Global-in-Time $H^1$-Stability of L2-1$_\sigma$ Method on General Nonuniform Meshes for Subdiffusion Equation

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Abstract

In this work the L2-1$_\sigma$ method on general nonuniform meshes is studied for the subdiffusion equation. When the time step ratio is no less than 0.475329, a bilinear form associated with the L2-1$_\sigma$ fractional-derivative operator is proved to be positive semidefinite and a new global-in-time $H^1$-stability of L2-1$_\sigma$ schemes is then derived under simple assumptions on the initial condition and the source term. In addition, the sharp $L^2$-norm convergence is proved under the constraint that the time step ratio is no less than 0.475329.

Keywords Subdiffusion equation · L2-1$_\sigma$ method · Nonuniform meshes · $H^1$-stability · Convergence

1 Introduction

In the past decade, many numerical methods have been proposed to solve the time-fractional diffusion equations [6, 21]. If the solution is sufficiently smooth (which requires the initial value to be smooth and satisfying some compatibility conditions), it has been proved that the L2-1$_\sigma$ scheme has second order accuracy [2] and the L2-type methods can achieve $(3 - \alpha)$-order accuracy [5, 20].

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 [25] prove the sharp error analysis of L1 scheme on graded meshes. Kopteva

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provides a different analysis framework of the L1 scheme on graded meshes in two and three spatial dimensions in [10]. Chen-Stynes [3] prove the second-order convergence of the L2-1_\sigma scheme on fitted meshes combining the graded meshes and quasiuniform meshes. Kopteva-Meng [12] 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 [11]. Liao-Li-Zhang establish the sharp error analysis for the L1 scheme of subdiffusion equation on general nonuniform meshes in [13] and then Liao-Mclean-Zhang study the L2-1_\sigma scheme in [14, 15], where a discrete Grönwall inequality is introduced. This analysis for general nonuniform meshes can be used to design adaptive strategies of time steps.

Taking into account the singularity of exact solution, Mustapha-Abdallah-Furati [22] analyze the global high-order convergence of the discontinuous Galerkin method for subdiffusion equation on graded mesh. Jin-Li-Zhou [7, 8] combine BDF (backward differentiation formula) CQ methods with corrections to achieve higher (more than two) order convergence which can also overcome the weak singularity problem for time-fractional diffusion equation.

In this work, we first study the H1-stability of the L2-1_\sigma method proposed initially in [2] 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 L2-1_\sigma fractional-derivative operator denoted by $L_k^{\alpha,*}$, we prove that the following bilinear form

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

is positive semidefinite under some mild restrictions (3.2) on time step ratios $\rho_k := \tau_k / \tau_{k-1}$ with $\tau_k$ the kth time step and $k \geq 2$. In fact, the positive semidefiniteness of $\mathcal{B}_n$ on general nonuniform meshes is an open problem as stated in the conclusion of [16], where the maximum principle and convergence analysis are provided for L2-1_\sigma scheme of the time-fractional Allen–Cahn equation but not the positive definiteness of L2-1_\sigma operator. On the positive definiteness, Karaa presents in [1, 9] a general criteria ensuring the positivity of quadratic forms that can be applied to the time-fractional operators such as the L1 formula. In [17], Liao-Tang-Zhou proves the positive definiteness of a new L1-type operator.

Based on the positive semidefiniteness of $\mathcal{B}_n$ associated with L2-1_\sigma operator, we propose a new global-in-time H1-stability result in Theorem 2 for the L2-1_\sigma scheme. In particular, when $\rho_k \geq 0.475329$ for $k \geq 2$, the restrictions (3.2) hold and the H1-stability can be ensured for all time.

Besides the global-in-time H1-stability of the L2-1_\sigma scheme in Theorem 2, we revisit the sharp convergence analysis in [15] by Liao-Mclean-Zhang. We provide a proof of sharp L2-norm convergence based on new properties of the L2-1_\sigma coefficients, where the restriction on time step ratios is relaxed from $\rho_k \geq 4/7$ in [15] to $\rho_k \geq 0.475329$.

In the numerical implementations, we compare the L2-1_\sigma schemes on the standard graded meshes [25] and the r-variable graded meshes (with varying grading parameter). According to our stability analysis, these methods are all H1-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 Sect. 2, the derivation, explicit expression and reformulation of L2-1_\sigma fractional-derivative operator are provided. In Sect. 3, we prove the positive semidefiniteness of the bilinear form $\mathcal{B}_n$ under some mild restrictions on the time step ratios.
In Sect. 4, we establish a new global-in-time $H^1$-stability of the L2-1$_\sigma$ 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 Sect. 5, we do some first numerical tests.

2 Discrete Fractional-Derivative Operator

In this part we show the derivation, explicit expression and reformulation of L2-1$_\sigma$ operator on an arbitrary nonuniform mesh.

We consider the L2-1$_\sigma$ approximation of the fractional-derivative operator defined by

$$\partial^\alpha_t u = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{u'(s)}{(t-s)^\alpha} \, ds.$$ 

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. [2] for this setting of $\sigma$). The fractional derivative $\partial^\alpha_t u(t)$ at $t = t_k^* := t_{k-1} + \sigma \tau_k$ could be approximated by the following L2-1$_\sigma$ fractional-derivative operator

$$L_k^\alpha u = \frac{1}{\Gamma(1-\alpha)} \left( \sum_{j=1}^{k-1} \int_{t_{j-1}}^{t_j} \frac{\partial_x H^j_x(s)}{(t_k^*-s)^\alpha} \, ds + \int_{t_{k-1}}^{t_k^*} \frac{\partial_x H^k_x(s)}{(t_k^*-s)^\alpha} \, ds \right)$$

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

$$H^j_x(t) = \frac{(t-t_j)(t-t_{j+1})}{(t_{j-1}-t_j)(t_{j-1}-t_{j+1})} u^{j-1} + \frac{(t-t_{j-1})(t-t_{j+1})}{(t_{j-1}-t_j)(t_{j-1}-t_{j+1})} u^j + \frac{(t-t_{j-1})(t-t_j)}{(t_{j+1}-t_{j-1})(t_{j+1}-t_j)} u^{j+1},$$

$$H^k_x(t) = \frac{t-t_k}{t_k-t_{k-1}} u^{k-1} + \frac{t-t_{k-1}}{t_k-t_{k-1}} u^k,$$

and

$$a_j^{(k)} = \int_{t_{j-1}}^{t_j} \frac{2s-t_j-t_{j+1}}{\tau_j(t_j+\tau_{j+1})(t_k^*-s)^\alpha} \, ds = \int_0^1 \frac{-2\tau_j(1-\theta) - \tau_j+1}{(\tau_j+\tau_{j+1})(t_k^*-t_{j-1} + \theta \tau_j)^\alpha} \, d\theta,$$

$$b_j^{(k)} = \int_{t_{j-1}}^{t_j} \frac{2s-t_j-t_{j+1}}{\tau_j t_{j+1}} \, ds = -\int_0^1 \frac{2\tau_j \theta - \tau_j - \tau_{j+1}}{\tau_{j+1}(t_k^*-t_{j-1} + \theta \tau_j)^\alpha} \, d\theta,$$

$$c_j^{(k)} = \int_{t_{j-1}}^{t_j} \frac{2s-t_j-t_{j+1}}{\tau_{j+1}(t_j+\tau_{j+1})(t_k^*-s)^\alpha} \, ds = \int_0^1 \frac{\tau_j^2 (2\theta - 1)}{\tau_{j+1}(t_j+\tau_{j+1})(t_k^*-t_{j-1} + \theta \tau_j)^\alpha} \, d\theta.$$
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 \( 1 \leq j \leq k - 1 \),

\[
\begin{align*}
a_j^{(k)} &= \frac{\tau_{j+1}}{(1-\alpha)\tau_j(\tau_j + \tau_{j+1})}(t_k^* - t_j)^{1-\alpha} - \frac{2\tau_j + \tau_{j+1}}{(1-\alpha)\tau_j(\tau_j + \tau_{j+1})}(t_k^* - t_{j-1})^{1-\alpha} \\
&\quad + \frac{2}{(2-\alpha)(1-\alpha)\tau_j(\tau_j + \tau_{j+1})} \left[(t_k^* - t_{j-1})^{2-\alpha} - (t_k^* - t_j)^{2-\alpha}\right], \\
c_j^{(k)} &= \frac{1}{(1-\alpha)\tau_{j+1}(\tau_j + \tau_{j+1})} \left[ -\tau_j((t_k^* - t_{j-1})^{1-\alpha} + (t_k^* - t_j)^{1-\alpha}) \\
&\quad + 2(2-\alpha)^{-1}(t_k^* - t_{j-1})^{2-\alpha} - (t_k^* - t_j)^{2-\alpha}\right].
\end{align*}
\]

We reformulate the discrete fractional derivative \( L_k^{\alpha,\sigma} \) in (2.1) as

\[
L_k^{\alpha,\sigma} u = \frac{1}{\Gamma(1-\alpha)} \left( c_{k-1}^{(k)} \delta_k u - a_k^{(\delta_1)} u + \sum_{j=2}^{k-1} d_{j+1}^{(k)} \delta_j u + \frac{\sigma^{1-\alpha}}{\Gamma(2-\alpha)\tau_k^\alpha} \delta_k u, \right) \tag{2.3}
\]

where \( \delta_j u = u^j - u^{j-1} \), \( d_j^{(k)} := c_j^{(k)} - a_j^{(k)} \). Here we make a convention that \( a_1^0 = 0 \) and \( c_0^1 = 0 \).

