ON STABILITY AND CONVERGENCE OF L2-1\(\sigma\) METHOD ON GENERAL NONUNIFORM MESHES FOR SUBDIFFUSION EQUATION

CHAOYU QUAN AND XU WU

Abstract. In this work the L2-1\(\sigma\) method on general nonuniform meshes is studied for the subdiffusion equation. Under some constraints on the time step ratio \(\rho_k\), for example \(\rho_k \geq 0.475329\) for all \(k \geq 2\), a crucial bilinear form associated with the L2-1\(\sigma\) fractional-derivative operator is proved to be positive semidefinite and the \(H^1\)-stability of L2-1\(\sigma\) schemes is then derived for all time under simple assumptions on the initial condition and the source term. In addition, we prove the sharp convergence when \(\rho_k \geq 0.475329\), which reduces the restriction \(\rho_k \geq 4/7\) proposed by Liao, McLean and Zhang in [SIAM J. Numer. Anal. 57 (2019), no. 1, 218–237].

1. Introduction

In the past decade, many numerical methods have been proposed to solve the time-fractional diffusion equations [20, 5]. Among these methods, the L1 scheme of \((2 - \alpha)\)-order has been well-developed by Langlands and Henry [11], Sun-Wu [24], and Lin-Xu [18], etc. Alikhanov proposes the L2-1\(\sigma\) scheme that has second order accuracy in time [1]. Gao-Sun-Zhang study an L2 method of \((3 - \alpha)\)-order on uniform meshes in [4] and later a slightly different L2 method is analyzed by Lv-Xu in [19].

Most of the aforementioned works have been concerned with solutions that are globally smooth. However, simple examples show that for given smooth data, the solutions to time-fractional problems typically have weak singularities. Some works start to focus on the numerical solution of more typical fractional problems whose solutions exhibit weak singularities. In particular, the L1, L2-1\(\sigma\) and L2 methods on the graded meshes have been developed. Stynes-Riordan-Gracia [23] prove the sharp error analysis of L1 scheme on graded meshes. Kopteva provides a different analysis framework of the L1 scheme on graded meshes in two and three spatial dimensions in [8]. Chen-Stynes [2] prove the second-order convergence of the L2-1\(\sigma\) scheme on fitted meshes combining the graded meshes and quasiuniform meshes. Kopteva-Meng [10] provide sharp pointwise-in-time error bounds for quasi-graded temporal meshes with arbitrary degree of grading for the L1 and L2-1\(\sigma\) schemes. Later Kopteva generalize this sharp pointwise error analysis to an L2-type scheme on quasi-graded meshes [9].

Liao-Li-Zhang establish the sharp error analysis for the L1 scheme of subdiffusion equation on general nonuniform meshes in [12] and then Liao-Mclean-Zhang study the L2-1\(\sigma\) scheme in [13, 14], where a discrete Gronwall inequality is introduced. This analysis for general nonuniform meshes can be used to design adaptive strategies of time steps.
In addition, we shall mention the convolution quadrature methods with corrections that can also overcome the weak singularity problem for time-fractional diffusion equation, see for example [6, 7] and the references therein.

In this work, we first study the $H^1$-stability of the $L_{2-1}^{1}$ method proposed initially in [1] on general nonuniform meshes for subdiffusion equation with homogeneous Dirichlet boundary condition:

$$\partial_t^{\alpha} u(t, x) = \Delta u(t, x) + f(t, x), \quad (t, x) \in (0, \infty) \times \Omega,$$

where $\Omega$ is a bounded Lipschitz domain in $\mathbb{R}^d$. For the $L_{2-1}^{1}$ fractional-derivative operator denoted by $L_{k}^{\alpha,*}$, we prove that the following bilinear form

$$B_n(v, w) = \sum_{k=1}^{n} \langle L_{k}^{\alpha,*} v, \delta_k w \rangle, \quad \delta_k w := w^k - w^{k-1}, \quad n \geq 1,$$

is positive semidefinite under the restrictions (3.2) on time step ratios $\rho_k := \tau_k / \tau_{k-1}$ with $\tau_k$ the $k$th time step and $k \geq 2$. Note that the positive semidefiniteness of $B_n$ on general nonuniform meshes is a challenging problem as stated in the conclusion of [15]. Based on this positive semidefiniteness, we propose the $H^1$-stability result in Theorem 4.1 for the $L_{2-1}^{1}$ scheme. In particular, when $\rho_k \geq 0.475329$ for $k \geq 2$, the restrictions (3.2) hold and the $H^1$-stability can be ensured for all time. We also mention our recent work [22], where the $H^1$-stability has been established for all time for an $L^2$-type scheme of the subdiffusion equation on general nonuniform meshes.

Besides the $H^1$-stability of the $L_{2-1}^{1}$ scheme in Theorem 4.1 we revisit the sharp convergence analysis in [14] by Liao-Mclean-Zhang. We provide a proof of sharp convergence based on some new properties of the $L_{2-1}^{1}$ coefficients, where the restriction on time step ratios is relaxed from $\rho_k \geq 4/7$ to $\rho_k \geq 0.475329$.

In the numerical implementations, we compare the $L_{2-1}^{1}$ schemes on the standard graded meshes [23] and the $r$-variable graded meshes (with varying grading parameter) proposed in [22]. According to our stability analysis, these methods are all $H^1$-stable. In our example, it can be observed that choosing proper $r$-variable graded meshes can lead to better numerical performance.

This work is organized as follows. In Section 2 the derivation, explicit expression and reformulation of $L_{2-1}^{1}$ fractional-derivative operator are provided. In Section 3 we prove the positive semidefiniteness of the bilinear form $B_n$ under some mild restrictions on the time step ratios. In Section 4 we establish the $H^1$-stability of the $L_{2-1}^{1}$ scheme for the subdiffusion equation, based on the positive semidefiniteness result. Moreover we show the global error estimate when $\rho_k \geq 0.475329$ under low regularity assumptions on the exact solution. In Section 5 we do some first numerical tests.

2. Discrete fractional-derivative operator

In this part we show the derivation, explicit expression and reformulation of $L_{2-1}^{1}$ operator on an arbitrary nonuniform mesh.

We consider the $L_{2-1}^{1}$ approximation of the fractional-derivative operator defined by

$$\partial_t^{\alpha} u = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{u'(s)}{(t-s)^\alpha} ds.$$
Take a nonuniform time mesh $0 = t_0 < t_1 < \ldots < t_{k-1} < t_k < \ldots$ with $k \geq 1$. Let $\tau_j = t_j - t_{j-1}$ and $\sigma = 1 - \alpha/2$ (c.f. [1] for this setting of $\sigma$). The fractional derivative $D^\alpha_t u(t)$ at $t = t^*_k := t_{k-1} + \sigma \tau_k$ could be approximated by the following L2-1,\sigma\text{ fractional-derivative operator}

\begin{equation}
\begin{aligned}
L^a_1u &= \frac{\sigma^{1-\alpha}(u^1 - u^0)}{\Gamma(2-\alpha)\tau_1^\alpha}, \\
L^a_ku &= \frac{1}{\Gamma(1-\alpha)} \left( \sum_{j=1}^{k-1} \int_{t_{j-1}}^{t_j} \frac{\partial_x H^2_j(s)}{(t_k^* - s)^\alpha} \, ds + \int_{t_{k-1}}^{t_k^*} \frac{\partial_x H^1_k(s)}{(t_k^* - s)^\alpha} \, ds \right) \\
&= \frac{1}{\Gamma(1-\alpha)} \left( \sum_{j=1}^{k-1} (a^j_k u^{j-1} + b^j_k u^j + c^j_k u^{j+1}) + \frac{\sigma^{1-\alpha}(u^k - u^{k-1})}{\Gamma(2-\alpha)\tau_k^\alpha} \right), 
\end{aligned}
\end{equation}

where for $1 \leq j \leq k - 1$,

\begin{align*}
H^2_j(t) &= \frac{(t - t_j)(t - t_{j+1})}{(t_{j-1} - t_j)(t_j - t_{j+1})} u^{j-1} + \frac{(t - t_{j-1})(t - t_{j+1})}{(t_j - t_{j-1})(t_j - t_{j+1})} u^j \\
&\quad\quad + \frac{(t - t_{j-1})(t - t_j)}{(t_{j+1} - t_j)(t_j - t_{j-1})} u^{j+1}, \\
H^1_k(t) &= \frac{t - t_k}{t_k - t_{k-1}} u^{k-1} + \frac{t - t_{k-1}}{t_k - t_{k-1}} u^k,
\end{align*}

and

\begin{align*}
a^j_k &= \int_{t_{j-1}}^{t_j} 2s - t_j - t_{j+1} \frac{1}{\tau_j(\tau_j + \tau_{j+1})(t_k^* - s)^\alpha} \, ds = \int_0^1 \frac{-2\tau_j(1-\theta) - \tau_{j+1}}{(\tau_j + \tau_{j+1})(t_k^* - (t_{j-1} + \theta \tau_j))^\alpha} \, d\theta, \\
b^j_k &= -\int_{t_{j-1}}^{t_j} 2s - t_{j-1} - t_{j+1} \frac{1}{\tau_j \tau_{j+1}(t_k^* - s)^\alpha} \, ds = -\int_0^1 \frac{2\tau_j \theta - \tau_{j+1}}{\tau_j + \theta \tau_j}(t_k^* - (t_{j-1} + \theta \tau_j))^\alpha \, d\theta, \\
c^j_k &= \int_{t_{j-1}}^{t_j} 2s - t_{j-1} - t_j \frac{1}{\tau_j + \tau_{j+1}(t_k^* - s)^\alpha} \, ds = \int_0^1 \frac{\tau_j^2(2\theta - 1)}{\tau_j + \theta \tau_{j+1}(t_k^* - (t_{j-1} + \theta \tau_j))^\alpha} \, d\theta.
\end{align*}

It can be verified that $a^j_k < 0$, $b^j_k > 0$, $c^j_k > 0$, and $a^j_k + b^j_k + c^j_k = 0$ for $1 \leq j \leq k - 1$.

