NUMERICAL APPROACH TO THE TIME-FRACTIONAL REACTION-DIFFUSION EQUATION

by

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The numerical solution to the time-fractional reaction-diffusion equation with boundary conditions is considered in this paper. By difference, the problem is transformed to solve a linear system whose coefficient matrices are Toeplitz-like, and the solution can be constructed directly. Numerical results are reported to show the feasibility of the proposed method.

Key words: *numerical solution, time-fractional reaction-diffusion equation, the linear equations, Toeplitz-like*

Introduction

In many applied domains such as physics, control and so on, some questions can be reduced to fractional differential equations [1-8]. More and more people have been interested by this topic in the last decades [9-16].

In this paper, we consider the following time-fractional reaction-diffusion equation (TFRDE):

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = b^2 \frac{\partial^2 u(x,t)}{\partial x^2} - c^2 u(x,t), \quad 0 \le x \le L, \quad 0 \le t \le T \tag{1}$$

with boundary conditions:

$$\begin{aligned} u(x,0) &= f(x), \quad 0 \le x \le L \\ u(0,t) &= u(L,t) = 0, \quad 0 \le t \le T \end{aligned} \tag{2}$$

where $[\partial^\alpha u(x, t)]/\partial t^\alpha$ denotes the Caputo fractional derivative [8] defined:

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial u(x_i,\tau)}{\partial \tau} \frac{\mathrm{d}\tau}{(t-\tau)^\alpha}, \quad 0 < \alpha < 1, \quad 0 < b^2, \quad 0 < c^2 \tag{3}$$

and $\Gamma(.)$ denotes gamma function. For simplicity, the time-fractional reaction-diffusion eq. (1) with boundary conditions (2) is marked as TFRDE (1).

In [7, 8], Liu and his collaborators give the differential discrete scheme for TFRDE (1). With their strategy, we intend to seek the numerical solutions to TFRDE (1). We continue along the same line of research of [11], that is, we consider the structure of the special matrix and use it to solve TFRDE (1). Our ideas are based on the following two observations:

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- By the difference to the Caputo fractional derivative (3), TFRDE (1) can be transformed to a set of linear equations with coefficient matrix A, and the major work is changed to express the inverse of matrix A.
- Note that the matrix A has the special structure, it is *Toeplitz-like*, symmetric and strictly diagonally dominant, so its inverse is directly constructed by Cholesky decomposition and the sum of the power of given matrix. Compared with the existing methods to ask for the solutions of TFRDE (1), our methods are easy to operate and the inverse can be constructed explicitly.

Notation. In the rest of paper, $R^{m\times n}$ denotes the space of real $m\times n$ matrix, O_n is zero matrix with order n. For any matrix $X\in R^{m\times n}$, X^T stands for its transpose. For any vector $v\in R^n$, $v(i)$ is its i^{th} component. The norm $\|\ \|_F$ is the Frobenius norm of matrix, while $\|\ \|_p$ is p-norm, and I_n is the identity matrix with order n.

The tridiagonal matrix and its inverse

The tridiagonal matrix with n-order has the following form:

$$T_n=\begin{pmatrix} a_1 & b_1 & & & \\ c_1 & a_2 & b_2 & & \\ & \ddots & \ddots & \ddots & \\ & & c_{n-2} & a_{n-1} & b_{n-1} \\ & & & c_{n-1} & a_n \end{pmatrix} \tag{4}$$

where $a_i, b_i, c_i, i=1,2,3,\cdots,n$ are parameters. If $b_i=c_i, i=1,2,\cdots n$, then T_n is symmetric. If :

$$a_i=a,\quad b_i=b,\quad c_i=c,\quad i=1,2,3,\cdots,n,$$

then T_n is Toeplitz-like. Now we introduce the following *Lemma*.

Lemma 1. Suppose the tridiagonal matrix T_n is symmetric and strictly diagonally dominant, and $a_i>0,\quad i=1,2,\cdots,n,$ then T_n is positive definite.

This *Lemma* can be proved by Disc Theorem [9], one can turn to [10] for details.

With *Lemma 1*, we have Cholesky decomposition [10] for T_n, that is, there exist matrices:

$$L_n=\begin{pmatrix} 1 & & & & \\ l_1 & 1 & & & \\ & \ddots & \ddots & \ddots & \\ & & l_{n-2} & 1 & \\ & & & l_{n-1} & 1 \end{pmatrix} \tag{5}$$

and

$$D_n=diag(d_1,d_2,\cdots,d_n)$$

such that

$$T_n=L_nD_nL_n^T \tag{6}$$

where the matrix L_n is a unit lower triangular matrix. To compute the inverse of T_n, we only need to express that of L_n. For this end, we introduce the following *Lemma*.

