An Efficient Numerical Method for Solving the Fractional Diffusion Equation

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Abstract

Fractional differential equations have recently been applied in various areas of engineering, science, finance, applied mathematics, bio-engineering and others. However, many researchers remain unaware of this field. In this paper, an efficient numerical method for solving the fractional diffusion equation (FDE) is considered. The fractional derivative is described in the Caputo sense. The method is based upon Legendre approximations. The properties of Legendre polynomials are utilized to reduce FDE to a system of ordinary differential equations, which solved by the finite difference method. Numerical solutions of FDE are presented and the results are compared with the exact solution.

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1 Introduction

Ordinary and partial fractional differential equations have been the focus of many studies due to their frequent appearance in various applications in fluid mechanics, viscoelasticity, biology, physics and engineering [1]. Consequently, considerable attention has been given to the solutions of fractional ordinary/partial differential equations of physical interest. Most fractional differential equations do not have exact solutions, so approximation and numerical techniques ([3]-[19]), must be used. Recently, several numerical methods to solve fractional differential equations have been given such as variational iteration method [8], homotopy perturbation method [20], Adomian decomposition method [9], homotopy analysis method [6] and collocation method [16]. We describe some necessary definitions and mathematical preliminaries of the fractional calculus theory required for our subsequent development.

Definition 1.1. The Caputo fractional derivative operator $D^\alpha$ of order $\alpha$ is defined in the following form:

$$D^\alpha f(x) = \frac{1}{\Gamma(m-\alpha)} \int_0^x \frac{f^{(m)}(t)}{(x-t)^{\alpha-m+1}} dt, \quad \alpha > 0,$$

where $m - 1 < \alpha \leq m$, $m \in \mathbb{N}$, $x > 0$.

Similar to integer-order differentiation, Caputo fractional derivative operator is a linear operation:

$$D^\alpha (\lambda f(x) + \mu g(x)) = \lambda D^\alpha f(x) + \mu D^\alpha g(x),$$

where $\lambda$ and $\mu$ are constants. For the Caputo’s derivative we have [15]:

$$D^\alpha C = 0, \quad C \text{ is a constant}, \quad (1)$$

$$D^\alpha x^n = \begin{cases} 0, & \text{for } n \in \mathbb{N}_0 \text{ and } n < \lceil \alpha \rceil; \\ \frac{\Gamma(n+1)}{\Gamma(n+1-\alpha)} x^{n-\alpha}, & \text{for } n \in \mathbb{N}_0 \text{ and } n \geq \lceil \alpha \rceil. \end{cases} \quad (2)$$

We use the ceiling function $\lceil \alpha \rceil$ to denote the smallest integer greater than or equal to $\alpha$. Also $\mathbb{N}_0 = \{0, 1, 2, \ldots\}$. Recall that for $\alpha \in \mathbb{N}$, the Caputo differential operator coincides with the usual differential operator of integer order.

For more details on fractional derivatives definitions and its properties see ([15], [17]).
The main goal in this paper is concerned with the application of Legendre pseudospectral method to obtain the numerical solution of the fractional diffusion equation of the form:

\[
\frac{\partial u(x,t)}{\partial t} = d(x,t) \frac{\partial^\alpha u(x,t)}{\partial x^\alpha} + s(x,t),
\]  

(3)
on a finite domain \(a < x < b, 0 \leq t \leq T\) and the parameter \(\alpha\) refers to the fractional order of spatial derivatives with \(1 \leq \alpha \leq 2\). The function \(s(x,t)\) is the source term.

We also assume an initial condition:

\[u(x,0) = u^0(x), \quad a < x < b,\]  

(4)
and the following Dirichlet boundary conditions:

\[u(a,t) = u(b,t) = 0.\]  

(5)

Note that \(\alpha = 2\), Eq. (3) is the classical diffusion equation:

\[
\frac{\partial u(x,t)}{\partial t} = d(x,t) \frac{\partial^2 u(x,t)}{\partial x^2} + s(x,t).
\]

Our idea is to apply the Legendre collocation method to discretize (3) to get a linear system of ordinary differential equations thus greatly simplifying the problem, and use the finite difference method (FDM) ([12]-[14]) to solve the resulting system.