Specifically speaking, we can figure out the explicit expressions of $a^j_k$ and $c^j_k$ as follows (note that $b^j_k = -a^j_k - c^j_k$): for $1 \leq j \leq k - 1$,

\begin{align*}
a^j_k &= \frac{\tau_{j+1}}{(1-\alpha)\tau_j (\tau_j + \tau_{j+1})} (t_k^* - t_j)^{1-\alpha} - \frac{2\tau_j + \tau_{j+1}}{(1-\alpha)\tau_j (\tau_j + \tau_{j+1})} (t_k^* - t_{j-1})^{1-\alpha} \\
&\quad\quad + \frac{2}{(2-\alpha)(1-\alpha)\tau_j (\tau_j + \tau_{j+1})} [(t_k^* - t_{j-1})^{2-\alpha} - (t_k^* - t_j)^{2-\alpha}], \\
c^j_k &= \frac{1}{(1-\alpha)\tau_{j+1} (\tau_j + \tau_{j+1})} \left[ -\tau_j ((t_k^* - t_{j-1})^{1-\alpha} + (t_k^* - t_j)^{1-\alpha}) \\
&\quad\quad + 2(2-\alpha)^{-1}((t_k^* - t_{j-1})^{2-\alpha} - (t_k^* - t_j)^{2-\alpha}) \right].
\end{align*}
We reformulate the discrete fractional derivative $L_k^{\alpha,*}$ in (2.3) as

$$L_1^{\alpha,*} u = \frac{\alpha^{1-\alpha}}{\Gamma(2-\alpha)t_1^{\alpha}} \delta_1 u,$$

$$L_k^{\alpha,*} u = \frac{1}{\Gamma(1-\alpha)} \left( c_{k-1}^j \delta_k u - a_j^k \delta_1 u + \sum_{j=2}^{k-1} d_j^k \delta_j u \right) + \frac{\alpha^{1-\alpha}}{\Gamma(2-\alpha)\tau_1^{\alpha}} \delta_k u, \quad k \geq 2,$$

where $\delta_j u = u^j - u^{j-1}$, $d_j^k := c_{j-1}^k - a_j^k$.

To establish the $H^1$-stability of $L_k^{\alpha,*}$ method for fractional-order parabolic problem, we shall prove the positive semidefiniteness of bilinear form $B_n$ defined in (1.2).

3. Positive semidefiniteness of bilinear form $B_n$

3.1. Properties of $L_2-1_\tau$ coefficients. Following [22], we propose the following properties of the $L_2-1_\tau$ coefficients $a_j^k$, $c_j^k$ and $d_j^k$ in (2.3), which will be useful to establish the positive semidefiniteness of bilinear form $B_n$.

**Lemma 3.1** (Properties of $a_j^k$, $c_j^k$ and $d_j^k$). For the $L_2-1_\tau$ coefficients given in (2.3), given a nonuniform mesh $\{\tau_j\}_{j\geq 1}$, the following properties hold:

- (P1) $a_j^k < 0$, $1 \leq j \leq k - 1$, $k \geq 2$;
- (P2) $a_{j+1}^k - a_j^k > 0$, $1 \leq j \leq k - 1$, $k \geq 2$;
- (P3) $a_{j+1}^k - a_j^k < 0$, $1 \leq j \leq k - 2$, $k \geq 3$;
- (P4) $a_{j+1}^k - a_j^k < a_{j+1}^{k+1} - a_j^{k+1}$, $1 \leq j \leq k - 2$, $k \geq 3$;
- (P5) $c_j^k > 0$, $1 \leq j \leq k - 1$, $k \geq 2$;
- (P6) $c_{j+1}^k - c_j^k < 0$, $1 \leq j \leq k - 1$, $k \geq 2$;
- (P7) $d_j^k > 0$, $2 \leq j \leq k - 1$, $k \geq 3$;
- (P8) $d_{j+1}^k - d_j^k < 0$, $2 \leq j \leq k - 1$, $k \geq 3$.

Furthermore, if the nonuniform mesh $\{\tau_j\}_{j\geq 1}$, with $\rho_j := \tau_j/\tau_{j-1}$ satisfies

$$\frac{1}{\rho_{j+1}} \geq \frac{1}{\rho_j^2(1 + \rho_j)} - 3, \quad \forall j \geq 2,$$

then the following properties of $d_j^k$ hold:

- (P9) $d_{j+1}^k - d_j^k > 0$, $2 \leq j \leq k - 2$, $k \geq 4$;
- (P10) $d_{j+1}^k - d_j^k > d_{j+1}^{k+1} - d_j^{k+1}$, $2 \leq j \leq k - 2$, $k \geq 4$.

**Proof.** The proof is the same as the proof of [22] Lemma 3.1] except replacing $t_k$ with $t_k^*$. We omit it here. \hfill \Box

**Theorem 3.2.** Consider a nonuniform mesh $\{\tau_k\}_{k\geq 1}$ satisfying that $k \geq 2$,

$$\left\{ \begin{array}{ll}
\rho_* < \rho_{k+1} & \leq \frac{\rho_*^2(1 + \rho_k)}{1 - 3\rho_*^2(1 + \rho_k)}, \\
\rho_* < \rho_{k+1} & < \eta, \\
\rho_* < \rho_{k+1}, & \eta \leq \rho_k,
\end{array} \right.$$ 

where $\rho_* \approx 0.356341$, and $\eta \approx 0.475329$. Then the for any function $u$ defined on $[0, \infty) \times \Omega$ and $n \geq 2$,

$$B_n(u, u) := \sum_{k=1}^{n} \langle L_k^{\alpha,*} u, \delta_k u \rangle \geq \sum_{k=1}^{n} \frac{g_k(\alpha)}{2\Gamma(2-\alpha)} \|\delta_k u\|_{L^2(\Omega)}^2 \geq 0,$$
We split $M(3.5)$ $M(3.4)$ $\psi(3.6)$ with $\alpha$ are always positive for $\beta \in \mathbb{R}$.

Proof. According to (2.3), we can rewrite $B_n(u, u)$ in the following matrix form

$$B_n(u, u) = \sum_{k=1}^{n} \langle \mathcal{L}_k u, \delta_k u \rangle = \frac{1}{\Gamma(1 - \alpha)} \int_{\Omega} \psi M \psi^T dx,$$

where $\psi = [\delta_1 u, \delta_2 u, \ldots, \delta_n u]$, and

$$M = \begin{pmatrix}
\frac{\sigma^{1-\alpha}}{(1-\alpha) \tau_1} & c_1 + \frac{\sigma^{1-\alpha}}{(1-\alpha) \tau_2} \\
-a_1^1 & c_1^2 + \frac{\sigma^{1-\alpha}}{(1-\alpha) \tau_2} \\
-a_2^1 & d_2^2 \\
\vdots & \vdots \\
-a_n^1 & d_n^2 \\
\end{pmatrix}.$$

We split $M$ as $M = A + B$, where

$$A = \begin{pmatrix}
\beta_1 \\
-a_1^2 & \beta_2 \\
\vdots & \vdots \\
-a_n^2 & \beta_n \\
\end{pmatrix},$$

and

$$B = \text{diag} \left( \frac{\sigma^{1-\alpha}}{(1-\alpha) \tau_1} - \beta_1, c_1^2 + \frac{\sigma^{1-\alpha}}{(1-\alpha) \tau_2} - \beta_2, \ldots, c_n^2 + \frac{\sigma^{1-\alpha}}{(1-\alpha) \tau_2} - \beta_n \right),$$

with

$$2\beta_1 = -a_1^2, \quad 2\beta_2 - d_2^1 = a_1^2 - a_1^1,$$

$$2\beta_k - d_k^{k+1} = d_k^{k-1} - d_{k-1}^{k+1}, \quad 3 \leq k \leq n - 1,$$

$$2\beta_n = d_n^{n-1}, \quad n \geq 3.$$

Consider the following symmetric matrix $S = A + A^T + \varepsilon e_n^T e_n$ with small constant $\varepsilon > 0$ and $e_n = (0, \ldots, 0, 1) \in \mathbb{R}^{1 \times n}$. According to Lemma 3.1 if the condition (3.1) holds, $S$ satisfies the following three properties:

1. $\forall 1 \leq j < i \leq n, S_{i-1, j} \geq S_{i, j};$
2. $\forall 1 < j \leq i \leq n, S_{i, j-1} < S_{i, j};$
3. $\forall 1 < j < i \leq n, S_{i, j-1} - S_{i-1, j-1} \leq S_{i-1, j} - S_{i, j}.$
Furthermore, we also reformulate (3.8) and (3.9)

We first provide two equivalent forms of \( a_j^k \) according to (2.2): \( \forall 1 \leq j \leq k - 1, \)

\[
a_j^k = \int_0^1 \frac{-2\tau_j(1 - s) - \tau_{j+1}}{(\tau_j + \tau_{j+1})(t_k^* - (t_{j-1} + s\tau_j))^{\alpha}} \, ds = \frac{1}{\tau_j + \tau_{j+1}} \int_0^1 (t_k^* - (t_{j-1} + s\tau_j))^{-\alpha} \, ds
\]

and

\[
\int_0^1 \frac{-2\tau_j(1 - s) - \tau_{j+1}}{(\tau_j + \tau_{j+1})(t_k^* - (t_{j-1} + s\tau_j))^{\alpha}} \, ds = \int_0^1 \frac{-2\tau_j s - \tau_{j+1}}{(\tau_j + \tau_{j+1})(t_k^* - t_j + s\tau_j)^{\alpha}} \, ds
\]

Furthermore, we also reformulate \( c_j^k \) in (2.2) as: \( \forall 1 \leq j \leq k - 1, \)

\[
c_j^k = \int_0^1 \frac{\tau_j^2(2s - 1)}{\tau_{j+1}(\tau_j + \tau_{j+1})(t_k^* - (t_{j-1} + s\tau_j))^{\alpha}} \, ds
\]

In the following content, we consider four cases: \( k = 1, k = 2, 3 \leq k \leq n - 1, \) and \( k = n. \)

**Case 1:** When \( k = 1, \) from (2.2) and \( 2\beta_1 = -a_1^2 \) in (3.6), we have

\[
[B]_{11} = \left( \frac{\sigma^{1-\alpha}}{(1 - \alpha)\tau_1^\alpha} - \frac{1}{2} \int_0^1 \frac{2\tau_1(1 - \theta) + \tau_2}{(\tau_1 + \tau_2)(t_2^* - (t_0 + \theta\tau_1))^{\alpha}} \, d\theta \right)
\]

\[
= \left( \frac{\sigma^{1-\alpha}}{(1 - \alpha)\tau_1^\alpha} - \frac{1}{2\tau_1^\alpha} \int_0^1 \frac{2s + \rho_2}{(1 + \rho_2)(\sigma\rho_2 + s)^{\alpha}} \, ds \right)
\]

\[
> \left( \frac{\sigma^{1-\alpha}}{(1 - \alpha)\tau_1^\alpha} - \frac{1}{2\tau_1^\alpha} \int_0^1 \frac{2s + \rho_2}{(1 + \rho_2)^{\alpha}} \, ds = \frac{1}{2(1 - \alpha)(\sigma\tau_1)} \left( 2\sigma - \frac{1 - \alpha}{\rho_2^2} \right) \right).
\]