Lemma 2. ([10], p 58) If $F \in R^{n\times n}$ and $\|F\|_p < 1$, then $I_n - F$ is non-singular and:

$$(I_n - F)^{-1} = \sum_{k=0}^{\infty} F^k$$

with

$$\left\|(I_n - F)^{-1}\right\|_p \le \frac{1}{1-\|F\|_p}$$

Denote by:

$$F = L_n - I_n$$

it is not difficult to verify:

$$F^n = O_n \quad \text{and} \quad \|F\|_p < 1$$

which implies:

$$L_n^{-1} = (I_n + F)^{-1} = I_n - F + F^2 - F^3 + \cdots + (-F)^{n-1} \tag{7}$$

Hence, the following theorem holds.

Theorem 1. Suppose the tridiagonal matrix T_n is symmetric and strictly diagonally dominant, and $a_i > 0, i = 1,2,3,\cdots,n$, then its inverse can be represented by:

$$T_n^{-1} = (L_n^{-1})^T D_n^{-1} L_n^{-1}$$

where L_n^{-1} satisfies (7).

Remark. For the given tridiagonal matrix T_n (specially Toeplitz-like matrix) which is symmetric and strictly diagonally dominant with $a_i > 0, i = 1,2,\cdots,n$, we present the representation to its inverse by Cholesky decomposition and (7). Compared with the existing methods, our methods are easy to operate and the inverse can be constructed explicitly.

The solution to TFRDE (1)

In this section, we apply *Theorem 1* to solve TFRDE (1). Set:

$$t_n = n\tau, \quad n = 0,1,2,\cdots,N \quad \text{and} \quad x_i = ih, \quad i = 0,1,2,\cdots m$$

where

$$\tau = \frac{T}{N} \quad \text{and} \quad h = \frac{L}{m}$$

then

$$\frac{\partial^\alpha u(x_i, t_{n+1})}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)} \int_0^{(n+1)\tau} \frac{\partial u(x_i,\tau)}{\partial \tau} \frac{\mathrm{d}\tau}{(t-\tau)^\alpha} \approx$$

$$\approx \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{n} \frac{u(x_i, t_{k+1}) - u(x_i, t_k)}{\tau} \int_{k\tau}^{(k+1)\tau} \frac{\mathrm{d}\tau}{(t-\tau)^\alpha} =$$

$$= \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{k=0}^{n} \frac{u(x_i, t_{k+1}) - u(x_i, t_k)}{\tau} [(n+1-k)^{1-\alpha} - (n-k)^{1-\alpha}] =$$

$$= \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{k=0}^{n} \frac{u(x_i, t_{n+1-k}) - u(x_i, t_{n-k})}{\tau} [(k+1)^{1-\alpha} - (k)^{1-\alpha}] .$$

Moreover,

$$\frac{\partial^2 u(x_i, t_{n+1})}{\partial x^2} = \frac{u(x_{i+1}, t_{n+1}) - 2u(x_i, t_{n+1}) + u(x_{i-1}, t_{n+1})}{h^2}$$

Set

$$u_i^n \approx u(x_i, t_n), \quad \mu = \frac{\tau^\alpha}{h^2}, \quad r = \mu b^2 \Gamma(2-\alpha), \quad s = c^2 \tau^\alpha \Gamma(2-\alpha)$$

and

$$c_k = 2k^{1-\alpha} - (k+1)^{1-\alpha} - (k-1)^{1-\alpha}, \quad b_k = (k+1)^{1-\alpha} - k^{1-\alpha}$$

we have

$$\begin{cases} Au^1 = u^0 \\ Au^{n+1} = \sum_{i=1}^{n} c_i u^{n+1-i} + b_n u^0 \\ u^0 = f \end{cases} \tag{8}$$

where

$$\mathrm{A} = \begin{pmatrix} 1+2r+s & -r & & & \\ -r & 1+2r+s & -r & & \\ & \ddots & \ddots & \ddots & \\ & & -r & 1+2r+s & -r \\ & & & -r & 1+2r+s \end{pmatrix} \tag{9}$$

and

$$u^n = \begin{pmatrix} u_1^n \\ u_2^n \\ \vdots \\ \vdots \\ u_{m-1}^n \end{pmatrix}, \quad f = \begin{pmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ \vdots \\ f(x_{m-1}) \end{pmatrix}, \quad n = 1, 2, 3 \cdots N$$

In [7], Yu and Liu have proved the solution of eq. (8) will converge to that of TFRDE (1), so we intend to seek the suitable methods to solve eq. (8). The main difficulty is how to get the inverse of the matrix A**.**

Note that the Toeplitz-like matrix A in eq. (9) is symmetric and strictly diagonally dominant, together with $1+2r+s>0,$ then A is positive definite. So A^{-1} can be constructed by *Theorem 1* directly.