Legendre polynomials are well known family of orthogonal polynomials on the interval \([-1, 1]\) that have many applications [16]. They are widely used because of their good properties in the approximation of functions. However, with our best knowledge, very little work was done to adapt this polynomials to the solution of fractional differential equations.

The organization of this paper is as follows. In the next section, the approximation of fractional derivative \(D^\alpha y(x)\) is obtained. Section 3 summarizes the application of Legendre collocation method to solve (3). As a result a system of ordinary differential equations is formed and the solution of the considered problem is introduced. In section 4, some numerical results are given to clarify the method. Also a conclusion is given in section 5. Note that we have computed the numerical results using Matlab programming.
2 Evaluation of the fractional derivative using Legendre Polynomials

The well known Legendre polynomials are defined on the interval $[-1, 1]$ and can be determined with the aid of the following recurrence formula [2]:

$$L_{k+1}(z) = \frac{2k + 1}{k + 1} z L_k(z) - \frac{k}{k + 1} L_{k-1}(z), \quad k = 1, 2, \ldots,$$

where $L_0(z) = 1$ and $L_1(z) = z$. In order to use these polynomials on the interval $x \in [0, 1]$ we define the so called shifted Legendre polynomials by introducing the change of variable $z = 2x - 1$. Let the shifted Legendre polynomials $L_k(2x - 1)$ be denoted by $P_k(x)$. Then $P_k(x)$ can be obtained as follows:

$$P_{k+1}(x) = \frac{(2k + 1)(2x - 1)}{(k + 1)} P_k(x) - \frac{k}{k + 1} P_{k-1}(x), \quad k = 1, 2, \ldots, \quad (6)$$

where $P_0(x) = 1$ and $P_1(x) = 2x - 1$. The analytic form of the shifted Legendre polynomials $P_k(x)$ of degree $k$ given by:

$$P_k(x) = \sum_{i=0}^{k} (-1)^{k+i} \frac{(k + i)! x^i}{(k - i)(i!)^2}. \quad (7)$$

Note that $P_k(0) = (-1)^k$ and $P_k(1) = 1$. The orthogonality condition is:

$$\int_0^1 P_i(x) P_j(x) \, dx = \begin{cases} \frac{1}{2i+1}, & \text{for } i = j; \\ 0, & \text{for } i \neq j. \end{cases} \quad (8)$$

The function $y(x)$, square integrable in $[0, 1]$, may be expressed in terms of shifted Legendre polynomials as:

$$y(x) = \sum_{i=0}^{\infty} y_i P_i(x),$$

where the coefficients $y_i$ are given by:

$$y_i = (2i + 1) \int_0^1 y(x) P_i(x) \, dx, \quad i = 1, 2, \ldots.$$ 

In practice, only the first $(m + 1)$-terms shifted Legendre polynomials are considered. Then we have:

$$y_m(x) = \sum_{i=0}^{m} y_i P_i(x). \quad (9)$$
In the following theorem we introduce an approximate formula of the fractional derivative of \(y(x)\).

**Theorem 2.1.** Let \(y(x)\) be approximated by shifted Legendre polynomials as (9) and also suppose \(\alpha > 0\) then:

\[
D^\alpha (y_m(x)) = \sum_{i=\lceil\alpha\rceil}^{m} y_i w_{i,k}^{(\alpha)} x^{k-\alpha},
\]

where \(w_{i,k}^{(\alpha)}\) is given by:

\[
w_{i,k}^{(\alpha)} = \frac{(-1)^{(i+k)}(i+k)!}{(i-k)!k!(1-\alpha)},
\]

**Proof.** Since the Caputo’s fractional differentiation is a linear operation we have:

\[
D^\alpha (y_m(x)) = \sum_{i=0}^{m} y_i D^\alpha (P_i(x)).
\]

Employing Eqs.(1)-(2) in Eq.(7) we have:

\[
D^\alpha P_i(x) = 0, \quad i = 0, 1, \ldots, \lceil\alpha\rceil - 1, \quad \alpha > 0.
\]

