Numerical approximations for fractional diffusion equations via splines

Ercília Sousa

CMUC, Department of Mathematics, University of Coimbra, 3001-454 Coimbra, Portugal

A R T I C L E   I N F O

Keywords:
Fractional diffusion
Integro-differential equations
Finite differences

A B S T R A C T

A one-dimensional fractional diffusion model is considered, where the usual second order derivative gives place to a fractional derivative of order $\alpha$, with $1 < \alpha \leq 2$. We consider the Caputo derivative as the space derivative, which is a form of representing the fractional derivative by an integral operator. An implicit numerical method is derived which uses a spline approximation for the Caputo derivative. The consistency and stability of the method are examined and numerical results are presented.

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1. Introduction

The derivation of numerical solutions to differential equations of integer order has been a topic in computational sciences for a long time. Fractional calculus is a natural extension of the integer order calculus and recently, a large number of applied problems have been formulated on fractional differential equations. There is a critical difference in the behavior of integer order derivatives and fractional order derivatives, which is, fractional derivatives are non-local. For that reason, new challenges appear when we try to derive numerical methods for this type of equations. Although in the past ten years many papers have appeared on numerical methods for fractional differential equations, there is still a lack of highly accurate numerical methods.

Fractional diffusion equations account for the typical anomalous features which are observed in many problems. Interesting reports about how fractional equations, which include anomalous diffusion, are a complementary tool in the description of anomalous transport processes are given, for instance, in [1,2].

Numerical approaches to different types of fractional diffusion models have been increasingly appearing in the literature. Recent work on numerical solutions for the fractional diffusion equation describing superdiffusion, the anomalous diffusion discussed here, can be found in [3,4]. Models describing subdiffusion are studied for instance in [5–8]. Several transport processes which include a fractional order diffusion derivative are studied in [9–13]. Other models consider also for advection a fractional derivative of order $0 < \alpha \leq 1$ [14,15]. The numerical methods developed up until now for fractional partial differential equations which involve a derivative of order $\alpha$, $1 < \alpha \leq 2$ are mainly of order one. A numerical method of order two can be found in [4], where a first order approximation of the fractional derivative is derived and a Richardson’s extrapolation is applied to achieve second order accuracy.

In this work we are concerned with a fractional diffusion model with a spatial derivative of fractional order $\alpha$, $1 < \alpha \leq 2$. When this fractional derivative replaces the second order derivative in a diffusion model it leads to superdiffusion. We present a numerical method with full discretization of second order by considering an implicit discretization in time and a second order approximation for the fractional derivative of order $\alpha$, $1 < \alpha \leq 2$.

Consider the one-dimensional fractional diffusion equation

$$\frac{\partial u}{\partial t}(x, t) = d(x) \frac{\partial^\alpha u}{\partial x^\alpha}(x, t) + p(x, t) \tag{1}$$
on the domain $a < x < b$, where $1 < \alpha \leq 2$ and $d(x) > 0$. We consider the initial condition
\[ u(x, 0) = f(x), \quad a < x < b \] (2)
and Dirichlet boundary conditions
\[ u(a, t) = g_a(t) \quad \text{and} \quad u(b, t) = g_b(t). \] (3)

The usual way of representing the fractional derivatives is by the Riemann–Liouville formula. The Riemann–Liouville fractional derivative of order $\alpha$, for $x \in [a, b]$, is defined by
\[ \frac{\partial^\alpha u}{\partial x^\alpha}(x, t) = \frac{1}{\Gamma(n - \alpha)} \frac{\partial^n}{\partial x^n} \int_a^x u(\xi, t)(x - \xi)^{n-\alpha-1}d\xi, \quad (n - 1 < \alpha < n) \] (4)
where $\Gamma(\cdot)$ is the Gamma function and $n = [\alpha] + 1$, with $[\alpha]$ denoting the integer part of $\alpha$.