To establish the global-in-time \( H^1 \)-stability of \( L_k^{\alpha,\sigma} \) method for fractional-order parabolic problem, we shall prove the positive semidefiniteness of \( \mathcal{B}_n \) defined in (1.2).

## 3 Positive Semidefiniteness of Bilinear Form \( \mathcal{B}_n \)

In this section, we first propose some properties of the \( L_k^{\alpha,\sigma} \) 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 \( \mathcal{B}_n \). Then we prove rigorously the positive semidefiniteness of bilinear form \( \mathcal{B}_n \) under some constraints of \( \rho_k, k \geq 2 \).

**Lemma 1** (Properties of \( a_j^{(k)}, c_j^{(k)} \) and \( d_j^{(k)} \)) For the \( L_k^{\alpha,\sigma} \) 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)** \( a_j^{(k+1)} - a_j^{(k)} > 0, 1 \leq j \leq k - 1, k \geq 2; \)
- **(P3)** \( a_j^{(k+1)} - a_j^{(k)} < 0, 1 \leq j \leq k - 2, k \geq 3; \)
- **(P4)** \( a_j^{(k+1)} - a_j^{(k)} < a_j^{(k+1)} - a_j^{(k+1)}, 1 \leq j \leq k - 2, k \geq 3; \)
- **(P5)** \( c_j^{(k)} > 0, 1 \leq j \leq k - 1, k \geq 2; \)
- **(P6)** \( c_j^{(k+1)} - c_j^{(k)} < 0, 1 \leq j \leq k - 1, k \geq 2; \)
- **(P7)** \( d_j^{(k)} > 0, 2 \leq j \leq k - 1, k \geq 3; \)
- **(P8)** \( d_j^{(k+1)} - d_j^{(k)} < 0, 2 \leq j \leq k - 1, k \geq 3. \)

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

\[
\frac{1}{\rho_{j+1}} \geq \frac{1}{\rho_j^2(1 + \rho_j)} - 3, \quad \forall j \geq 2, \tag{3.1}
\]
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 [24, Lemma 3.1] except replacing \( t_k \) with \( t_k^* \). We omit it here. \( \square \)

**Theorem 1** Consider a nonuniform mesh \( \{ \tau_k \}_{k \geq 1} \) satisfying that \( k \geq 2, \)

\[
\begin{align*}
\rho_* &< \rho_{k+1} \leq \frac{\rho_k^2 (1 + \rho_k)}{1 - 3 \rho_k^2 (1 + \rho_k)}, \quad \rho_* < \rho_k < \eta, \quad (3.2) \\
\rho_* &< \rho_{k+1}, \quad \eta \leq \rho_k,
\end{align*}
\]

where \( \rho_* \approx 0.356341, \) and \( \eta \approx 0.475329. \) Then the for any function \( u \) defined on \( [0, \infty) \times \Omega \) and \( n \geq 1, \)

\[
\mathcal{B}_n(u, u) = \sum_{k=1}^{n} \langle L_k^{\alpha, u}, \delta_k u \rangle \geq \sum_{k=1}^{n} \frac{g_k(\alpha)}{2 \Gamma(2 - \alpha)} \| \delta_k u \|_{L^2(\Omega)}^2 \geq 0, \quad (3.3)
\]

where

\[
g_k(\alpha) = \begin{cases}
\frac{1}{(\sigma_1^2)^{\alpha}} \left( 2 \sigma - \frac{1 - \alpha}{\sigma_2^2} \right), & k = 1, \\
(1 - \alpha) c_{k-1}^{(k)} + \frac{1}{(\sigma_2)^2} \left( 2 \sigma - (1 - \alpha) - \frac{c(1-\alpha)}{1+\rho_k+1+\rho_k} \int_0^1 \frac{1}{\sigma(x)^{1+\alpha}} \mathrm{d}x \right), & 2 \leq k \leq n - 1, \\
(1 - \alpha) c_{n-1}^{(n)} + \frac{1}{(\sigma_2)^2} (2 \sigma - (1 - \alpha)), & k = n \neq 2,
\end{cases} \quad (3.4)
\]

are always positive for \( \alpha \in (0, 1). \)

**Proof** According to (2.3), we can rewrite \( \mathcal{B}_n(u, u) \) in the following matrix form

\[
\mathcal{B}_n(u, u) = \sum_{k=1}^{n} \langle L_k^{\alpha, u}, \delta_k u \rangle = \frac{1}{\Gamma(1 - \alpha)} \int_\Omega \psi \mathbf{M} \psi^T \mathrm{d}x,
\]

where \( \psi = [\delta_1 u, \delta_2 u, \cdots, \delta_n u], \) and

\[
\mathbf{M} = \begin{pmatrix}
\frac{\sigma^{1-\alpha}}{(1-\alpha)^{\frac{1}{\Gamma_1}}}
& -d_1^{(2)} c_1^{(2)} + \frac{\sigma^{1-\alpha}}{(1-\alpha)^{\frac{1}{\Gamma_2}}}
& \cdots
& -d_1^{(n)} c_1^{(n)} + \frac{\sigma^{1-\alpha}}{(1-\alpha)^{\frac{1}{\Gamma_n}}}
\end{pmatrix}, \quad (3.5)
\]

We split \( \mathbf{M} \) as \( \mathbf{M} = \mathbf{A} + \mathbf{B}, \) where

\[
\mathbf{A} = \begin{pmatrix}
\beta_1
& -d_1^{(2)} \beta_2
& \cdots
& -d_1^{(n)} \beta_n
\end{pmatrix},
\]

\[
\mathbf{B} = \begin{pmatrix}
d_1^{(2)}
& d_2^{(3)}
& \cdots
& d_{n-1}^{(n)}
\end{pmatrix}.
\]
and
\[
\mathbf{B} = \text{diag}\left( \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_1^\alpha} - \beta_1, \ c_1^{(2)} \right) + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_2^\alpha} - \beta_2, \ldots, \ c_{n-1}^{(n)} + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_n^\alpha} - \beta_n \right),
\]
with
\[
2\beta_1 = -a_1^{(2)}, \quad 2\beta_2 - d_2^{(3)} = a_1^{(3)} - a_1^{(2)},
\]
\[
2\beta_k - d_k^{(k+1)} = d_{k-1}^{(k)} - d_{k-1}^{(k+1)}, \quad 3 \leq k \leq n - 1,
\]
\[
2\beta_n = d_{n-1}^{(n)}, \quad n \geq 3.
\]

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

1. \( \forall \ 1 \leq j < i \leq n, \ [\mathbf{S}]_{i,j-1} \geq [\mathbf{S}]_{i,j}; \)
2. \( \forall \ 1 < j \leq i \leq n, \ [\mathbf{S}]_{i,j-1} < [\mathbf{S}]_{i,j}; \)
3. \( \forall \ 1 < j < i \leq n, \ [\mathbf{S}]_{i,j-1} - [\mathbf{S}]_{i,j} \leq [\mathbf{S}]_{i,j-1} - [\mathbf{S}]_{i,j}. \)

From [23, Lemma 2.1], \( \mathbf{S} \) is positive definite. Let \( \varepsilon \to 0 \). We can claim that \( \mathbf{A} + \mathbf{A}^T \) is positive semidefinite.

In the following we will prove \( [\mathbf{B}]_{kk} \geq 0, \ k \geq 1 \), under some constraints on \( \rho_k \). We first provide two equivalent forms of \( a_j^{(k)} \) according to (2.2): \( \forall 1 \leq j \leq k - 1, \)
\[
a_j^{(k)} = \int_0^1 \frac{-2\tau_j (1 - s) - \tau_{j+1}}{(\tau_j + \tau_{j+1})(\int_0^{\tau_{j+1}} - (t_{j+1} - s\tau_j))^{\alpha}} \, ds
\]
\[
= \frac{1}{\tau_j + \tau_{j+1}} \int_0^1 (t_k^s - (t_{j+1} + s\tau_j))^{-\alpha} d\tau j s^2 - (2\tau_j + \tau_{j+1}) s \geq 0 \]
\[
= - (t_k^s - t_j)^{-\alpha} + \frac{\alpha \tau_j}{\tau_j + \tau_{j+1}} \int_0^1 (\tau_j + \tau_{j+1} + s\tau_j)(1 - s)(t_k^s - t_j + s\tau_j)^{-\alpha-1} \, ds \quad (3.7)
\]
and
\[
a_j^{(k)} = \int_0^1 \frac{-2\tau_j (1 - s) - \tau_{j+1}}{(\tau_j + \tau_{j+1})(\int_0^{\tau_{j+1}} - (t_{j+1} + s\tau_j))^{\alpha}} \, ds = \int_0^1 \frac{-2\tau_j s - \tau_{j+1}}{(\tau_j + \tau_{j+1})(t_k^s - t_j + s\tau_j)} \, ds
\]
\[
= \frac{1}{\tau_j + \tau_{j+1}} \int_0^1 (t_k^s - t_j + s\tau_j)^{-\alpha} d(-\tau j s^2 - \tau_{j+1} s) \geq 0 \]
\[
= -(t_k^s - t_{j+1})^{-\alpha} - \frac{\alpha \tau_j}{\tau_j + \tau_{j+1}} \int_0^1 (\tau_j + \tau_{j+1} + s\tau_j)(1 - s)(t_k^s - t_{j+1} + s\tau_j)^{-\alpha-1} \, ds. \quad (3.8)
\]

