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A Novel Numerical Approach to Time-Fractional Parabolic Equations with Nonsmooth Solutions

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Abstract. This paper is concerned with numerical solutions of time-fractional parabolic equations. Due to the Caputo time derivative being involved, the solutions of equations are usually singular near the initial time $t = 0$ even for a smooth setting. Based on a simple change of variable $s = t^\beta$, an equivalent s-fractional differential equation is derived and analyzed. Two type finite difference methods based on linear and quadratic approximations in the s-direction are presented, respectively, for solving the s-fractional differential equation. We show that the method based on the linear approximation provides the optimal accuracy $\mathcal{O}(N^{-(2-\alpha)})$ where N is the number of grid points in temporal direction. Numerical examples for both linear and nonlinear fractional equations are presented in comparison with $L1$ methods on uniform meshes and graded meshes, respectively. Our numerical results show clearly the accuracy and efficiency of the proposed methods.

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1. Introduction

Time-fractional differential equations have attracted much attention in the last two decades since many physical models can be described more precisely in this way. Here,

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we consider the time-fractional parabolic equations in the form

$$\mathcal{D}_t^\alpha u + \mathcal{L}u = f, \quad x \in \Omega \times (0,T] \tag{1.1}$$

with the initial and boundary conditions given by

$$\begin{aligned} u(x,0) &= u_0(x), \quad x \in \Omega, \\ u(x,t) &= 0, \qquad\quad x \in \partial\Omega \times [0,T], \end{aligned} \tag{1.2}$$

where $\mathcal{L}$ is a second-order linear and strongly elliptic differential operator on $\bar{\Omega}$. Since we mainly focus on finite difference discretization, we simply assume that $\Omega = [0,b]^d$, where d denotes the dimension. The Caputo fractional derivative $\mathcal{D}_t^\alpha$ is defined by

$$\mathcal{D}_t^\alpha u(x,t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial u(x,z)}{\partial z} \frac{1}{(t-z)^\alpha} dz, \quad 0 < \alpha < 1, \tag{1.3}$$

where $\Gamma(\cdot)$ denotes the usual Gamma function.

Numerous effort has been devoted to developing effective numerical methods and rigorous numerical analysis for the time fractional differential equation (1.1)-(1.2). Clearly, the accuracy of numerical methods heavily relies on the regularity of the solution of the equation. Theoretical analysis based on assumption of the solution being smooth was done by many authors for different applications and different numerical methods. Unlike regular differential equations ($\alpha = 1$), the solution of the time-fractional differential equations may not be smooth even for a smooth setting (for source term, the boundary/initial conditions and compatibility conditions), see [5, 6, 15,16,24,28,30,36,37] for detailed discussion. For certain simple time-independent elliptic operator $\mathcal{L}$, with a standard separation of variable, the solution of (1.1)-(1.2) can be given [35] in terms of the expansion of eigenpairs $(\lambda_k, \psi_k(x))$ of the corresponding steady state problem by

$$u(x,t) = \sum_{k=1}^\infty \big[(u_0,\psi_k) E_{\alpha,1}(-\lambda_k t^\alpha) + J_k(t)\big] \psi_k(x), \tag{1.4}$$

where

$$\begin{aligned} J_k(t) &= \int_0^t z^{\alpha-1} E_{\alpha,\alpha}(-\lambda_k z^\alpha) f_k(t-z) dz, \\ f_k(t) &= \int_\Omega f(x,t)\psi_k(x) dx, \quad E_{\alpha,\beta}(z) := \sum_{k=0}^\infty \frac{z^k}{\Gamma(\alpha k + \beta)} \end{aligned}$$

defines the classical Mittag-Leffler function. More details can be found in [36]. From (1.4) one can see that the solution has a singular layer near $t = 0$, in which the optimal error estimate of the $L1$ scheme on a uniform temporal mesh is [14, 37]

$$\max_{1 \le n \le N} \|e^n\| \le \mathcal{O}(\tau^\alpha). \tag{1.5}$$

To deal with the initial layer, one often uses a nonuniform mesh with more mesh points in the layer. In fact, numerical approximation based on a graded mesh has been applied for solving integro-differential equations for several decades (see [32, 39] for weakly singular Volterra integral equations). A second-order numerical method on a graded mesh was presented by McLean and Mustapha [33] for a fractional wave equation. More recently this technique has been used in [37] for solving time-fractional differential equations (1.1), in which an $L1$ scheme on the graded mesh $t_j = T(\frac{j}{N})^\gamma, j = 0, \ldots, N$, was proposed where $\gamma > 1$ denotes a mesh scaling. Analysis of the $L1$ finite difference method on such graded meshes was done in [37], where they presented the error estimate

$$\max_{1\le n\le N} \|e^n\| \le CN^{-\min\{2-\alpha,\gamma\alpha\}} \tag{1.6}$$

in the time direction, which is optimal when $\gamma \ge \frac{(2-\alpha)}{\alpha}$. Recently, a curvilinear approximation on a graded mesh was introduced in [11] for an equivalent form of the fractional equation (1.1). The optimal error estimate of the graded mesh method with the scaling $\gamma = \frac{1}{\alpha}$ was established.

Since the singularity concerned arises at the initial time, a simple and natural manner is a time re-scaling. In terms of a simple change of variable $t = s^\beta$ in the time direction, we derive a new and equivalent time re-scaled fractional (s-fractional) differential equation. Numerical approximations to the s-fractional differential equation are more efficient. In particular, we present two type finite difference methods based on linear and quadratic approximations, respectively, to the s-fractional differential equation. The method based on the linear approximation ($L1$ scheme) is equivalent to one proposed in [11] by using a curvilinear approximation on a graded mesh, while the optimal error estimate $\mathcal{O}(N^{-(2-\alpha)})$ established in this paper requires weaker regularity assumptions. The proposed method based on a quadratic approximation is more efficient for the s-fractional differential equation. Since the solution of the equation satisfies an extra homogeneous Neumann initial condition, a $(3-\alpha)$-order approximation can be generated without any initial iteration as required previously, see [27]. More important is that the proposed s-fractional differential equation provides more information and regularity at $t = 0$. The method is applicable for nonlinear time fractional differential equations by noting the structure of the solution as presented in [8].

The $L1$ scheme is one of the most popular approximations to time fractional differential operators due to its ease of implementation. The scheme has been extensively investigated by combining with many commonly-used spatial approximations for time fractional parabolic PDEs (see [10, 20, 25, 27, 37] for $L1$ finite difference methods, [14, 22, 40] for $L1$ finite element methods and [13, 27, 34] for others). Under assumptions of the solution being smoothness, error analysis of $L1$ methods was made by several authors [27, 37, 38]. More recently, a framework of numerical analysis for graded mesh methods was presented in [17]. Extension to high-order schemes can also be found in [1,7,19,26,27,31]. Besides, the approach of change of variable is also applied in the numerical solutions of the Volterra integral equations with a weakly singular kernel [3]. However, the convergence results as well as their proof are different.

The outline of the paper is as follows. In the next section, we derive a s-fractional differential equation in terms of the change of variable. The existence, uniqueness and regularity of the solution of the s-fractional differential equation are analyzed. In Section 3, we present two finite difference schemes to the s-fractional differential operator on a uniform mesh, with linear and quadratic approximation, respectively. The optimal error estimate of the $L1$ finite difference method is established under weaker regularity assumptions. In Section 4, we present three numerical examples, one linear equation and two nonlinear equations. Numerical results are given in comparison with those obtained by $L1$ methods with both uniform and graded meshes. Our numerical results clearly show the accuracy and efficiency of methods uniformly for any $0 < \alpha < 1$.

2. A re-scaled time-fractional differential equation

Based on the observation of the expansion (1.4), we introduce the change of variable

$$t = s^{\frac{1}{\beta}} \tag{2.1}$$

with which and $v(x,s) := u(x, s^{\frac{1}{\beta}})$, we have

$$\begin{aligned}\mathcal{D}_t^\alpha u &= \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{u_z(x,z)dz}{(t-z)^\alpha} \\ &= \frac{1}{\Gamma(1-\alpha)} \int_0^s \frac{v_r(x,r)dr}{\left(s^{\frac{1}{\beta}} - r^{\frac{1}{\beta}}\right)^\alpha} =: D_s^\alpha v.\end{aligned} \tag{2.2}$$

An equivalent re-scaled time-fractional (s-fractional) differential equation is defined by

$$D_s^\alpha v + \mathcal{L}v = f, \quad (x,s) \in \Omega \times (0, T^\alpha] \tag{2.3}$$

with the initial and boundary conditions

$$\begin{aligned} &v(x,0) = u_0(x), \quad x \in \Omega, \\ &v(x,s) = 0, \qquad x \in \partial\Omega, \quad 0 \le s \le T^\alpha. \end{aligned} \tag{2.4}$$

For simplicity, we assume in this section that

$$\mathcal{L}u = -u_{xx} + p(x)u,$$

where $p(x) \ge 0$ is smooth.