We can also represent the fractional derivative by the Grünwald–Letnikov formula, that is,
\[ \frac{\partial^\alpha u}{\partial x^\alpha}(x, t) = \lim_{\Delta x \to 0} \frac{1}{\Delta x^\alpha} \sum_{k=0}^{[\alpha]} (-1)^k \binom{\alpha}{k} u(x - k\Delta x, t). \quad (\alpha > 0). \] (5)

Numerical discretizations of the fractional derivative obtained up until now through the Grünwald–Letnikov formula led to first order accurate approximations and this can be seen as a disadvantage. Another representation of the fractional derivative was proposed by Caputo,
\[ \frac{\partial^\alpha u}{\partial x^\alpha}(x, t) = \frac{1}{\Gamma(n - \alpha)} \int_a^x \frac{\partial^n u}{\partial \xi^n}(\xi, t)(x - \xi)^{n-\alpha-1}d\xi, \quad (n - 1 < \alpha < n). \] (6)

The most well-known advantage of the Caputo representation over the Riemann–Liouville representation is related to the fact that very frequently the Laplace transform method is used for solving fractional differential equations. The Laplace transform of the Riemann–Liouville derivative leads to boundary conditions containing the limit values of the Riemann–Liouville fractional derivatives at the lower terminal $x = a$. Mathematically such problems can be solved, but there is no physical interpretation for such type of conditions. On the other hand, the Laplace transform of the Caputo derivative imposes boundary conditions involving integer order derivatives. Properties about the fractional derivatives can be found for instance in [16–18].

The plan of the paper is as follows. In Section 2, we derive the linear spline approximation of the Caputo derivative. The full discretization of the fractional diffusion equation is given in Section 3, where we apply Crank–Nicolson in time. In Section 4, we present results concerning the consistency and stability of the numerical method. In Section 5, numerical results are shown which confirm that the numerical method is second order accurate and in Section 6, some conclusions are given.

2. The spline approximation of the Caputo derivative

In this section we derive a numerical approximation to the fractional derivative for $a < x < b$ [19]. Consider the Caputo derivative,
\[ \frac{\partial^\alpha u}{\partial x^\alpha}(x, t) = \frac{1}{\Gamma(2 - \alpha)} \int_a^x \frac{\partial^2 u}{\partial \xi^2}(\xi, t)(x - \xi)^{1-\alpha}d\xi, \quad 1 < \alpha < 2. \] (7)

Let us define the mesh points $x_j = a + j\Delta x$, $j = 0, 1, \ldots, N$ where $\Delta x$ denotes the uniform space step. For $x_j$, $j = 1, 2, \ldots, N - 1$ we need to calculate the integral on (7). We compute these integrals by approximating the second order derivative by a linear spline $s_j(\xi)$, whose nodes and knots are chosen at $x_k$, $k = 0, 1, 2, \ldots, j$, that is, an approximation to the integral in (7) becomes
\[ I_j = \frac{1}{\Gamma(2 - \alpha)} \int_a^{x_j} s_j(\xi)(x - \xi)^{1-\alpha}d\xi, \quad (8) \]
where the spline $s_j(\xi)$ is of the form
\[ s_j(\xi) = \sum_{k=0}^{j} \frac{\partial^2 u}{\partial \xi^2}(x_k, t)s_{j,k}(\xi), \] (9)
with $s_{j,k}(\xi)$, in each interval $[x_{k-1}, x_{k+1}]$, for $1 \leq k \leq j - 1$, given by
\[ s_{j,k}(\xi) = \begin{cases} \frac{\xi - x_{k-1}}{x_k - x_{k-1}}, & x_{k-1} \leq \xi \leq x_k \\ \frac{x_{k+1} - \xi}{x_{k+1} - x_k}, & x_k \leq \xi \leq x_{k+1} \\ 0, & \text{otherwise.} \end{cases} \]
For \( k = 0 \) and \( k = j \), \( s_{j,k}(\xi) \) is of the form

\[
\begin{align*}
    s_{j,0}(\xi) &= \begin{cases} 
        \frac{x_{j} - \xi}{x_{j} - x_{0}}, & x_{0} \leq \xi \leq x_{1}, \\
        0, & \text{otherwise}
    \end{cases}, \\
    s_{j,j}(\xi) &= \begin{cases} 
        \frac{\xi - x_{j-1}}{x_{j} - x_{j-1}}, & x_{j-1} \leq \xi \leq x_{j}, \\
        0, & \text{otherwise}
    \end{cases}.
\end{align*}
\]