Furthermore, we also reformulate \( c_j^{(k)} \) in (2.2) as: \( \forall 1 \leq j \leq k - 1, \)
\[
c_j^{(k)} = \int_0^1 \frac{\tau_j^2 (2s - 1)}{(\tau_j + \tau_{j+1})(t_k^s - (t_{j+1} + s\tau_j))^{\alpha}} \, ds
\]
\[
= \frac{\tau_j^2}{\tau_j + \tau_{j+1}} \int_0^1 (t_k^s - (t_{j+1} + s\tau_j))^{-\alpha} d(s^2 - s) \quad (3.9)
\]
\[
= \frac{\alpha \tau_j^3}{\tau_j + \tau_{j+1}} \int_0^1 s(1 - s)(t_k^s - t_j + s\tau_j)^{-\alpha-1} \, ds.
\]
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

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

$$= \frac{\sigma^{1-\alpha}}{(1 - \alpha)\tau_1^\alpha} - \frac{1}{2\tau_1^\alpha} \int_0^1 \frac{2s + \rho_2}{(1 + \rho_2)(\sigma \rho_2 + s)} ds$$

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

To ensure $[\mathbf{B}]_{11} \geq 0$, we impose

$$2\sigma - \frac{1 - \alpha}{\rho_2^\alpha} \geq 0. \quad (3.10)$$

**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 (1) gives

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

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

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

Using the forms (3.7) for $a_1^{(2)}$, $a_1^{(3)}$ and (3.8) for $a_2^{(3)}$, we can derive

$$a_1^{(2)} - a_1^{(3)} + a_2^{(3)} = -(\sigma \tau_2)^{-\alpha} + \frac{\alpha \tau_1}{\tau_1 + \tau_2} \int_0^1 (\tau_1 + \tau_2 + s \tau_1)(1 - s)(t_2^* - t_1 + s \tau_1)^{-\alpha - 1} ds$$

$$- \frac{\alpha \tau_1}{\tau_1 + \tau_2} \int_0^1 (\tau_1 + \tau_2 + s \tau_1)(1 - s)(t_3^* - t_1 + s \tau_1)^{-\alpha - 1} ds$$

$$- \frac{\alpha \tau_2}{\tau_2 + \tau_3} \int_0^1 (\tau_2 + \tau_3 - s \tau_2)(1 - s)(t_3^* - t_3 - s \tau_2)^{-\alpha - 1} ds$$

$$= -(\sigma \tau_2)^{-\alpha} - \frac{\alpha}{(1 + \rho_3)\tau_2^\alpha} \int_0^1 s(\rho_3 + s)(\sigma \rho_3 + s)^{-\alpha - 1} ds$$

$$- (\sigma \tau_2)^{-\alpha} - \frac{\alpha}{(1 + \rho_3)\sigma \tau_2^\alpha \rho_3^\alpha} \int_0^1 s(\rho_3 + s) \frac{\sigma \rho_3 + s}{\sigma \rho_3 + s} ds. \quad (3.12)$$

Substituting (3.12) into (3.11) yields

$$\mathbf{B}t_{22} \geq \frac{1}{2}c_1^{(2)} + \frac{1}{2(1 - \alpha)(\sigma \tau_2)^\alpha} \left(2\sigma - (1 - \alpha) - \frac{\alpha(1 - \alpha)}{(1 + \rho_3)\rho_3^\alpha} \int_0^1 s(\rho_3 + s) \frac{\sigma \rho_3 + s}{\sigma \rho_3 + s} ds\right).$$

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

$$2\sigma - (1 - \alpha) - \frac{\alpha(1 - \alpha)}{(1 + \rho_3)\rho_3^\alpha} \int_0^1 s(\rho_3 + s) \frac{\sigma \rho_3 + s}{\sigma \rho_3 + s} ds \geq 0. \quad (3.13)$$
Case 3 When $3 \leq k \leq n - 1$, using $2\beta_k = a^{(k+1)}_k + a^{(k)}_k - d^{(k+1)}_{k-1}$ in (3.6) and $d^{(k)}_j = c^{(k)}_{j-1} - a^{(k)}_j$, we have

$$[B]_{kk} = \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau^\alpha_k} + \frac{1}{2}c^{(k)}_{k-1} - \frac{1}{2}(c^{(k)}_{k-1} - d^{(k+1)}_{k-1} - d^{(k)}_{k} + d^{(k+1)}_{k})$$

$$= \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau^\alpha_k} + \frac{1}{2}c^{(k)}_{k-1} + \frac{1}{2}[(c^{(k)}_{k-1} - c^{(k+1)}_{k-1}) - (c^{(k)}_{k-2} - c^{(k+1)}_{k-2})$$

$$+ (-a^{(k+1)}_{k-1} + a^{(k)}_{k-1} + a^{(k)}_{k-1})].$$

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

$$(c^{(k)}_{k-1} - c^{(k+1)}_{k-1}) - (c^{(k)}_{k-2} - c^{(k+1)}_{k-2}) + (-a^{(k+1)}_{k-1} + a^{(k)}_{k-1} + a^{(k)}_{k-1})$$

$$= \frac{\alpha\tau^3_{k-1}}{\tau_k(\tau_{k-1} + \tau_k)} \int_0^1 s(1-s) \left[ (t^*_k - t_{k-1} + s\tau_{k-1})^{-\alpha - 1} - (t^*_k - t_{k-1} + s\tau_{k-1})^{-\alpha - 1} \right] ds$$

$$+ \frac{\alpha\tau^3_{k-1}}{\tau_{k-1} + \tau_k} \int_0^1 (\tau_{k-1} + \tau_k + s\tau_{k-1})(1-s) \left[ (t^*_k - t_{k-1} + s\tau_{k-1})^{-\alpha - 1} - (t^*_k - t_{k-1} + s\tau_{k-1})^{-\alpha - 1} \right] ds$$

$$- (\sigma\tau_k)^{-\alpha} - \frac{\alpha\tau_k}{\tau_k + \tau_{k+1}} \int_0^1 (\tau_k + \tau_{k+1} - s\tau_k)(1-s)(t^*_k - t_{k-1} - s\tau_k)^{-\alpha - 1} ds$$

$$> -(\sigma\tau_k)^{-\alpha} - \frac{\alpha\tau_k}{\tau_k + \tau_{k+1}} \int_0^1 s(\tau_{k+1} + s\tau_k)(\sigma\tau_{k+1} + s\tau_k)^{-\alpha - 1} ds$$

$$= -(\sigma\tau_k)^{-\alpha} - \frac{\alpha}{(1 + \rho_{k+1})\tau^\alpha_k} \int_0^1 s(\rho_{k+1} + s)(\sigma\rho_{k+1} + s)^{-\alpha - 1} ds$$

$$- (\sigma\tau_k)^{-\alpha} - \frac{\alpha}{(1 + \rho_{k+1})(\sigma\tau_k)^\alpha\rho^\alpha_{k+1}} \int_0^1 s(\rho_{k+1} + s)\rho^\alpha_{k+1} + s)^{-\alpha - 1} ds,$$

(3.15)

where we use the forms (3.7) for $a^{(k)}_{k-1}$, $a^{(k+1)}_{k-1}$ and (3.8) for $d^{(k)}_k$. The first inequality in (3.15) can be derived as follows. For fixed $j$, it is easy to see that

$$(t^*_k - t_{k-1} + s\tau_{k-1})^{-\alpha - 1} - (t^*_k - t_{k-1} + s\tau_{k-1})^{-\alpha - 1} > 0$$

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

$$\int_0^1 (\tau_{k-1} + \tau_k + s\tau_{k-1})(1-s)[(t^*_k - t_{k-1} + s\tau_{k-1})^{-\alpha - 1} - (t^*_k - t_{k-1} + s\tau_{k-1})^{-\alpha - 1}] ds$$