Also, for \(i = \lceil\alpha\rceil, \ldots, m\), by using Eqs.(1)-(2) and (7) we get:

\[
D^\alpha P_i(x) = \sum_{k=\lceil\alpha\rceil}^{i} \frac{(-1)^{(i+k)}(i+k)!}{(i-k)!(k)!} D^\alpha (x^k) = \sum_{k=\lceil\alpha\rceil}^{i} \frac{(-1)^{(i+k)}(i+k)!}{(i-k)!k!(1-\alpha)} x^{k-\alpha}.
\]

A combination of Eqs.(12), (13) and (14) leads to the desired result.

**Example 2.2.** Consider the case when \(y(x) = x^2\) and \(m = 2\), the shifted series of \(x^2\) is:

\[
x^2 = \frac{1}{3} P_0(x) + \frac{1}{2} P_1(x) + \frac{1}{6} P_2(x).
\]

Hence,

\[
D^{\frac{1}{2}} x^2 = \sum_{i=1}^{2} \sum_{k=1}^{i} y_i w_i^{(\frac{1}{2})} x^{k-\frac{1}{2}}, \quad \text{where,} \quad w_1^{(\frac{1}{2})} = \frac{2}{\Gamma(\frac{3}{2})}, \quad w_2^{(\frac{1}{2})} = \frac{-6}{\Gamma(\frac{3}{2})}, \quad w_2^{(\frac{1}{2})} = \frac{12}{\Gamma(\frac{5}{2})}.
\]

Therefore:

\[
D^{\frac{1}{2}} x^2 = x^{-\frac{1}{2}}[y_1 w_1^{(\frac{1}{2})} x + y_2 w_2^{(\frac{1}{2})} x + y_2 w_2^{(\frac{1}{2})} x^2] = \frac{2}{\Gamma(\frac{5}{2})} x^{\frac{3}{2}}.
\]
3 Solution of the fractional diffusion equation

Consider the fractional diffusion equation of type given in Eq.(3). In order to use Legendre collocation method, we first approximate \( u(x, t) \) as:

\[
u_m(x, t) = \sum_{i=0}^{m} u_i(t) P_i(x).
\]  \( \text{(15)} \)

From Eqs.(3), (15) and Theorem 2.1 we have:

\[
\sum_{i=0}^{m} \frac{du_i(t)}{dt} P_i(x) = d(x, t) \sum_{i=\lceil \alpha \rceil}^{m} \sum_{k=\lceil \alpha \rceil}^{i} u_i(t) w_{i,k}^{(\alpha)} x^{k-\alpha} + s(x, t), \quad \text{(16)}
\]

we now collocate Eq.(16) at \((m + 1 - \lceil \alpha \rceil)\) points \( x_p \) as:

\[
\sum_{i=0}^{m} \dot{u}_i(t) P_i(x_p) = d(x_p, t) \sum_{i=\lceil \alpha \rceil}^{m} \sum_{k=\lceil \alpha \rceil}^{i} u_i(t) w_{i,k}^{(\alpha)} x_p^{k-\alpha} + s(x_p, t), \quad p = 0, 1, ..., m - \lceil \alpha \rceil. \quad \text{(17)}
\]

For suitable collocation points we use roots of shifted Legendre polynomial \( P_{m+1-\lceil \alpha \rceil}(x) \).

Also, by substituting Eqs.(15) and (10) in the boundary conditions (5) we can obtain \([\alpha]\) equations as follows:

\[
\sum_{i=0}^{m} (-1)^i u_i(t) = 0, \quad \sum_{i=0}^{m} u_i(t) = 0. \quad \text{(18)}
\]

Eq.(17), together with \([\alpha]\) equations of the boundary conditions (18), give \((m + 1)\) of ordinary differential equations which can be solved, for the unknown \( u_i, i = 0, 1, ..., m \), using the finite difference method, as described in the following section.