To ensure \([B]_{11} \geq 0,\) we impose

\[
2\sigma - \frac{1 - \alpha}{\rho_2^2} \geq 0.
\]
Case 2: When $k = 2$, combining $2\beta_2 - d_2^3 = a_1^3 - a_1^2$ in (3.6) and the property (P6) in Lemma 3.1 gives

$$[B]_{22} = c_1^2 + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_2^2} - \frac{1}{2}(d_2^3 + a_1^3 - a_1^2)$$

(3.11)

$$\geq \frac{1}{2}c_1^2 + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_2^2} + \frac{1}{2}(a_1^2 - a_1^3 + a_2^3) + \frac{1}{2}(c_1^2 - c_3^2)$$

To make sure $[B]_{22} \geq 0$, we impose

$$2\sigma - (1-\alpha) - \frac{\alpha(1-\alpha)}{(1+\rho_3)\rho_3^2}\int_0^1 s(\rho_3 + s)\frac{s}{\sigma\rho_3 + s} ds \geq 0.$$  

(3.13)

Case 3: When $3 \leq k \leq n - 1$, using $2\beta_k = d_k^{k+1} + d_{k-1}^{k+1} - d_{k-1}^{k+1}$ in (3.6) and $d_j = c_{j-1}^k - a_j^k$, we have

$$[B]_{kk} = \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_k^2} + \frac{1}{2}c_{k-1}^k + \frac{1}{2}(c_{k-1}^k - d_k^{k+1} - d_{k-1}^{k+1})$$

(3.14)

$$= \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_k^2} + \frac{1}{2}c_{k-1}^k + \frac{1}{2}[(c_{k-1}^k - c_{k-1}^{k+1} - (c_{k-1}^k - c_{k-1}^{k+1} + (a_{k-1}^{k+1} + a_{k}^{k+1} + a_{k-1}^{k+1})].$$

From (3.7) - (3.9), if (3.1) holds for $j = k - 1$, we have

$$\int_0^1 s(\rho_3 + s)\frac{s}{\sigma\rho_3 + s} ds \geq 0.$$  

(3.15)
Then we can get the following result:

Moreover the convexity of the function $t^{-\alpha} - (t^*_{k+1} - t_{k-1} + s\tau_{k-1})^{-\alpha-1}$ can be derived as follows. For fixed $\tau$, we use the forms (3.7) for $a_k^{k+1}$ and (3.8) for $a_k^{k+1}$. The first inequality in (3.15) can be derived as follows. For fixed $j$, it is easy to see that

$$\int_0^1 (t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} - (t_{k+1}^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} ds > 0$$

decreases w.r.t. $s$ and $\int_0^1 (1 - 3s)(1 - s) = 0$, thus

$$\int_0^1 (1 - s)(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} - (t_{k+1}^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} ds \geq \int_0^1 (4\tau_{k-1} + 3\tau_k)(1 - s)(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} - (t_{k+1}^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} ds.$$

Moreover the convexity of the function $t^{-\alpha}$ gives

$$(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} - (t_{k+1}^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} > (t_k^* - t_{k-2} + s\tau_{k-2})^{-\alpha-1} - (t_{k+1}^* - t_{k-2} + s\tau_{k-2})^{-\alpha-1},$$

Then we can get the following result:

$$\int_0^1 (1 - s)(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} - (t_{k+1}^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} ds \geq \int_0^1 (4\tau_{k-1} + 3\tau_k)(1 - s)(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} - (t_{k+1}^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} ds.$$

Moreover the convexity of the function $t^{-\alpha}$ gives

$$(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} - (t_{k+1}^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} > (t_k^* - t_{k-2} + s\tau_{k-2})^{-\alpha-1} - (t_{k+1}^* - t_{k-2} + s\tau_{k-2})^{-\alpha-1},$$

Then we can get the following result:

$$\int_0^1 s(1 - s)\left[(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} - (t_{k+1}^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1}\right] ds$$
as (3.1) for \(j = k - 1\) gives
\[
\frac{\tau_k^3}{\tau_k \left( \tau_k + \tau_k \right)} \geq \frac{\tau_k^3}{\tau_k \left( \tau_k + \tau_k \right)} + \frac{4\tau_k - 3\tau_k \tau_k \geq 0.}
\]
Combining (3.15) with (3.14) yields
\[
[B]_{kk} \geq \frac{1}{2} c_k^2 - \frac{1}{2} \frac{1}{\tau_k + \tau_k} \left( 2\sigma - (1 - \alpha) - \frac{\alpha(1 - \alpha)}{(1 + \rho_k + \rho_k \alpha)} \right) \int_0^1 s \left( \rho_k + s \right) ds.
\]
Thus, to ensure \(B_{kk} \geq 0\) for \(3 \leq k \leq n - 1\), it is sufficient to impose
\[
\frac{1}{\rho_k} \geq \frac{1}{\rho_k - 1 \pm (1 + \rho_k) - 3},
\]
(3.16)
\[
2\sigma - (1 - \alpha) - \frac{\alpha(1 - \alpha)}{(1 + \rho_k + \rho_k \alpha)} \int_0^1 s \left( \rho_k + s \right) ds \geq 0.
\]
**Case 4:** When \(k = n\), we show \([B]_{nn} \geq 0\) under some constraints on \(\rho_n\). From (3.6), (3.7) and (3.9), we can derive
(3.17)
\[
[B]_{nn} = c_n^2 - \frac{1}{(1 - \alpha)\tau_n^\alpha} \left[ \frac{\sigma^\alpha}{\tau_n^\alpha} - \frac{1}{(1 - \alpha)\tau_n^\alpha} \left( c_n^2 - a_n^2 \right) \right]
\]
\[
= \frac{1}{2} c_n^2 - \frac{1}{2} \frac{\sigma^\alpha}{\tau_n^\alpha} + \frac{1}{2} \left( c_n^2 - c_n^2 + a_n^2 \right) + \frac{1}{2} \left( \tau_n + \tau_n + \tau_n \right) \int_0^1 s \left( 1 - s \right) (t^n_e - t_n - s \tau_n)^{-\alpha} ds
\]
\[
- \frac{\alpha \tau_n}{\tau_n \left( \tau_n + \tau_n - 1 \right)} \int_0^1 s \left( 1 - s \right) (t^n_e - t_n - s \tau_n - 1)^{-\alpha} ds
\]
\[
- \left( \sigma \tau_n \right)^{-\alpha} + \frac{\alpha \tau_n}{\tau_n \left( \tau_n + \tau_n \right)} \int_0^1 \left( \tau_n + \tau_n + s \tau_n - 1 \right) (1 - s) \left( t^n_e - t_n - s \tau_n - 1 \right)^{-\alpha} ds
\]
\[
\geq \frac{1}{2} c_n^2 - \frac{1}{2} \frac{1}{(1 - \alpha)\sigma \tau_n^\alpha} \left( 2\sigma - (1 - \alpha) \right),
\]
if (3.1) holds for \(j = n - 1\). The proof of the last inequality in (3.17) is similar to the previous proof of (3.15), where we use the facts
\[
\int_0^1 (\tau_n + \tau_n + s \tau_n - 1) (1 - s) (t^n_e - t_n - s \tau_n - 1)^{-\alpha} ds
\]
\[
\geq \int_0^1 (4 \tau_n + 3 \tau_n) s (1 - s) (t^n_e - t_n - s \tau_n)^{-\alpha} ds,
\]
and
\[
(t^n_e - t_n - s \tau_n - 1)^{-\alpha} > (t^n_e - t_n - s \tau_n - 2)^{-\alpha}.
\]
We omit the details here. To ensure \([B]_{nn} \geq 0\), it is sufficient to impose
(3.18)
\[
\frac{1}{\rho_n} \geq \frac{1}{\rho_n^2 (1 + \rho_n)} - 3, \quad 2\sigma - (1 - \alpha) \geq 0.
\]
Combining (3.10), (3.13), (3.16) and (3.18), we can conclude that if the condition (3.1) holds for $3 \leq k \leq n$ and

\begin{equation}
2\sigma - \frac{1 - \alpha}{\rho^2} \geq 0,
\end{equation}

\begin{equation}
2\sigma - (1 - \alpha) - \frac{\alpha(1 - \alpha)}{(1 + \rho_{k+1})\rho_{k+1}^2} \int_0^1 \frac{s(\rho_{k+1} + s)}{\sigma\rho_{k+1} + s} \, ds \geq 0, \quad 2 \leq k \leq n - 1,
\end{equation}

then $[B]_{kk} \geq 0$, $k \geq 1$. We have proved the following results:

- Positive semidefiniteness of $A + A^T$: (3.1) holds;
- Positive definiteness of $B$: (3.19) holds and (3.1) holds for $3 \leq k \leq n$;

which ensure

$$M + M^T = (A + A^T) + 2B \geq 2B \geq (1 - \alpha)^{-1}\text{diag} (g_1(\alpha), g_2(\alpha), \ldots, g_n(\alpha)) \geq 0,$$

where $g_k(\alpha)$ is given in (3.4). In the following content, we just simplify the above constraints for the positive semidefiniteness of $M + M^T$.