We define the following $\mathcal{L}^p$ norm based on the expansion of the eigenpairs (λ_i, ψ_i) in (1.4),

$$\|g\|_{\mathcal{L}^p} = \left(\sum_{i=1}^\infty \lambda_i^{2p} |(g, \psi_i)|^2 \right)^{\frac{1}{2}}. \tag{2.5}$$

By [35, Theorem 16], there exists a constant C such that

$$|E_{\alpha_1,\alpha_2}(-r)| \le \frac{C}{1+r}, \quad \text{for} \quad 0 < \alpha_1 < 2, \quad \alpha_2 \in \mathbb{R}, \quad \text{and all} \quad r \ge 0. \tag{2.6}$$

The existence, uniqueness and regularity of the solution of the time-fractional equation (1.1)-(1.2) were investigated by several authors [27,30,35,37].

Lemma 2.1 ([37]). *Assume that*

$$\|u_0\|_{\mathcal{L}^{\frac{5}{2}}} + \|f(\cdot,t)\|_{\mathcal{L}^{\frac{5}{2}}} + \|f_t(\cdot,t)\|_{\mathcal{L}^{\frac{1}{2}}} + t^{\eta}\|f_{tt}(\cdot,t)\|_{\mathcal{L}^{\frac{1}{2}}} \le C_1 \tag{2.7}$$

for all $t \in (0,T]$ *and some* $0<\eta<1$, *where* C_1 *is a constant independent of* t. *Then, the time fractional differential equation* (1.1)-(1.2) *has a unique solution satisfying*

$$\left|\frac{\partial^k u}{\partial x^k}(x,t)\right| \le C_2, \qquad \textit{for} \quad k=0,1,2,3,4, \tag{2.8}$$

$$\left|\frac{\partial^l u}{\partial t^l}(x,t)\right| \le C_2(1+t^{\alpha-l}), \quad \textit{for} \quad l=1,2 \tag{2.9}$$

for all $x\in[0,1]$ *and* $t\in(0,T]$, *where* C_2 *is a constant independent of* x *and* t.

In the following lemma, we present the corresponding results for the s-fractional differential equation (2.3)-(2.4) for $\beta=\alpha$.

Lemma 2.2. *Under the assumption* (2.7) *in Lemma* 2.1, *the* s*-fractional differential equation* (2.3)-(2.4) *has a unique solution satisfying*

$$\left|\frac{\partial^k v}{\partial x^k}(x,s)\right| \le C_3, \qquad \textit{for} \quad k=0,1,2,3,4, \tag{2.10}$$

$$\left|\frac{\partial^l v}{\partial s^l}(x,s)\right| \le C_3\left(1+s^{\frac{1}{\alpha}+1-l}\right) < \infty, \quad \textit{for} \quad l=1,2 \tag{2.11}$$

for all $s\in(0,T^{\alpha}]$, *where* C_3 *is a constant independent of* x *and* s.

Proof. By (1.4),

$$\begin{aligned} v(x,s) = u\big(x,s^{\frac{1}{\alpha}}\big) &= \sum_{i=1}^{\infty}(u_0,\psi_i)E_{\alpha,1}(-\lambda_i s)\psi_i(x) \\ &\quad + \frac{1}{\alpha}\sum_{i=1}^{\infty}\left[\int_0^s E_{\alpha,\alpha}(-\lambda_i z) f_i\big(s^{\frac{1}{\alpha}}-z^{\frac{1}{\alpha}}\big)dz\right]\psi_i(x) \\ &=: v_1(x,s)+v_2(x,s). \end{aligned} \tag{2.12}$$

By (2.6) and (2.7), we can see that v satisfies (2.10) and v_1 satisfies (2.11). It remains to prove that v_2 satisfies (2.11). From (2.12),

$$\begin{aligned} \frac{\partial v_2}{\partial s} &= \sum_{i=1}^{\infty}\left[\frac{1}{\alpha}E_{\alpha,\alpha}(-\lambda_i s)f_i(0) + \frac{1}{\alpha^2}\int_0^s E_{\alpha,\alpha}(-\lambda_i z) f_i'\big(s^{\frac{1}{\alpha}}-z^{\frac{1}{\alpha}}\big)s^{\frac{1}{\alpha}-1}dz\right]\psi_i(x) \\ &\le C + Cs^{\frac{1}{\alpha}-1}\int_0^s \sum_{i=1}^{\infty}\left|f_i'\big(s^{\frac{1}{\alpha}}-z^{\frac{1}{\alpha}}\big)\right|dz \end{aligned}$$

$$
\begin{aligned}
&\le C + Cs^{\frac{1}{\alpha}-1}\int_0^s \sqrt{\sum_{i=1}^{\infty}\frac{1}{\lambda_i}}\sqrt{\sum_{i=1}^{\infty}\lambda_i\left(f_i'\big(s^{\frac{1}{\alpha}}-z^{\frac{1}{\alpha}}\big)\right)^2}dz\\
&\le C + Cs^{\frac{1}{\alpha}-1}\int_0^s \left\|f_t\big(\cdot, s^{\frac{1}{\alpha}}-z^{\frac{1}{\alpha}}\big)\right\|_{\mathcal{L}^{\frac{1}{2}}} dz\\
&\le C\big(1+s^{\frac{1}{\alpha}}\big),
\end{aligned}
$$

where we have noted $\lambda_i \ge Ci^2$ [4] and used (2.7). Moreover, we have

$$
\begin{aligned}
\frac{\partial^2 v_2}{\partial s^2} =& \sum_{i=1}^{\infty}\Bigg[\int_0^s E_{\alpha,\alpha}(-\lambda_i z)\left[f_i''\big(s^{\frac{1}{\alpha}}-z^{\frac{1}{\alpha}}\big)\frac{1}{\alpha^3}s^{\frac{2}{\alpha}-2}+f_i'\big(s^{\frac{1}{\alpha}}-z^{\frac{1}{\alpha}}\big)\frac{1-\alpha}{\alpha^2}s^{\frac{1}{\alpha}-2}\right]dz\\
&\qquad + \frac{1}{\alpha^2}E_{\alpha,\alpha}(-\lambda_i s)f_i'(0)s^{\frac{1}{\alpha}-1}\Bigg]\psi_i(x)\\
&\le Cs^{\frac{1}{\alpha}-2}\sum_{i=1}^{\infty}\int_0^s\left(\left|f_i''\big(s^{\frac{1}{\alpha}}-z^{\frac{1}{\alpha}}\big)s^{\frac{1}{\alpha}}\right|+\left|f_i'\big(s^{\frac{1}{\alpha}}-z^{\frac{1}{\alpha}}\big)\right|\right)dz + C\\
&\le Cs^{\frac{1}{\alpha}-2}\int_0^s\left(s^{\frac{1}{\alpha}}\left\|f_{tt}\big(\cdot, s^{\frac{1}{\alpha}}-z^{\frac{1}{\alpha}}\big)\right\|_{\mathcal{L}^{\frac{1}{2}}}+\left\|f_t\big(\cdot, s^{\frac{1}{\alpha}}-z^{\frac{1}{\alpha}}\big)\right\|_{\mathcal{L}^{\frac{1}{2}}}\right)dz + C\\
&\le Cs^{\frac{1}{\alpha}-2}\int_0^s\left(\big(s^{\frac{1}{\alpha}}-z^{\frac{1}{\alpha}}\big)^{-1}s^{\frac{1}{\alpha}}+1\right)dz + C\\
&\le Cs^{\frac{1}{\alpha}-2}\left(\frac{1}{\alpha}B\Big(1,\frac{1}{\alpha},1-\eta\Big)s^{\frac{(1-\eta)}{\alpha}+1}+s\right)+C\\
&\le C\left(1+s^{\frac{1}{\alpha}-1}\right),
\end{aligned}
$$

where $0<\eta<1$ is defined in (2.7). The proof is complete. □

Lemma 2.1 was proved in [37] for $\mathcal{L}u = pu_{xx} + c(x)u$ with a positive constant p. The results in above two lemmas may be extended to some time-independent second-order elliptic partial differential operator in a rectangle or cube. For general multi-dimensional cases, we may have the following regularity

$$
\begin{aligned}
&\left\|\frac{\partial^k v}{\partial x^k}(x,s)\right\|_{L^2(\Omega)} \le C_3, && \text{for} \quad k=0,1,2,3,4,\\
&\left\|\frac{\partial^l v}{\partial s^l}(x,s)\right\|_{L^2(\Omega)} \le C_3\left(1+s^{\frac{1}{\alpha}+1-l}\right)<\infty, && \text{for} \quad l=1,2
\end{aligned}
$$

in L^2-norm since the orthonormal basis may not be bounded uniformly in spatial direction under $L^\infty(\Omega)$-norm.

