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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

Mathematics Subject Classification (2000) 35R11 · 65M12

1 Introduction

In the past decade, many numerical methods have been proposed to solve the time-fractional diffusion equations [31, 8]. If the solution is sufficiently smooth (which requires the initial value to be smooth and satisfying some compatibility conditions), the L1 scheme has $(2 - \alpha)$ order accuracy, see the works of Langlands and Henry [16], Sun-Wu [36], and Lin-Xu [25]. Alikhanov proposes the L2-1 $_{\sigma}$ scheme

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having second order accuracy in time [3]. Gao-Sun-Zhang study an L2 method of $(3 - \alpha)$ -order on uniform meshes in [7] and later a slightly different L2 method is analyzed by Lv-Xu in [30]. In addition to the Lagrangian interpolation methods, the discontinous Galerkin methods is analyzed by Mustapha-Abdallah-Furati [32] and the convolution quadrature (CQ) scheme is studied by Jin-Li-Zhou [9], both of which can obtain the desired high-order accuracy.

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_σ , and L2 methods on the graded meshes have been developed. Stynes-Riordan-Gracia [35] 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 [13]. Chen-Stynes [5] prove the second-order convergence of the L2- 1_σ scheme on fitted meshes combining the graded meshes and quasiuniform meshes. Kopteva-Meng [15] provide sharp pointwise-in-time error bounds for quasi-graded temporal meshes with arbitrary degree of grading for the L1 and L2- 1_σ schemes. Later Kopteva generalize this sharp pointwise error analysis to an L2-type scheme on quasi-graded meshes [14]. Liao-Li-Zhang establish the sharp error analysis for the L1 scheme of subdiffusion equation on general nonuniform meshes in [18] and then Liao-Mclean-Zhang study the L2- 1_σ scheme in [19, 20], 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 [32] analyze the global high-order convergence of the discontinuous Galerkin method for subdiffusion equation on graded mesh. The CQ methods provides a flexible framework for constructing high-order methods to approximate the fractional derivative, developed by Lubich in [26, 27, 28]. Along this way, Lubich-Sloan-Thomée [29] analyze first and second order CQ schemes for subdiffusion equation. In recent years, Jin-Li-Zhou [9, 11] 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. Banjai and López-Fernández [4] provide an arbitrarily high-order accuracy algorithm for subdiffusion equation based on Runge-Kutta CQ. In addition, the CQ methods have also been developed to solve nonlinear subdiffusion equations (see [10, 1, 38, 17]).

In this work, we first study the H^1 -stability of the L2- 1_σ method proposed initially in [3] 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 Ω is a bounded Lipschitz domain in \mathbb{R}^d . For the L2- 1_σ fractional-derivative operator denoted by $L_k^{\alpha,*}$, we prove that the following bilinear form

$$\mathcal{B}_n(v, w) = \sum_{k=1}^n \langle L_k^{\alpha,*} v, \delta_k w \rangle, \quad \delta_k w := w^k - w^{k-1}, \quad n \geq 1, \quad (1.1)$$

is positive semidefinite under the restrictions (3.2) on time step ratios $\rho_k := \tau_k / \tau_{k-1}$ with τ_k the k th 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 [21], 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 [12, 2] a general criteria ensuring the positivity of quadratic forms that can be applied to the time-fractional operators such as the L1 formula. In [22], 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* H^1 -stability result in Theorem 4.1 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 H^1 -stability can be ensured for all time.

Besides the global-in-time H^1 -stability of the L2-1 $_{\sigma}$ scheme in Theorem 4.1, we revisit the sharp convergence analysis in [20] by Liao-Mclean-Zhang. We provide a proof of sharp L^2 -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 [20] to $\rho_k \geq 0.475329$.

In the numerical implementations, we compare the L2-1 $_{\sigma}$ schemes on the standard graded meshes [35] and the r -variable graded meshes (with varying grading parameter) proposed in [34]. 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 L2-1 $_{\sigma}$ fractional-derivative operator are provided. In Section 3, we prove the positive semidefiniteness of the bilinear form \mathcal{B}_n under some mild restrictions on the time step ratios. In Section 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 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 L2-1 $_{\sigma}$ operator on an arbitrary nonuniform mesh.

We consider the L2-1 $_{\sigma}$ 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 $0 = t_0 < t_1 < \dots < t_{k-1} < t_k < \dots$ with $k \geq 1$. Let $\tau_j = t_j - t_{j-1}$ and $\sigma = 1 - \alpha/2$ (c.f. [3] for this setting of σ). The fractional derivative $\partial_t^{\alpha} u(t)$ at $t = t_k^* := t_{k-1} + \sigma \tau_k$ could be approximated by the following L2-1 $_{\sigma}$

fractional-derivative operator

$$\begin{aligned} L_k^{\alpha,*} u &= \frac{1}{\Gamma(1-\alpha)} \left(\sum_{j=1}^{k-1} \int_{t_{j-1}}^{t_j} \frac{\partial_s H_2^j(s)}{(t_k^*-s)^\alpha} ds + \int_{t_{k-1}}^{t_k^*} \frac{\partial_s H_1^k(s)}{(t_k^*-s)^\alpha} ds \right) \\ &= \frac{1}{\Gamma(1-\alpha)} \left(\sum_{j=1}^{k-1} (a_j^k u^{j-1} + b_j^k u^j + c_j^k u^{j+1}) \right) + \frac{\sigma^{1-\alpha} (u^k - u^{k-1})}{\Gamma(2-\alpha) \tau_k^\alpha}, \end{aligned} \quad (2.1)$$

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

$$\begin{aligned} H_2^j(t) &= \frac{(t-t_j)(t-t_{j+1})}{(t_{j-1}-t_j)(t_{j-1}-t_{j+1})} u^{j-1} + \frac{(t-t_{j-1})(t-t_{j+1})}{(t_j-t_{j-1})(t_j-t_{j+1})} u^j \\ &\quad + \frac{(t-t_{j-1})(t-t_j)}{(t_{j+1}-t_{j-1})(t_{j+1}-t_j)} u^{j+1}, \\ H_1^k(t) &= \frac{t-t_k}{t_{k-1}-t_k} u^{k-1} + \frac{t-t_{k-1}}{t_k-t_{k-1}} u^k, \end{aligned}$$

and

$$\begin{aligned} a_j^k &= \int_{t_{j-1}}^{t_j} \frac{2s-t_j-t_{j+1}}{\tau_j(\tau_j+\tau_{j+1})} \frac{1}{(t_k^*-s)^\alpha} ds = \int_0^1 \frac{-2\tau_j(1-\theta)-\tau_{j+1}}{(\tau_j+\tau_{j+1})(t_k^*-(t_{j-1}+\theta\tau_j))^\alpha} d\theta, \\ b_j^k &= - \int_{t_{j-1}}^{t_j} \frac{2s-t_{j-1}-t_{j+1}}{\tau_j\tau_{j+1}} \frac{1}{(t_k^*-s)^\alpha} ds = - \int_0^1 \frac{2\tau_j\theta-\tau_j-\tau_{j+1}}{\tau_{j+1}(t_k^*-(t_{j-1}+\theta\tau_j))^\alpha} d\theta, \\ c_j^k &= \int_{t_{j-1}}^{t_j} \frac{2s-t_{j-1}-t_j}{\tau_{j+1}(\tau_j+\tau_{j+1})} \frac{1}{(t_k^*-s)^\alpha} ds = \int_0^1 \frac{\tau_j^2(2\theta-1)}{\tau_{j+1}(\tau_j+\tau_{j+1})(t_k^*-(t_{j-1}+\theta\tau_j))^\alpha} d\theta. \end{aligned} \quad (2.2)$$

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

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

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

$$L_k^{\alpha,*} u = \frac{1}{\Gamma(1-\alpha)} \left(c_{k-1}^k \delta_k u - a_1^k \delta_1 u + \sum_{j=2}^{k-1} d_j^k \delta_j u \right) + \frac{\sigma^{1-\alpha}}{\Gamma(2-\alpha) \tau_k^\alpha} \delta_k u, \quad (2.3)$$

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

To establish the global-in-time H^1 -stability of L2-1 $_{\sigma}$ method for fractional-order parabolic problem, we shall prove the positive semidefiniteness of \mathcal{B}_n defined in (1.1).