From (8) and (9) and after some calculations we obtain

\[
l_{j} = \frac{1}{\Gamma(2 - \alpha)} \sum_{k=0}^{j} \frac{\partial^{2}u}{\partial \xi^{2}}(x_{k}, t) \int_{a}^{s_{j}} (x_{j} - \xi)^{1-\alpha} s_{j,k}(\xi) d\xi
\]

\[
= \frac{\Delta x^{2-\alpha}}{\Gamma(4 - \alpha)} \sum_{k=0}^{j} \frac{\partial^{2}u}{\partial \xi^{2}}(x_{k}, t) a_{j,k},
\]

where

\[
a_{j,k} = \begin{cases} 
        (j - 1)^{3-\alpha} - j^{2-\alpha}(j - 3 + \alpha), & k = 0 \\
        (j - k + 1)^{3-\alpha} - 2(j - k)^{3-\alpha} + (j - k - 1)^{3-\alpha}, & 1 \leq k \leq j - 1 \\
        1, & k = j.
    \end{cases}
\]

Let us assume there are approximations \( U^n := \{U^n_i\} \) to the values \( u(x_i, t_n) \), where \( t_n = n\Delta t \), \( n \geq 0 \) and \( \Delta t \) is the uniform time step. For the mesh points \( x_i, k = 1, \ldots, N - 1 \) the second order derivative of (11) can be approximated by \( \Delta^2 U^n_i / \Delta x^2 \)

where \( \Delta^2 \) is the central second order differential operator

\[
\Delta^2 U^n = U^n_{i+1} - 2U^n_i + U^n_{i-1}.
\]

Additionally, we also need to know the value of the second order derivative at the boundary point \( x_0 \).

The second order derivative can be approximated by \( \delta_0 U_0 / \Delta x^2 \) where \( \delta_0 \) is the operator

\[
\delta_0 U^n = 2U^n_1 - 5U^n_2 + 4U^n_3 - U^n_4.
\]

A discrete approximation at a boundary point is usually called a numerical boundary condition.

Finally, the approximation of \( l_j \) for \( t = t_n \) can be written as

\[
l_j \simeq \frac{\Delta x^{2-\alpha}}{\Gamma(4 - \alpha)} \left\{ a_{j,0}\delta_0 U^n_0 + \sum_{k=1}^{j} a_{j,k}\delta^2 U^n_k \right\}.
\]

In the next section we describe the full discretization of the differential equation and write the matricial form of our numerical method.

3. The numerical scheme

We discretize the spatial \( \alpha \)-order derivative following the steps of the previous section. The discretization in time consists of the Crank–Nicolson numerical method. We consider the time discretization \( 0 \leq t_n \leq T \). Additionally, let \( d_j = d(x_j) \), \( p^n_j = p(x_j, t_n) \) and \( n^{-1/2} = p(x_j, t_{n+1/2}) \), where \( t_{n+1/2} = t_n + (1/2)\Delta t \). For the uniform space step \( \Delta x \) and time step \( \Delta t \), let \( \mu_j^n = d_j\Delta t / \Delta x^\alpha \). The fractional differential operator is defined as

\[
\delta_\alpha U^n = \frac{1}{\Gamma(4 - \alpha)} \left\{ a_{j,0}\delta_0 U^n_0 + \sum_{k=1}^{j} a_{j,k}\delta^2 U^n_k \right\}.
\]

Note that for \( \alpha = 2 \), the operator (14) is the central second order operator \( \delta^2 U^n_j \), that is, \( \delta_\alpha U^n_j = U^n_{j+1} - 2U^n_j + U^n_{j-1} \).