Numerical example

For any matrix $A \in R^{n\times n},$ two errors of its inverse A^{-1} are denoted by:

$$\varepsilon_{\text{left}}(A^{-1}) = \| A^{-1} \cdot A - I_n \|_F$$

and

$$\varepsilon_{\text{right}}(A^{-1}) = \| A \cdot A^{-1} - I_n \|_F$$

respectively.

We report the numerical results for the inverse of tridiagonal matrix and the numerical solutions to TFRDE (1). All examples are performed by MATLAB 7.4 on a personal computer of the Intel Core CPU i5 5300U with 4G memory.

Example 1. In this example, we test *Theorem 1* in chapter *The solution to TFRDE (1)*, the tridiagonal matrix T_n is constructed by:

$$T_n = diag(a) - diag(b,-1) - diag(b,1)$$

where

$$a = (a_1, a_2, \cdots, a_n), \quad b = (b_1, b_2, \cdots, b_n)$$

satisfy

$$a_i = 2b_i + r, \quad i = 1, 2, \cdots, n-1$$

$$a_n = 2b_{n-1} + r$$

As n increases, the errors $\varepsilon_{\text{left}}(A^{-1}),\ \varepsilon_{\text{right}}(A^{-1}),\ \varepsilon_{\text{left}}(L_n^{-1}),$ and $\varepsilon_{\text{right}}(L_n^{-1})$ can all reach the precision 10^{-16}, but change a little. In tab. 1, we list $\varepsilon_{\text{left}}(A^{-1}),\ \varepsilon_{\text{right}}(A^{-1}),$ $\varepsilon_{\text{left}}(L_n^{-1}),$ and $\varepsilon_{\text{right}}(L_n^{-1})$ for different values of n, respectively.

Table 1. The inverse of tridiagonal matrix T_n

n	$\varepsilon_{\text{left}}(L_n^{-1})$	$\varepsilon_{\text{right}}(L_n^{-1})$	$\varepsilon_{\text{left}}(A_n^{-1})$	$\varepsilon_{\text{right}}(A_n^{-1})$
100	$1.34\cdot 10^{-16}$	$1.36\cdot 10^{-16}$	$4.34\cdot 10^{-16}$	$4.35\cdot 10^{-16}$
200	$1.64\cdot 10^{-16}$	$1.61\cdot 10^{-16}$	$5.64\cdot 10^{-16}$	$5.65\cdot 10^{-16}$
300	$1.98\cdot 10^{-16}$	$1.99\cdot 10^{-16}$	$4.98\cdot 10^{-16}$	$4.98\cdot 10^{-16}$
400	$1.01\cdot 10^{-16}$	$1.05\cdot 10^{-16}$	$3.46\cdot 10^{-16}$	$3.47\cdot 10^{-16}$
500	$1.74\cdot 10^{-16}$	$1.75\cdot 10^{-16}$	$5.79\cdot 10^{-16}$	$5.78\cdot 10^{-16}$
700	$1.79\cdot 10^{-16}$	$1.78\cdot 10^{-16}$	$7.79\cdot 10^{-16}$	$7.78\cdot 10^{-16}$

Example 2. In this example, we test our algorithm for TFRDE (1). Let a = 0.4, b = 1, c = 1, τ = 0.0025, L = 2.

Initial condition is set as:

$$u(x,0) = f(x) = \begin{cases} 2x, & 0 \le x \le \dfrac{1}{2} \\ \dfrac{4-2x}{3}, & \dfrac{1}{2} \le x \le 2 \end{cases}$$

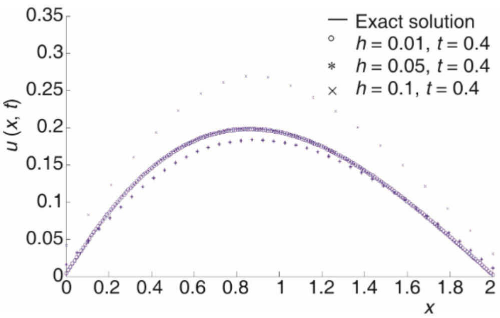

Figure 1. The solution to TFRDE (1)

We solve the inverse of A in (9) by *Theorem 1*, and ask for the solution of TFRDE (1) by (8). In fig. 1, we fix t = 0.4**,** and let h be 0.01, 0.05, and 0.1, respectively. We find the computational value u^n converges to the exact solution step-wisely.

Conclusions

In this paper we present the inverse of the tridiagonal matrix by Cholesky decomposition and the sum of the power of given matrix, and construct the solutions to TFRDE (1) directly. Compared with the existing methods, our methods are easy to operate and the inverse can be constructed explicitly.

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