3 Positive semidefiniteness of bilinear form \mathcal{B}_n

In this section, we first propose some properties of the L2-1 $_{\sigma}$ 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 ρ_k , $k \geq 2$.

Lemma 3.1 (Properties of a_j^k , c_j^k and d_j^k) *For the L2-1 $_{\sigma}$ 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) $a_{j+1}^k - a_j^k < 0$, $1 \leq j \leq k-2$, $k \geq 3$;
- (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) $c_j^{k+1} - c_j^k < 0$, $1 \leq j \leq k-1$, $k \geq 2$;
- (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

$$\frac{1}{\rho_{j+1}} \geq \frac{1}{\rho_j^2(1+\rho_j)} - 3, \quad \forall j \geq 2, \quad (3.1)$$

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 [34, Lemma 3.1] except replacing t_k with t_k^* . We omit it here.

Theorem 3.1 *Consider a nonuniform mesh $\{\tau_k\}_{k \geq 1}$ satisfying that $k \geq 2$,*

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

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

$$g_k(\alpha) = \begin{cases} \frac{1}{(\sigma\tau_1)^\alpha} \left(2\sigma - \frac{1-\alpha}{\rho_2^\alpha} \right), & k=1, \\ (1-\alpha)c_{k-1}^k + \frac{1}{(\sigma\tau_k)^\alpha} \left(1 - \frac{\alpha(1-\alpha)}{(1+\rho_{k+1})\rho_{k+1}^\alpha} \int_0^1 \frac{s(\rho_{k+1}+s)}{\sigma\rho_{k+1}+s} ds \right), & 2 \leq k \leq n-1, \\ (1-\alpha)c_{n-1}^n + \frac{1}{(\sigma\tau_n)^\alpha}, & k=n \neq 2, \end{cases} \quad (3.4)$$

are always positive for $\alpha \in (0, 1)$ and $\sigma = 1 - \alpha/2$.

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

$$\mathcal{B}_n(u, u) = \sum_{k=1}^n \langle L_k^{\alpha,*} u, \delta_k u \rangle = \frac{1}{\Gamma(1-\alpha)} \int_{\Omega} \psi \mathbf{M} \psi^T dx,$$

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

$$\mathbf{M} = \begin{pmatrix} \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_1^\alpha} & & & & \\ -a_1^2 & c_1^2 + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_2^\alpha} & & & \\ -a_1^3 & d_2^3 & c_2^3 + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_3^\alpha} & & \\ \vdots & \vdots & \ddots & \ddots & \\ -a_1^n & d_2^n & \cdots & d_{n-1}^n & c_{n-1}^n + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_n^\alpha} \end{pmatrix}. \quad (3.5)$$

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

$$\mathbf{A} = \begin{pmatrix} \beta_1 & & & & \\ -a_1^2 & \beta_2 & & & \\ -a_1^3 & d_2^3 & \beta_3 & & \\ \vdots & \vdots & \ddots & \ddots & \\ -a_1^n & d_2^n & \cdots & d_{n-1}^n & \beta_n \end{pmatrix},$$

and

$$\mathbf{B} = \text{diag} \left(\frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_1^\alpha} - \beta_1, c_1^2 + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_2^\alpha} - \beta_2, \dots, c_{n-1}^n + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_n^\alpha} - \beta_n \right),$$

with

$$\begin{aligned} 2\beta_1 &= -a_1^2, & 2\beta_2 - d_2^3 &= a_1^3 - a_1^2, \\ 2\beta_k - d_k^{k+1} &= d_{k-1}^k - d_{k-1}^{k+1}, & 3 \leq k \leq n-1, \\ 2\beta_n &= d_{n-1}^n, & n \geq 3. \end{aligned} \quad (3.6)$$

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 $\mathbf{e}_n = (0, \dots, 0, 1) \in \mathbb{R}^{1 \times n}$. According to Lemma 3.1, if the condition (3.1) holds, \mathbf{S} satisfies the following three properties:

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

From [33, Lemma 2.1], \mathbf{S} is positive definite. Let $\varepsilon \rightarrow 0$. 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 ρ_k . We first provide two equivalent forms of a_j^k according to (2.2): $\forall 1 \leq j \leq k-1$,

$$\begin{aligned} a_j^k &= \int_0^1 \frac{-2\tau_j(1-s) - \tau_{j+1}}{(\tau_j + \tau_{j+1})(t_k^* - (t_{j-1} + s\tau_j))^\alpha} ds \\ &= \frac{1}{\tau_j + \tau_{j+1}} \int_0^1 (t_k^* - (t_{j-1} + s\tau_j))^{-\alpha} d(\tau_j s^2 - (2\tau_j + \tau_{j+1})s) \\ &= -(t_k^* - t_j)^{-\alpha} + \frac{\alpha\tau_j}{\tau_j + \tau_{j+1}} \int_0^1 (\tau_j + \tau_{j+1} + s\tau_j)(1-s)(t_k^* - t_j + s\tau_j)^{-\alpha-1} ds \end{aligned} \quad (3.7)$$

and

$$\begin{aligned} a_j^k &= \int_0^1 \frac{-2\tau_j(1-s) - \tau_{j+1}}{(\tau_j + \tau_{j+1})(t_k^* - (t_{j-1} + s\tau_j))^\alpha} ds = \int_0^1 \frac{-2\tau_j s - \tau_{j+1}}{(\tau_j + \tau_{j+1})(t_k^* - t_j + s\tau_j)^\alpha} ds \\ &= \frac{1}{\tau_j + \tau_{j+1}} \int_0^1 (t_k^* - t_j + s\tau_j)^{-\alpha} d(-\tau_j s^2 - \tau_{j+1}s) \\ &= -(t_k^* - t_{j-1})^{-\alpha} - \frac{\alpha\tau_j}{\tau_j + \tau_{j+1}} \int_0^1 (\tau_j + \tau_{j+1} - s\tau_j)(1-s)(t_k^* - t_{j-1} - s\tau_j)^{-\alpha-1} ds. \end{aligned} \quad (3.8)$$

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

$$\begin{aligned} c_j^k &= \int_0^1 \frac{\tau_j^2(2s-1)}{\tau_{j+1}(\tau_j + \tau_{j+1})(t_k^* - (t_{j-1} + s\tau_j))^\alpha} ds \\ &= \frac{\tau_j^2}{\tau_{j+1}(\tau_j + \tau_{j+1})} \int_0^1 (t_k^* - (t_{j-1} + s\tau_j))^{-\alpha} d(s^2 - s) \\ &= \frac{\alpha\tau_j^3}{\tau_{j+1}(\tau_j + \tau_{j+1})} \int_0^1 s(1-s)(t_k^* - t_j + s\tau_j)^{-\alpha-1} ds. \end{aligned} \quad (3.9)$$

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

$$\begin{aligned} [\mathbf{B}]_{11} &= \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_1^\alpha} - \frac{1}{2} \int_0^1 \frac{2\tau_1(1-\theta) + \tau_2}{(\tau_1 + \tau_2)(t_2^* - (t_0 + \theta\tau_1))^\alpha} d\theta \\ &= \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_1^\alpha} - \frac{1}{2\tau_1^\alpha} \int_0^1 \frac{2s + \rho_2}{(1+\rho_2)(\sigma\rho_2 + s)^\alpha} ds \\ &> \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_1^\alpha} - \frac{1}{2\tau_1^\alpha(\sigma\rho_2)^\alpha} \int_0^1 \frac{2s + \rho_2}{(1+\rho_2)} ds = \frac{1}{2(1-\alpha)(\sigma\tau_1)^\alpha} \left(2\sigma - \frac{1-\alpha}{\rho_2^\alpha} \right). \end{aligned}$$