3. Finite difference methods

Let $s_n = \frac{T^\alpha n}{N}, n = 0, \ldots, N$, denote a uniform mesh on $[0, T^\alpha]$ with $\tau_s = s_k - s_{k-1}$. For the one-dimensional s-fractional parabolic equation (2.3)-(2.4) with

$$\mathcal{L}v = -v_{xx}, \quad x \in (0,1) \tag{3.1}$$

we use a standard second-order finite difference approximation

$$v_{xx}(x_j) \approx \delta_x^2 v_j^n := \frac{1}{h^2}\left(v_{j+1}^n - 2v_j^n + v_{j-1}^n\right) \tag{3.2}$$

on a uniform mesh $x_j = \frac{j}{M}$, $j = 0, \ldots, M$, with $h = x_j - x_{j-1}$. We consider two $L1$ schemes below.

3.1. $L1$-scheme

Based on a piecewise linear interpolation on s direction, we define an $L1$ scheme to the s-fractional differential operator in (2.2) with $\beta = \alpha$ by

$$\begin{aligned} D_{s_n}^\alpha v &= \frac{1}{\Gamma(1-\alpha)} \sum_{k=1}^{n} \frac{1}{\tau_s}\big(v(x, s_k) - v(x, s_{k-1})\big) \int_{s_{k-1}}^{s_k} \frac{dz}{\left(s_n^{\frac{1}{\alpha}} - z^{\frac{1}{\alpha}}\right)^\alpha} + Q^n \\ &= \sum_{k=1}^{n} a_{n,k-1}\big(v(x, s_k) - v(x, s_{k-1})\big) + Q^n, \end{aligned} \tag{3.3}$$

where

$$\begin{aligned} a_{n,k-1} &= \frac{1}{\tau_s \Gamma(1-\alpha)} \int_{s_{k-1}}^{s_k} \frac{dz}{\left(s_n^{\frac{1}{\alpha}} - z^{\frac{1}{\alpha}}\right)^\alpha} \\ &= \frac{\alpha}{\tau_s \Gamma(1-\alpha)} \int_{\widetilde{t}_{k-1}}^{\widetilde{t}_k} \frac{dt}{(\widetilde{t}_n - t)^\alpha t^{1-\alpha}}, \quad \widetilde{t}_k = s_k^{\frac{1}{\alpha}} \end{aligned} \tag{3.4}$$

and Q^n denotes the corresponding truncation error. With a change of variable, $a_{n,k-1}$ can be expressed by

$$\begin{aligned} a_{n,k-1} &= \frac{\alpha}{\tau_s \Gamma(1-\alpha)} \int_{\frac{\widetilde{t}_{k-1}}{\widetilde{t}_n}}^{\frac{\widetilde{t}_k}{\widetilde{t}_n}} \frac{dz}{(1-z)^\alpha z^{1-\alpha}} \\ &= \frac{\alpha}{\tau_s \Gamma(1-\alpha)} \left(B\left(\frac{\widetilde{t}_k}{\widetilde{t}_n}, \alpha, 1-\alpha\right) - B\left(\frac{\widetilde{t}_{k-1}}{\widetilde{t}_n}, \alpha, 1-\alpha\right) \right), \end{aligned} \tag{3.5}$$

where $B(z, \alpha, 1-\alpha)$ is the incomplete beta function, i.e.,

$$B(z, a, b) = \int_0^z x^{a-1}(1-x)^{b-1} dx. \tag{3.6}$$

Efficient numerical algorithms for the evaluation of beta functions can be found in literatures (see [12] and references therein).

It is noted that the above $L1$ scheme is equivalent to a curvilinear interpolation approximation

$$u \approx \frac{t^\alpha - t_{k-1}^\alpha}{t_k^\alpha - t_{k-1}^\alpha} u(x, t_k) + \frac{t_k^\alpha - t^\alpha}{t_k^\alpha - t_{k-1}^\alpha} u(x, t_{k-1})$$

for the time-fractional equation on the graded mesh $t_k = T(\frac{k}{N})^{\frac{1}{\alpha}}$, which was derived in [11] from a different form of the time-fractional differential equation with the curvilinear interpolation, while the analysis presented in [11] requires stronger regularity conditions.

Based on the finite difference approximation in (3.2), an $L1$ finite difference method is given by

$$\begin{aligned} &a_{n,n-1} v_j^n - \sum_{k=1}^{n-1} (a_{n,k} - a_{n,k-1}) v_j^k - a_{n,0} v_j^0 = \delta_x^2 v_j^n + F(x_j, s_n), \\ &v_0^n = 0, \quad v_M^n = 0, \quad v_j^0 = u_0(x_j), \quad j = 1, \ldots, M-1, \quad n = 1, \ldots, N. \end{aligned} \tag{3.7}$$

3.2. High-order scheme

In this subsection, we present a high-order approximation to the s-fractional differential equation in terms of the change of variable (2.1) with $\beta = \frac{\alpha}{2}$ with which the s-fractional differential equation is defined by

$$\widetilde{D}_{s_n}^\alpha \widetilde{v} := \frac{1}{\Gamma(1-\alpha)} \int_0^{s_n} \frac{\widetilde{v}_z(x, z) dz}{\big(s_n^{\frac{2}{\alpha}} - z^{\frac{2}{\alpha}}\big)^\alpha}, \tag{3.8}$$

where $\widetilde{v}(x, s) := u(x, s^{\frac{2}{\alpha}})$.

Similar to the regularity analysis in Lemma 2.2, we can see that

$$\left| \frac{\partial^l \widetilde{v}}{\partial s^l}(x, s) \right| \le \widetilde{C}_3 \big(1 + s^{\frac{2}{\alpha} - l}\big) \quad \text{for} \quad l = 1, 2, 3. \tag{3.9}$$

Remark 3.1. From (2.1) we can see that in this case,

$$\widetilde{v}_s(x, s) = \frac{2 s^{\frac{2}{\alpha} - 1}}{\alpha} u_t\big(x, s^{\frac{2}{\alpha}}\big), \tag{3.10}$$

which together with (3.9) further leads to

$$\widetilde{v}_s(x, 0) = 0. \tag{3.11}$$

The above extra initial condition will be used in the first step of our high-order approximation.

We introduce a quadratic approximation to $\widetilde{v}$ interpolating at the three points $\{s_{k-1}, s_k, s_{k+1}\}$ by

$$\begin{aligned} H^k(s) = &\widetilde{v}^k - \frac{1}{\tau_s}\big(\widetilde{v}^k - \widetilde{v}^{k-1}\big)(s_k - s) - \frac{1}{\tau_s^2}\big(\widetilde{v}^{k+1} - 2\widetilde{v}^k + \widetilde{v}^{k-1}\big) \\ &\times \frac{1}{2}(s_k - s)(s - s_{k-1}), \end{aligned} \tag{3.12}$$

where $\widetilde{v}^k := \widetilde{v}(x, s_k)$. For the first interval $(0, s_1)$, we present a Hermite type approximation to $\widetilde{v}$

$$G(s) = \Big[\widetilde{v}^1 - \widetilde{v}^0 - s_1\widetilde{v}_s^0\Big]\left(\frac{s}{s_1}\right)^2 + \widetilde{v}_s^0 + \widetilde{v}^0 = \big(\widetilde{v}^1 - \widetilde{v}^0\big)\left(\frac{s}{s_1}\right)^2 + \widetilde{v}^0, \tag{3.13}$$

where we have used (3.11). With (3.12)-(3.13), a high-order approximation to the s-fractional differential operator (3.8) is defined by