$$\geq \int_0^1 (4\tau_{k-1} + 3\tau_k)s(1-s)[(t^*_k - t_{k-1} + s\tau_{k-1})^{-\alpha - 1} - (t^*_k - t_{k-1} + s\tau_{k-1})^{-\alpha - 1}] ds.$$
Moreover the convexity of the function \( t^{-1-\alpha} \) gives
\[
(t_k^n - t_{k-1} + s \tau_{k-1})^{-\alpha-1} - (t_{k+1}^n - t_{k-1} + s \tau_{k-1})^{-\alpha-1} \\
> (t_k^n - t_{k-2} + s \tau_{k-2})^{-\alpha-1} - (t_{k+1}^n - t_{k-2} + s \tau_{k-2})^{-\alpha-1},
\]
Then we can get the following result:
\[
\frac{\alpha \tau_k^3}{\tau_k(\tau_k-1 + \tau_k)} \int_0^1 \frac{1}{(1-s)} \left[ (t_k^n - t_{k-1} + s \tau_{k-1})^{-\alpha-1} \right. \\
- (t_{k+1}^n - t_{k-1} + s \tau_{k-1})^{-\alpha-1} \] \] 
\[ 
- (t_k^n - t_{k-2} + s \tau_{k-2})^{-\alpha-1} - (t_{k+1}^n - t_{k-2} + s \tau_{k-2})^{-\alpha-1} \right] ds \\
+ \frac{\alpha \tau_k^3}{\tau_k(\tau_k-1 + \tau_k)} \int_0^1 \left[ (t_k^n - t_{k-1} + s \tau_{k-1})^{-\alpha-1} \right. \\
- (t_{k+1}^n - t_{k-1} + s \tau_{k-1})^{-\alpha-1} \] \] 
\[ 
\left[ (t_k^n - t_{k-1} + s \tau_{k-1})^{-\alpha-1} - (t_{k+1}^n - t_{k-1} + s \tau_{k-1})^{-\alpha-1} \right] ds \geq 0,
\]
as (3.1) for \( j = k - 1 \) gives
\[
\frac{\tau_k^3}{\tau_k(\tau_k-1 + \tau_k)} - \frac{\tau_{k-1}^3}{\tau_k(\tau_k-1 + \tau_k)} - \frac{(4\tau_{k-2} + 3\tau_k-1)\tau_k}{\tau_k(\tau_k-1 + \tau_k)} \geq 0.
\]
Combining (3.15) with (3.14) yields
\[
B_{kk} \geq \frac{1}{2} c^{(k)}_{k-1} + \frac{1}{2(1-\alpha)(\sigma \tau_k^\alpha)} \left[ 2\sigma - (1-\alpha) - \frac{\alpha(1-\alpha)}{(1+\rho_{k+1})\rho_{k+1}^\alpha} \int_0^1 \frac{s(\rho_{k+1} + s)}{\sigma \rho_{k+1} + s} ds \right].
\]
Thus, to ensure \( [B]_{kk} \geq 0 \) for \( 3 \leq k \leq n - 1 \), it is sufficient to impose
\[
\frac{1}{\rho_k} \geq \frac{1}{\rho_{k-1}^2(1 + \rho_{k-1})} - 3, \\
2\sigma - (1-\alpha) - \frac{\alpha(1-\alpha)}{(1+\rho_{k+1})\rho_{k+1}^\alpha} \int_0^1 \frac{s(\rho_{k+1} + s)}{\sigma \rho_{k+1} + s} ds \geq 0.
\]
**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
\[
[B]_{nn} = c^{(n)}_{n-1} + \frac{\sigma^{1-\alpha}}{(1-\alpha)^{\tau_n^\alpha}} - \frac{1}{2} (c^{(n)}_{n-2} - a^{(n)}_{n-1}) \\
= \frac{1}{2} c^{(n)}_{n-1} + \frac{\sigma^{1-\alpha}}{(1-\alpha)^{\tau_n^\alpha}} + \frac{1}{2} (c^{(n)}_{n-2} - c^{(n)}_{n-2} + a^{(n)}_{n-1}) \\
= \frac{1}{2} c^{(n)}_{n-1} + \frac{\sigma^{1-\alpha}}{(1-\alpha)^{\tau_n^\alpha}} + \frac{1}{2} \left( \frac{\alpha \tau_{n-1}^3}{\tau_n(\tau_{n-1} + \tau_n)} \right) \int_0^1 \frac{s(1-s)(t_n^n - t_{n-1} + s \tau_{n-1})^{-\alpha-1}}{\sigma \tau_{n-1} + s} ds.
\]
which ensure We omit the details here. To ensure 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

\[
\int_0^1 (\tau_n - \tau_n + \tau_n - 1 - s)(\tau_n - \tau_n + s - 1) - \alpha^{-1} ds
\]

and

\[
(\tau_n - \tau_n + s - 1)^{-\alpha^{-1}} > (\tau_n - \tau_n + s - 2)^{-\alpha^{-1}}.
\]

We omit the details here. To ensure \([B]_{nn} \geq 0\), it is sufficient to impose

\[
\frac{1}{\rho_n} \geq \frac{1}{\rho_n^2(1 + \rho_n - 1)} - 3, \quad 2\alpha - (1 - \alpha) \geq 0.
\]

Combining (3.10), (3.13), (3.16) and (3.18), we can conclude that if the condition (3.1) holds for \( 2 \leq k \leq n - 1 \) and

\[
2\alpha = \frac{1 - \alpha}{\rho_{n-1}^2(1 + \rho_n - 1)} \geq 0,
\]

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

then \([B]_{kk} \geq 0, \quad k \geq 1\). 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 \( 2 \leq k \leq n - 1 \);

which ensure

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

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 Fig. 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: for \( j \geq 2 \),

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

$$2\sigma - \frac{1 - \alpha}{\rho_*^2} \geq 2 - \alpha - \frac{1 - \alpha}{\rho_*^2} \geq 0, \quad 2\sigma - (1 - \alpha) = 1,$$

and for $2 \leq k \leq n - 1$, we have

$$2\sigma - (1 - \alpha) - \frac{\alpha(1 - \alpha)}{(1 + \rho_{k+1})\rho_{k+1}^\alpha} \int_0^1 \frac{s(\rho_{k+1} + s)}{\sigma \rho_{k+1} + s} \, ds \geq 1 - \frac{\alpha(1 - \alpha)}{(1 + \rho_{k+1})\rho_{k+1}^\alpha} \int_0^1 \frac{s(\rho_{k+1} + s)}{\rho_{k+1} + s} \, ds \geq 1 - \frac{\alpha(1 - \alpha)}{(1 + \rho_*)\rho_*^\alpha} \geq 1 - \frac{1}{4(1 + \rho_*)\rho_*^\alpha} \geq 0.$$

In summary, if (3.20) holds, then

$$\mathcal{B}_n(u, u) = \sum_{k=1}^n \langle L_k^{\alpha, n} u, \delta_k u \rangle \geq \sum_{k=1}^n \frac{g_k(\alpha)}{2\Gamma(2 - \alpha)} \| \delta_k u \|^2_{L^2(\Omega)} \geq 0,$$

with $g_k(\alpha)$ given in (3.4).

**Remark 1** 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 $\mathcal{B}_n(u, u)$ (3.3) can be guaranteed.
4 Stability and Convergence of L2-1\(\sigma\) Method for Subdiffusion Equation

We consider the following subdiffusion equation:

\[
\begin{align*}
\partial_t^\sigma u(t, x) &= \Delta u(t, x) + f(t, x), \quad (t, x) \in (0, \infty) \times \Omega, \\
\partial_t u(t, x) &= 0, \quad (t, x) \in (0, \infty) \times \partial \Omega, \\
\partial_t u(0, x) &= u^0(x), \quad x \in \Omega,
\end{align*}
\]

(4.1)

where \(\Omega\) is a bounded Lipschitz domain in \(\mathbb{R}^d\). Given an arbitrary nonuniform mesh \(\{\tau_k\}_{k \geq 1}\), the L2-1\(\sigma\) scheme of this subdiffusion equation is written as

\[
\begin{align*}
L_k^{u_{\alpha, \eta}} u &= (1 - \alpha/2) \Delta u^k + \alpha/2 \Delta u^{k-1} + f^k, \quad \text{in } \Omega, \\
u^k &= 0, \quad \text{on } \partial \Omega,
\end{align*}
\]

(4.2)

where \(f^k = f(t^*_k, \cdot)\).

4.1 Global-in-Time \(H^1\)-Stability of L2-1\(\sigma\) Scheme for Subdiffusion Equation

Theorem 2 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 \(u^0 \in H^1_0(\Omega)\). 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 L2-1\(\sigma\) scheme (4.2) satisfies the following global-in-time \(H^1\)-stability

\[
\|\nabla u^n\|_{L^2(\Omega)} \leq \|\nabla u^0\|_{L^2(\Omega)} + 2C_f C_\Omega,
\]

where \(C_f = 2\|f\|_{L^\infty([0, \infty); L^2(\Omega))} + \|f\|_{BV([0, \infty); L^2(\Omega))}\), \(C_\Omega\) is the Sobolev embedding constant depending on \(\Omega\) and the spatial dimension \(d\).