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 (3.1) gives

$$\begin{aligned} [\mathbf{B}]_{22} &= c_1^2 + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_2^\alpha} - \frac{1}{2}(d_2^3 + a_1^3 - a_1^2) \\ &= \frac{1}{2}c_1^2 + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_2^\alpha} + \frac{1}{2}(a_1^2 - a_1^3 + a_2^3) + \frac{1}{2}(c_1^2 - c_1^3) \\ &\geq \frac{1}{2}c_1^2 + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_2^\alpha} + \frac{1}{2}(a_1^2 - a_1^3 + a_2^3). \end{aligned} \quad (3.11)$$

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

$$\begin{aligned} a_1^2 - a_1^3 + a_2^3 &= -(\sigma\tau_2)^{-\alpha} + \frac{\alpha\tau_1}{\tau_1 + \tau_2} \int_0^1 (\tau_1 + \tau_2 + s\tau_1)(1-s)(t_2^* - t_1 + s\tau_1)^{-\alpha-1} ds \\ &\quad - \frac{\alpha\tau_1}{\tau_1 + \tau_2} \int_0^1 (\tau_1 + \tau_2 + s\tau_1)(1-s)(t_3^* - t_1 + s\tau_1)^{-\alpha-1} ds \\ &\quad - \frac{\alpha\tau_2}{\tau_2 + \tau_3} \int_0^1 (\tau_2 + \tau_3 - s\tau_2)(1-s)(t_3^* - t_1 - s\tau_2)^{-\alpha-1} ds \\ &> -(\sigma\tau_2)^{-\alpha} - \frac{\alpha\tau_2}{\tau_2 + \tau_3} \int_0^1 (\tau_2 + \tau_3 - s\tau_2)(1-s)(\tau_2 + \sigma\tau_3 - s\tau_2)^{-\alpha-1} ds \\ &= -(\sigma\tau_2)^{-\alpha} - \frac{\alpha}{(1+\rho_3)\tau_2^\alpha} \int_0^1 s(\rho_3 + s)(\sigma\rho_3 + s)^{-\alpha-1} ds \\ &> -(\sigma\tau_2)^{-\alpha} - \frac{\alpha}{(1+\rho_3)(\sigma\tau_2)^\alpha\rho_3^\alpha} \int_0^1 \frac{s(\rho_3 + s)}{\sigma\rho_3 + s} ds. \end{aligned} \quad (3.12)$$

Substituting (3.12) into (3.11) yields

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

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

$$2\sigma - (1-\alpha) - \frac{\alpha(1-\alpha)}{(1+\rho_3)\rho_3^\alpha} \int_0^1 \frac{s(\rho_3 + s)}{\sigma\rho_3 + s} ds \geq 0. \quad (3.13)$$

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

$$\begin{aligned} [\mathbf{B}]_{kk} &= \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_k^\alpha} + \frac{1}{2}c_{k-1}^k + \frac{1}{2}(c_{k-1}^k - d_k^{k+1} - d_{k-1}^k + d_{k-1}^{k+1}) \\ &= \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_k^\alpha} + \frac{1}{2}c_{k-1}^k + \frac{1}{2}[(c_{k-1}^k - c_{k-1}^{k+1}) - (c_{k-2}^k - c_{k-2}^{k+1}) + (-a_{k-1}^{k+1} + a_k^{k+1} + a_{k-1}^k)]. \end{aligned} \quad (3.14)$$

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

$$\begin{aligned}
& (c_{k-1}^k - c_{k-1}^{k+1}) - (c_{k-2}^k - c_{k-2}^{k+1}) + (-a_{k-1}^{k+1} + a_k^{k+1} + a_{k-1}^k) \\
&= \frac{\alpha \tau_{k-1}^3}{\tau_k(\tau_{k-1} + \tau_k)} \int_0^1 s(1-s) \left[(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} - (t_{k+1}^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} \right] ds \\
&\quad - \frac{\alpha \tau_{k-2}^3}{\tau_{k-1}(\tau_{k-2} + \tau_{k-1})} \int_0^1 s(1-s) \left[(t_k^* - t_{k-2} + s\tau_{k-2})^{-\alpha-1} \right. \\
&\quad \left. - (t_{k+1}^* - t_{k-2} + s\tau_{k-2})^{-\alpha-1} \right] ds \\
&\quad + \frac{\alpha \tau_{k-1}}{\tau_{k-1} + \tau_k} \int_0^1 (\tau_{k-1} + \tau_k + s\tau_{k-1})(1-s) \left[(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} \right. \\
&\quad \left. - (t_{k+1}^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} \right] ds \\
&\quad - (\sigma \tau_k)^{-\alpha} - \frac{\alpha \tau_k}{\tau_k + \tau_{k+1}} \int_0^1 (\tau_k + \tau_{k+1} - s\tau_k)(1-s)(t_{k+1}^* - t_{k-1} - s\tau_k)^{-\alpha-1} ds \\
&> -(\sigma \tau_k)^{-\alpha} - \frac{\alpha \tau_k}{\tau_k + \tau_{k+1}} \int_0^1 s(\tau_{k+1} + s\tau_k)(\sigma \tau_{k+1} + s\tau_k)^{-\alpha-1} ds \\
&= -(\sigma \tau_k)^{-\alpha} - \frac{\alpha}{(1+\rho_{k+1})\tau_k^\alpha} \int_0^1 s(\rho_{k+1} + s)(\sigma \rho_{k+1} + s)^{-\alpha-1} ds \\
&> -(\sigma \tau_k)^{-\alpha} - \frac{\alpha}{(1+\rho_{k+1})(\sigma \tau_k)^\alpha \rho_{k+1}^\alpha} \int_0^1 \frac{s(\rho_{k+1} + s)}{\sigma \rho_{k+1} + s} ds,
\end{aligned} \tag{3.15}$$

where we use the forms (3.7) for a_{k-1}^k , a_{k-1}^{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

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

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

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

Moreover the convexity of the function $t^{-1-\alpha}$ gives

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

Then we can get the following result:

$$\begin{aligned}
& \frac{\alpha \tau_{k-1}^3}{\tau_k(\tau_{k-1} + \tau_k)} \int_0^1 s(1-s) \left[(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} - (t_{k+1}^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} \right] ds \\
& - \frac{\alpha \tau_{k-2}^3}{\tau_{k-1}(\tau_{k-2} + \tau_{k-1})} \int_0^1 s(1-s) \left[(t_k^* - t_{k-2} + s\tau_{k-2})^{-\alpha-1} \right. \\
& \quad \left. - (t_{k+1}^* - t_{k-2} + s\tau_{k-2})^{-\alpha-1} \right] ds \\
& + \frac{\alpha \tau_{k-1}}{\tau_{k-1} + \tau_k} \int_0^1 (\tau_{k-1} + \tau_k + s\tau_{k-1})(1-s) \left[(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} \right. \\
& \quad \left. - (t_{k+1}^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} \right] ds \\
& > \alpha \left(\frac{\tau_{k-1}^3}{\tau_k(\tau_{k-1} + \tau_k)} - \frac{\tau_{k-2}^3}{\tau_{k-1}(\tau_{k-2} + \tau_{k-1})} + \frac{(4\tau_{k-1} + 3\tau_k)\tau_{k-1}}{\tau_{k-1} + \tau_k} \right) \int_0^1 s(1-s) \\
& \quad \left[(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} - (t_{k+1}^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} \right] ds \geq 0,
\end{aligned}$$

as (3.1) for $j = k - 1$ gives

$$\frac{\tau_{k-1}^3}{\tau_k(\tau_{k-1} + \tau_k)} - \frac{\tau_{k-2}^3}{\tau_{k-1}(\tau_{k-2} + \tau_{k-1})} + \frac{(4\tau_{k-1} + 3\tau_k)\tau_{k-1}}{\tau_{k-1} + \tau_k} \geq 0.$$