$$\begin{aligned} \widetilde{D}_{s_n}^{\alpha}\widetilde{v} = &\frac{1}{\Gamma(1-\alpha)}\left(\sum_{k=2}^{n}\int_{s_{k-1}}^{s_k}\frac{\partial_z H^{k-1}(z)dz}{\big(s_n^{\frac{2}{\alpha}} - z^{\frac{2}{\alpha}}\big)^{\alpha}} + \int_{s_0}^{s_1}\frac{\partial_z G(z)dz}{\big(s_n^{\frac{2}{\alpha}} - z^{\frac{2}{\alpha}}\big)^{\alpha}}\right) + \widetilde{Q}^n \\ = &\frac{1}{\Gamma(1-\alpha)}\sum_{k=2}^{n}\left(\frac{1}{\tau_s}\big(\widetilde{v}^{k-1} - \widetilde{v}^{k-2}\big)\int_{s_{k-1}}^{s_k}\frac{dz}{\big(s_n^{\frac{2}{\alpha}} - z^{\frac{2}{\alpha}}\big)^{\alpha}}\right. \\ &\left. + \frac{1}{\tau_s^2}\big(\widetilde{v}^k - 2\widetilde{v}^{k-1} + \widetilde{v}^{k-2}\big)\int_{s_{k-1}}^{s_k}\frac{\big(z - s_{k-\frac{3}{2}}\big)dz}{\big(s_n^{\frac{2}{\alpha}} - z^{\frac{2}{\alpha}}\big)^{\alpha}}\right) \\ &+ \frac{2(\widetilde{v}^1 - \widetilde{v}^0)}{\tau_s^2\Gamma(1-\alpha)}\int_{s_0}^{s_1}\frac{sdz}{\big(s_n^{\frac{2}{\alpha}} - z^{\frac{2}{\alpha}}\big)^{\alpha}} + \widetilde{Q}^n \\ = &\sum_{k=2}^{n-2}\Big(\widetilde{b}_{n,k+1} - 2\widetilde{b}_{n,k} + \widetilde{b}_{n,k-1} + \frac{1}{2}\widetilde{a}_{n,k-1} - \frac{1}{2}\widetilde{a}_{n,k+1}\Big)\widetilde{v}^k \\ &+ \Big(\widetilde{b}_{n,n-2} - 2\widetilde{b}_{n,n-1} + \frac{1}{2}\widetilde{a}_{n,n-2}\Big)\widetilde{v}^{n-1} + \Big(\widetilde{b}_{n,n-1} + \frac{1}{2}\widetilde{a}_{n,n-1}\Big)\widetilde{v}^n \\ &+ \Big(\widetilde{b}_{n,1} - 2\widetilde{b}_{n,0} - \frac{1}{2}\widetilde{a}_{n,1}\Big)\widetilde{v}^0 + \Big(\widetilde{b}_{n,2} - 2\widetilde{b}_{n,1} + 2\widetilde{b}_{n,0} - \frac{1}{2}\widetilde{a}_{n,2}\Big)\widetilde{v}^1 + \widetilde{Q}^n \end{aligned} \tag{3.14}$$

for $n = 2, \ldots, N$ and

$$\widetilde{D}_{s_1}^{\alpha}\widetilde{v} = \frac{1}{\Gamma(1-\alpha)}\int_{s_0}^{s_1}\frac{\partial_z G(z)dz}{\big(s_1^{\frac{2}{\alpha}} - z^{\frac{2}{\alpha}}\big)^{\alpha}} + \widetilde{Q}^1 = 2\widetilde{b}_{1,0}\big(\widetilde{v}^1 - \widetilde{v}^0\big) + \widetilde{Q}^1 \tag{3.15}$$

for $n = 1$, where $\widetilde{Q}^n$ denotes the truncation error. The coefficients $\widetilde{a}_{n,k}$ and $\widetilde{b}_{n,k}$ are defined by

$$\widetilde{a}_{n,k} := \frac{1}{\tau_s\Gamma(1-\alpha)}\int_{s_k}^{s_{k+1}}\frac{dz}{\big(s_n^{\frac{2}{\alpha}} - z^{\frac{2}{\alpha}}\big)^{\alpha}} = \frac{\alpha}{2n\tau_s^2\Gamma(1-\alpha)}$$

$$\times\left[B\left(\left(\frac{k+1}{n}\right)^{\frac{2}{\alpha}},\frac{\alpha}{2},1-\alpha\right)-B\left(\left(\frac{k}{n}\right)^{\frac{2}{\alpha}},\frac{\alpha}{2},1-\alpha\right)\right], \tag{3.16}$$

$$\begin{aligned}\widetilde{b}_{n,k} :=& \frac{1}{\tau_s^2\Gamma(1-\alpha)}\int_{s_k}^{s_{k+1}}\frac{(z-s_k)dz}{\left(s_n^{\frac{2}{\alpha}}-z^{\frac{2}{\alpha}}\right)^{\alpha}}=\frac{\alpha}{2\tau_s^2\Gamma(1-\alpha)}\\ &\times\left[B\left(\left(\frac{k+1}{n}\right)^{\frac{2}{\alpha}},\alpha,1-\alpha\right)-B\left(\left(\frac{k}{n}\right)^{\frac{2}{\alpha}},\alpha,1-\alpha\right)\right.\\ &\left.-\frac{k}{n}B\left(\left(\frac{k+1}{n}\right)^{\frac{2}{\alpha}},\frac{\alpha}{2},1-\alpha\right)+\frac{k}{n}B\left(\left(\frac{k}{n}\right)^{\frac{2}{\alpha}},\frac{\alpha}{2},1-\alpha\right)\right],\end{aligned} \tag{3.17}$$

respectively. A high-order method for the s-fractional equation is

$$\begin{aligned}&\sum_{k=2}^{n-2}\left(\widetilde{b}_{n,k+1}-2\widetilde{b}_{n,k}+\widetilde{b}_{n,k-1}+\frac{1}{2}\widetilde{a}_{n,k-1}-\frac{1}{2}\widetilde{a}_{n,k+1}\right)\widetilde{v}_j^k\\ &+\left(\widetilde{b}_{n,n-2}-2\widetilde{b}_{n,n-1}+\frac{1}{2}\widetilde{a}_{n,n-2}\right)\widetilde{v}_j^{n-1}+\left(\widetilde{b}_{n,n-1}+\frac{1}{2}\widetilde{a}_{n,n-1}\right)\widetilde{v}_j^n\\ &+\left(\widetilde{b}_{n,1}-2\widetilde{b}_{n,0}-\frac{1}{2}\widetilde{a}_{n,1}\right)\widetilde{v}_j^0+\left(\widetilde{b}_{n,2}-2\widetilde{b}_{n,1}+2\widetilde{b}_{n,0}-\frac{1}{2}\widetilde{a}_{n,2}\right)\widetilde{v}_j^1\\ =&\ \delta_x^2\widetilde{v}_j^n+f\left(x_j,s_n^{\frac{2}{\alpha}}\right),\\ &\widetilde{v}_0^n=0,\quad \widetilde{v}_M^n=0,\quad \widetilde{v}_j^0=u_0(x_j),\quad j=1,\ldots,M-1,\quad n=1,\ldots,N.\end{aligned} \tag{3.18}$$

3.3. Analysis

Here we present optimal error analysis for the $L1$ finite difference method (3.7) under a weaker regularity condition. It is easy to see that the truncation error of the method in spatial direction is

$$\left|v_{xx}(x_j,s_n)-\delta_x^2 v(x_j,s_n)\right|\le Ch^2\,. \tag{3.19}$$

On the other hand, the truncation error in temporal direction is defined by

$$\begin{aligned}Q^n(x_j)=&\ D_{s_n}^{\alpha}v(x_j,s)-\sum_{i=1}^{n}a_{n,i-1}\big(v(x_j,s_i)-v(x_j,s_{i-1})\big)\\ =&\ \frac{1}{\Gamma(1-\alpha)}\sum_{i=0}^{n-1}\int_{s_i}^{s_{i+1}}\frac{1}{\left(s_n^{\frac{1}{\alpha}}-y^{\frac{1}{\alpha}}\right)^{\alpha}}\left(v_y(x_j,y)-\frac{1}{\tau_s}\big(v(x_j,s_{i+1})-v(x_j,s_i)\big)\right)dy\\ =:&\ \frac{1}{\Gamma(1-\alpha)}\sum_{i=0}^{n-1}T_n^i(x_j),\quad n>0.\end{aligned} \tag{3.20}$$

The extension to multi-dimensional problems is straightforward and numerical methods by combining the $L1$ approximation with other classical methods in spatial directions can be defined similarly.