Proof Multiplying (4.2) with \(\delta_k u\), integrating over \(\Omega\), and summing up the derived equations over \(k\) yield

\[
\sum_{k=1}^{n} \langle L_k^{u_{\alpha, \eta}} u, \delta_k u \rangle = \sum_{k=1}^{n} \langle (1 - \alpha/2) \Delta u^k + \alpha/2 \Delta u^{k-1}, \delta_k u \rangle + \sum_{k=1}^{n} \langle f^k, \delta_k u \rangle
\]

\[
= -\frac{1}{2} \|\nabla u^n\|^2_{L^2(\Omega)} + \frac{1}{2} \|\nabla u^0\|^2_{L^2(\Omega)} - \frac{1 - \alpha}{2} \sum_{k=1}^{n} \|\nabla \delta_k u\|^2_{L^2(\Omega)}
\]

\[
+ \langle f^n, u^n \rangle - \langle f^1, u^0 \rangle - \sum_{k=2}^{n} \langle \delta_k f, u^{k-1} \rangle.
\]

Applying the Cauchy–Schwarz inequality yields

\[
\langle f^n, u^n \rangle - \langle f^1, u^0 \rangle + \sum_{k=2}^{n} \langle \delta_k f, u^{k-1} \rangle
\]

\[
\leq (2\|f\|_{L^\infty([0, \infty); L^2(\Omega))} + \|f\|_{BV([0, \infty); L^2(\Omega))}) \max_{0 \leq k \leq n} \|u^k\|_{L^2(\Omega)}
\]

\[
\leq C_f C_\Omega \max_{0 \leq k \leq n} \|\nabla u^k\|_{L^2(\Omega)},
\]

where \(C_f = 2\|f\|_{L^\infty([0, \infty); L^2(\Omega))} + \|f\|_{BV([0, \infty); L^2(\Omega))}\), and \(C_\Omega\) is the Sobolev embedding constant depending on \(\Omega\) and the spatial dimension. From Theorem 1, we then have for
Assume that the solution of subdiffusion equation satisfies
\[ \frac{2C_f C_{Ω}}{0 \leq k \leq n} \| \nabla u^k \|_{L^2(Ω)} \]
which indicates
\[ \| \nabla u^0 \|_{L^2(Ω)}^2 + 2C_f C_{Ω} \max_{0 \leq k \leq n} \| \nabla u^k \|_{L^2(Ω)}. \]

For any \( N \geq 1 \), we take \( \max_{0 \leq n \leq N} \) on both sides of (4.3), to obtain
\[ \max_{0 \leq n \leq N} \| \nabla u^n \|_{L^2(Ω)} \leq \| \nabla u^0 \|_{L^2(Ω)}^2 + 2C_f C_{Ω} \max_{0 \leq n \leq N} \| \nabla u^n \|_{L^2(Ω)}, \]
which indicates
\[ \max_{0 \leq n \leq N} \| \nabla u^n \|_{L^2(Ω)} \leq \| \nabla u^0 \|_{L^2(Ω)} + 2C_f C_{Ω}. \]

The proof is completed. \( \square \)

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

According to [26],
\[ \int_0^T \int_Ω \frac{d}{dt} u(t, x) \partial_t u(t, x) \, dx \, dt \geq 0, \]
and moreover,
\[ \int_0^T \int_Ω f(t, x) \partial_t u(t, x) \, dx \, dt = \left( \int_Ω f(t, x) u(t, x) \, dx \right) \bigg|_0^T - \int_0^T \int_Ω \partial_t f(t, x) u(t, x) \, dx \, dt \leq \left( 2\| f \|_{L^∞((0, ∞); L^2(Ω))} + \int_0^∞ \| \partial_t f(t, x) \|_{L^2(Ω)} \, dt \right) C_{Ω} \| \nabla u \|_{L^∞((0, T); L^2(Ω))} \]
\[ =: C_{cont}^f C_{Ω} \| \nabla u \|_{L^∞((0, T); L^2(Ω))}. \]

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

**Remark 3** In the case of \( α = 1 \), i.e., the standard diffusion equation, the energy stability (or \( H^1 \)-stability) has been established for the second order BDF2 schemes in [19, Theorem 2.1] and for the third order BDF3 schemes in [18, Theorem 3.1] on general nonuniform meshes.
4.2 Sharp Convergence of L2-1 Scheme for Subdiffusion Equation

We show the error estimate of the L2-1 scheme (4.2) for the subdiffusion equation (4.1), that is different from the one in [14, 15]. To be precise we will reduce the restriction on time step ratios from \( \rho_k \geq 4/7 \) in [15] to \( \rho_k \geq 0.475329 \). We first reformulate the discrete fractional operator (2.3):

\[
L_{k}^{α,σ}u = \frac{1}{\Gamma(1-α)} \left( [M]_{k,k}u^k - \sum_{j=2}^{k} ([M]_{k,j} - [M]_{k,j-1})u^{j-1} - [M]_{k,1}u^0 \right),
\]

where \( M \) is given by (3.5). We now give some properties on \([M]_{k,j}\).

**Lemma 2** Under the condition (3.2), the following properties of \([M]_{k,j}\) given by (3.5) hold:

1. For all \( 2 \leq j \leq k-1 \),

\[
[M]_{k,j} - [M]_{k,j-1} \geq \frac{\alpha \tau_j}{\tau_j + \tau_{j+1}} \int_{\tau_j}^{1} (\tau_j + \tau_{j+1} - s\tau_j)(1-s)(t^*_k - t_{j-1} - s\tau_j)^{-α-1} ds,
\]

and

\[
[M]_{k,k} - [M]_{k,k-1} \geq \frac{\alpha}{2(1-α)(\sigma \tau_k)^α}.
\]

2. Moreover, if \( \rho_k \geq η \approx 0.475329 \) for all \( k \geq 2 \), then

\[
\frac{1-α}{σ}[M]_{k,k} - [M]_{k,k-1} \geq 0.
\]

Here \( η \) is the real root of \( 1 - 3ρ^2(1+ρ) = 0 \).

**Proof** From (3.5), for \( 1 \leq j \leq k-1 \),

\[
M_{k,j} \geq -a_{j}^{(k)} = \frac{2τ_j(1-θ) + τ_{j+1}}{τ_j + τ_{j+1}} \frac{1}{(t^*_k - (t_{j-1} + θ\tau_j))^α} dθ
\]

\[
\geq \frac{ρ_{j+1}}{1 + ρ_{j+1}} \int_{0}^{1} \frac{1}{(t^*_k - (t_{j-1} + θ\tau_j))^α} dθ \geq \frac{ρ_{j+1}}{1 + ρ_{j+1}} \int_{t_{j-1}}^{t_j} (t^*_k - s)^{-α} ds,
\]

and for \( j = k \),

\[
[M]_{k,k} = c_{k-1}^{(k)} + \frac{σ^{1-α}}{(1-α)τ_k^α} \geq \frac{σ^{1-α}}{(1-α)τ_k^α} = \frac{1}{τ_k} \int_{t_{k-1}}^{t_k} (t^*_k - s)^{-α} ds.
\]

The inequality (4.4) holds.

For \( 2 \leq j \leq k-1 \), according to (3.7) – (3.9),
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)

$$[\mathbf{M}]_{2,2} - [\mathbf{M}]_{2,1} = c_1^{(2)} + \frac{\sigma^{1-\alpha}}{1 - \alpha} \tau_2^\alpha + a_1^{(2)} \geq \frac{\sigma^{1-\alpha}}{1 - \alpha} \tau_2^\alpha - \frac{1}{(\sigma \tau_2)^\alpha} = \frac{\alpha}{2(1 - \alpha)(\sigma \tau_2)^\alpha},$$

where we use the fact $\sigma = 1 - \alpha/2$. Moreover when $j = k \geq 3$, we have

$$[\mathbf{M}]_{k,k} - [\mathbf{M}]_{k,k-1}$$

$$= \frac{\sigma^{1-\alpha}}{1 - \alpha} \tau_k^\alpha + (c_k^{(k)} - c_{k-2}^{(k)} + d_k^{(k)})$$

$$- \frac{\alpha \tau_{k-1}^\alpha}{(\sigma \tau_k)^\alpha} \left( \int_0^1 s(1 - s)(t_k^* - t_{k-1} + s \tau_{k-1})^{-\alpha-1} \, ds \right) + \left( \int_0^1 \frac{\alpha \tau_{k-2}^\alpha}{\tau_{k-1}(\tau_{k-2} + \tau_{k-1})} s(1 - s)(t_{k-2}^* - t_{k-1} + s \tau_{k-2})^{-\alpha-1} \, ds \right) >$$

$$\frac{\sigma^{1-\alpha}}{1 - \alpha} \tau_k^\alpha - \frac{1}{(\sigma \tau_k)^\alpha} = \frac{\alpha}{2(1 - \alpha)(\sigma \tau_k)^\alpha},$$

when the condition (3.2) holds. This inequality coincide with (3.17) by replacing $n$ with $k$. For the property (Q3), the case of $k = 2$ is trivial. In the case of $k \geq 3$, we have

$$\frac{1 - \alpha}{\sigma} [\mathbf{M}]_{k,k} - [\mathbf{M}]_{k,k-1}$$

$$\geq (\sigma \tau_k)^{-\alpha} - c_{k-2}^{(k)} + d_{k-1}^{(k)}$$

$$= (\sigma \tau_k)^{-\alpha} - \frac{\alpha \tau_{k-2}^\alpha}{\tau_{k-1}(\tau_{k-2} + \tau_{k-1})} \left( \int_0^1 s(1 - s)(t_k^* - t_{k-2} + s \tau_{k-2})^{-\alpha-1} \, ds \right) + \left( \int_0^1 \frac{\alpha \tau_{k-1}^\alpha}{\tau_{k-1}(\tau_{k-2} + \tau_{k-1})} s(1 - s)(t_k^* - t_{k-1} + s \tau_{k-1})^{-\alpha-1} \, ds \right) >$$

$$\alpha \left( \frac{\tau_{k-1}(4 \tau_{k-1} + 3 \tau_k)}{\tau_{k-1} + \tau_k} - \frac{\tau_{k-2}^2}{\tau_{k-1}(\tau_{k-2} + \tau_{k-1})} \right) \int_0^1 s(1 - s)(t_k^* - t_{k-1} + s \tau_{k-1})^{-\alpha-1} \, ds.$$

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where we use the facts
\[ \int_0^1 (\tau_{k-1} + \tau_k + s\tau_{k-1})(1 - s)(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha - 1} \, ds \]
\[ \geq (4\tau_{k-1} + 3\tau_k) \int_0^1 s(1 - s)(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha - 1} \, ds, \]
\[ (t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha} \geq (t_k^* - t_{k-2} + s\tau_{k-2})^{-\alpha - 1}, \]
and
\[ \frac{\tau_{k-1}(4\tau_{k-1} + 3\tau_k)}{\tau_{k-1} + \tau_k} - \frac{s\tau_{k-2}^3}{\tau_{k-1} - 1 + (\tau_{k-2} + \tau_{k-1})} \geq 0, \]
when \( \rho_k \geq \eta \approx 0.475329 \) for all \( k \geq 2 \).