Combining (3.15) with (3.14) yields

$$[\mathbf{B}]_{kk} \geq \frac{1}{2} c_{k-1}^k + \frac{1}{2(1-\alpha)(\sigma\tau_k)^\alpha} \left(2\sigma - (1-\alpha) - \frac{\alpha(1-\alpha)}{(1+\rho_{k+1})\rho_{k+1}^\alpha} \int_0^1 \frac{s(\rho_{k+1}+s)}{\sigma\rho_{k+1}+s} ds \right).$$

Thus, to ensure $[\mathbf{B}]_{kk} \geq 0$ for $3 \leq k \leq n-1$, it is sufficient to impose

$$\begin{aligned}
\frac{1}{\rho_k} & \geq \frac{1}{\rho_{k-1}^2(1+\rho_{k-1})} - 3, \\
2\sigma - (1-\alpha) - \frac{\alpha(1-\alpha)}{(1+\rho_{k+1})\rho_{k+1}^\alpha} \int_0^1 \frac{s(\rho_{k+1}+s)}{\sigma\rho_{k+1}+s} ds & \geq 0.
\end{aligned} \tag{3.16}$$

Case 4: When $k = n$, we show $[\mathbf{B}]_{nn} \geq 0$ under some constraints on ρ_n . From (3.6), (3.7) and (3.9), we can derive

$$\begin{aligned}
& [\mathbf{B}]_{nn} \\
&= c_{n-1}^n + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_n^\alpha} - \frac{1}{2}(c_{n-2}^n - a_{n-1}^n) \\
&= \frac{1}{2}c_{n-1}^n + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_n^\alpha} + \frac{1}{2}(c_{n-1}^n - c_{n-2}^n + a_{n-1}^n) \\
&= \frac{1}{2}c_{n-1}^n + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_n^\alpha} + \frac{1}{2}\left(\frac{\alpha\tau_{n-1}^3}{\tau_n(\tau_{n-1}+\tau_n)} \int_0^1 s(1-s)(t_n^* - t_{n-1} + s\tau_{n-1})^{-\alpha-1} ds\right. \\
&\quad - \frac{\alpha\tau_{n-2}^3}{\tau_{n-1}(\tau_{n-2}+\tau_{n-1})} \int_0^1 s(1-s)(t_n^* - t_{n-2} + s\tau_{n-2})^{-\alpha-1} ds - (\sigma\tau_n)^{-\alpha} \\
&\quad \left.+ \frac{\alpha\tau_{n-1}}{\tau_{n-1}+\tau_n} \int_0^1 (\tau_{n-1} + \tau_n + s\tau_{n-1})(1-s)(t_n^* - t_{n-1} + s\tau_{n-1})^{-\alpha-1} ds\right) \\
&> \frac{1}{2}c_{n-1}^n + \frac{1}{2(1-\alpha)(\sigma\tau_n)^\alpha} (2\sigma - (1-\alpha)),
\end{aligned} \tag{3.17}$$

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

$$\begin{aligned}
& \int_0^1 (\tau_{n-1} + \tau_n + s\tau_{n-1})(1-s)(t_n^* - t_{n-1} + s\tau_{n-1})^{-\alpha-1} ds \\
& \geq \int_0^1 (4\tau_{n-1} + 3\tau_n)s(1-s)(t_n^* - t_{n-1} + s\tau_{n-1})^{-\alpha-1} ds,
\end{aligned}$$

and

$$(t_n^* - t_{n-1} + s\tau_{n-1})^{-\alpha-1} > (t_n^* - t_{n-2} + s\tau_{n-2})^{-\alpha-1}.$$

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

$$\frac{1}{\rho_n} \geq \frac{1}{\rho_{n-1}^2(1+\rho_{n-1})} - 3, \quad 2\sigma - (1-\alpha) \geq 0. \tag{3.18}$$

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

$$\begin{aligned}
& 2\sigma - \frac{1-\alpha}{\rho_2^\alpha} \geq 0, \\
& 2\sigma - (1-\alpha) - \frac{\alpha(1-\alpha)}{(1+\rho_{k+1})\rho_{k+1}^\alpha} \int_0^1 \frac{s(\rho_{k+1}+s)}{\sigma\rho_{k+1}+s} ds \geq 0, \quad 2 \leq k \leq n-1, \\
& 2\sigma - (1-\alpha) \geq 0,
\end{aligned} \tag{3.19}$$

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

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

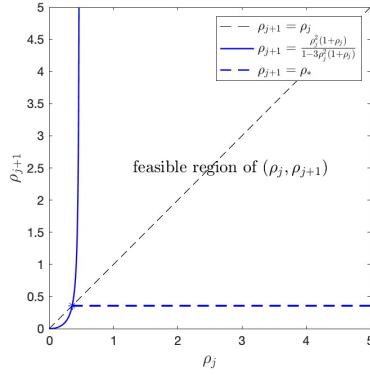


Fig. 3.1 Feasible region of (ρ_j, ρ_{j+1}) , on the right-hand side of the blue solid curve and above the blue dashed line, obtained from the constraint (3.20) for $j \geq 2$. The blue star marker denotes (ρ_*, ρ_*) .

which ensure

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

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

The condition (3.1) actually says that (ρ_j, ρ_{j+1}) lies on the right-hand side of the blue solid curve in Figure 3.1. 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 $\rho_* \geq \rho_j \geq \rho_{j+1} \geq \rho_{j+2} \geq \dots$ and τ_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 $j \geq 2$,

$$\begin{cases} \rho_* < \rho_{j+1} \leq \frac{\rho_j^2(1 + \rho_j)}{1 - 3\rho_j^2(1 + \rho_j)}, & \rho_* < \rho_j < \eta, \\ \rho_* < \rho_{j+1}, & \eta \leq \rho_j, \end{cases} \quad (3.20)$$

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

$$2\sigma - \frac{1 - \alpha}{\rho_2^\alpha} \geq 2 - \alpha - \frac{1 - \alpha}{\rho_*^\alpha} \geq 0, \quad 2\sigma - (1 - \alpha) = 1,$$

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

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

In summary, if (3.20) holds, then

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

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

Remark 3.1 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:

$$\begin{aligned} \partial_t^{\alpha} u(t, x) &= \Delta u(t, x) + f(t, x), \quad (t, x) \in (0, \infty) \times \Omega, \\ u(t, x) &= 0, \quad (t, x) \in (0, \infty) \times \partial\Omega, \\ u(0, x) &= u^0(x), \quad x \in \Omega, \end{aligned} \tag{4.1}$$

where Ω 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

$$\begin{aligned} L_k^{\alpha,*} u &= (1 - \alpha/2)\Delta u^k + \alpha/2\Delta u^{k-1} + f^k, \quad \text{in } \Omega, \\ u^k &= 0, \quad \text{on } \partial\Omega, \end{aligned} \tag{4.2}$$

where $f^k = f(\tau_k^*, \cdot)$.

4.1 Global-in-time H^1 -stability of L2-1 $_{\sigma}$ scheme for subdiffusion equation

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 $u^0 \in H_0^1(\Omega)$. 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 depends on the source term f , C_{Ω} is the Sobolev embedding constant depending on Ω and the spatial dimension d .