Lemma 3.1. *For $n \geq 1$, there holds*

$$\frac{CN}{n} \leq a_{n,0} \leq \cdots \leq a_{n,i-1} \leq a_{n,i} \quad \textit{for} \quad 0 \leq i \leq n-1. \tag{3.21}$$

Proof. By (3.5), for $n \geq 2$ we have

$$\begin{aligned} a_{n,0} &= \frac{\alpha}{\tau_s \Gamma(1-\alpha)} \int_0^{\frac{\widetilde{t}_1}{\widetilde{t}_n}} \frac{dz}{(1-z)^{\alpha} z^{1-\alpha}} \\ &\geq \frac{1}{\tau_s \Gamma(1-\alpha)} \left(\frac{\widetilde{t}_1}{\widetilde{t}_n} \right)^{\alpha} \geq \frac{N}{n\Gamma(1-\alpha)}, \end{aligned} \tag{3.22}$$

and for $n = 1$,

$$a_{1,0} = \frac{\alpha}{\tau_s \Gamma(1-\alpha)} \int_0^1 \frac{dz}{(1-z)^{\alpha} z^{1-\alpha}} = N\Gamma(1+\alpha). \tag{3.23}$$

On the other hand, using (3.4) and the monotonicity of the function $(s_n^{\frac{1}{\alpha}} - z^{\frac{1}{\alpha}})^{-\alpha}$, we see that, for $j \geq 1$,

$$a_{n,j-1} \leq a_{n,j}.$$

The proof is complete. □

An estimate of Q^n is given in the following lemma.

Lemma 3.2. *Assume*

$$\begin{aligned} \left| \frac{\partial^k v}{\partial x^k}(x,s) \right| &\leq C_3, & \textit{for} \quad k = 0,1,2,3,4, \\ \left| \frac{\partial^l v}{\partial s^l}(x,s) \right| &\leq C_3\big(1 + s^{\frac{1}{\alpha}-l}\big), & \textit{for} \quad l = 1,2. \end{aligned}$$

Then

$$|Q^n(x_j)| \leq \frac{C_4}{nN^{1-\alpha}}, \quad 1 \leq n \leq N, \quad 1 \leq j \leq M-1, \tag{3.24}$$

where C_4 is a constant independent of n, N and j.

Proof. For $1 \leq i \leq n-2$, by (3.20) and using integration by parts, we get

$$\begin{aligned} \big|T_n^i(x_j)\big| &= \int_{s_i}^{s_{i+1}} s^{\frac{1}{\alpha}-1} \Big(s_n^{\frac{1}{\alpha}} - s^{\frac{1}{\alpha}}\Big)^{-\alpha-1} \\ &\quad \times \left[v(x_j,s) - v(x_j,s_i) - \frac{1}{\tau_s}\big(v(x_j,s_{i+1}) - v(x_j,s_i)\big)(s-s_i) \right] ds \\ &\leq C\tau_s^2 \int_{s_i}^{s_{i+1}} s^{\frac{1}{\alpha}-1} \Big(s_n^{\frac{1}{\alpha}} - s^{\frac{1}{\alpha}}\Big)^{-\alpha-1} |v_{ss}(x_j,\xi_i)| ds \\ &\leq C\tau_s^2 \Big(1 + s_i^{\frac{1}{\alpha}-2}\Big) \int_{s_i}^{s_{i+1}} s^{\frac{1}{\alpha}-1} \Big(s_n^{\frac{1}{\alpha}} - s^{\frac{1}{\alpha}}\Big)^{-\alpha-1} ds \\ &\leq C\tau_s^2 \Big(1 + s_i^{\frac{1}{\alpha}-2}\Big) \int_{\widetilde{t}_i}^{\widetilde{t}_{i+1}} (\widetilde{t}_n - z)^{-\alpha-1} dz, \end{aligned} \tag{3.25}$$

where we have used (3.9). By noting the fact that

$$\widetilde{t}_{i+1}-\widetilde{t}_i=s_{i+1}^{\frac{1}{\alpha}}-s_i^{\frac{1}{\alpha}}\le\frac{1}{\alpha}\tau_s^{\frac{1}{\alpha}}(i+1)^{\frac{1}{\alpha}-1},$$

we have

$$\begin{aligned}\sum_{i=1}^{[\frac{n}{2}]-1}\left|T_n^i(x_j)\right|&\le C\tau_s^2\sum_{i=1}^{[\frac{n}{2}]-1}\Big(1+s_i^{\frac{1}{\alpha}-2}\Big)\frac{\widetilde{t}_{i+1}-\widetilde{t}_i}{(\widetilde{t}_n-\widetilde{t}_{i+1})^{\alpha+1}}\\&\le C\tau_s\sum_{i=1}^{[\frac{n}{2}]-1}\Big(1+i^{\frac{1}{\alpha}-2}\tau_s^{\frac{1}{\alpha}-2}\Big)\frac{(i+1)^{\frac{1}{\alpha}-1}}{(n/2)^{1+\frac{1}{\alpha}}}\\&\le C\left(\frac{\tau_s}{n}+\frac{\tau_s^{\frac{1}{\alpha}-1}}{n^{3-\frac{1}{\alpha}}}\right),\end{aligned}\tag{3.26}$$

$$\begin{aligned}\sum_{i=[\frac{n}{2}]}^{n-2}\left|T_n^i(x_j)\right|&\le C\tau_s^2\Big(1+s_n^{\frac{1}{\alpha}-2}\Big)\sum_{i=[\frac{n}{2}]}^{n-2}\int_{\widetilde{t}_i}^{\widetilde{t}_{i+1}}(\widetilde{t}_n-z)^{-\alpha-1}dz\\&\le C\tau_s^2\Big(1+s_n^{\frac{1}{\alpha}-2}\Big)(\widetilde{t}_n-\widetilde{t}_{n-1})^{-\alpha}\\&\le C\tau_s^2\Big(1+s_n^{\frac{1}{\alpha}-2}\Big)\Big(\tau_s^{\frac{1}{\alpha}}n^{\frac{1}{\alpha}-1}\Big)^{-\alpha}\\&\le C\Big(\tau_s n^{\alpha-1}+\tau_s^{\frac{1}{\alpha}-1}n^{\alpha+\frac{1}{\alpha}-3}\Big).\end{aligned}\tag{3.27}$$

Moreover, by (3.20), there exist $\xi_1,\xi_2\in(0,s_1)$ such that

$$\begin{aligned}\left|T_1^0(x_j)\right|&=\left|\int_0^{s_1}\frac{1}{\big(s_1^{\frac{1}{\alpha}}-y^{\frac{1}{\alpha}}\big)^{\alpha}}\left[v_s(x_j,y)-\frac{1}{\tau_s}\big(v(x_j,s_1)-v(x_j,0)\big)\right]dy\right|\\&\le|v_s(x_j,\xi_1)-v_s(x_j,\xi_2)|\int_0^{s_1}\frac{1}{\big(s_1^{\frac{1}{\alpha}}-y^{\frac{1}{\alpha}}\big)^{\alpha}}dy\\&\le C\int_0^{\tau_s}|v_{ss}(x_j,y)|dy\int_0^1 z^{\alpha-1}(1-z)^{-\alpha}dz\\&\le C\Big(\tau_s+\tau_s^{\frac{1}{\alpha}-1}\Big),\end{aligned}\tag{3.28}$$

where we have used (3.9) again. By (3.25) we get

$$\begin{aligned}\left|T_n^0(x_j)\right|&=\left|\int_0^{\tau_s}s^{\frac{1}{\alpha}-1}\Big(s_n^{\frac{1}{\alpha}}-s^{\frac{1}{\alpha}}\Big)^{-\alpha-1}\left[v(x_j,s)-v(x_j,0)-\frac{1}{\tau_s}\big(v(x_j,s_1)-v(x_j,0)\big)s\right]ds\right|\\&\le\frac{1}{2}\int_0^{\tau_s}s^{\frac{1}{\alpha}-1}\Big(s_n^{\frac{1}{\alpha}}-s^{\frac{1}{\alpha}}\Big)^{-\alpha-1}\left[\int_0^s|v_{ss}(x_j,z)|zdz\right]ds\\&\le C\int_0^{\tau_s}s^{\frac{1}{\alpha}-1}\Big(s_n^{\frac{1}{\alpha}}-s^{\frac{1}{\alpha}}\Big)^{-\alpha-1}\big(s^2+s^{\frac{1}{\alpha}}\big)ds\end{aligned}$$