The condition (3.1) actually says that $(\rho_j, \rho_{j+1})$ lies on the right-hand side of the blue solid curve in Figure 1. Let $\rho_* \approx 0.356341$ be the root of $\rho(1+\rho) = 1 - 3\rho^2(1+\rho)$. It can be found that if $\rho_j \leq \rho_*$ for some $j$, then $\rho_* \geq \rho_j \geq \rho_{j+1} \geq \rho_{j+2} \geq \ldots$ and $\tau_j$ will shrink to 0 quickly as $j$ increases. This doesn’t make sense in practice. We shall impose $\rho_j > \rho_*$, $\forall j \geq 2$. As a consequence, we have the following constraints:

\begin{equation}
\begin{aligned}
\rho_* &< \rho_{j+1} \leq \frac{\rho_j^2(1 + \rho_j)}{1 - 3\rho_j^2(1 + \rho_j)}, & \rho_* < \rho_j < \eta, \\
\rho_* &< \rho_{j+1}, & \eta \leq \rho_j,
\end{aligned}
\end{equation}

where $\eta \approx 0.475329$ be the unique positive root of $1 - 3\rho^2(1 + \rho) = 0$.
We now prove that \((3.20)\) leads to \((3.19)\) when \(\sigma = 1 - \alpha/2 \geq 1/2\). In fact, it is easy to check that
\[
2\sigma - \frac{1 - \alpha}{\rho^2} \geq 2 - \alpha - \frac{1 - \alpha}{\rho^*} \geq 0, \quad 2\sigma - (1 - \alpha) = 1,
\]
and for \(2 \leq k \leq n - 1\), we have
\[
2\sigma - (1 - \alpha) - \frac{\alpha(1 - \alpha)}{(1 + \rho_{k+1})\rho^*_k} \int_0^1 s(\rho_{k+1} + s) \sigma \rho_{k+1} + s \, ds \geq 1 - \frac{\alpha(1 - \alpha)}{(1 + \rho_{k+1})\rho^*_k} \geq 1 - \frac{1}{4(1 + \rho_*)\rho_*} \geq 0.
\]
In summary, if \((3.20)\) holds, then
\[
B_n(u, u) = \sum_{k=1}^n (L_k^\alpha u, \delta_k u) \geq \sum_{k=1}^n \frac{g_k(\alpha)}{2\Gamma(2 - \alpha)} \|\delta_k u\|^2_{L^2(\Omega)} \geq 0,
\]
with \(g_k(\alpha)\) given in \((3.4)\).

\[\square\]

**Remark 3.3.** If \(\rho_k \geq \eta \approx 0.475329\) for all \(k \geq 2\), then the condition \((3.2)\) holds, for which the positive semidefiniteness of bilinear form \(B_n(u, u)\) \((3.3)\) can be guaranteed.

4. **Stability and Convergence of L2-1σ Method for Subdiffusion Equation**

We consider the following subdiffusion equation:
\[
\begin{align*}
\partial_t^\alpha u(t, x) &= \Delta u(t, x) + f(t, x), \quad (t, x) \in (0, \infty) \times \Omega, \\
u(t, x) &= 0, \quad (t, x) \in (0, \infty) \times \partial \Omega, \\
\eta(0, x) &= \eta_0(x), \quad x \in \Omega,
\end{align*}
\]
(4.1)
where \(\Omega\) is a bounded Lipschitz domain in \(\mathbb{R}^d\). Given an arbitrary nonuniform mesh \(\{\tau_k\}_{k \geq 1}\), the L2-1σ scheme of this subdiffusion equation is written as
\[
L_k^{\alpha, *} u = (1 - \alpha/2)\Delta u^k + \alpha/2\Delta u^{k-1} + f^k, \quad \text{in } \Omega,
\]
(4.2)
where \(f^k = f(t_k^*, \cdot)\).

4.1. **H1-stability of the L2-1σ scheme.**

**Theorem 4.1.** Assume that \(f(t, x) \in L^\infty([0, \infty); L^2(\Omega)) \cap BV([0, \infty); L^2(\Omega))\) is a bounded variation function in time and \(u^0 \in H^{1/2}_0(\Omega)\). If the nonuniform mesh \(\{\tau_k\}_{k \geq 1}\) satisfies \((3.2)\) (for example \(\rho_k \geq \eta \approx 0.475329\) for \(k \geq 2\)), then the numerical solution \(u^n\) of the L2-1σ scheme \((4.2)\) satisfies the following H1-stability
\[
\|\nabla u^n\|_{L^2(\Omega)} \leq \|\nabla u^0\|_{L^2(\Omega)} + 2C_fC_\Omega,
\]
where \(C_f\) depends on the source term \(f\), \(C_\Omega\) is the Sobolev embedding constant depending on \(\Omega\) and the spatial dimension \(d\).
Proof. When \( n = 1 \), we have
\[
(4.3) \quad \frac{\sigma^1 - \alpha \delta_k u}{\Gamma(2 - \alpha) \tau_1^a} = (1 - \alpha/2) \Delta u^1 + \alpha/2 \Delta u^0 + f^1.
\]
Multiplying (4.3) with (4.4) and summing up the derived equations over \( C \) where
\[
\frac{\sigma^1 - \alpha \delta_k u}{\Gamma(2 - \alpha) \tau_1^a} = -\frac{1}{2} \| \nabla u^1 \|^2_{L^2(\Omega)} + \frac{1}{2} \| \nabla u^0 \|^2_{L^2(\Omega)} - \frac{1}{2} \| \nabla \delta_k u \|^2_{L^2(\Omega)} + \langle f^1, \delta_k u \rangle.
\]
Applying Cauchy–Schwarz inequality, we can derive
\[
\| \nabla u^1 \|^2_{L^2(\Omega)} \leq \| \nabla u^0 \|^2_{L^2(\Omega)} + 4 \| f \|_{L^\infty((0,\infty);L^2(\Omega))} \max_{0 \leq k \leq 1} \| u_k \|_{L^2(\Omega)}
\]
\[
\leq \| \nabla u^0 \|^2_{L^2(\Omega)} + 4 \| f \|_{L^\infty((0,\infty);L^2(\Omega))} C_\Omega \max_{0 \leq k \leq 1} \| u_k \|_{L^2(\Omega)},
\]
where \( C_\Omega \) is the Sobolev embedding constant depending on \( \Omega \) and the spatial dimension.

Now we turn to the case \( n \geq 2 \). Multiplying (4.2) with \( \delta_k u \), integrating over \( \Omega \), and summing up the derived equations over \( k \) yield
\[
\sum_{k=1}^n \langle L_k^n u, \delta_k u \rangle = \sum_{k=1}^n \left( (1 - \alpha/2) \Delta u_k + \alpha/2 \Delta u_k^{k-1}, \delta_k u \right) + \sum_{k=1}^n \langle f^k, \delta_k u \rangle
\]
\[
= -\frac{1}{2} \| \nabla u^n \|^2_{L^2(\Omega)} + \frac{1}{2} \| \nabla u^0 \|^2_{L^2(\Omega)} - \frac{1}{2} \sum_{k=1}^n \| \nabla \delta_k u \|^2_{L^2(\Omega)}
\]
\[
+ \langle f^n, u^n \rangle - \langle f^1, u^0 \rangle - \sum_{k=2}^n \langle \delta_k f, u^{k-1} \rangle.
\]
Applying the Cauchy–Schwarz inequality yields
\[
\langle f^n, u^n \rangle - \langle f^1, u^0 \rangle + \sum_{k=2}^n \langle \delta_k f, u^{k-1} \rangle
\]
\[
\leq \left( 2 \| f \|_{L^\infty((0,\infty);L^2(\Omega))} + \| f \|_{BV((0,\infty);L^2(\Omega))} \right) \max_{0 \leq k \leq n} \| u_k \|_{L^2(\Omega)}
\]
\[
\leq C_f C_\Omega \max_{0 \leq k \leq n} \| \nabla u_k \|_{L^2(\Omega)},
\]
where \( C_f = 2 \| f \|_{L^\infty((0,\infty);L^2(\Omega))} + \| f \|_{BV((0,\infty);L^2(\Omega))} \). From Theorem 3.2 we then have for \( n \geq 2 \),
\[
(4.5) \quad \| \nabla u^n \|^2_{L^2(\Omega)} \leq \| \nabla u^0 \|^2_{L^2(\Omega)} - (1 - \alpha) \sum_{k=1}^n \| \nabla \delta_k u \|^2_{L^2(\Omega)} - \sum_{k=1}^n \frac{g_k(\alpha)}{\Gamma(2 - \alpha)} \| \delta_k u \|^2_{L^2(\Omega)}
\]
\[
+ 2 C_f C_\Omega \max_{0 \leq k \leq n} \| \nabla u_k \|_{L^2(\Omega)}
\]
\[
\leq \| \nabla u^0 \|^2_{L^2(\Omega)} + 2 C_f C_\Omega \max_{0 \leq k \leq n} \| \nabla u_k \|_{L^2(\Omega)}.
\]
Note that (4.4) implies that (4.5) also holds for \( n = 1 \). For any \( N \geq 1 \), we take \( \max_{0 \leq n \leq N} \) on both sides of (4.5) to obtain
\[
\max_{0 \leq n \leq N} \| \nabla u^n \|^2_{L^2(\Omega)} \leq \| \nabla u^0 \|^2_{L^2(\Omega)} + 2 C_f C_\Omega \max_{0 \leq n \leq N} \| \nabla u^n \|_{L^2(\Omega)},
\]
which indicates
\[
\max_{0 \leq n \leq N} \| \nabla u^n \|_{L^2(\Omega)} \leq C_f C_\Omega + \sqrt{(C_f C_\Omega)^2 + \| \nabla u^0 \|^2_{L^2(\Omega)}} \leq \| \nabla u^n \|_{L^2(\Omega)} + 2C_f C_\Omega.
\]

The proof is completed. \hfill \Box

Remark 4.2. Assume that the solution of subdiffusion equation satisfies \( u(t, x) \in C([0, \infty); H^1_0(\Omega)) \cap C^1((0, \infty); H^1_0(\Omega)) \) and the source term satisfies \( f(t, x) \in C([0, \infty); L^2(\Omega)), \ \partial_t f(t, x) \in L^1([0, \infty); L^2(\Omega)) \). For any fixed \( T > 0 \), multiplying the first equation of (4.1) with \( \partial_t u(t, x) \) and integrating over \((0, T) \times \Omega\) yield
\[
\int_0^T \int_{\Omega} \partial_t^2 u(t, x) \partial_t u(t, x) \, dx \, dt = \frac{1}{2} \int_0^T \int_{\Omega} \partial_t |\nabla u(t, x)|^2 \, dx \, dt + \int_0^T \int_{\Omega} f(t, x) \partial_t u(t, x) \, dx \, dt.
\]

According to [25],
\[
\int_0^T \int_{\Omega} \partial_t^2 u(t, x) \partial_t u(t, x) \, dx \, dt \geq 0,
\]
and moreover,
\[
\int_0^T \int_{\Omega} f(t, x) \partial_t u(t, x) \, dx \, dt
\]
\[
= \left( \int_{\Omega} f(t, x) u(t, x) \, dx \right) \bigg|_0^T - \int_0^T \int_{\Omega} \partial_t f(t, x) u(t, x) \, dx \, dt
\]
\[
\leq \left( 2 \| f \|_{L^\infty([0, \infty); L^2(\Omega))} + \int_0^\infty \| \partial_t f(t, x) \|_{L^2(\Omega)} \, dt \right) C_\Omega \| \nabla u \|_{L^\infty([0, T]; L^2(\Omega))}
\]
\[
=: C_f^{cont} C_\Omega \| \nabla u \|_{L^\infty([0, T]; L^2(\Omega))}.
\]

Thus we derive the \( H^1 \)-stability at the continuous level
\[
\| \nabla u(T, x) \|_{L^2(\Omega)} \leq \| \nabla u(0, x) \|_{L^2(\Omega)} + 2C_f^{cont} C_\Omega, \quad \forall \ T > 0,
\]
which corresponds to our \( H^1 \)-stability result in Theorem 4.1 for the L2-1\( _\sigma \) scheme of the subdiffusion equation (4.1).