Consider the following three standard Lagrange interpolation operators with the following interpolation points:
\[ \Pi_{1,j} : t_{j-1}, t_j, \quad \Pi_{2,j} : t_{j-1}, t_j, t_{j+1}, \quad \Pi_{1,j}^* : t_{j-1}, t_j^*, t_j. \]
As stated in [12], when \( \sigma = 1 - \alpha / 2 \),
\[ \int_{t_{k-1}}^{t_k^*} (\Pi_{1,k}v - \Pi_{2,k}v)\prime(s)(t_k^* - s)^{-\alpha} \, ds = 0. \]
We now analyze the approximation error of the discrete fractional operator in the following lemma.

**Lemma 3** Given a function \( u \) satisfying \( |\partial_i^m u(t)| \leq C_m(1 + t^{\alpha - m}) \) for \( m = 1, 3 \) and nonuniform mesh \( \{\tau_k\}_{k \geq 1} \) satisfying condition (3.2), the approximation error is given by
\[ r_k := \frac{1}{\Gamma(1 - \alpha)} \int_0^{t_{k-1}^*} (t_k^*-s)^{-\alpha} \partial_s[u(s) - I_2u(s)] \, ds, \quad k \geq 1, \]
(4.6)
where \( I_2u = \Pi_{2,j}u \) on \( (t_{j-1}, t_j) \) for \( j < k \) and \( I_2u = \Pi_{2,k}u \) on \( (t_{k-1}, t_k^*) \). Then for \( k \geq 1 \),
\[ |r_k| \leq \frac{C}{\Gamma(1 - \alpha)} \left( [M]_{j,1} (t_2^* / \alpha + t_2) + \sum_{j=2}^k ([M]_{j,j-1} - [M]_{k,j}) (1 + \rho_{j+1})(1 + t_{j-1}^{\alpha - 3}) \right) t_j^3 \]
(4.7)
where \( C \) is a constant depending on \( C_m \) for \( m = 1, 3 \).

**Proof** The case of \( k = 1 \) is not difficult to prove. We now consider the case of \( k \geq 2 \). Let \( \chi(s) := u - I_2u \). Three subcases are discussed in the following content.

**Subcase 1** On the interval \( (t_0, t_1) \), we have
\[ \partial_s I_2u(s) = \frac{2s - t_1 - t_2}{\tau_1(\tau_1 + \tau_2)} u(t_0) - \frac{2s - t_2}{\tau_1 \tau_2} u(t_1) + \frac{2s - t_1}{\tau_2(\tau_1 + \tau_2)} u(t_2) \]
that is linear w.r.t. \( s \). Then we have
\[ |\partial_s I_2u(s)| \leq \max\{|\partial_s I_2u(t_0)|, |\partial_s I_2u(t_1)|\} \leq C_1 \frac{1 + \rho_2}{\tau_1 \rho_2} (t_2 + t_2^* / \alpha), \]

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where we use the facts

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

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

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

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

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

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

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

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

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

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

Therefore, we have

\[
|\partial_s \chi(s)| \leq |\partial_s u| + |\partial_s I_2 u| \leq C_1 \left( s^{\alpha - 1} + 1 + \frac{1 + \rho_2}{\tau_1\rho_2} (t_2 + t_2^\alpha / \alpha) \right),
\]

which yields

\[
\left| \frac{1}{\Gamma(1 - \alpha)} \int_0^{t_1} (t_k^\alpha - s)^{-\alpha} \partial_s \chi(s) \, ds \right|
\]

\[
\leq \frac{C_1}{\Gamma(1 - \alpha)} \left( \int_0^{t_1} s^{\alpha - 1} (t_k^\alpha - s)^{-\alpha} \, ds + \frac{\tau_1 + (1 + \rho_2) / \rho_2 (t_2 + t_2^\alpha / \alpha)}{\tau_1} \int_0^{t_1} (t_k^\alpha - s)^{-\alpha} \, ds \right)
\]

\[
\leq \frac{C_1}{\Gamma(1 - \alpha)} \left( \frac{\tau_1^\alpha}{\alpha(t_k^\alpha - \tau_1)^\alpha} + \frac{\tau_1 + (1 + \rho_2) / \rho_2 (t_2 + t_2^\alpha / \alpha)}{\tau_1} \int_0^{t_1} (t_k^\alpha - s)^{-\alpha} \, ds \right)
\]

\[
\leq \frac{C (t_2^\alpha / \alpha + t_2)}{\Gamma(1 - \alpha)} [\mathbf{M}]_{k,1},
\]

where \( C \) is an absolute constant only depending on \( C_1 \). In the last inequality of (4.8), we use the fact

\[
[\mathbf{M}]_{k,1} \geq \frac{\rho_2}{(1 + \rho_2) \tau_1} \int_0^{t_1} (t_k^\alpha - s)^{-\alpha} \, ds \geq \frac{\rho_2}{(1 + \rho_2) (t_k^\alpha / \alpha)}
\]

\[
\geq \frac{\rho_2^{1+\alpha}}{(1 + \rho_2)(2 + \rho_2)^\alpha (t_k^\alpha - \tau_1)^\alpha} \geq \frac{\rho_2^{1+\alpha}}{(1 + \rho_2)(2 + \rho_2)^\alpha (t_k^\alpha - \tau_1)^\alpha}
\]

obtained from the inequality (4.5).
Subcase 2 On the interval \((t_{j-1}, t_j), 2 \leq j \leq k - 1,\)

\[ |\chi(s)| = \left| \frac{u^{(3)}(\xi)}{6} (s - t_{j-1})(s - t_j)(s - t_{j+1}) \right| \leq C_3 (1 + t_{j-1}^{a-3})(s - t_{j-1})(s - t_j)(s - t_{j+1}), \]

where \(\xi \in (t_{j-1}, t_{j+1}).\) Then we have

\[
\frac{1}{\Gamma(1 - \alpha)} \int_{t_{j-1}}^{t_j} (t_k^* - s)^{-\alpha} \partial_s \chi(s) \, ds = \left| \frac{-\alpha}{\Gamma(1 - \alpha)} \int_{t_{j-1}}^{t_j} (t_k^* - s)^{-1} \chi(s) \, ds \right|
\]

\[
\leq \frac{C_3 \alpha (1 + t_{j-1}^{a-3}) \int_{t_{j-1}}^{t_j} (t_k^* - s)^{-\alpha - 1} (s - t_{j-1})(s - t_j)(s - t_{j+1}) \, ds}{\Gamma(1 - \alpha)}
\]

\[
= \frac{C_3 \alpha (1 + t_{j-1}^{a-3}) \tau_j^3}{\Gamma(1 - \alpha)} \int_{t_{j-1}}^{t_j} s(t_{j+1} - s)\tau_j(1 - s) - s\tau_j)^{-\alpha - 1} \, ds
\]

\[
\leq \frac{C_3 (1 + \rho_{j+1})(1 + t_{j-1}^{a-3}) \tau_j^3}{\Gamma(1 - \alpha)} ([M]_{k,j} - [M]_{k,j-1}),
\]

(4.9)

from (Q2) in Lemma 2.

Subcase 3 On the interval \((t_{k-1}, t_k^*),\)

\[ |\chi(s)| \leq \frac{C_3 (1 + t_{k-1}^{a-3})(s - t_{k-1})(t_k^* - s)(t_k - s) \leq C_3 (1 + t_{k-1}^{a-3}) \tau_k^2 (t_k^* - s), \]

which yields

\[
\frac{1}{\Gamma(1 - \alpha)} \int_{t_{k-1}}^{t_k} (t_k^* - s)^{-\alpha} \partial_s \chi(s) \, ds = \left| \frac{-\alpha}{\Gamma(1 - \alpha)} \int_{t_{k-1}}^{t_k} (t_k^* - s)^{-1} \chi(s) \, ds \right|
\]

\[
\leq \frac{C_3 \alpha (1 + t_{k-1}^{a-3}) \tau_k^2}{\Gamma(1 - \alpha)} \int_{t_{k-1}}^{t_k} (t_k^* - s)^{-\alpha} \, ds = \frac{2C_3 \sigma (1 + t_{k-1}^{a-3}) \tau_k^3}{\Gamma(1 - \alpha)} \frac{\alpha}{2(1 - \alpha)(\sigma \tau_k)^{\alpha}}
\]

\[
\leq \frac{2C_3 \sigma (1 + t_{k-1}^{a-3}) \tau_k^3}{\Gamma(1 - \alpha)} ([M]_{k,k} - [M]_{k,k-1})
\]

(4.10)

from (Q2) in Lemma 2.