$$\leq C\Big(\tau_s^2+\tau_s^{\frac{1}{\alpha}}\Big)\int_0^{\tau_s^{\frac{1}{\alpha}}}(\widetilde{t}_n-y)^{-\alpha-1}dy\leq C\frac{\tau_s+\tau_s^{\frac{1}{\alpha}-1}}{n^{1+\frac{1}{\alpha}}},\tag{3.29}$$

and by (3.20),

$$\begin{aligned}\big|T_n^{n-1}(x_j)\big|&=\left|\int_{s_{n-1}}^{s_n}\frac{1}{\big(s_n^{\frac{1}{\alpha}}-y^{\frac{1}{\alpha}}\big)^{\alpha}}\Big(v_s(x_j,y)-\frac{1}{\tau_s}\big(v(x_j,s_n)-v(x_j,s_{n-1})\big)\Big)dy\right|\\&\leq C\tau_s\Big(1+s_n^{\frac{1}{\alpha}-2}\Big)\int_{s_{n-1}}^{s_n}\frac{1}{\big(s_n^{\frac{1}{\alpha}}-y^{\frac{1}{\alpha}}\big)^{\alpha}}dy\\&\leq C\tau_s\Big(1+s_n^{\frac{1}{\alpha}-2}\Big)\int_{\widetilde{t}_{n-1}}^{\widetilde{t}_n}\frac{dz}{(\widetilde{t}_n-z)^{\alpha}z^{1-\alpha}}\\&\leq C\tau_s\Big(1+s_n^{\frac{1}{\alpha}-2}\Big)\frac{(\widetilde{t}_n-\widetilde{t}_{n-1})^{1-\alpha}}{\widetilde{t}_{n-1}^{1-\alpha}}\\&\leq C\Big(\tau_s n^{\alpha-1}+\tau_s^{\frac{1}{\alpha}-1}n^{\alpha+\frac{1}{\alpha}-3}\Big).\end{aligned}\tag{3.30}$$

Combining the above estimates, we arrive at

$$|Q^n(x_j)|\leq C\Big(\tau_s^{\frac{1}{\alpha}-1}n^{\alpha+\frac{1}{\alpha}-3}+\tau_s n^{\alpha-1}\Big)\leq\frac{C}{nN^{1-\alpha}}.\tag{3.31}$$

The proof is complete. □

Let $e_j^n=v(x_j,s_n)-v_j^n=u(x_j,s_n^{\frac{1}{\alpha}})-v_j^n$ denote an error function. From (3.7), we see that e_j^n satisfies the equation

$$\begin{aligned}&a_{n,n-1}e_j^n-\sum_{k=1}^{n-1}(a_{n,k}-a_{n,k-1})e_j^k=\delta_x^2e_j^n+Q^n(x_j)+\mathcal{O}\big(h^2\big),\\&e_0^n=e_M^n=0,\quad e_j^0=0,\quad j=1,\dots,M-1,\quad n=1,\dots,N.\end{aligned}\tag{3.32}$$

We present an optimal error estimate below.

Theorem 3.1. *Under the assumptions of Lemma* 3.2*,*

$$\max_{1\leq n\leq N}\max_{0\leq j\leq M}|e_j^n|\leq C_5\big(h^2+N^{-(2-\alpha)}\big),\tag{3.33}$$

where C_5 is a constant independent of h and N.

Proof. Let

$$\big|e_m^k\big|:=\max_{0\leq j\leq M}\max_{1\leq n\leq N}\big|e_j^n\big|>0.$$

By (3.32) and Theorem 3.2, we have

$$\left|\big(a_{k,k-1}-\delta_x^2\big)e_m^k+\sum_{i=1}^{k-1}e_m^i(a_{k,i-1}-a_{k,i})\right|\leq\frac{C}{kN^{1-\alpha}}+Ch^2.$$

Since $\delta_x^2 e_m^k \ge 0$ for $e_m^k \le 0$ and $\delta_x^2 e_m^k \le 0$ for $e_m^k \ge 0$, we have $e_m^k \delta_x^2 e_m^k \le 0$. By Lemma 3.1, we find that

$$\begin{aligned} a_{k,k-1}\big(e_m^k\big)^2 &\le e_m^k(a_{k,k-1}-\delta_x^2)e_m^k = \big|e_m^k\big|\big|\left(a_{k,k-1}-\delta_x^2\right)e_m^k\big| \\ &\le \big|e_m^k\big|\left(|e_m^k|\sum_{i=1}^{k-1}(a_{k,i}-a_{k,i-1}) + \frac{C}{kN^{1-\alpha}} + Ch^2\right) \\ &\le (a_{k,k-1}-a_{k,0})\big(e_m^k\big)^2 + \big|e_m^k\big|\left(\frac{C}{kN^{1-\alpha}} + Ch^2\right), \end{aligned}$$

which in turn shows that

$$\big|e_m^k\big| \le \frac{1}{a_{k,0}}\left(\frac{C}{kN^{1-\alpha}} + Ch^2\right) \le C\big(h^2 + N^{-(2-\alpha)}\big).$$

The proof is complete. □

4. Numerical examples

In this section, we present three numerical examples to show the efficiency and convergence rate of two methods presented in this paper for time-fractional differential equations in comparison with the $L1$ method based on uniform meshes and graded meshes proposed in [37] with the optimal parameter $\gamma_{\text{opt}} = \frac{(2-\alpha)}{\alpha}$. The computations for Examples 4.1 and 4.2 are performed by using Matlab, while FEniCS is used for Example 4.3.

Example 4.1. We consider the following time fractional parabolic equation

$$\mathcal{D}_t^\alpha u = \partial_x^2 u + f(x,t), \qquad x \in (0,\pi), \quad 0 < t \le 1, \tag{4.1}$$

$$u(x,0) = 0, \qquad x \in (0,\pi), \tag{4.2}$$

$$u(0,t) = 0, \quad u(\pi,t) = 0 \tag{4.3}$$

with the exact solution

$$u(x,t) = \big(t^\alpha + c_0 t^{2\alpha} + c_1\left(t + t^3\right)\big)\sin x. \tag{4.4}$$

The function f is given from the exact solution. The equation was investigated numerically in [37], by using the traditional $L1$ finite difference method with $\alpha = 0.4, 0.6$. Here, we apply the $L1$ finite difference method for the time-fractional equation (4.1)-(4.3) on uniform mesh as well as the optimal graded mesh and the $L1$ method defined in (3.7) for the corresponding s-fractional equation with $N = 64, 128, 256, 512, 1024, 2048$. Since the convergence rate is $\mathcal{O}(h^2 + N^{-(2-\alpha)})$, we take $M = 5N$ to observe the convergence rate in temporal direction. We define

$$e_u^N = \max_{1\le n\le N}\max_{0\le j\le M}\big|u_j^n - u(x_j,t_n)\big|,$$

$$e_v^N = \max_{1\le n\le N}\max_{0\le j\le M}\left|v_j^n - v(x_j,s_n)\right|,$$

where u_j^n and v_j^n denote the numerical solutions of the $L1$ finite difference method for (4.1)-(4.3) and for the corresponding s-fractional equation, respectively.

We first test the case $(c_0,c_1)=(0,1)$ and present in Table 1 numerical errors for $\alpha=0.6,0.4,0.2,0.1$. We see clearly that the $L1$ method with uniform meshes produces errors of order $\mathcal{O}(N^{-\alpha})$, worse than the other two methods for all values of α. The optimal rate $\mathcal{O}(N^{-(2-\alpha)})$ can be observed from numerical results for both the $L1$ method on graded meshes and the scheme (3.7), while the latter shows better performance. These numerical results confirm our theoretical analysis.

Then we test the cases $(c_0,c_1)=(0,0)$ and $(c_0,c_1)=(1,0)$ for $N=128,256,512$ by the $L1$ method on graded meshes and the scheme (3.7). Numerical results are presented in Tables 2 and 3, respectively. For the former, the exact solutions of the time fractional equation (1.1) and the s-fractional equation (2.3) are

$$u(x,t)=t^{\alpha}\sin x,\quad v(x,s)=s\sin x.$$

Since the $L1$ method in (3.7) is based on a linear approximation to the variable v, no error in temporal direction arises from the scheme (3.7). Therefore, in this case the convergence rate of the scheme (3.7) is the same as the convergence rate in spatial

Table 1: Errors e_u^N and e_v^N and convergence rates in temporal direction (Example 4.1).