We have the following implicit numerical method

\[
\left( 1 - \frac{\mu_j^n}{2} \delta_\alpha \right) U^{n+1}_j = \left( 1 + \frac{\mu_j^n}{2} \delta_\alpha \right) U^n_j + \Delta t p^n_{j+1/2}.
\]

The numerical method can be written in the matricial form

\[
\left( I - \frac{\mu_j^n}{2} \delta_\alpha \right) U^{n+1} = \left( I + \frac{\mu_j^n}{2} \delta_\alpha \right) U^n + \frac{\mu_j^n}{2\Gamma(4 - \alpha)} (b^{n+1} + b^n) + p^{n+1/2},
\]

where \( U^n = [U^n_1 \ldots U^n_{N-1}]^T \), \( p^n = [\Delta t p^n_{1/2} \ldots \Delta t p^n_{N-1}]^T \), \( b^n \) contains the boundary values, \( \mu^n \) is a diagonal matrix with entries \( \mu_j^n \) and \( Q \) is related to the fractional operator.
The matrix \( Q \) has the structure \( Q = B + N \), where the matrix \( B \) is related to the operator \( \delta_0 \) and the matrix \( N \) is related to the operator \( \delta_0 \). The matrix \( B = [b_{j,k}] \) is of the form:

\[
b_{j,k} = \begin{cases} 
-2a_{j,1}, & j = 1, k = 1 \\
-2a_{j,1} + a_{j,2}, & 2 \leq j \leq N - 1, k = 1 \\
a_{j,k-1} - 2a_{j,k} + a_{j,k+1}, & k \leq j - 1, k \geq 2 \\
a_{j,j-1} - 2a_{j,j}, & k = j, k \geq 2 \\
a_{j,j}, & k = j + 1, k \geq 2 \\
0, & k > j + 1, k \geq 2. 
\end{cases}
\]

If we assume we have a numerical boundary condition of the form (13) we have, for \( 1 \leq j \leq N - 1 \),

\[
n_{j,k} = \begin{cases} 
-5a_{j,0}, & k = 1 \\
4a_{j,0}, & k = 2 \\
-a_{j,0}, & k = 3 \\
0, & k \geq 4, 
\end{cases} \quad b_j^n = \begin{cases} 
(2a_{j,0} + a_{j,1})U_0^n, & j = 1, \ldots, N - 2 \\
(2a_{j,0} + a_{j,1})U_0^n + a_{j,j}U_N^n, & j = N - 1. 
\end{cases}
\]

Note that \( U_0^n = g_a(t_n) \) and \( U_N^n = g_b(t_n) \).

4. Accuracy and stability

In this section we prove the convergence of the numerical methods by showing that they are consistent and stable. First, we start to study the consistency of the numerical methods and lastly we present the stability result.

Let \( C^4[a, b] \) be the linear space of real valued functions on \([a, b]\) that have continuous fourth order derivatives.

**Theorem 1.** Let \( u^\alpha(x) \) be a function in \( C^4[a, b] \) and \( 1 < \alpha < 2 \). Consider the discrete operator \( \delta_0 \) defined by

\[
\delta_0 u^\alpha(x) = \frac{1}{\Gamma(4-\alpha)} \left( a_{j,0} \delta_0 u^\alpha(x_0) + \sum_{k=1}^{j} a_{j,k} \delta^2 u^\alpha(x_k) \right),
\]

where \( \delta_0 u^\alpha(x_k) = 2u^\alpha(x_k) - 5u^\alpha(x_{k+1}) + 4u^\alpha(x_{k+2}) - u^\alpha(x_{k+3}) \) and \( \delta^2 u^\alpha(x_k) = u^\alpha(x_{k+1}) - 2u^\alpha(x_k) + u^\alpha(x_{k-1}) \). Then

\[
\frac{1}{\Delta x^\alpha} \delta_0 u^\alpha(x_j) = \frac{\partial^\alpha u^\alpha}{\partial x^\alpha}(x_j) + \epsilon_1(x_j) + \epsilon_2(x_j)
\]

with

\[
\max_{a \leq x \leq b} |\epsilon_p(x_j)| \leq \frac{(b - a)^{2-\alpha}}{\Gamma(3 - \alpha)} \Theta(\Delta x^2), \quad p = 1, 2.
\]

**Proof.** Considering the definition of the operator \( \delta_0 \), we have

\[
\frac{1}{\Delta x^\alpha} \delta_0 u^\alpha(x_j) = \frac{\Delta x^{2-\alpha}}{\Gamma(4 - \alpha)} \left( a_{j,0} \delta_0 u^\alpha(x_0) + \sum_{k=1}^{j} a_{j,k} \delta^2 u^\alpha(x_k) \right).
\]