4 Numerical results

In this section, we implement the proposed method to solve FDE (3) with \( \alpha = 1.8 \), of the form:

\[
\frac{\partial u(x, t)}{\partial t} = d(x, t) \frac{\partial^{1.8} u(x, t)}{\partial x^{1.8}} + s(x, t),
\]
defined on a finite domain $0 < x < 1$ and $t > 0$.
with the coefficient function: $d(x, t) = \Gamma(1.2)x^{1.8}$,
and the source function: $s(x, t) = 3x^2(2x - 1)e^{-t}$,
with initial condition: $u(x, 0) = x^2(1 - x)$,
and Dirichlet conditions: $u(0, t) = u(1, t) = 0$.
Note that the exact solution to this problem is: $u(x, t) = x^2(1 - x)e^{-t}$,
which can be verified by applying the fractional differential formula (2).
We apply the method with $m = 3$, and approximate the solution as follows:
\[
  u_3(x, t) = \sum_{i=0}^{3} u_i(t)P_i(x).
\] (19)

Using Eq.(17) we have:
\[
  \sum_{i=0}^{3} \hat{u}_i(t)P_i(x_p) = d(x_p, t) \sum_{i=2}^{3} \sum_{k=2}^{i} u_i(t) w_{i,k}^{(1,8)} x_p^{k-1.8} + s(x_p, t), \quad p = 0, 1,
\] (20)
where $x_p$ are roots of shifted Legendre polynomial $P_2(x)$, i.e.
\[ x_0 = 0.211324, \quad x_1 = 0.788675. \]

By using Eqs.(18) and (20) we obtain the following system of ordinary differential equations:
\[
  \hat{u}_0(t) + k_1 \hat{u}_1(t) + k_2 \hat{u}_2(t) = R_1 u_2(t) + R_2 u_3(t) + s_0(t), \quad (21)
\]
\[
  \hat{u}_0(t) + k_{11} \hat{u}_1(t) + k_{22} \hat{u}_2(t) = R_{11} u_2(t) + R_{22} u_3(t) + s_1(t), \quad (22)
\]
\[
  u_0(t) - u_1(t) + u_2(t) - u_3(t) = 0, \quad (23)
\]
\[
  u_0(t) + u_1(t) + u_2(t) + u_3(t) = 0, \quad (24)
\]
where:
\[
  k_1 = P_1(x_0), \quad k_2 = P_3(x_0), \quad k_{11} = P_1(x_1), \quad k_{22} = P_3(x_1),
\]
\[
  R_1 = d(x_0, t) w_{2,2}^{(1,8)} x_0^{0.2}, \quad R_2 = d(x_0, t) [w_{3,2}^{(1,8)} x_0^{0.2} + w_{3,3}^{(1,8)} x_0^{1.2}] ,
\]
\[
  R_{11} = d(x_1, t) w_{2,2}^{(1,8)} x_1^{0.2}, \quad R_{22} = d(x_1, t) [w_{3,2}^{(1,8)} x_1^{0.2} + w_{3,3}^{(1,8)} x_1^{1.2}] .
\]

Now, we use FDM to solve the system (21)-(24). We will use the following notations: $t_i = i\Delta t$ to be the integration time $0 \leq t_i \leq T$, $\Delta t = T/N$, for $i = 0, 1, ..., N$. 
Define \( u^n_i = u_i(t_n) \), \( s^n_i = s_i(t_n) \). Then the system (21)-(24), is discretized in time and takes the following form:

\[
\frac{u^n_0 - u^{n-1}_0}{\Delta t} + k_1 \frac{u^n_1 - u^{n-1}_1}{\Delta t} + k_2 \frac{u^n_3 - u^{n-1}_3}{\Delta t} = R^n_1 u^n_2 + R^n_2 u^n_3 + s^n_0, \tag{25}
\]

\[
\frac{u^n_0 - u^{n-1}_0}{\Delta t} + k_{11} \frac{u^n_1 - u^{n-1}_1}{\Delta t} + k_{22} \frac{u^n_3 - u^{n-1}_3}{\Delta t} = R^n_{11} u^n_2 + R^n_{22} u^n_3 + s^n_1, \tag{26}
\]

\[
u^n_0 - u^n_1 + u^n_2 - u^n_3 = 0, \tag{27}
\]

\[
u^n_0 + u^n_1 + u^n_2 + u^n_3 = 0. \tag{28}
\]