	N	$\alpha=0.6$		$\alpha=0.4$		$\alpha=0.2$		$\alpha=0.1$	
		error	order	error	order	error	order	error	order
e_u^N uniform mesh	64	2.00e-02	–	4.21e-02	–	5.62e-02	–	4.30e-02	–
	128	1.35e-02	0.57	3.31e-02	0.35	5.08e-02	0.15	4.12e-02	0.06
	256	9.03e-03	0.58	2.58e-02	0.36	4.58e-02	0.15	3.94e-02	0.06
	512	6.02e-03	0.59	1.99e-02	0.37	4.11e-02	0.16	3.77e-02	0.07
	1024	4.00e-03	0.59	1.54e-02	0.38	3.68e-02	0.16	3.60e-02	0.07
	2048	2.65e-03	0.59	1.18e-02	0.38	3.28e-02	0.16	3.43e-02	0.07
e_u^N graded mesh [37]	64	6.22e-03	–	4.98e-03	–	5.39e-03	–	6.92e-03	–
	128	2.43e-03	1.35	1.77e-03	1.49	1.82e-03	1.56	2.43e-03	1.51
	256	9.40e-04	1.37	6.14e-04	1.53	5.91e-04	1.63	7.93e-04	1.62
	512	3.61e-04	1.38	2.10e-04	1.55	1.86e-04	1.67	2.47e-04	1.68
	1024	1.38e-04	1.39	7.12e-05	1.56	5.75e-05	1.70	7.44e-05	1.73
	2048	5.25e-05	1.39	2.40e-05	1.57	1.75e-05	1.72	2.20e-05	1.76
e_v^N scheme (3.7)	64	6.17e-03	–	4.00e-03	–	3.61e-03	–	4.50e-03	–
	128	2.39e-03	1.37	1.39e-03	1.53	1.17e-03	1.63	1.46e-03	1.63
	256	9.16e-04	1.38	4.74e-04	1.55	3.67e-04	1.67	4.52e-04	1.69
	512	3.50e-04	1.39	1.61e-04	1.56	1.13e-04	1.70	1.36e-04	1.73
	1024	1.33e-04	1.39	5.40e-05	1.57	3.44e-05	1.72	4.02e-05	1.76
	2048	5.07e-05	1.40	1.81e-05	1.58	1.03e-05	1.73	1.17e-05	1.78

Table 2: Errors e_u^N and e_v^N and convergence rates in temporal direction (Example 4.1).

	N	$\alpha=0.6$		$\alpha=0.4$		$\alpha=0.2$		$\alpha=0.1$	
		error	order	error	order	error	order	error	order
e_u^N	128	6.09e-04	–	2.81e-04	–	1.38e-04	–	9.68e-05	–
graded	256	2.39e-04	1.35	9.62e-05	1.55	4.32e-05	1.68	2.94e-05	1.72
mesh [37]	512	9.27e-05	1.37	3.27e-05	1.56	1.33e-05	1.69	8.81e-06	1.74
e_v^N	128	2.99e-07	–	3.18e-07	–	3.24e-07	–	3.21e-07	–
scheme	256	7.48e-08	2.00	7.94e-08	2.00	8.09e-08	2.00	8.03e-08	2.00
(3.7)	512	1.87e-08	2.00	1.98e-08	2.00	2.04e-08	1.99	2.02e-08	1.99

Table 3: Errors e_u^N and e_v^N and convergence rates in temporal direction (Example 4.1).

	N	$\alpha=0.6$		$\alpha=0.4$		$\alpha=0.2$		$\alpha=0.1$	
		error	order	error	order	error	order	error	order
e_u^N	128	5.98e-04	–	2.87e-04	–	1.97e-04	–	1.73e-04	–
graded	256	2.36e-04	1.34	9.78e-05	1.55	6.03e-05	1.71	5.14e-05	1.75
mesh [37]	512	9.20e-05	1.36	3.32e-05	1.56	1.82e-05	1.73	1.50e-05	1.78
e_v^N	128	3.79e-04	–	8.49e-05	–	1.67e-05	–	5.37e-06	–
scheme	256	1.44e-04	1.39	2.86e-05	1.57	5.13e-06	1.71	1.60e-06	1.75
(3.7)	512	5.48e-05	1.40	9.56e-06	1.58	1.56e-06	1.72	4.70e-07	1.76

direction, i.e., second order, which can be observed clearly from Table 2. For the case $(c_0, c_1) = (1, 0)$, we can see from Table 3 that the scheme (3.7) shows much better performance than the graded mesh method, although both have the convergence rate of $\mathcal{O}(N^{2-\alpha})$.

Moreover, since the solution of the equation has its singularity around $t = 0$, we further present in Fig. 1 numerical errors of the graded mesh method and the scheme (3.7) in the initial time period $t \in [0, 0.2]$. All three cases are tested with $\alpha = 0.5$ and

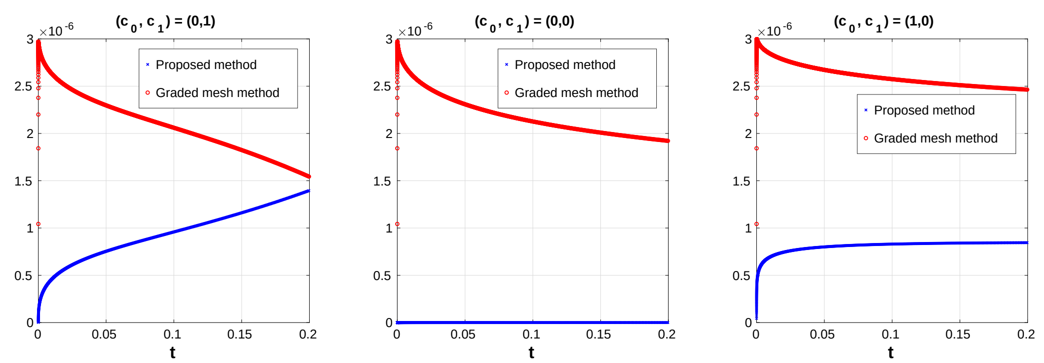

Figure 1: Errors of graded meshes and proposed methods for $t \in (0, 0.2)$ (Example 4.1).

Table 4: Errors $e_{\widetilde{v}}^N$ and convergence rates in temporal direction (Example 4.1).

	N	$\alpha=0.6$		$\alpha=0.4$		$\alpha=0.2$		$\alpha=0.1$	
		error	order	error	order	error	order	error	order
	64	1.46e-03	–	1.37e-03	–	2.22e-03	–	4.49e-03	–
	128	2.87e-04	2.34	2.49e-04	2.46	4.00e-04	2.47	9.04e-04	2.31
$e_{\widetilde{v}}^N$	256	5.60e-05	2.36	4.36e-05	2.51	6.66e-05	2.58	1.58e-04	2.52
scheme	512	1.08e-05	2.38	7.49e-06	2.54	1.06e-05	2.65	2.53e-05	2.64
(3.18)	1024	2.06e-06	2.39	1.27e-06	2.56	1.64e-06	2.69	3.87e-06	2.71
	2048	3.92e-07	2.39	2.13e-07	2.57	2.51e-07	2.71	5.82e-07	2.73

$N=2048$. The scheme (3.7) provides a better approximation in the initial time period.

Finally we solve the system (4.1)-(4.3) by the proposed high-order method defined in (3.18) for $\alpha=0.1,0.2,0.4,0.6$ with $N=64,128,256,512,1024,2048$, respectively. Since the scheme is of second order accuracy in the spatial direction, we take $M=\lfloor(\frac{N}{2})^{1.5-\frac{\alpha}{2}}\rfloor$ in our numerical simulations, where $\lfloor x\rfloor=\max\{m\in\mathbb{Z}\mid m\le x\}$. We present our numerical results in Table 4. It can be observed that the scheme (3.18) provides a higher-order accuracy for all α although the exact solution has strong singularity at initial moment. In particular, numerical results show the optimal convergence rate $\mathcal{O}(N^{-(3-\alpha)})$ for $\alpha=0.4,0.6$ and a rate slightly lower than the optimal one for $\alpha=0.1$. The latter may require smaller time steps to yield the optimal convergence rate.