Now, using Taylor expansion arguments it is easy to check that

\[
\frac{1}{\Delta x^2} \delta_0 u^\alpha(x_0) = \frac{d^2 u}{dx^2}(x_0) + \Theta(\Delta x^2); \quad \frac{1}{\Delta x^2} \delta^2 u^\alpha(x_k) = \frac{d^2 u}{dx^2}(x_k) + \Theta(\Delta x^2).
\]

Therefore

\[
\frac{1}{\Delta x^\alpha} \delta_0 u^\alpha(x_j) = \frac{\Delta x^{2-\alpha}}{\Gamma(4 - \alpha)} \sum_{k=0}^{j} a_{j,k} \left( \frac{d^2 u}{dx^2}(x_k) + \Theta(\Delta x^2) \right)
\]

\[
= \frac{\Delta x^{2-\alpha}}{\Gamma(4 - \alpha)} \sum_{k=0}^{j} a_{j,k} \frac{d^2 u}{dx^2}(x_k) + \epsilon_1(x_j)
\]

with

\[
\epsilon_1(x_j) = \frac{\Delta x^{2-\alpha}}{\Gamma(4 - \alpha)} \sum_{k=0}^{j} a_{j,k} \Theta(\Delta x^2) = \frac{(x_j - a)^{2-\alpha}}{\Gamma(3 - \alpha)} \Theta(\Delta x^2).
\]
We can write
\[
\frac{1}{\Delta x^\alpha} \delta_a u^n(x_j) = \frac{1}{\Gamma(2 - \alpha)} \int_a^{x_j} s_j(\xi)(x_j - \xi)^{1-\alpha} d\xi + \epsilon_1(x_j)
\]
and therefore
\[
\frac{1}{\Gamma(2 - \alpha)} \int_a^{x_j} \frac{d^2u^n}{dx^2}(\xi)(x_j - \xi)^{1-\alpha} d\xi + \epsilon_2(x_j) + \epsilon_1(x_j),
\]
for
\[
\epsilon_2(x_j) = \frac{1}{\Gamma(2 - \alpha)} \left| \int_a^{x_j} s_j(\xi)(x_j - \xi)^{1-\alpha} d\xi - \int_a^{x_j} \frac{d^2u^n}{dx^2}(\xi)(x_j - \xi)^{1-\alpha} d\xi \right|
\]
and henceforth
\[
\epsilon_2(x_j) \leq \frac{1}{\Gamma(2 - \alpha)} \max_{a \leq \xi \leq b} \left| \frac{d^2u^n}{dx^2}(\xi) - s_j(\xi) \right| \frac{\int_a^{x_j} (x_j - \xi)^{1-\alpha} d\xi}{\int_a^{x_j} (x_j - \xi)^{1-\alpha} d\xi).
\]
The function \(s_j(\xi)\) is a piecewise linear approximation for \(\frac{d^2u^n}{dx^2}\) and it is known that
\[
\max_{a \leq \xi \leq b} \left| \frac{d^2u^n}{dx^2}(\xi) - s_j(\xi) \right| = O(\Delta x^2)
\]
and therefore
\[
\epsilon_2(x_j) \leq \frac{(x_j - a)^{2-\alpha}}{\Gamma(3 - \alpha)} \cdot O(\Delta x^2). \quad \square
\]
The next result presents the order of the truncation error for the numerical scheme.

**Proposition 2.** The truncation error of the method (15) is of order \(O(\Delta x^2) + O(\Delta t^2)\).

**Proof.** Let \(u = u(x, t)\) be a solution to the fractional partial differential equation and note that the truncation error for the numerical method (15) is given by
\[
\tau_j^n = \frac{u_{j+1}^n - u_j^n}{\Delta t} - \frac{d_j}{2\Delta x^\alpha} (\delta_a u_{j+1}^n + \delta_a u_j^n) - p_j^{n+1/2}.
\]
Using the previous theorem we have
\[
\tau_j^n = \left( \frac{\partial}{\partial t} \right)_j^{n+1/2} + O(\Delta t^2) - d_j \left( \frac{\partial^\alpha u}{\partial x^\alpha} \right)_j^{n+1/2} + O(\Delta x^2) + O(\Delta t^2) - p_j^{n+1/2}
\]
\[
= \left( \frac{\partial}{\partial t} \right)_j^{n+1/2} - d_j \left( \frac{\partial^\alpha u}{\partial x^\alpha} \right)_j^{n+1/2} - p_j^{n+1/2} + O(\Delta t^2) + O(\Delta x^2),
\]
and therefore \(\tau_j^n = O(\Delta t^2) + O(\Delta x^2). \quad \square\)