Remark 4.3. In the case of \( \alpha = 1 \), i.e., the standard diffusion equation, the energy stability (or \( H^1 \)-stability) has been established for the second order BDF2 schemes in [14, Theorem 2.1] and for the third order BDF3 schemes in [16, Theorem 3.1] on general nonuniform meshes.

4.2. Global convergence of the L2-1\( _\sigma \) scheme. We show the error estimate of the L2-1\( _\sigma \) scheme for the subdiffusion equation (4.1), that is different from the one in [14, Theorem 2.1]. To be precise we will reduce the restriction on time step ratios from \( \rho_k \geq 4/7 \) in [14] to \( \rho_k \geq 0.475329 \). We first reformulate the discrete fractional operator (2.3):
\[
L_k^{\alpha, \sigma} u = \frac{1}{\Gamma(1 - \alpha)} \left( [M]_{k,j} u^n - \sum_{j=2}^k ([M]_{k,j} - [M]_{k,j-1}) u^{n-j} - [M]_{k,1} u^0 \right),
\]
where \( M \) is given by (3.5). We now give some properties on \([M]_{k,j}\).

Lemma 4.4. Under the condition (3.2), the following properties of \([M]_{k,j}\) given by (3.5) hold:
\[(Q1)\]
\[|M|_{k,j} \geq \frac{\rho_\ast}{(1 + \rho_\ast)\tau_j} \int_{t_j-1}^{\min\{t_j, t_k\}} (t_k^* - s)^{-\alpha} ds, \quad 1 \leq j \leq k.\]

\[(Q2)\] For all \(2 \leq j \leq k - 1,\)
\[|M|_{k,j} - |M|_{k,j-1} \geq \frac{\alpha \tau_j}{\tau_j + \tau_{j+1}} \int_0^1 (\tau_j + \tau_{j+1} - s\tau_j)(1 - s)(t_k^* - t_{j-1} - s\tau_j)^{-\alpha - 1} ds,\]
and
\[|M|_{k,k} - |M|_{k,k-1} \geq \frac{\alpha}{2(1 - \alpha)(\sigma\tau_k)^\alpha}.\]

\[(Q3)\] Moreover, if \(\rho_k \geq \eta \approx 0.475329\) for all \(k \geq 2,\) then
\[\frac{1 - \alpha}{\sigma} |M|_{k,k} - |M|_{k,k-1} \geq 0.\]
Here \(\eta\) is the real root of \(1 - 3\rho^2(1 + \rho) = 0.\)

**Proof.** From \([3.5]\), for \(1 \leq j \leq k - 1,\)
\[|M|_{k,j} \geq -a_j^n = \int_0^1 \frac{2\tau_j(1 - \theta) + \tau_{j+1}}{(\tau_j + \tau_{j+1})(t_k^* - (t_{j-1} + \theta\tau_j))^{\alpha}} d\theta\]
\[\geq \frac{\rho_{j+1}}{1 + \rho_{j+1}} \int_0^1 \frac{1}{(t_k^* - (t_{j-1} + \theta\tau_j))^{\alpha}} d\theta \geq \frac{\rho_\ast}{(1 + \rho_\ast)\tau_j} \int_{t_{j-1}}^{t_j} (t_k^* - s)^{-\alpha} ds,\]
and for \(j = k,\)
\[|M|_{k,k} = c_{k-1}^\ast + \frac{\sigma^{1-\alpha}}{(1 - \alpha)\tau_k^n} \geq \frac{\sigma^{1-\alpha}}{(1 - \alpha)\tau_k^n} = \frac{1}{\tau_k} \int_{t_{k-1}}^{t_k} (t_k^* - s)^{-\alpha} ds.\]
The inequality \((4.6)\) holds.
For \(2 \leq j \leq k - 1,\) according to \([3.7, 3.9],\)
\[|M|_{k,j} - |M|_{k,j-1}\]
\[= \frac{\alpha \tau_j^3}{\tau_j(\tau_{j-1} + \tau_j)} \int_0^1 s(1 - s)(t_k^* - t_{j-1} + s\tau_{j-1})^{-\alpha - 1} ds\]
\[- \frac{\alpha \tau_j^2}{\tau_{j-1}(\tau_{j-2} + \tau_{j-1})} \int_0^1 s(1 - s)(t_k^* - t_{j-2} + s\tau_{j-2})^{-\alpha - 1} ds\]
\[+ \frac{\alpha \tau_j}{\tau_{j-1} + \tau_j} \int_0^1 (\tau_j + \tau_{j+1} + s\tau_j)(1 - s)(t_k^* - t_{j-1} + s\tau_{j-1})^{-\alpha - 1} ds\]
\[+ \frac{\alpha \tau_j}{\tau_j + \tau_{j+1}} \int_0^1 (\tau_j + \tau_{j+1} + s\tau_j)(1 - s)(t_k^* - t_{j-1} - s\tau_j)^{-\alpha - 1} ds,\]
under the condition \((3.2)\) (for simplicity we make a convention that \(\tau_0 = 0\)). Note that \((3.2)\) indicates the sum of first three terms is positive, using the techniques in \((3.17)\). When \(j = k = 2,\) we obtain from \((3.7)\)
\[|M|_{2,2} - |M|_{2,1} = c_1^2 + \frac{\sigma^{1-\alpha}}{(1 - \alpha)\tau_2^n} + a_1^2 \geq \frac{\sigma^{1-\alpha}}{(1 - \alpha)\tau_2^n} - \frac{1}{(\sigma\tau_2)^\alpha} = \frac{\alpha}{2(1 - \alpha)(\sigma\tau_2)^\alpha}.\]
where we use the fact \( \sigma = 1 - \alpha/2 \). Moreover when \( j = k \geq 3 \), we have
\[
[M]_{k,k} - [M]_{k,k-1} = \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_k^\alpha} + (c_{k-1} - c_{k-2} + a_{k-1})
\]
\[
= \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_k^\alpha} + \left( \frac{\alpha\tau_k^3}{\tau_k(\tau_k - \tau_k)} \right) \int_0^1 s(1-s)(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} \, ds
\]
\[
- \frac{\alpha\tau_k^3}{\tau_{k-1}(\tau_k - \tau_{k-1})} \int_0^1 s(1-s)(t_k^* - t_{k-2} + s\tau_{k-2})^{-\alpha-1} \, ds
\]
\[
- (\sigma\tau_k)^{-\alpha} + \frac{\alpha\tau_k}{\tau_{k-1} + \tau_k} \int_0^1 (\tau_k - \tau_k + s\tau_{k-1})(1-s)(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} \, ds
\]
\[
> \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_k^\alpha} - \frac{1}{(\sigma\tau_k)^\alpha} = \frac{\alpha}{2(1-\alpha)(\sigma\tau_k)^\alpha},
\]
when the condition (3.2) holds. This inequality coincide with (3.17) by replacing \( \alpha \) with \( k \).

For the property (Q3), the case of \( k = 2 \) is trivial. In the case of \( k \geq 3 \), we have
\[
\frac{1-\alpha}{\sigma}[M]_{k,k} - [M]_{k,k-1}
\]
\[
\geq (\sigma\tau_k)^{-\alpha} - c_{k-2} + a_{k-1}
\]
\[
= (\sigma\tau_k)^{-\alpha} - \frac{\alpha\tau_k^3}{\tau_{k-1}(\tau_k - \tau_{k-1})} \int_0^1 s(1-s)(t_k^* - t_{k-2} + s\tau_{k-2})^{-\alpha-1} \, ds
\]
\[
- (\sigma\tau_k)^{-\alpha} + \frac{\alpha\tau_k}{\tau_{k-1} + \tau_k} \int_0^1 (\tau_k - \tau_k + s\tau_{k-1})(1-s)(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} \, ds
\]
\[
> \alpha \left( \frac{\tau_k - 4\tau_k + 3\tau_k}{\tau_{k-1} + \tau_k} - \frac{\tau_k^3}{\tau_{k-1}(\tau_k - \tau_{k-1})} \right) \int_0^1 s(1-s)(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} \, ds
\]
\[
\geq 0,
\]
where we use the facts
\[
\int_0^1 (\tau_{k-1} + \tau_k + s\tau_{k-1})(1-s)(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} \, ds
\]
\[
\geq (4\tau_{k-1} + 3\tau_k) \int_0^1 s(1-s)(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} \, ds,
\]
\[
(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} \geq (t_k^* - t_{k-2} + s\tau_{k-2})^{-\alpha-1},
\]
and
\[
\frac{\tau_{k-1}(4\tau_{k-1} + 3\tau_k)}{\tau_{k-1} + \tau_k} - \frac{\tau_k^3}{\tau_{k-1}(\tau_k - \tau_{k-1})} \geq 0,
\]
when \( \rho_k \geq \eta \approx 0.475329 \) for all \( k \geq 2 \).

\[\square\]

Consider the following three standard Lagrange interpolation operators with the following interpolation points:
\[
\Pi_{1,j} : t_{j-1}, t_j, \quad \Pi_{2,j} : t_{j-1}, t_j, t_{j+1}, \quad \Pi_{3,j} : t_{j-1}, t_j, t_{j+1}.
\]
As stated in [10], when $\sigma = 1 - \alpha/2$, 
\[
\int_{t_{k-1}}^{t_k} (\Pi_{1,k} v - \Pi_{2,k} v)'(s)(t_k - s)^{-\alpha} \, ds = 0.
\]

We now analyze the approximation error of the discrete fractional operator in the following lemma.