Example 4.2. We study a nonlinear time fractional parabolic initial and boundary value problem

$$\mathcal{D}_t^\alpha u = u_{xx}+\lambda u+\rho u\big(1-u^2\big), \quad x\in(0,\pi), \quad 0<t\le 1, \tag{4.5}$$

$$u(x,0)=\sin x, \qquad x\in(0,\pi), \tag{4.6}$$

$$u(0,t)=u(\pi,t)=0 \tag{4.7}$$

with $\lambda=-3$ and $\rho=1$.

For dealing with the nonlinear term, a classical second order extrapolation linearization [9, 18] is used in our computation, with which a linearized $L1$ finite difference equation is defined by

$$\widetilde{a}_{n,n-1}v_j^n-\sum_{k=1}^{n-1}(\widetilde{a}_{n,k}-\widetilde{a}_{n,k-1})v_j^k-\widetilde{a}_{n,0}v_j^0-\delta_x^2v_j^n=\lambda v_j^n+\rho\left(v_j^n-\left(2v_j^{n-1}-v_j^{n-2}\right)^3\right),$$

$$v_0^n=v_M^n=0, \quad v_j^0=\sin x_j, \quad j=1,\dots,M-1, \quad n=1,\dots,N,$$

where $x_j=\frac{\pi j}{M}$. We solve the initial and boundary value problem (4.5) by the linearized $L1$ finite difference method. Here the numerical solution on the fine mesh $N=2048$ and $M=4N$ is used as a benchmark solution.

Table 5: Errors e_v^N and convergence rates in temporal direction (Example 4.2).

N	$\alpha=0.6$		$\alpha=0.4$		$\alpha=0.2$		$\alpha=0.1$	
scheme (3.7)	error	order	error	order	error	order	error	order
8	2.82e-02	–	1.47e-02	–	4.29e-03	–	1.28e-03	–
16	1.24e-02	1.18	5.59e-03	1.40	1.60e-03	1.43	4.37e-04	1.55
32	5.14e-03	1.27	2.16e-03	1.37	5.90e-04	1.44	1.69e-04	1.37
64	2.04e-03	1.33	7.93e-04	1.45	2.06e-04	1.52	6.12e-05	1.47
128	7.88e-04	1.37	2.79e-04	1.50	6.93e-05	1.57	2.11e-05	1.53
256	2.94e-04	1.42	9.47e-05	1.56	2.23e-05	1.63	6.88e-06	1.62
scheme (3.18)	error	order	error	order	error	order	error	order
8	2.71e-03	–	1.63e-03	–	1.16e-03	–	1.08e-03	–
16	5.29e-04	2.36	2.64e-04	2.63	1.39e-04	3.06	1.06e-04	3.35
32	9.62e-05	2.46	4.02e-05	2.72	1.76e-05	2.98	1.24e-05	3.10
64	1.76e-05	2.45	6.29e-06	2.68	2.36e-06	2.90	1.56e-06	2.99
128	3.24e-06	2.44	1.00e-06	2.65	3.28e-07	2.85	2.04e-07	2.93
256	5.89e-07	2.46	1.59e-07	2.66	4.59e-08	2.83	2.74e-08	2.90

We present numerical results of the schemes (3.7) and (3.18) in Table 5 with $N = 8, 16, 32, 64, 128, 256$ and $M = 4N$ for the $L1$ scheme and $M = 6N$ for the high-order scheme in our computation. Numerical results show that the scheme (3.7) is convergent and stable for all values of α. One can observe the convergence rates $\mathcal{O}(N^{-(2-\alpha)})$ clearly for $\alpha = 0.6, 0.4, 0.2$. For $\alpha = 0.1$, the convergence rate at $N = 256$ is a little lower than the optimal one, while the rate as N increases. For the high-order method (3.18), we observe the optimal convergence order $\mathcal{O}(N^{-(3-\alpha)})$ for all α.

Example 4.3. The last example is the nonlinear time-fractional Fisher equation

$$\mathcal{D}_t^\alpha u = \Delta u + u(1-u) + f(x,t), \qquad x \in \Omega := (0,1)\times(0,1), \quad 0 < t \le 1, \tag{4.8}$$

$$u(x,0) = 0, \qquad x \in \Omega, \tag{4.9}$$

$$u(x,t) = 0, \qquad x \in \partial\Omega, \quad 0 < t \le 1. \tag{4.10}$$

The initial and boundary value problem (4.8)-(4.10) was originally proposed to describe the spatial and temporal propagation of a virile gene. Later, it was revised by providing some characteristics of memory embedded into the system [2]. The problem was investigated numerically by many authors, e.g., see [21] for an $L1$ finite difference method with a uniform mesh. We calculate the right-hand side f of (4.8) based on the exact solution

$$u = \left(t^\alpha + t^2\right)\sin(\pi x_1)\sin(\pi x_2).$$

The $L1$ scheme (3.7) can be combined with any other methods in spatial direction. Here, we solve the initial and boundary value problem (4.8)-(4.10) by an $L1$ FEM, in which the $L1$ approximation (3.7) is used in temporal direction and a linear FE approximation is applied in spatial direction.

Table 6: Errors $\|e_h^N\|_{L^\infty}$ and convergence rates in temporal direction (Example 4.3).

N	$\alpha=0.6$		$\alpha=0.4$		$\alpha=0.2$		$\alpha=0.1$	
	error	order	error	order	error	order	error	order
16	2.96e-03	–	5.18e-03	–	1.57e-02	–	3.86e-02	–
32	9.48e-04	1.64	1.51e-03	1.78	4.99e-03	1.66	1.55e-02	1.32
64	3.11e-04	1.61	4.29e-04	1.82	1.42e-03	1.81	4.97e-03	1.64
128	1.05e-04	1.57	1.21e-04	1.82	3.84e-04	1.89	1.42e-03	1.81

Let $\mathcal{T}_h = \{x_{1i}, x_{2j}\}_{i,j=0}^M$ denote a uniform triangular mesh on $\Omega := [0,1]\times[0,1]$ with $M+1$ vertices in each spatial direction. We denote by V_h the linear Lagrange finite element subspaces of $H_0^1(\Omega)$ on the partition $\mathcal{T}_h$. Applying the Newton's linearization to approximate the nonlinear term, a linearized $L1$ FEM is to find $v_h^n \in V_h$ such that for $n = 1,\dots,N$,

$$(\widetilde{a}_{n,n-1}v_h^n, \omega_h) + (\nabla v_h^n, \nabla\omega_h) - \Big(\big(1-2v_h^{n-1}\big)v_h^n, \omega_h\Big) \tag{4.11}$$

$$= \left(\sum_{k=1}^{n-1}(\widetilde{a}_{n,k}-\widetilde{a}_{n,k-1})v_h^k + \widetilde{a}_{n,0}v_h^0, \omega_h\right) - \Big(\big(v_h^{n-1}\big)^2, \omega_h\Big) + (f^n, \omega_h)\,, \quad \forall\,\omega_h \in V_h.$$

Since the accuracy of the $L1$ scheme is in order of $\mathcal{O}(N^{-(2-\alpha)})$, the global accuracy of the $L1$ FEM is assumed to be the same as the $L1$ finite difference method. We apply the $L1$ FEM for solving the initial and boundary value problem (4.8)-(4.10) with $N = 16, 32, 64, 128$ and $\alpha = 0.6, 0.4, 0.2, 0.1$, respectively. Similarly, we take $M = 4N$ to observe the convergence rate in temporal direction. We present numerical errors in Table 6 where

$$\big\|e_h^N\big\|_{L^\infty} = \max_{1\le n\le N}\max_{0\le j\le M}\Big|v_h^n(x_i,y_j) - u\Big(x_i, y_j, s_n^{\frac{1}{\alpha}}\Big)\Big|.$$

We can see clearly that the proposed method is convergent and stable for all values of α.

5. Conclusions

We have derived a re-scaled time-fractional (s-fractional) differential equation in terms of a simple change of variable. A class of finite difference methods are introduced for s-fractional differential equations to handle the singularity of the solution at initial time. Numerical experiments for two types finite difference methods with linear and quadratic approximations, respectively, are presented. Numerical results show that both methods provide the optimal convergence rates in temporal direction uniformly for $0 < \alpha < 1$, while theoretical analysis has been given only for the $L1$ finite difference method (3.7) under weaker regularity assumptions. Also the proposed methods can be easily combined with any other numerical approximations in spatial direction, such as FEM, spectral method and DG.

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