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

$$\begin{aligned} \sum_{k=1}^n \langle L_k^{\alpha} u, \delta_k u \rangle &= \sum_{k=1}^n \langle (1 - \alpha/2)\Delta u^k + \alpha/2\Delta u^{k-1}, \delta_k u \rangle + \sum_{k=1}^n \langle f^k, \delta_k u \rangle \\ &= -\frac{1}{2} \|\nabla u^n\|_{L^2(\Omega)}^2 + \frac{1}{2} \|\nabla u^0\|_{L^2(\Omega)}^2 - \frac{1-\alpha}{2} \sum_{k=1}^n \|\nabla \delta_k u\|_{L^2(\Omega)}^2 \\ &\quad + \langle f^n, u^n \rangle - \langle f^1, u^0 \rangle - \sum_{k=2}^n \langle \delta_k f, u^{k-1} \rangle. \end{aligned}$$

Applying the Cauchy–Schwarz inequality yields

$$\begin{aligned} & \langle f^n, u^n \rangle - \langle f^1, u^0 \rangle + \sum_{k=2}^n \langle \delta_k f, u^{k-1} \rangle \\ & \leq \left(2\|f\|_{L^\infty([0,\infty);L^2(\Omega))} + \|f\|_{BV([0,\infty);L^2(\Omega))} \right) \max_{0 \leq k \leq n} \|u^k\|_{L^2(\Omega)} \\ & \leq C_f C_\Omega \max_{0 \leq k \leq n} \|\nabla u^k\|_{L^2(\Omega)}, \end{aligned}$$

where $C_f = 2\|f\|_{L^\infty([0,\infty);L^2(\Omega))} + \|f\|_{BV([0,\infty);L^2(\Omega))}$, and C_Ω is the Sobolev embedding constant depending on Ω and the spatial dimension. From Theorem 3.1, we then have for $n \geq 1$,

$$\begin{aligned} \|\nabla u^n\|_{L^2(\Omega)}^2 & \leq \|\nabla u^0\|_{L^2(\Omega)}^2 - (1-\alpha) \sum_{k=1}^n \|\nabla \delta_k u\|_{L^2(\Omega)}^2 - \sum_{k=1}^n \frac{g_k(\alpha)}{\Gamma(2-\alpha)} \|\delta_k u\|_{L^2(\Omega)}^2 \\ & \quad + 2C_f C_\Omega \max_{0 \leq k \leq n} \|\nabla u^k\|_{L^2(\Omega)} \\ & \leq \|\nabla u^0\|_{L^2(\Omega)}^2 + 2C_f C_\Omega \max_{0 \leq k \leq n} \|\nabla u^k\|_{L^2(\Omega)}. \end{aligned} \tag{4.3}$$

For any $N \geq 1$, we take $\max_{0 \leq n \leq N}$ on both sides of (4.3), to obtain

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

which indicates

$$\max_{0 \leq n \leq N} \|\nabla u^n\|_{L^2(\Omega)} \leq C_f C_\Omega + \sqrt{(C_f C_\Omega)^2 + \|\nabla u^0\|_{L^2(\Omega)}^2} \leq \|\nabla u^0\|_{L^2(\Omega)} + 2C_f C_\Omega.$$

The proof is completed.

Remark 4.1 Assume that the solution of subdiffusion equation satisfies $u(t,x) \in C([0,\infty);H_0^1(\Omega)) \cap C^1((0,\infty);H_0^1(\Omega))$ 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

$$\begin{aligned} & \int_0^T \int_\Omega \partial_t^\alpha u(t,x) \partial_t u(t,x) \, dx dt \\ & = \frac{1}{2} \int_0^T \int_\Omega \partial_t |\nabla u(t,x)|^2 \, dx dt + \int_0^T \int_\Omega f(t,x) \partial_t u(t,x) \, dx dt. \end{aligned}$$

According to [37],

$$\int_0^T \int_\Omega \partial_t^\alpha u(t,x) \partial_t u(t,x) \, dx dt \geq 0,$$

and moreover,

$$\begin{aligned}
& \int_0^T \int_{\Omega} f(t, x) \partial_t u(t, x) \, dx dt \\
&= \left(\int_{\Omega} f(t, x) u(t, x) \, dx \right) \Big|_0^T - \int_0^T \int_{\Omega} \partial_t f(t, x) u(t, x) \, dx dt \\
&\leq \left(2 \|f\|_{L^\infty([0, \infty); L^2(\Omega))} + \int_0^\infty \|\partial_t f(t, x)\|_{L^2(\Omega)} \, dt \right) C_\Omega \|\nabla u\|_{L^\infty([0, T]; L^2(\Omega))} \\
&=: C_f^{cont} C_\Omega \|\nabla u\|_{L^\infty([0, T]; L^2(\Omega))}.
\end{aligned}$$

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 σ scheme of the subdiffusion equation (4.1).

Remark 4.2 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 [24, Theorem 2.1] and for the third order BDF3 schemes in [23, Theorem 3.1] on general nonuniform meshes.

4.2 Sharp convergence of L2-1 σ scheme for subdiffusion equation

We show the error estimate of the L2-1 σ scheme (4.2) for the subdiffusion equation (4.1), that is different from the one in [20, 19]. To be precise we will reduce the restriction on time step ratios from $\rho_k \geq 4/7$ in [20] to $\rho_k \geq 0.475329$. We first reformulate the discrete fractional operator (2.3):

$$L_k^{\alpha,*} u = \frac{1}{\Gamma(1-\alpha)} \left([\mathbf{M}]_{k,k} u^k - \sum_{j=2}^k ([\mathbf{M}]_{k,j} - [\mathbf{M}]_{k,j-1}) u^{j-1} - [\mathbf{M}]_{k,1} u^0 \right),$$

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

Lemma 4.1 *Under the condition (3.2), the following properties of $[\mathbf{M}]_{k,j}$ given by (3.5) hold:*

(Q1)

$$[\mathbf{M}]_{k,j} \geq \frac{\rho_*}{(1+\rho_*)\tau_j} \int_{t_{j-1}}^{\min\{t_j, t_k^*\}} (t_k^* - s)^{-\alpha} \, ds, \quad 1 \leq j \leq k. \quad (4.4)$$

(Q2) *For all $2 \leq j \leq k-1$,*

$$[\mathbf{M}]_{k,j} - [\mathbf{M}]_{k,j-1} \geq \frac{\alpha \tau_j}{\tau_j + \tau_{j+1}} \int_0^1 (\tau_j + \tau_{j+1} - s\tau_j)(1-s)(t_k^* - t_{j-1} - s\tau_j)^{-\alpha-1} \, ds,$$

and

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

(Q3) Moreover, if $\rho_k \geq \eta \approx 0.475329$ for all $k \geq 2$, then

$$\frac{1-\alpha}{\sigma} [\mathbf{M}]_{k,k} - [\mathbf{M}]_{k,k-1} \geq 0.$$

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

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

$$\begin{aligned} [\mathbf{M}]_{k,j} &\geq -a_j^n = \int_0^1 \frac{2\tau_j(1-\theta) + \tau_{j+1}}{(\tau_j + \tau_{j+1})(t_k^* - (t_{j-1} + \theta\tau_j))^\alpha} d\theta \\ &\geq \frac{\rho_{j+1}}{1+\rho_{j+1}} \int_0^1 \frac{1}{(t_k^* - (t_{j-1} + \theta\tau_j))^\alpha} d\theta \geq \frac{\rho_*}{(1+\rho_*)\tau_j} \int_{t_{j-1}}^{t_j} (t_k^* - s)^{-\alpha} ds, \end{aligned} \quad (4.5)$$

and for $j = k$,

$$[\mathbf{M}]_{k,k} = c_{k-1}^k + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_k^\alpha} \geq \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_k^\alpha} = \frac{1}{\tau_k} \int_{t_{k-1}}^{t_k^*} (t_k^* - s)^{-\alpha} ds.$$

The inequality (4.4) holds.