**Lemma 4.5.** Given a function $u$ satisfying $|\partial_s^\alpha u(t)| \leq C(1 + t^{\alpha-1})$ for $l = 1, 3$ and nonuniform mesh $\{\tau_k\}_{k \geq 1}$ satisfying condition [3.2], the approximation error is given by

\[
(4.8) \quad r_k := \frac{1}{\Gamma(1 - \alpha) \Gamma(\alpha)} \int_0^{t_k} (t_k - s)^{-\alpha} \partial_s[u(s) - I_2 u(s)] \, ds, \quad k \geq 1,
\]

where $I_2 u = \Pi_{2,j} u$ on $(t_{j-1}, t_j)$ for $j < k$ and $I_2 u = \Pi_{2,k} u$ on $(t_{k-1}, t_k)$. Then for $k \geq 1$,

\[
(4.9) \quad |r_k| \leq \frac{C}{\Gamma(1 - \alpha)} \left( |M|_{k,1} (t_2^{\alpha}/\alpha + t_2) + \sum_{j=2}^k (|M|_{k,j} - |M|_{k,j-1})(1 + \rho_{j+1})(1 + t_j^{\alpha-3})r_j^3 \right),
\]

where $C$ is a constant depending on $C_l$ for $l = 1, 3$ and $\rho_{k+1} = 1$.

**Proof.** The case of $k = 1$ is trivial. We now consider the case of $k \geq 2$. Let $\chi(s) := u - I_2 u$. Three subcases are discussed in the following content.

1. **Subcase 1.** On the interval $(t_0, t_1)$, we have

\[
\partial_s I_2 u(s) = \frac{2s - t_1 - t_2}{\tau_1(\tau_1 + \tau_2)} u(t_0) - \frac{2s - t_2}{\tau_1 \tau_2} u(t_1) + \frac{2s - t_1}{\tau_2(\tau_1 + \tau_2)} u(t_2)
\]

that is linear w.r.t. $s$. Then we have

\[
|\partial_s I_2 u(s)| \leq \max\{|\partial_s I_2 u(t_0)|, |\partial_s I_2 u(t_1)|\} \leq C_1 \frac{1 + \rho_2^2}{\tau_1 \rho_2},
\]

where we use the facts

\[
\partial_s I_2 u(t_0) = -\frac{2\tau_1 + \tau_2}{\tau_1(\tau_1 + \tau_2)} u(t_0) + \frac{\tau_1 + \tau_2}{\tau_1 \tau_2} u(t_1) - \frac{\tau_1}{\tau_2(\tau_1 + \tau_2)} u(t_2)
\]

\[
= -\frac{2\tau_1 + \tau_2}{\tau_1(\tau_1 + \tau_2)} (u(t_0) - u(t_1)) + \frac{\tau_1}{\tau_2(\tau_1 + \tau_2)} (u(t_1) - u(t_2))
\]

\[
\leq \left( \frac{2\tau_1 + \tau_2}{\tau_1(\tau_1 + \tau_2)} + \frac{\tau_1}{\tau_2(\tau_1 + \tau_2)} \right) \max\{|u(t_0) - u(t_1)|, |u(t_1) - u(t_2)|\}
\]

\[
= \frac{\tau_1 + \tau_2}{\tau_1 \tau_2} \max\{|u(t_0) - u(t_1)|, |u(t_1) - u(t_2)|\},
\]

\[
\partial_s I_2 u(t_1) = -\frac{\tau_2}{\tau_1(\tau_1 + \tau_2)} u(t_0) - \frac{\tau_1 - \tau_2}{\tau_1 \tau_2} u(t_1) + \frac{\tau_1}{\tau_2(\tau_1 + \tau_2)} u(t_2)
\]

\[
= -\frac{\tau_2}{\tau_1(\tau_1 + \tau_2)} (u(t_0) - u(t_1)) - \frac{\tau_1}{\tau_2(\tau_1 + \tau_2)} (u(t_1) - u(t_2))
\]

\[
\leq \left( \frac{\tau_2}{\tau_1(\tau_1 + \tau_2)} + \frac{\tau_1}{\tau_2(\tau_1 + \tau_2)} \right) \max\{|u(t_0) - u(t_1)|, |u(t_1) - u(t_2)|\}
\]

\[
= \frac{\tau_1^2 + \tau_2^2}{\tau_1 \tau_2(\tau_1 + \tau_2)} \max\{|u(t_0) - u(t_1)|, |u(t_1) - u(t_2)|\},
\]

...
\[|u(t_0) - u(t_1)| = \left| \int_0^{t_1} \partial_s u(s) \, ds \right| \leq C_1(\tau_1 + \tau_1^\alpha / \alpha),\]
\[|u(t_1) - u(t_2)| = \left| \int_{t_1}^{t_2} \partial_s u(s) \, ds \right| \leq C_1(\tau_2 + (t_2^\alpha - t_1^\alpha) / \alpha).\]

Therefore, we have
\[|\partial_s \chi(s)| \leq |\partial_s u| + |\partial_s I_2u| \leq C_1 \left( s^{\alpha - 1} + 1 + \frac{1 + \rho_2}{\tau_1 \rho_2} (t_2 + t_2^\alpha / \alpha) \right),\]
which yields
\[(4.10)\]
\[\left| \frac{1}{\Gamma(1 - \alpha)} \int_0^{t_1} (t_k^\alpha - s)^{-\alpha} \partial_s \chi(s) \, ds \right| \leq \frac{C_1}{\Gamma(1 - \alpha)} \left( \int_0^{t_1} s^{\alpha - 1} (t_k^\alpha - s)^{-\alpha} \, ds + \frac{\tau_1 + (1 + \rho_2) / \rho_2 (t_2 + t_2^\alpha / \alpha)}{\tau_1} \int_0^{t_1} (t_k^\alpha - s)^{-\alpha} \, ds \right) \leq \frac{C_1}{\Gamma(1 - \alpha)} \left( \frac{\tau_1^\alpha}{\alpha (t_k^\alpha - \tau_1)^\alpha} + \frac{\tau_1 + (1 + \rho_2) / \rho_2 (t_2 + t_2^\alpha / \alpha)}{\tau_1} \int_0^{t_1} (t_k^\alpha - s)^{-\alpha} \, ds \right) \leq \frac{C(t_2^\alpha + t_2)}{\Gamma(1 - \alpha)} |M|_{k,1},\]
where \(C\) is an absolute constant only depending on \(C_1\). In the last inequality of (4.10), we use the fact
\[|M|_{k,1} \geq \frac{\rho_2}{(1 + \rho_2) \tau_1} \int_0^{t_1} (t_k^\alpha - s)^{-\alpha} \, ds \geq \frac{\rho_2}{(1 + \rho_2) (t_k^\alpha)^\alpha} \geq \frac{\rho_2^{1-\alpha}}{(1 + \rho_2) (2 + \rho_2)^\alpha (t_k^\alpha - \tau_1)^\alpha} \geq (1 + \rho_2) (2 + \rho_2)^\alpha (t_k^\alpha - \tau_1)^\alpha \]
obtained from the inequality (4.7).

**Subcase 2.** On the interval \((t_{j-1}, t_j), 2 \leq j \leq k - 1,\)
\[|\chi(s)| = \frac{|u^{(3)}(\xi)|}{6} (s - t_{j-1})(s - t_j) \leq C_3 (t_{j-1}^\alpha)(s - t_{j-1})(s - t_j)(s - t_{j+1}),\]
where \(\xi \in (t_{j-1}, t_{j+1})\). Then we have
\[(4.11) \left| \frac{1}{\Gamma(1 - \alpha)} \int_{t_{j-1}}^{t_j} (t_k^\alpha - s)^{-\alpha} \partial_s \chi(s) \, ds \right| = \left| \frac{-\alpha}{\Gamma(1 - \alpha)} \int_{t_{j-1}}^{t_j} (t_k^\alpha - s)^{-\alpha-1} \chi(s) \, ds \right| \leq \frac{C_3 \alpha (1 + t_{j-1}^\alpha)^3}{\Gamma(1 - \alpha)} \int_{t_{j-1}}^{t_j} (t_k^\alpha - s)^{-\alpha-1} (s - t_{j-1})(s - t_j)(s - t_{j+1}) \, ds \leq \frac{C_3 \alpha (1 + t_{j-1}^\alpha)^3 \tau_j^3}{\Gamma(1 - \alpha)} \int_0^1 s(\tau_j + \tau_{j+1} - s \tau_j)(1 - s)(t_k^\alpha - t_{j-1} - s \tau_j)^{-\alpha-1} \, ds \leq \frac{C_3 (1 + \rho_{j+1})(1 + t_{j-1}^\alpha) \tau_j^3}{\Gamma(1 - \alpha)} (|M|_{k,j} - |M|_{k,j-1}),\]
from (Q2) in Lemma 4.4.

**Subcase 3.** On the interval \((t_{k-1}, t_k),\)
\[|\chi(s)| \leq C_3 (1 + t_{k-1}^\alpha)(s - t_{k-1})(t_k^\alpha - s) \leq C_3 (1 + t_{k-1}^\alpha) \tau_k^2 (t_k^\alpha - s),\]
which yields
(4.12)
\[
\frac{1}{\Gamma(1 - \alpha)} \int_{t_k-1}^{t_k} (t^*_k - s)^{-\alpha} \partial_s \chi(s) \, ds = \frac{-\alpha}{\Gamma(1 - \alpha)} \int_{t_k-1}^{t_k} (t^*_k - s)^{-\alpha - 1} \chi(s) \, ds
\]
\[
\leq C_3 \alpha (1 + \frac{t^*_{k-3}}{t^*_k})^2 \int_{t_k-1}^{t_k} (t^*_k - s)^{-\alpha} \, ds = \frac{2C_3 \sigma (1 + \frac{t^*_{k-3}}{t^*_k})^2}{\Gamma(1 - \alpha)} \frac{\alpha}{2(1 - \alpha)(\sigma \tau_k)^\alpha}
\]
\[
\leq \frac{2C_3 \sigma (1 + \frac{t^*_{k-3}}{t^*_k})^3}{\Gamma(1 - \alpha)} ([M]_{k,k} - [M]_{k,k-1})
\]
from (Q2) in Lemma 4.4.

Combining (4.10), (4.11) and (4.12) we obtain the estimation (4.9) of approximation error.

Theorem 4.6. Assume that \( u \in C^3([0, T], H^1_\sigma(\Omega)) \) and \( |\partial^l u(t)| \leq C_l (1 + t^{-\alpha}) \), for \( l = 1, 2, 3 \) for \( 0 < t \leq T \). If the nonuniform mesh satisfies \( \rho_k \geq \eta \approx 0.475329 \), then the numerical solutions of \( L^2_{-1,\sigma} \) scheme (4.2) have the following global error estimate
\[
\max_{1 \leq k \leq n} \| u(t_k) - u^k \|_{L^2(\Omega)}
\]
\[
\leq C \left( t_2^*/\alpha + t_2 + \frac{1}{2} \max_{2 \leq k \leq n} (1 + \rho_{k+1})(1 + \frac{t^*_{k-3}}{t^*_k})^{\alpha/2} \cdot \frac{\alpha}{2(1 - \alpha)} \right)
\]
where \( C \) is a constant depending only on \( C_1, l = 1, 2, 3 \) and \( \Omega \).