Let us now, turn to the stability analysis. The numerical method can be written in the form of a matrix iteration, that is,
\[
U^{n+1} = AU^n + v^n, \quad n = 0, 1, 2, \ldots
\]
where \(A\) is an \((N - 1) \times (N - 1)\) matrix given by
\[
A = \left( I - \frac{\mu^\alpha}{2\Gamma(4 - \alpha)} Q \right)^{-1} \left( I + \frac{\mu^\alpha}{2\Gamma(4 - \alpha)} Q \right)
\]
(18)
and \(v^n\) includes boundary conditions and source terms.

Any errors \(E^n\) in a calculation based on (17) will grow according to
\[
E^{n+1} = A E^n, \quad n = 0, 1, 2, \ldots
\]
where \(E^n = u^n - U^n\) with \(u^n, U^n\) the exact and numerical solutions of (17), respectively, at \(t = n\Delta t\).

Denoting the spectral radius of \(A\) by \(\rho(A)\), we recall that, for any \(A \in \mathbb{R}^{(N-1) \times (N-1)}\)
\[
A^m \to 0 \quad \text{as} \quad m \to \infty \quad \text{if and only if} \quad \rho(A) < 1.
\]
A criterion for regulating the error growth governed by (19) is therefore given by \(\rho(A) < 1\).
Let us consider the matrix $Q = B + N$. It can easily be seen computationally that the real parts of the eigenvalues of the matrix $Q$ are negative. We plot in Figs. 1–2 the real parts of the eigenvalues of the matrix $Q$. In Fig. 2 we show in more detail the maximum value the real parts can take for different values of $\alpha$ and for matrices of size $N = 50$ and $N = 500$, respectively.

**Proposition 3.** If the real parts of the eigenvalues of $Q$ are negative then for $A$ defined by (18) we have $\rho(A) < 1$.

**Proof.** Note that $\lambda$ is an eigenvalue of the matrix $\frac{\mu}{\Gamma(\alpha)}Q$ if and only if $(1 + \lambda)/(1 - \lambda)$ is an eigenvalue of $A$. Since the eigenvalues $\lambda$ have negative real parts, it comes that $|(1 + \lambda)/(1 - \lambda)| < 1$. Therefore the spectral radius of the matrix $A$ is less than one. □

5. Numerical results

Consider the problem with initial condition $u(x, 0) = x^4$, $0 < x < 1$ and boundary conditions $u(0, t) = 0$ and $u(1, t) = e^{-t}$. In our tests we consider the numerical boundary condition (13).

Let $d(x) = \frac{1}{\mu} \Gamma(5 - \alpha)x^\alpha$ and $p(x, t) = -2e^{-t}x^4$. The exact solution of the problem is of the form $u(x, t) = e^{-t}x^4$.

Consider the vectors $U_{app} = (U(x_0, t), \ldots, U(x_N, t))$, where $U$ is the approximated solution and $u_{ex} = (u(x_0, t), \ldots, u(x_N, t))$, where $u$ is the exact solution. The error is defined by

$$\|u_{ex}(\Delta x) - U_{app}(\Delta x)\|_\infty,$$

where $\| \cdot \|_\infty$ is the $l_\infty$ norm.

In Tables 1 and 2, we show the implicit scheme is second order convergent and this is in agreement with the order of the truncation error.

6. Conclusions

We have presented an implicit numerical method for the fractional diffusion equation by using the Crank–Nicolson discretization in time. The discretization of the fractional derivative is done by using spline approximations and is second
order accurate. Therefore, the full scheme is second order accurate in time and space and unconditionally stable as expected when a Crank–Nicolson discretization in time is applied.

References