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

$$\begin{aligned} &[\mathbf{M}]_{k,j} - [\mathbf{M}]_{k,j-1} \\ &= \frac{\alpha\tau_{j-1}^3}{\tau_j(\tau_{j-1} + \tau_j)} \int_0^1 s(1-s)(t_k^* - t_{j-1} + s\tau_{j-1})^{-\alpha-1} ds \\ &\quad - \frac{\alpha\tau_{j-2}^3}{\tau_{j-1}(\tau_{j-2} + \tau_{j-1})} \int_0^1 s(1-s)(t_k^* - t_{j-2} + s\tau_{j-2})^{-\alpha-1} ds \\ &\quad + \frac{\alpha\tau_{j-1}}{\tau_{j-1} + \tau_j} \int_0^1 (\tau_{j-1} + \tau_j + s\tau_{j-1})(1-s)(t_k^* - t_{j-1} + s\tau_{j-1})^{-\alpha-1} ds \\ &\quad + \frac{\alpha\tau_j}{\tau_j + \tau_{j+1}} \int_0^1 (\tau_j + \tau_{j+1} - s\tau_j)(1-s)(t_k^* - t_{j-1} - s\tau_j)^{-\alpha-1} ds \\ &\geq \frac{\alpha\tau_j}{\tau_j + \tau_{j+1}} \int_0^1 (\tau_j + \tau_{j+1} - s\tau_j)(1-s)(t_k^* - t_{j-1} - s\tau_j)^{-\alpha-1} ds, \end{aligned}$$

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

$$\begin{aligned}
& [\mathbf{M}]_{k,k} - [\mathbf{M}]_{k,k-1} \\
&= \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_k^\alpha} + (c_{k-1}^k - c_{k-2}^k + a_{k-1}^k) \\
&= \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_k^\alpha} + \left(\frac{\alpha\tau_{k-1}^3}{\tau_k(\tau_{k-1} + \tau_k)} \int_0^1 s(1-s)(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} ds \right. \\
&\quad - \frac{\alpha\tau_{k-2}^3}{\tau_{k-1}(\tau_{k-2} + \tau_{k-1})} \int_0^1 s(1-s)(t_k^* - t_{k-2} + s\tau_{k-2})^{-\alpha-1} ds \\
&\quad \left. - (\sigma\tau_k)^{-\alpha} + \frac{\alpha\tau_{k-1}}{\tau_{k-1} + \tau_k} \int_0^1 (\tau_{k-1} + \tau_k + s\tau_{k-1})(1-s)(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} ds \right) \\
&> \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_k^\alpha} - \frac{1}{(\sigma\tau_k)^\alpha} = \frac{\alpha}{2(1-\alpha)(\sigma\tau_k)^\alpha},
\end{aligned}$$

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 not difficult to obtain. In the case of $k \geq 3$, we have

$$\begin{aligned}
& \frac{1-\alpha}{\sigma} [\mathbf{M}]_{k,k} - [\mathbf{M}]_{k,k-1} \\
&\geq (\sigma\tau_k)^{-\alpha} - c_{k-2}^k + a_{k-1}^k \\
&= (\sigma\tau_k)^{-\alpha} - \frac{\alpha\tau_{k-2}^3}{\tau_{k-1}(\tau_{k-2} + \tau_{k-1})} \int_0^1 s(1-s)(t_k^* - t_{k-2} + s\tau_{k-2})^{-\alpha-1} ds \\
&\quad - (\sigma\tau_k)^{-\alpha} + \frac{\alpha\tau_{k-1}}{\tau_{k-1} + \tau_k} \int_0^1 (\tau_{k-1} + \tau_k + s\tau_{k-1})(1-s)(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} ds \\
&> \alpha \left(\frac{\tau_{k-1}(4\tau_{k-1} + 3\tau_k)}{\tau_{k-1} + \tau_k} - \frac{\tau_{k-2}^3}{\tau_{k-1}(\tau_{k-2} + \tau_{k-1})} \right) \int_0^1 s(1-s)(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} ds \\
&\geq 0,
\end{aligned}$$

where we use the facts

$$\begin{aligned}
& \int_0^1 (\tau_{k-1} + \tau_k + s\tau_{k-1})(1-s)(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} ds \\
&\geq (4\tau_{k-1} + 3\tau_k) \int_0^1 s(1-s)(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} ds, \\
&(t_k^* - t_{k-1} + s\tau_{k-1})^{-\alpha-1} \geq (t_k^* - t_{k-2} + s\tau_{k-2})^{-\alpha-1},
\end{aligned}$$

and

$$\frac{\tau_{k-1}(4\tau_{k-1} + 3\tau_k)}{\tau_{k-1} + \tau_k} - \frac{\tau_{k-2}^3}{\tau_{k-1}(\tau_{k-2} + \tau_{k-1})} \geq 0,$$

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:

$$\Pi_{1,j} : t_{j-1}, t_j, \quad \Pi_{2,j} : t_{j-1}, t_j, t_{j+1}, \quad \Pi_{2,j}^* : t_{j-1}, t_j^*, t_j.$$

As stated in [15], 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 4.2 *Given a function u satisfying $|\partial_t^m u(t)| \leq C_m(1+t^{\alpha-m})$ for $m = 1, 3$ and nonuniform mesh $\{\tau_k\}_{k \geq 1}$ satisfying condition (3.2), the approximation error is given by*

$$r_k := \frac{1}{\Gamma(1-\alpha)} \int_0^{t_k^*} (t_k^* - s)^{-\alpha} \partial_s [u(s) - I_2 u(s)] ds, \quad k \geq 1, \quad (4.6)$$

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 $k \geq 1$,

$$|r_k| \leq \frac{C}{\Gamma(1-\alpha)} \left([\mathbf{M}]_{k,1} (t_2^\alpha / \alpha + t_2) + \sum_{j=2}^k ([\mathbf{M}]_{k,j} - [\mathbf{M}]_{k,j-1}) (1 + \rho_{j+1}) (1 + t_{j-1}^{\alpha-3}) \tau_j^3 \right), \quad (4.7)$$

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

Proof The case of $k = 1$ is not difficult to prove. We now consider the case of $k \geq 2$. Let $\chi(s) := u - I_2 u$. Three subcases are discussed in the following content.

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

$$|\partial_s I_2 u(s)| \leq \max\{|\partial_s I_2 u(t_0)|, |\partial_s I_2 u(t_1)|\} \leq C_1 \frac{1+\rho_2}{\tau_1\rho_2} (t_2 + t_2^\alpha / \alpha),$$

