the formula
\[
\|U\|_{\infty, \eta_0} := \sup_{\eta \in [0, \eta_0]} |U(\eta)|.
\]

Definition
A function $U : [0, \infty] \to [0, \infty]$ is called \textbf{admissible} if it is bounded along with its first derivative, nonincreasing and vanishing at infinity.

Theorem
Let $U$ be admissible and fix $\eta_0 > 0$ such that $E_{\eta_0} := \sup_{\eta \in [0, \eta_0]} |\eta/U'(\eta)|$ is finite. We then have
\[
\left\| D(U) - \tilde{D}(U) \right\|_{\infty, \eta_0} \leq E_{\eta_0} \left( 2A(\alpha) \|U\|_{\infty} + B(\alpha) \eta_0 \|U'\|_{\infty} \right),
\]
where $A(\alpha)$ and $B(\alpha)$ are $O(1 - \alpha)$ as $\alpha \to 1$ and explicitly known.
Main results. Regularization

- Differentiation is not a stable operation, thus we have to regularize our formula for $D$.
- Let $U^\delta$ be the moisture with a measurement noise, i.e. \( \| U - U^\delta \|_\infty \leq \delta \).
- Introduce a **regularization strategy** for $U'$ (ex. finite difference)
  \[
  \| U' - (U^\delta)'_h \|_\infty \leq R(h, \delta),
  \]
  for which there exists $h_0 = h_0(\delta)$ such as $R(h_0(\delta), \delta) \to 0$ as $\delta \to 0$.
  Moreover, $(U^\delta)'_h$ is a **stable** operator for each $h > 0$. 

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Main results. Regularization

Theorem
Let $D_h$ be a family of regularization operators for the diffusivity and fix $\eta_0 > 0$. Then for $U \in \mathcal{X}$ such that there exists an $\epsilon > 0$ with
$\epsilon \leq \inf_{\eta \in [0, \eta_0]} |U'(\eta)| < \infty$ we have

$$\|D(U) - D_h(U^\delta)\|_{\infty, \eta_0} \leq \frac{1}{\epsilon} \left[ D_s \left( 1 + \frac{R(h, \delta) + \|U'\|_{\infty}}{\epsilon} \right) R(h, \delta) ight. $$

$$\left. + \frac{\eta_0}{\Gamma(2 - \alpha)} \left( \delta + \frac{\delta + \|U\|_{\infty}}{\epsilon} R(h, \delta) \right) \right].$$

Theorem
Let the assumptions of the above Theorem be fulfilled. If the regularization strategy is such that $R(h_0(\delta), \delta) = O(\delta^\mu)$ for $\delta \to 0$ then

$$\|D(U) - D_h(U^\delta)\|_{\infty, \eta_0} = O(\delta^\mu) \quad \text{as} \quad \delta \to 0.$$
Numerical methods

- This is a work in progress but we have some preliminary results.
- Discretization of the E-K operator

\[ I_c^{a,b} U(\eta) = \sum_{i=0}^{n-1} w_{n,i} U(\eta_i) + R_n(\eta). \]

We have several schemes for choosing \( w_{n,i} \) along with exact asymptotic behaviour of \( R_n \) as \( n \to \infty \).

- Our results can be applied to any integro-differential equations with E-K operator. The relevant work:

Numerical methods

The second problem is a numerical solution of

\[ y(z) = \left( \int_0^z G(z, t) F^\alpha y(t) dt \right)^{\frac{1}{m+1}}, \]

which is not easy since the nonlinearity is not Lipschitzian.

The above equation appears in the above integral formulation of time-fractional porous medium equation.

Results:

- Convergence of a family of finite-difference schemes.
- An explicit construction of a convergent method.

Main assumption: kernel has to be positively bounded from below (now working how to remove this: for anomalous diffusion we have \( G(z, u) \leq C(z - u)^{1-\alpha} \)). The relevant work:

Numerical methods

- The crucial step of the convergence proof is done with aid of the following Gronwall-Bellman's Lemma.

**Lemma**

Let \( \{e_n\}, n = 1, 2, \ldots \) be a sequence of positive numbers satisfying

\[
e_n \leq \frac{1}{n} \left( A \sum_{i=1}^{n-1} e_i + B \right), \quad n \geq 2,
\]

for \( A > 0 \). If we define

\[
M := \max\{e_1, B\} \times \begin{cases} 
\frac{1}{-A\zeta(1-A)}, & 0 < A < 1 \\
1, & A \geq 1,
\end{cases}
\]

then

\[
e_n \leq \frac{M}{n^{1-A}}. \tag{3}
\]
Numerical methods: a sketch of the proof

- The method’s error can be estimated as follows

\[(m + 1)\xi_n^m |e_n| \leq (m + 1)\xi_n^m |y(nh) − y_n|\]

\[= |y(nh)^{m+1} − y_n^{m+1}| \leq hWD \sum_{i=1}^{n-1} |e_i| + \delta(h)\]

- Some work is required to estimate \(\xi_n\) in terms of \(y(nh)\). Then, a comparison theorem for integral equations helps us to obtain a recurrence inequality only for \(e_i\).

- Gronwall-Bellman’s Lemma gives the assertion.

- In the above way we can prove the following estimate

\[|e_n| \leq \text{const.} \times h^{1-\frac{C}{m}} \max\{h^p, \delta(h)h^{-1}\} \quad \text{as} \quad h \to 0^+ \quad \text{with} \quad nh \to x_n,\]

where \(|e_1| = O(h^p)\) as \(h \to 0^+\) with \(p > 0\) and \(C\) is a (known) constant.
Numerical example

- Consider the following equation

\[ y(x)^{m+1} = \int_0^x y(t) \, dt, \quad x \in [0, 1], \]

which can be readily solved with

\[ y(x) = \left( \frac{m}{m + 1} x \right)^{\frac{1}{m}}. \]

- Our theorem gives us the order of convergence equal to at least \( 1 - \frac{1}{m} \) (which is not large, though).

- To calculate the numerical order of convergence we use Aitken’s method based on Richardson’s extrapolation. As a quadrature we use the midpoint’s method.

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References