Combining (4.8), (4.9) and (4.10) we obtain the estimation (4.7) of approximation error.

\[ \square \]

**Theorem 3** Assume that \(u \in C^3((0, T], H_0^1(\Omega))\) and \(\left| \partial_t^m u(t) \right| \leq C_m (1 + t^{a-m}),\) for \(m = 1, 2, 3\) 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

\[
\max\limits_{1 \leq k \leq n} \| u(t_k) - u^k \|_{L^2(\Omega)} \leq C \left( t_2^2/\alpha + t_2 + \frac{1}{1 - \alpha} \max\limits_{2 \leq k \leq n} (1 + \rho_{k+1})(1 + t_{k-1}^{a-3})(t_k^*)^\alpha \tau_k^{\alpha} \right.
\]

\[
+ \left. (t_1^\alpha/\alpha + \tau_1)^{\alpha/2} + \sqrt{\Gamma(1 - \alpha)} \max\limits_{2 \leq k \leq n} (t_k^{\alpha/2})(1 + t_{k-1}^{a-2})^2 \right).
\]

where \(C\) is a constant depending only on \(C_m, m = 1, 2, 3\) and \(\Omega.\)

**Proof** Let \(e_k := u(t_k) - u^k.\) We have

\[
L^\alpha \ast e = \Delta e_k^\ast - r_k + \Delta R_k^e,
\]

(4.11)
where \( e^*_k := (1 - \alpha/2)e^k + \alpha/2e^{k-1} \), \( r_k \) is given in (4.6), and \( R^*_k := u(t^*_k) - ((1 - \alpha/2)u(t_k) + \alpha/2u(t_{k-1})) \). Multiplying (4.11) with \( e^*_k \) and integrating over \( \Omega \) yield
\[
(L^*_k, e^*_k) = -\|\nabla e^*_k\|^2_{L^2(\Omega)} - (r_k, e^*_k) - (\nabla R^*_k, \nabla e^*_k).
\] (4.12)

According to [2, Lemma 1] as well as Lemma 2, we can derive
\[
(L^*_k, e^*_k) = \frac{1}{\Gamma(1 - \alpha)} \sum_{j=1}^k [M]_{k,j} \langle (e^j - e^{j-1}), (1 - \alpha/2)e^k + \alpha/2e^{k-1} \rangle
\]
\[
\geq \frac{1}{2\Gamma(1 - \alpha)} \sum_{j=1}^k [M]_{k,j} \left( \|e^j\|^2_{L^2(\Omega)} - \|e^{j-1}\|^2_{L^2(\Omega)} \right).
\]

Applying Cauchy-Schwarz inequality in (4.12) yields
\[
\sum_{j=1}^k [M]_{k,j} \left( \|e^j\|^2_{L^2(\Omega)} - \|e^{j-1}\|^2_{L^2(\Omega)} \right) \leq 2\Gamma(1 - \alpha) \|r_k\|_{L^2(\Omega)} \|e^*_k\|_{L^2(\Omega)}
\]
\[
+ \Gamma(1 - \alpha) \|R^*_k\|^2_{H^1(\Omega)}.
\] (4.13)

We define a lower triangular \( P \) matrix such that
\[
P M = E_L
\]
where
\[
E_L = \begin{pmatrix}
1 & & & \\
1 & 1 & & \\
& \ddots & \ddots & \\
& & 1 & 1 & 1
\end{pmatrix}.
\]

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 [14]. It can be easily checked that \([P]_{k,l} \geq 0\) due to the monotonicity properties of \( M \). From (4.13) we can derive that \( \forall 1 \leq k \leq n, \)
\[
\|e^k\|^2_{L^2(\Omega)} \leq 2\Gamma(1 - \alpha) \sum_{l=1}^k [P]_{k,l} \|r_l\|_{L^2(\Omega)} \|e^*_l\|_{L^2(\Omega)} + \Gamma(1 - \alpha) \sum_{l=1}^k [P]_{k,l} \|R^*_l\|^2_{H^1(\Omega)}
\]
\[
\leq 2\Gamma(1 - \alpha) \left( \max_{1 \leq l \leq k} \|e^*_l\|_{L^2(\Omega)} \right) \sum_{l=1}^k [P]_{k,l} \|r_l\|_{L^2(\Omega)} + \Gamma(1 - \alpha) \sum_{l=1}^k [P]_{k,l} \|R^*_l\|^2_{H^1(\Omega)},
\] (4.14)

where we use
\[
\sum_{l=1}^k [P]_{k,l} \sum_{j=1}^l [M]_{l,j} \left( \|e^j\|^2_{L^2(\Omega)} - \|e^{j-1}\|^2_{L^2(\Omega)} \right)
\]
\[
= \sum_{j=1}^k \left( \|e^j\|^2_{L^2(\Omega)} - \|e^{j-1}\|^2_{L^2(\Omega)} \right) \sum_{l=j}^k [P]_{k,l}[M]_{l,j}
\]
where we use (Q1) in Lemma 2 for the inequality of upper bound of 

\[ \left\| e_j \right\|_{L^2(\Omega)}^2 - \left\| e_{j-1} \right\|_{L^2(\Omega)}^2 = \left\| e^k \right\|_{L^2(\Omega)}^2. \]

According to Lemma 3,

\[
\Gamma (1 - \alpha) \sum_{l=1}^{k} |P|_{l,j} \| r_j \|
\leq C |\Omega| \sum_{l=1}^{k} |P|_{l,j} \left( |M|_{l,1} (t^2_j / \alpha + t_2) + \sum_{j=2}^{l} (|M|_{l,j} - |M|_{l,j-1}) (1 + \rho_{j+1} (1 + t^\alpha_{j-1} \tau_j^3)) \right)
\]

\[
= C |\Omega| \left( (t^2_j / \alpha + t_2) + \sum_{j=2}^{k} (1 + \rho_{j+1} (1 + t^\alpha_{j-1} \tau_j^3)) \sum_{l=j}^{k} |P|_{l,j} (|M|_{l,j} - |M|_{l,j-1}) \right)
\]

\[
= C |\Omega| \left( (t^2_j / \alpha + t_2) + \sum_{j=2}^{k} (1 + \rho_{j+1} (1 + t^\alpha_{j-1} \tau_j^3)) |P|_{k,j-1} |M|_{j-1,j-1} \right)
\]

\[
= C |\Omega| \left( (t^2_j / \alpha + t_2) + \sum_{j=2}^{k} |P|_{k,j-1} |M|_{j-1,j-1} \frac{|M|_{j-1,j-1} (1 + \rho_{j+1} (1 + t^\alpha_{j-1} \tau_j^3))}{|M|_{j-1,j-1}} \right)
\]

\[
\leq C |\Omega| \left( (t^2_j / \alpha + t_2) + \frac{1}{1 - \alpha} \max_{2 \leq j \leq k} \frac{|M|_{j-1,j-1} (1 + \rho_{j+1} (1 + t^\alpha_{j-1} \tau_j^3))}{|M|_{j-1,j-1}} \right)
\]

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

\[
M_t \quad j,j = c_{j-1}^{(j)} + \frac{\sigma^{1-\alpha}}{(1-\alpha) \tau_j^\alpha} (4.15)
\]

\[
\int_{0}^{1} \frac{\tau_j^2 (2\theta - 1)}{\tau_j (\tau_j+1 + \tau) (t^\alpha_j - (t_j-2 + \theta \tau_j-1)^\alpha)} d\theta + \frac{\sigma^{1-\alpha}}{(1-\alpha) \tau_j^\alpha}
\]

\[
\leq \frac{1}{\rho_j (1 + \rho_{j+1} (\sigma \tau_j)^\alpha) + \frac{\sigma^{1-\alpha}}{(1-\alpha) \tau_j^\alpha}} \leq \frac{1}{\eta (1 + \eta) (\sigma \tau_j)^\alpha} + \frac{\sigma^{1-\alpha}}{(1-\alpha) \tau_j^\alpha},
\]

\[
|M|_{j,1} \geq \frac{\eta}{(1 + \eta) \tau_1} \int_{0}^{t_1} (t^\alpha_j - s)^{-\alpha} ds \geq \frac{\eta}{(1 + \eta) (t^\alpha_j)^{-\alpha}}.
\]

where we use (Q1) in Lemma 2 for the inequality of \( |M|_{j,1} \).

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

\[
\| R_j^* \|_{H^1(\Omega)} \leq C (\tau_j^\alpha / \alpha + \tau_1), \quad \| R_j^* \|_{H^1(\Omega)} \leq C (1 + \tau^\alpha_{j-1} \tau_j^2), \quad 2 \leq j \leq k.
\]
Then we have
\[
\sum_{l=1}^{k} [P]_{k,l} \| R_l^n \|_{H^1(\Omega)}^2 \leq C \left( \left[ P \right]_{k,1} \left[ M \right]_{1,1} + \sum_{l=2}^{k} \left[ P \right]_{k,l} \left[ M \right]_{1,2} \right) \left( (1 + \frac{\alpha^2 - 2}{\alpha - 1}) \frac{\tau_l^2}{\alpha} \right)^2 \right) \leq C \left( \left[ M \right]_{1,1} \left( \frac{\tau_l^2}{\alpha} \right)^2 + \max_{2 \leq l \leq k} \left[ M \right]_{1,2} \left( (1 + \frac{\alpha^2 - 2}{\alpha - 1}) \frac{\tau_l^2}{\alpha} \right)^2 \right) \leq C \left( \left( 1 - \alpha \right) \frac{\tau_l^2}{\alpha} + \max_{2 \leq l \leq k} \left( \frac{\tau_l^2}{\alpha} \right)^2 \right),
\]
where we use \([M]_{l,2} \geq [M]_{l,1}\) and (4.15).