where we use the facts

$$\begin{aligned}
\partial_s I_2 u(t_0) &= -\frac{2\tau_1 + \tau_2}{\tau_1(\tau_1 + \tau_2)} u(t_0) + \frac{\tau_1 + \tau_2}{\tau_1 \tau_2} u(t_1) - \frac{\tau_1}{\tau_2(\tau_1 + \tau_2)} u(t_2) \\
&= -\frac{2\tau_1 + \tau_2}{\tau_1(\tau_1 + \tau_2)} (u(t_0) - u(t_1)) + \frac{\tau_1}{\tau_2(\tau_1 + \tau_2)} (u(t_1) - u(t_2)) \\
&\leq \left(\frac{2\tau_1 + \tau_2}{\tau_1(\tau_1 + \tau_2)} + \frac{\tau_1}{\tau_2(\tau_1 + \tau_2)} \right) \max\{|u(t_0) - u(t_1)|, |u(t_1) - u(t_2)|\} \\
&= \frac{\tau_1 + \tau_2}{\tau_1 \tau_2} \max\{|u(t_0) - u(t_1)|, |u(t_1) - u(t_2)|\}, \\
\partial_s I_2 u(t_1) &= -\frac{\tau_2}{\tau_1(\tau_1 + \tau_2)} u(t_0) - \frac{\tau_1 - \tau_2}{\tau_1 \tau_2} u(t_1) + \frac{\tau_1}{\tau_2(\tau_1 + \tau_2)} u(t_2) \\
&= -\frac{\tau_2}{\tau_1(\tau_1 + \tau_2)} (u(t_0) - u(t_1)) - \frac{\tau_1}{\tau_2(\tau_1 + \tau_2)} (u(t_1) - u(t_2)) \\
&\leq \left(\frac{\tau_2}{\tau_1(\tau_1 + \tau_2)} + \frac{\tau_1}{\tau_2(\tau_1 + \tau_2)} \right) \max\{|u(t_0) - u(t_1)|, |u(t_1) - u(t_2)|\} \\
&= \frac{\tau_1^2 + \tau_2^2}{\tau_1 \tau_2 (\tau_1 + \tau_2)} \max\{|u(t_0) - u(t_1)|, |u(t_1) - u(t_2)|\}, \\
|u(t_0) - u(t_1)| &= \left| \int_0^{t_1} \partial_s u(s) ds \right| \leq C_1 (\tau_1 + t_1^\alpha / \alpha), \\
|u(t_1) - u(t_2)| &= \left| \int_{t_1}^{t_2} \partial_s u(s) ds \right| \leq C_1 (\tau_2 + (t_2^\alpha - t_1^\alpha) / \alpha).
\end{aligned}$$

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

$$\begin{aligned}
&\left| \frac{1}{\Gamma(1-\alpha)} \int_0^{t_1} (t_k^* - s)^{-\alpha} \partial_s \chi(s) ds \right| \\
&\leq \frac{C_1}{\Gamma(1-\alpha)} \left(\int_0^{t_1} s^{\alpha-1} (t_k^* - s)^{-\alpha} ds + \frac{\tau_1 + (1+\rho_2)/\rho_2 (t_2 + t_2^\alpha / \alpha)}{\tau_1} \int_0^{t_1} (t_k^* - s)^{-\alpha} ds \right) \\
&\leq \frac{C_1}{\Gamma(1-\alpha)} \left(\frac{\tau_1^\alpha}{\alpha(t_k^* - \tau_1)^\alpha} + \frac{\tau_1 + (1+\rho_2)/\rho_2 (t_2 + t_2^\alpha / \alpha)}{\tau_1} \int_0^{t_1} (t_k^* - s)^{-\alpha} ds \right) \\
&\leq \frac{C(t_2^\alpha / \alpha + t_2)}{\Gamma(1-\alpha)} [\mathbf{M}]_{k,1},
\end{aligned} \tag{4.8}$$

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

$$\begin{aligned}
[\mathbf{M}]_{k,1} &\geq \frac{\rho_2}{(1+\rho_2)\tau_1} \int_0^{t_1} (t_k^* - s)^{-\alpha} ds \geq \frac{\rho_2}{(1+\rho_2)(t_k^*)^\alpha} \\
&\geq \frac{\rho_2^{1+\alpha}}{(1+\rho_2)(2+\rho_2)^\alpha (t_k^* - \tau_1)^\alpha} \geq \frac{\rho_*^{1+\alpha}}{(1+\rho_*)(2+\rho_*)^\alpha (t_k^* - \tau_1)^\alpha}
\end{aligned}$$

obtained from the inequality (4.5).

Subcase 2. On the interval (t_{j-1}, t_j) , $2 \leq j \leq k-1$,

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

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

$$\begin{aligned} & \left| \frac{1}{\Gamma(1-\alpha)} \int_{t_{j-1}}^{t_j} (t_k^* - s)^{-\alpha} \partial_s \chi(s) ds \right| = \left| \frac{-\alpha}{\Gamma(1-\alpha)} \int_{t_{j-1}}^{t_j} (t_k^* - s)^{-\alpha-1} \chi(s) ds \right| \quad (4.9) \\ & \leq \frac{C_3 \alpha (1+t_{j-1}^{\alpha-3})}{\Gamma(1-\alpha)} \int_{t_{j-1}}^{t_j} (t_k^* - s)^{-\alpha-1} (s-t_{j-1})(s-t_j)(s-t_{j+1}) ds \\ & = \frac{C_3 \alpha (1+t_{j-1}^{\alpha-3}) \tau_j^3}{\Gamma(1-\alpha)} \int_0^1 s(\tau_j + \tau_{j+1} - s\tau_j)(1-s)(t_k^* - t_{j-1} - s\tau_j)^{-\alpha-1} ds \\ & \leq \frac{C_3 (1+\rho_{j+1}) (1+t_{j-1}^{\alpha-3}) \tau_j^3}{\Gamma(1-\alpha)} ([\mathbf{M}]_{k,j} - [\mathbf{M}]_{k,j-1}), \end{aligned}$$

from (Q2) in Lemma 4.1.

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

$$|\chi(s)| \leq C_3 (1+t_{k-1}^{\alpha-3}) (s-t_{k-1}) (t_k^* - s) (t_k - s) \leq C_3 (1+t_{k-1}^{\alpha-3}) \tau_k^2 (t_k^* - s),$$

which yields

$$\begin{aligned} & \left| \frac{1}{\Gamma(1-\alpha)} \int_{t_{k-1}}^{t_k^*} (t_k^* - s)^{-\alpha} \partial_s \chi(s) ds \right| = \left| \frac{-\alpha}{\Gamma(1-\alpha)} \int_{t_{k-1}}^{t_k^*} (t_k^* - s)^{-\alpha-1} \chi(s) ds \right| \\ & \leq \frac{C_3 \alpha (1+t_{k-1}^{\alpha-3}) \tau_k^2}{\Gamma(1-\alpha)} \int_{t_{k-1}}^{t_k^*} (t_k^* - s)^{-\alpha} ds = \frac{2C_3 \sigma (1+t_{k-1}^{\alpha-3}) \tau_k^3}{\Gamma(1-\alpha)} \frac{\alpha}{2(1-\alpha)(\sigma \tau_k)^\alpha} \\ & \leq \frac{2C_3 \sigma (1+t_{k-1}^{\alpha-3}) \tau_k^3}{\Gamma(1-\alpha)} ([\mathbf{M}]_{k,k} - [\mathbf{M}]_{k,k-1}) \end{aligned} \quad (4.10)$$

from (Q2) in Lemma 4.1.

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

Theorem 4.2 Assume that $u \in C^3((0, T], H_0^1(\Omega))$ and $|\partial_t^m u(t)| \leq C_m (1+t^{\alpha-m})$, 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 L2-1_σ scheme (4.2) have the following global error estimate

$$\begin{aligned} & \max_{1 \leq k \leq n} \|u(t_k) - u^k\|_{L^2(\Omega)} \\ & \leq C \left(t_2^\alpha / \alpha + t_2 + \frac{1}{1-\alpha} \max_{2 \leq k \leq n} (1+\rho_{k+1})(1+t_{k-1}^{\alpha-3})(t_{k-1}^*)^\alpha \tau_k^3 \tau_{k-1}^{-\alpha} \right. \\ & \quad \left. + (\tau_1^\alpha / \alpha + \tau_1) \tau_1^{\alpha/2} + \sqrt{\Gamma(1-\alpha)} \max_{2 \leq k \leq n} (t_k^*)^{\alpha/2} (1+t_{k-1}^{\alpha-2}) \tau_k^2 \right), \end{aligned}$$

where C is a constant depending only on C_m , $m=1, 2, 3$ and Ω .