Proof. Let \( e^k := u(t_k) - u^k \). We have
(4.13)
\[
L^* e = \Delta e^k + r_k + \Delta R^*_k,
\]
where \( e^k := (1 - \alpha/2)e^k + \alpha/2e^{k-1} \), \( r_k \) is given in (4.8), and \( R^*_k := u(t_k^*) - ((1 - \alpha/2)u(t_k) + \alpha/2u(t_{k-1})) \). Multiplying (4.13) with \( e^k \) and integrating over \( \Omega \) yield
(4.14)
\[
\langle L^* e, e^k \rangle = -\| \nabla e^k \|_{L^2(\Omega)}^2 - \langle r_k, e^k \rangle - \langle \nabla R^*_k, \nabla e^k \rangle.
\]

According to Lemma 1 as well as Lemma 4.4 we can derive
\[
\langle L^* e, e^k \rangle = \frac{1}{\Gamma(1 - \alpha)} \sum_{j=1}^{k} [M]_{k,j} \langle (e^j - e^{j-1}), (1 - \alpha/2)e^k + \alpha/2e^{k-1} \rangle
\]
\[
\geq \frac{1}{2\Gamma(1 - \alpha)} \sum_{j=1}^{k} [M]_{k,j} \left( \| e^j \|_{L^2(\Omega)}^2 - \| e^{j-1} \|_{L^2(\Omega)}^2 \right).
\]
Applying Cauchy-Schwarz inequality in (4.14) yields
(4.15)
\[
\sum_{j=1}^{k} [M]_{k,j} \left( \| e^j \|_{L^2(\Omega)}^2 - \| e^{j-1} \|_{L^2(\Omega)}^2 \right) \leq 2\Gamma(1 - \alpha) \| r_k \|_{L^2(\Omega)} \| e^k \|_{L^2(\Omega)} + (1 - \alpha) \| R^*_k \|_{H^1(\Omega)}^2.
\]

We define a lower triangular \( P \) matrix such that
\[
PM = E_k
where

\[
E_L = \begin{pmatrix}
1 & 1 & \cdots & 1 \\
1 & 1 & \cdots & 1 \\
\vdots & \vdots & \ddots & \vdots \\
1 & 1 & \cdots & 1
\end{pmatrix}.
\]

In other words,

\[
\sum_{l=j}^{k} |P|_{k,l} |M|_{l,j} = 1, \quad \forall 1 \leq j \leq k \leq n.
\]

Here \( P \) is called complementary discrete convolution kernel in the work [13]. It can be easily checked that \(|P|_{k,l} \geq 0\) due to the monotonicity properties of \( M \). From (4.15) we can derive that \( \forall 1 \leq k \leq n, \)

(4.16)

\[
\|e^k\|_{L^2(\Omega)}^2 \leq 2\Gamma(1 - \alpha) \sum_{l=1}^{k} |P|_{k,l} \|r_l\|_{L^2(\Omega)} \|e_l^i\|_{L^2(\Omega)} + \Gamma(1 - \alpha) \sum_{l=1}^{k} |P|_{k,l} \|R_l^i\|_{H^1(\Omega)}^2,
\]

where we use

\[
\sum_{l=1}^{k} |P|_{k,l} \sum_{j=1}^{l} |M|_{l,j} \left( \|e^j\|_{L^2(\Omega)}^2 - \|e^{j-1}\|_{L^2(\Omega)}^2 \right)
= \sum_{j=1}^{k} \left( \|e^j\|_{L^2(\Omega)}^2 - \|e^{j-1}\|_{L^2(\Omega)}^2 \right) \sum_{l=j}^{k} |P|_{k,l} |M|_{l,j}
= \sum_{j=1}^{k} \left( \|e^j\|_{L^2(\Omega)}^2 - \|e^{j-1}\|_{L^2(\Omega)}^2 \right) = \|e^k\|_{L^2(\Omega)}^2.
\]

According to Lemma 4.5

\[
\Gamma(1 - \alpha) \sum_{l=1}^{k} |P|_{k,l} \|r_l\|
\leq C|\Omega| \sum_{l=1}^{k} |P|_{k,l} \left( |M|_{l,1} (t_2^o / \alpha + t_2) + \sum_{j=2}^{l} (|M|_{l,j} - |M|_{l,j-1}) (1 + \rho_{j+1}) (1 + t_{j-3}^o / \alpha t_2) \tau_j^3 \right)
= C|\Omega| \left( (t_2^o / \alpha + t_2) + \sum_{j=2}^{k} (1 + \rho_{j+1}) (1 + t_{j-3}^o / \alpha t_2) \tau_j^3 \sum_{l=j}^{k} |P|_{k,l} (|M|_{l,j} - |M|_{l,j-1}) \right)
= C|\Omega| \left( (t_2^o / \alpha + t_2) + \sum_{j=2}^{k} (1 + \rho_{j+1}) (1 + t_{j-3}^o / \alpha t_2) \tau_j^3 |P|_{k,j-1} |M|_{j-1,j-1} \right)
= C|\Omega| \left( (t_2^o / \alpha + t_2) + \sum_{j=2}^{k} |P|_{k,j-1} |M|_{j-1,j-1} \frac{|M|_{j-1,j-1}}{|M|_{j-1,1}} (1 + \rho_{j+1}) (1 + t_{j-3}^o / \alpha t_2) \tau_j^3 \right)
\leq C|\Omega| \left( (t_2^o / \alpha + t_2) + \max_{2 \leq j \leq k} \frac{|M|_{j-1,j-1}}{|M|_{j-1,1}} (1 + \rho_{j+1}) (1 + t_{j-3}^o / \alpha t_2) \tau_j^3 \right)
\]
\[ \leq C|\Omega| \left( t^2_2/\alpha + t_2 + \frac{1}{1 - \alpha} \max_{1 \leq j \leq n} (1 + \rho_{j+1})(1 + t^{\alpha-3}_{j-1})(t^*_j)^\alpha t^3_j \right), \]

where \( C \) is a constant only depending on \( C_1 \). The last inequality is obtained by the following upper bound of \( [M]_{j,j} \) and lower bound of \( [M]_{j,1} \):

\[
[M]_{j,j} = c_{j-1}^j + \frac{\sigma^{1-\alpha}}{(1-\alpha)t^*_j^\alpha} \]
\[
\leq \int_0^1 \frac{\tau^2_{j-1}(2\theta - 1)}{\tau_j(t^*_{j-1} + \tau_j)(t^*_j - (t^*_{j-2} + \theta t_{j-1}))^\alpha} d\theta + \frac{\sigma^{1-\alpha}}{(1-\alpha)t^*_j^\alpha} \]
\[
\leq \rho_j(1 + \rho_j)(\sigma t^*_j)^\alpha + \frac{\sigma^{1-\alpha}}{(1-\alpha)t^*_j^\alpha} \leq \frac{1}{\eta(1 + \eta)(\sigma t^*_j)^\alpha} + \frac{\sigma^{1-\alpha}}{(1-\alpha)t^*_j^\alpha}, \]

where we use (Q1) in Lemma 4.4 for the inequality of \( [M]_{j,j} \).

Using the Taylor formula with integral remainder for \( R_j^* \) gives

\[ R_j^* = -\alpha/2 \int_{t_{j-1}}^{t_j} (s - t_{j-1})u''(s) \, ds - (1 - \alpha/2) \int_{t_j}^{t_{j+1}} (t_j - s)u''(s) \, ds, \quad 1 \leq j \leq k. \]

Under the regularity assumption, we have

\[ \|R_1^*\|_{H^1(\Omega)} \leq C(\tau^*_{j_1}/\alpha + \tau_1), \quad \|R_j^*\|_{H^1(\Omega)} \leq C(1 + t^{\alpha-2}_{j-1})t^*_j, \quad 2 \leq j \leq k. \]

Then we have

\[ \sum_{l=1}^k [P]_{k,l} \|R_l^*\|_{H^1(\Omega)}^2 \]
\[ \leq C \left( [P]_{k,1} [M]_{1,1} \left( \tau^*_{1}/\alpha + \tau_1 \right)^2 + \sum_{l=2}^k [P]_{k,l} [M]_{l,2} \left( (1 + t^{\alpha-2}_{l-1})t^*_l \right)^2 \right) \]
\[ \leq C \left( \frac{1}{[M]_{1,1}} \left( \tau^*_{1}/\alpha + \tau_1 \right)^2 + \max_{2 \leq l \leq k} \frac{1}{[M]_{l,2}} \left( (1 + t^{\alpha-2}_{l-1})t^*_l \right)^2 \right) \]
\[ \leq C \left( (1 - \alpha)\tau^*_{1}(\tau^*_{1}/\alpha + \tau_1)^2 + \max_{2 \leq l \leq k} \left( (1 + t^{\alpha-2}_{l-1})t^*_l \right)^2 \right), \]

where we use \( [M]_{l,2} \geq [M]_{l,1} \) and (4.17).