Taking the max for \(1 \leq k \leq n\) on both sides of (4.14), we can derive
\[
\max_{1 \leq k \leq n} \| e_k \|_{L^2(\Omega)} \leq C \left( \frac{t_2^2}{\alpha} + \frac{1}{1 - \alpha} \max_{2 \leq k \leq n} (1 + \rho_{k+1})(1 + \frac{\alpha^2 - 3}{\alpha - 1})(1 + \frac{\alpha^2 - 2}{\alpha - 1})(t_{k-1}^\alpha) \tau_k \tau_{k-1}^\alpha \right) + \left( \frac{\tau_l^2}{\alpha} \right)^2 + \sqrt{1 - \alpha} \max_{2 \leq k \leq n} \left( \frac{\tau_l^2}{\alpha} \right)^2 \right) \right) \leq \left( \left( \frac{j}{K} \right)^r T, \quad \tau_j = t_j - t_{j-1} = \left( \left( \frac{j}{K} \right)^r - \left( \frac{j-1}{K} \right)^r \right) \right) T,
\]
(4.17)
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 (4.16) can be estimated as follows:
\[
\begin{align*}
(1 + \rho_{k+1})(1 + \frac{\alpha^2 - 3}{\alpha - 1})(1 + \frac{\alpha^2 - 2}{\alpha - 1})(t_{k-1}^\alpha) \tau_k \tau_{k-1}^\alpha & \leq C t_{k-1}^{2\alpha - 3} \tau_k^{3 - \alpha} \\
& = C t_{k-1}^{2\alpha - 3} (t_k - t_{k-1})^{3 - \alpha} = C (t_{k-1}^\alpha (t_k/t_{k-1} - 1))^{3 - \alpha} \\
& = C t_{k-1}^{\alpha} ((1 + 1/(k - 1))^r - 1)^{3 - \alpha} \\
& \leq C r^{3 - \alpha} T^\alpha \frac{(k - 1)^{r - (3 - \alpha)}}{K^\alpha} = \frac{C_{T,1} K^{\min[\alpha,3 - \alpha]}}{K^\alpha}
\end{align*}
\]
(4.18)
and
\[
\begin{align*}
(t_l^\alpha)^{2}(1 + \frac{\alpha^2 - 2}{\alpha - 1}) \tau_k^2 & \leq C t_{k-1}^{2\alpha - 2} \tau_k^2 = C t_{k-1}^{\alpha - 2} (t_k - t_{k-1})^2 = C t_{k-1}^{\alpha} (t_k/t_{k-1} - 1)^2 \\
& = C T^\alpha \frac{(k - 1)^{r - (\alpha - 2)}}{K^\alpha} \left( (1 + 1/(k - 1))^r - 1 \right)^2 \leq C r^2 T^\alpha \frac{(k - 1)^{r - (\alpha - 2)}}{K^\alpha} = \frac{C_{T,2} K^{\min[\alpha,2 - \alpha]}}{K^\alpha},
\end{align*}
\]
(4.19)
In (4.18) and (4.19), \(C_{T,1}\) and \(C_{T,2}\) only depend on \(T\). Therefore, if \(u\) satisfies the regularity assumptions in Theorem 3, then we have the following error estimate of numerical solutions of the L2-1\(_\sigma\) scheme on the graded mesh with grading parameter \(r\):
\[
\max_{1 \leq k \leq K} \| u(t_k) - u^k \|_{L^2(\Omega)} \leq \frac{\tilde{C}}{K^{\min[\alpha,2 - \alpha]}},
\]
(4.20)
where \(\tilde{C}\) depends on \(C_m\) with \(m = 1, 2, 3, \alpha\) and \(\Omega\).
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 \( \alpha = 0.3 \)

| \( K \)  | \( r = 1 \)    | \( r = 2 \)    | \( r = 2/\alpha \) | \( r = 3/\alpha \) |
|--------|----------------|----------------|-------------------|-------------------|
| 40     | 2.3600e–2      | 1.3254e–2      | 2.7182e–4        | 5.6542e–4        |
| 80     | 2.2505e–2      | 9.4767e–3      | 7.4873e–5        | 1.5847e–4        |
| 160    | 2.0661e–2      | 6.5872e–3      | 1.9983e–5        | 4.2808e–5        |
| 320    | 1.8461e–2      | 4.9467e–3      | 5.2316e–6        | 1.1281e–5        |
| 480    | 1.7117e–2      | 3.5761e–3      | 1.9335           | 5.1370e–6        |
| 640    | 1.6165e–2      | 3.0338e–3      | 1.9408           | 2.9371e–6        |

Remark 4 When \( \alpha \to 1^- \), the constant \( \tilde{C} \) in (4.20) will tend to infinity. However, using the technique by Chen-Stynes in [4], 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 \( L^2_{-1.\alpha} \) scheme (4.2) of the subdiffusion equation (4.1).

As in [3, 15], the discrete coefficients \( a_j^{(k)} \) and \( c_j^{(k)} \) in (2.2) are computed by adaptive Gauss-Kronrod quadrature, to avoid roundoff error problems.

5.1 1D Example

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

The graded mesh (4.17) 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 \( \max_{1 \leq k \leq K} \| u(t_k) - u^k \|_{L^2(\Omega)} \). Tables 1, 2 and 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 (4.20) derived from Theorem 3.

In [10, 25], 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 Tables 1, 2 and 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, for this example, we use the following \( r \)-variable graded mesh

\[
\begin{align*}
    r_j &= 2/\alpha + 1.5 - \frac{3(j - 1)}{K - 1}, \\
    t_j &= \left( \frac{j}{K} \right)^{r_j} T, \\
    \tau_j &= t_j - t_{j-1} = \left[ \left( \frac{j}{K} \right)^{r_j} - \left( \frac{j-1}{K} \right)^{r_{j-1}} \right] T.
\end{align*}
\]

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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 \( \alpha = 0.5 \)

| \( K \) | \( r = 1 \) | \( r = 2 \) | \( r = 2/\alpha \) | \( r = 3/\alpha \) |
|-------|--------|--------|----------------|----------------|
| 40    | 1.857e-2 | 3.918e-3 | 2.2728e-4 | 3.5987e-4 |
| 80    | 1.4568e-2 | 2.0105e-3 | 9.628e-4 | 9.908e-5 |
| 160   | 1.1059e-2 | 1.0182e-3 | 9.908e-4 | 1.9524e-4 |
| 320   | 8.2145e-3 | 5.1239e-4 | 3.7186e-6 | 2.6590e-5 |
| 480   | 6.8534e-3 | 3.4232e-4 | 1.6536e-6 | 7.0116e-6 |
| 640   | 6.0116e-3 | 8.2145e-3 | 9.908e-5 | 1.9524e-4 |

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 \( \alpha = 0.7 \)

| \( K \) | \( r = 1 \) | \( r = 2 \) | \( r = 2/\alpha \) | \( r = 3/\alpha \) |
|-------|--------|--------|----------------|----------------|
| 40    | 8.3068e-3 | 7.3797e-4 | 1.7758e-4 | 1.5861e-4 |
| 80    | 5.4221e-3 | 2.8495e-4 | 4.6703e-5 | 4.3872e-5 |
| 160   | 3.4582e-3 | 1.0874e-4 | 1.1903e-5 | 1.1918e-5 |
| 320   | 2.1753e-3 | 4.1317e-5 | 2.9940e-6 | 3.1981e-6 |
| 480   | 1.6518e-3 | 2.3437e-5 | 1.3323e-6 | 1.4809e-6 |
| 640   | 1.3569e-3 | 1.5672e-5 | 1.9970 | 1.8608 |

Fig. 2 Time steps (left), pointwise \( L^2 \)-errors (middle), and maximum \( L^2 \)-errors (right) of the \( L^2 \)-1 scheme in 1D on the \( r \)-variable graded mesh (5.1) and the standard graded meshes (4.17) with \( r = 2/\alpha, \ 3/\alpha (\alpha = 0.7) \)

In Fig. 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 (4.17) 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 Fig. 2, the maximum \( L^2 \)-error for the \( r \)-variable graded mesh is smaller than the standard graded meshes with \( r = 2/\alpha, \ 3/\alpha \).
Fig. 3  Pointwise $L^2$-errors (left) with $K = 640$ and maximum $L^2$-errors (right) of L2-$1_\sigma$ scheme in 2D on the $r$-variable graded mesh (5.1) and the graded mesh (4.17) with $r = 2/\alpha$ ($\alpha = 0.7$)

5.2 2D Example

In the 2D case, we set $f(t, x, y) = (\Gamma(1 + \alpha) + 2t^\alpha) \sin(x) \sin(y)$ and then the exact solution $u(t, x, y) = t^\alpha \sin(x) \sin(y)$. 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 Fig. 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 (4.17) 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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Declarations

Conflict of interest  The authors have not disclosed any competing interests.

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