We can write the above system (25)-(28) in the following matrix form:

\[
\begin{pmatrix}
1 & k_1 & - \tau R^n_1 & k_2 - \tau R^n_2 \\
1 & k_{11} & - \tau R^n_{11} & k_{22} - \tau R^n_{22} \\
1 & 1 & 1 & -1 \\
1 & 1 & 1 & 1
\end{pmatrix}
\begin{pmatrix}
u^n_0 \\
u^n_1 \\
u^n_2 \\
u^n_3
\end{pmatrix} =
\begin{pmatrix}
1 & k_1 & 0 & k_2 \\
1 & k_{11} & 0 & k_{22} \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
u^{n-1}_0 \\
u^{n-1}_1 \\
u^{n-1}_2 \\
u^{n-1}_3
\end{pmatrix} +
\begin{pmatrix}
s^n_0 \\
s^n_1 \\
0 \\
0
\end{pmatrix}. \tag{29}
\]

We will use the notation for the above system:

\[
AU^n = BU^{n-1} + S^n, \quad \text{or}, \quad U^n = A^{-1} BU^{n-1} + A^{-1} S^n, \tag{30}
\]

where

\[
U^n = (u^n_0, u^n_1, u^n_2, u^n_3)^T \quad \text{and} \quad S^n = (s^n_0, s^n_1, 0, 0)^T.
\]

The obtained numerical results by means of the proposed method are shown in Table 1 and Figures 1 and 2. In the Table 1, the absolute error between the exact solution \( u_{ex} \) and the approximate solution \( u_{approx} \) at \( m = 3 \) and \( m = 5 \) with the final time \( T = 2 \) are given. Also, in the Figures 1 and 2, comparison between the exact and approximate solution with \( m = 5 \) and time step \( \tau = 0.0025 \), at \( T = 1 \), and \( T = 2 \), respectively, are presented.
Table 1: The absolute error between the exact and approximate solution at \( m = 3, m = 5 \) and \( T = 2 \).

| x | \(| u_{\text{ex}} - u_{\text{approx}}| \text{ at } m = 3 \) | \(| u_{\text{ex}} - u_{\text{approx}}| \text{ at } m = 5 \) |
|---|---|---|
| 0.0 | 4.483787e-03 | 2.726496e-04 |
| 0.1 | 4.479660e-03 | 3.455890e-04 |
| 0.2 | 4.201329e-03 | 3.809670e-04 |
| 0.3 | 3.695172e-03 | 3.809103e-04 |
| 0.4 | 3.007566e-03 | 3.514280e-04 |
| 0.5 | 2.184889e-03 | 3.009263e-04 |
| 0.6 | 1.273510e-03 | 2.387121e-04 |
| 0.7 | 0.319831e-03 | 1.735125e-04 |
| 0.8 | 0.629793e-03 | 1.119821e-04 |
| 0.9 | 1.528978e-03 | 0.572150e-04 |
| 1.0 | 2.331347e-03 | 0.072566e-04 |

5 Conclusion

The properties of the Legendre polynomials are used to reduce the fractional diffusion equation to the solution of system of ordinary differential equations which solved by using FDM. The fractional derivative is considered in the Caputo sense. The solution obtained using the suggested method is in very excellent agreement with the already existing ones and show that this approach can be solved the problem effectively. Although we only considered a model problem in this paper, the main idea and the used techniques in this work are also applicable to many other problems. It is evident that the overall errors can be made smaller by adding new terms from the series (15). Comparisons are made between approximate solutions and exact solutions to illustrate the validity and the great potential of the technique.

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Figure 1: Comparison between the exact and approximate solution at $T = 1$ with $\tau = 0.0025$, $m = 5$.

Figure 2: Comparison between the exact and approximate solution at $T = 2$ with $\tau = 0.0025$, $m = 5$. 
References