Taking the max for \( 1 \leq k \leq n \) on both sides of (4.16), we can derive (4.18)

\[ \max_{1 \leq k \leq n} \|e_k\|_{L^2(\Omega)} \leq C \left( t^2_2/\alpha + t_2 + \frac{1}{1 - \alpha} \max_{2 \leq k \leq n} (1 + \rho_{k+1})(1 + t^{\alpha-3}_{k-1})(t^*_k)^\alpha t^3_k \right) \]
\[ + \left( \tau^*_{1}/\alpha + \tau_1 \right)\tau^*_{1}/2 + \sqrt{\Gamma(1 - \alpha)} \max_{2 \leq k \leq n} \left( t^*_k \right)^{\alpha/2} \leq C \left( \tau^*_{1}/\alpha + \tau_1 \right)^{\alpha/2} \]

In the case of graded mesh with grading parameter \( r \),

\[ t_j = \left( \frac{j}{K} \right)^r T, \quad \tau_j = t_j - t_{j-1} = \left[ \left( \frac{j}{K} \right)^r - \left( \frac{j-1}{K} \right)^r \right] T, \]
where $K$ is the total time step number, $1 \leq j \leq K$, $t_K = T$. As a consequence, the two terms after max operations in (4.18) can be estimated as follows:

\[
(1 + r_k)(1 + t^\alpha_{k-1}^*(t_k - t_{k-1})^2)^{\alpha/2} \leq C T_k^\alpha \min\{r, 2\}
\]

using the technique by Chen-Stynes in [3], one can obtain

\[
\begin{align*}
&\tilde{C}T_k^\alpha \min\{r, 2\} \leq |C|, \\
&|C| \leq C_{T,1} K r^\alpha \leq C_{T,2} K r^\alpha \min\{r, 2\},
\end{align*}
\]

In (4.20) and (4.21), $C_{T,1}$ and $C_{T,2}$ only depend on $T$. Therefore, if $u$ satisfies the regularity assumptions in Theorem 4.6 then we have the following error estimate of numerical solutions of the L2-1 regularity assumptions in Theorem 4.6, then we have the following error estimate of

\[
\begin{align*}
&\text{max}_{1 \leq j \leq K} \|u(t_k) - u^k\|_{L^2(\Omega)} \leq \tilde{C} K r^\alpha \min\{r, 2\},
\end{align*}
\]

where $\tilde{C}$ depends on $C_l$ with $l = 1, 2, 3, \alpha$ and $\Omega$.

**Remark 4.7.** When $\alpha \to 1^-$, the constant $\tilde{C}$ in (4.22) will tend to infinity. However, using the technique by Chen-Stynes in [3], one can obtain $\alpha$-robust error estimate in the sense that $\tilde{C}$ won’t tend to infinity when $\alpha \to 1^-$.}

5. **Numerical Tests**

In this section, we provide some numerical tests on the L2-1, scheme (4.2) on the subdiffusion equation (4.1).

As in [13, 2], the discrete coefficients $a^k_j$ and $b_j^k$ in (4.2) are computed by adaptive Gauss–Kronrod quadrature, to avoid roundoff error problems.

5.1. **1D example.** We first test the convergence rate of a 1D example, where $\Omega = [0, 2\pi]$, $T = 1$, $u^0(x) \equiv 0$, and $f(t, x) = (1 + \alpha) t^\alpha \cos(x)$. It can be checked that the exact solution is $u(t, x) = t^\alpha \cos(x)$.

The graded mesh (4.19) with grading parameter $r$ and time step number $K$ is adopted in time. We use the central finite difference method in space with grid spacing $h = 2\pi/10000$. The maximum $L_2$-error is computed by $\max_{1 \leq k \leq K} \|u(t_k) - u^k\|_{L^2(\Omega)}$. Table 1-3 present the maximum $L_2$-errors for $\alpha = 0.3, 0.5, 0.7$ and $r = 1, 2, 2/\alpha, 3/\alpha$ respectively. It can be observed that the convergence rates are consistent with (4.22) derived from Theorem 4.6.

In [23, 8], the authors state that the large value of $r$ in the graded mesh increases the temporal mesh width near the final time $t = T$ which can lead to large errors. Indeed, when $r = 3/\alpha$, the errors seem larger than the case of $r = 2/\alpha$, as observed in Table 1-3. We then propose to use the graded mesh with varying grading parameter $r_j$ (dependent on the time), called $r$-variable graded mesh. In particular,
Table 1. $\max_{1 \leq k \leq K} \| u(t_k) - u^k \|_{L^2(\Omega)}$ for the graded meshes with different grading parameters and time step numbers where $\alpha = 0.3$.

| $K$   | $K = 40$ | $K = 80$ | $K = 160$ | $K = 320$ | $K = 480$ | $K = 640$ |
|-------|----------|----------|----------|----------|----------|----------|
| $r = 1$ | 2.3600e-2 | 2.2505e-2 | 2.0661e-2 | 1.8461e-2 | 1.7117e-2 | 1.6165e-2 |
| order | - | 0.0685 | 0.1233 | 0.1625 | 0.1863 | 0.1988 |
| $r = 2$ | 1.3254e-2 | 9.4767e-3 | 6.5872e-3 | 4.9467e-3 | 3.5761e-3 | 3.0338e-3 |
| order | - | 0.4841 | 0.5247 | 0.5508 | 0.5650 | 0.5716 |
| $r = 2/\alpha$ | 2.7182e-4 | 7.4873e-5 | 1.9983e-5 | 5.2316e-6 | 2.3816e-6 | 1.6165e-6 |
| order | - | 1.8601 | 1.9056 | 1.9335 | 1.9408 | 1.9334 |
| $r = 3/\alpha$ | 5.6542e-4 | 1.5847e-4 | 4.2808e-5 | 1.1281e-5 | 5.1370e-6 | 2.9371e-6 |
| order | - | 1.8351 | 1.8883 | 1.9239 | 1.9403 | 1.9432 |

Table 2. $\max_{1 \leq k \leq K} \| u(t_k) - u^k \|_{L^2(\Omega)}$ for the graded meshes with different grading parameters and time step numbers where $\alpha = 0.5$.

| $K$   | $K = 40$ | $K = 80$ | $K = 160$ | $K = 320$ | $K = 480$ | $K = 640$ |
|-------|----------|----------|----------|----------|----------|----------|
| $r = 1$ | 1.8575e-2 | 1.4568e-2 | 1.1059e-2 | 8.2145e-3 | 6.8534e-3 | 6.0116e-3 |
| order | - | 0.3506 | 0.3976 | 0.4290 | 0.4468 | 0.4555 |
| $r = 2$ | 3.9186e-3 | 2.0105e-3 | 1.0182e-3 | 5.1239e-4 | 3.4232e-4 | 2.5701e-4 |
| order | - | 0.9628 | 0.9815 | 0.9908 | 0.9947 | 0.9963 |
| $r = 2/\alpha$ | 2.2728e-4 | 5.8725e-5 | 1.4830e-5 | 3.7186e-6 | 1.6536e-6 | 9.3037e-7 |
| order | - | 1.9524 | 1.9854 | 1.9957 | 1.9986 | 1.9993 |
| $r = 3/\alpha$ | 3.5987e-4 | 9.9080e-5 | 2.6590e-5 | 7.0116e-6 | 3.2025e-6 | 1.8379e-6 |
| order | - | 1.8608 | 1.8977 | 1.9231 | 1.9327 | 1.9302 |

Table 3. $\max_{1 \leq k \leq K} \| u(t_k) - u^k \|_{L^2(\Omega)}$ for the graded meshes with different grading parameters and time step numbers where $\alpha = 0.7$.

| $K$   | $K = 40$ | $K = 80$ | $K = 160$ | $K = 320$ | $K = 480$ | $K = 640$ |
|-------|----------|----------|----------|----------|----------|----------|
| $r = 1$ | 8.3068e-3 | 5.4221e-3 | 3.4582e-3 | 2.1753e-3 | 1.6518e-3 | 1.3569e-3 |
| order | - | 0.6154 | 0.6488 | 0.6688 | 0.6790 | 0.6883 |
| $r = 2$ | 7.3797e-4 | 2.8495e-4 | 1.0874e-4 | 4.1317e-5 | 2.3437e-5 | 1.5672e-5 |
| order | - | 1.3729 | 1.3898 | 1.3961 | 1.3983 | 1.3989 |
| $r = 2/\alpha$ | 1.7758e-4 | 4.6703e-5 | 1.1903e-5 | 2.9940e-6 | 1.3323e-6 | 7.4975e-7 |
| order | - | 1.9269 | 1.9721 | 1.9913 | 1.9970 | 1.9985 |
| $r = 3/\alpha$ | 1.5861e-4 | 4.3872e-5 | 1.1918e-5 | 3.1981e-6 | 1.4809e-6 | 8.6093e-7 |
| order | - | 1.8541 | 1.8802 | 1.8978 | 1.8987 | 1.8855 |

For this example, we use the following $r$-variable graded mesh

$$r_j = 2/\alpha + 1.5 - \frac{3(j - 1)}{K - 1},$$

$$t_j = \left( \frac{j}{K} \right)^{r_j} T,$$

$$\tau_j = t_j - t_{j-1} = \left[ \left( \frac{j}{K} \right)^{r_j} - \left( \frac{j - 1}{K} \right)^{r_{j-1}} \right] T.$$
In Figure 2, we compare the time steps, the pointwise $L^2$-errors, and the maximum $L^2$-errors of the $r$-variable graded mesh (5.1) and the standard graded meshes (4.19) with $r = 2/\alpha$, $3/\alpha$. Here we set $\alpha = 0.7$ and for the left and middle subfigures $K = 640$. From the middle of Figure 2 the maximum $L^2$-error for the $r$-variable graded mesh is smaller than the standard graded meshes with $r = 2/\alpha$, $3/\alpha$.

Figure 2. Time steps (left), pointwise $L^2$-errors (middle), and maximum $L^2$-errors (right) of the L2-1$_\sigma$ scheme in 1D on the $r$-variable graded mesh (5.1) and the graded meshes (4.19) with $r = 2/\alpha$, $3/\alpha$.

5.2. 2D example. In the 2D case, we set $f(t, x) = (\Gamma(1 + \alpha) + 2t^\alpha) \sin(x) \sin(y)$ and then the exact solution $u(t, x) = t^{\alpha} \sin(x) \sin(y)$. In this example, we set periodic boundary condition for the subdiffusion equation. We take $T = 1$ and $\alpha = 0.7$. Here we use Fourier spectral method in the domain $\Omega = [0, 2\pi]^2$ with $256 \times 256$ Fourier modes. In Figure 3, we show the pointwise $L^2$-errors (with $K = 640$) and the maximum $L^2$-errors of the L2-1$_\sigma$ schemes on the standard graded meshes (4.19) with $r = 2/\alpha$ and the $r$-variable graded mesh (5.1). One can observe that the $r$-variable graded mesh performs better than the graded mesh for this example.

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Figure 3. Pointwise $L^2$-errors (left) with $K = 640$ and maximum $L^2$-errors (right) of $L^2$-1$_r$ scheme in 2D on the $r$-variable graded mesh \([5.1]\) and the graded mesh \([4.19]\) with $r = 2/\alpha$ ($\alpha = 0.7$).

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SUSTech International Center for Mathematics, Southern University of Science and Technology, Shenzhen, China.

Email address: quancy@sustech.edu.cn

Department of Mathematics, Harbin Institute of Technology, Harbin 150001, China; Department of Mathematics, Southern University of Science and Technology, Shenzhen, China.

Email address: 11849596@mail.sustech.edu.cn