Proof Let $e^k := u(t_k) - u^k$. We have

$$L_k^{\alpha,*} e = \Delta e_k^* - r_k + \Delta R_k^*, \quad (4.11)$$

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 Ω yield

$$\langle L_k^{\alpha,*} e, e_k^* \rangle = -\|\nabla e_k^*\|_{L^2(\Omega)}^2 - \langle r_k, e_k^* \rangle - \langle \nabla R_k^*, \nabla e_k^* \rangle. \quad (4.12)$$

According to [3, Lemma 1] as well as Lemma 4.1, we can derive

$$\begin{aligned} \langle L_k^{\alpha,*} e, e_k^* \rangle &= \frac{1}{\Gamma(1-\alpha)} \sum_{j=1}^k [\mathbf{M}]_{k,j} \langle (e^j - e^{j-1}), (1 - \alpha/2)e^k + \alpha/2e^{k-1} \rangle \\ &\geq \frac{1}{2\Gamma(1-\alpha)} \sum_{j=1}^k [\mathbf{M}]_{k,j} \left(\|e^j\|_{L^2(\Omega)}^2 - \|e^{j-1}\|_{L^2(\Omega)}^2 \right). \end{aligned}$$

Applying Cauchy-Schwarz inequality in (4.12) yields

$$\begin{aligned} &\sum_{j=1}^k [\mathbf{M}]_{k,j} \left(\|e^j\|_{L^2(\Omega)}^2 - \|e^{j-1}\|_{L^2(\Omega)}^2 \right) \\ &\leq 2\Gamma(1-\alpha) \|r_k\|_{L^2(\Omega)} \|e_k^*\|_{L^2(\Omega)} + \Gamma(1-\alpha) \|R_k^*\|_{H^1(\Omega)}^2. \end{aligned} \quad (4.13)$$

We define a lower triangular \mathbf{P} matrix such that

$$\mathbf{PM} = \mathbf{E}_L$$

where

$$\mathbf{E}_L = \begin{pmatrix} 1 & & & \\ 1 & 1 & & \\ \vdots & \vdots & \ddots & \\ 1 & 1 & \cdots & 1 \end{pmatrix}.$$

In other words,

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

Here \mathbf{P} is called complementary discrete convolution kernel in the work [19]. It can be easily checked that $[\mathbf{P}]_{k,l} \geq 0$ due to the monotonicity properties of \mathbf{M} . From (4.13) we can derive that $\forall 1 \leq k \leq n$,

$$\begin{aligned} &\|e^k\|_{L^2(\Omega)}^2 \\ &\leq 2\Gamma(1-\alpha) \sum_{l=1}^k [\mathbf{P}]_{k,l} \|r_l\|_{L^2(\Omega)} \|e_l^*\|_{L^2(\Omega)} + \Gamma(1-\alpha) \sum_{l=1}^k [\mathbf{P}]_{k,l} \|R_l^*\|_{H^1(\Omega)}^2 \\ &\leq 2\Gamma(1-\alpha) \left(\max_{1 \leq l \leq k} \|e_l^*\|_{L^2(\Omega)} \right) \sum_{l=1}^k [\mathbf{P}]_{k,l} \|r_l\|_{L^2(\Omega)} + \Gamma(1-\alpha) \sum_{l=1}^k [\mathbf{P}]_{k,l} \|R_l^*\|_{H^1(\Omega)}^2, \end{aligned} \quad (4.14)$$

where we use

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

According to Lemma 4.2,

$$\begin{aligned} & \Gamma(1-\alpha) \sum_{l=1}^k [\mathbf{P}]_{k,l} \|r_l\| \\ & \leq C|\Omega| \sum_{l=1}^k [\mathbf{P}]_{k,l} \left([\mathbf{M}]_{l,1} (t_2^\alpha / \alpha + t_2) + \sum_{j=2}^l ([\mathbf{M}]_{l,j} - [\mathbf{M}]_{l,j-1}) (1 + \rho_{j+1}) (1 + t_{j-1}^{\alpha-3}) \tau_j^3 \right) \\ &= C|\Omega| \left((t_2^\alpha / \alpha + t_2) + \sum_{j=2}^k (1 + \rho_{j+1}) (1 + t_{j-1}^{\alpha-3}) \tau_j^3 \sum_{l=j}^k [\mathbf{P}]_{k,l} ([\mathbf{M}]_{l,j} - [\mathbf{M}]_{l,j-1}) \right) \\ &= C|\Omega| \left((t_2^\alpha / \alpha + t_2) + \sum_{j=2}^k (1 + \rho_{j+1}) (1 + t_{j-1}^{\alpha-3}) \tau_j^3 [\mathbf{P}]_{k,j-1} [\mathbf{M}]_{j-1,j-1} \right) \\ &= C|\Omega| \left((t_2^\alpha / \alpha + t_2) + \sum_{j=2}^k [\mathbf{P}]_{k,j-1} [\mathbf{M}]_{j-1,1} \frac{[\mathbf{M}]_{j-1,j-1}}{[\mathbf{M}]_{j-1,1}} (1 + \rho_{j+1}) (1 + t_{j-1}^{\alpha-3}) \tau_j^3 \right) \\ &\leq C|\Omega| \left((t_2^\alpha / \alpha + t_2) + \max_{2 \leq j \leq k} \frac{[\mathbf{M}]_{j-1,j-1}}{[\mathbf{M}]_{j-1,1}} (1 + \rho_{j+1}) (1 + t_{j-1}^{\alpha-3}) \tau_j^3 \right) \\ &\leq C|\Omega| \left((t_2^\alpha / \alpha + t_2) + \frac{1}{1-\alpha} \max_{2 \leq j \leq k} (1 + \rho_{j+1}) (1 + t_{j-1}^{\alpha-3}) (t_{j-1}^*)^\alpha \tau_j^3 \tau_{j-1}^{-\alpha} \right), \end{aligned}$$

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

$$\begin{aligned} [\mathbf{M}]_{j,j} &= c_{j-1}^j + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_j^\alpha} \\ &= \int_0^1 \frac{\tau_{j-1}^2 (2\theta - 1)}{\tau_j(\tau_{j-1} + \tau_j)(t_j^* - (t_{j-2} + \theta\tau_{j-1}))^\alpha} d\theta + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_j^\alpha} \quad (4.15) \\ &\leq \frac{1}{\rho_j(1+\rho_j)(\sigma\tau_j)^\alpha} + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_j^\alpha} \leq \frac{1}{\eta(1+\eta)(\sigma\tau_j)^\alpha} + \frac{\sigma^{1-\alpha}}{(1-\alpha)\tau_j^\alpha}, \\ [\mathbf{M}]_{j,1} &\geq \frac{\eta}{(1+\eta)\tau_1} \int_0^{t_j^*} (t_j^* - s)^{-\alpha} ds \geq \frac{\eta}{(1+\eta)(t_j^*)^\alpha}, \end{aligned}$$

where we use (Q1) in Lemma 4.1 for the inequality of $[\mathbf{M}]_{j,1}$.

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

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

Under the regularity assumption, we have

$$\|R_1^*\|_{H^1(\Omega)} \leq C(\tau_1^\alpha/\alpha + \tau_1), \quad \|R_j^*\|_{H^1(\Omega)} \leq C(1 + t_{j-1}^{\alpha-2}) \tau_j^2, \quad 2 \leq j \leq k.$$

Then we have

$$\begin{aligned} & \sum_{l=1}^k [\mathbf{P}]_{k,l} \|R_l^*\|_{H^1(\Omega)}^2 \\ & \leq C \left([\mathbf{P}]_{k,1} [\mathbf{M}]_{1,1} \frac{1}{[\mathbf{M}]_{1,1}} (\tau_1^\alpha/\alpha + \tau_1)^2 + \sum_{l=2}^k [\mathbf{P}]_{k,l} [\mathbf{M}]_{l,2} \frac{1}{[\mathbf{M}]_{l,2}} ((1 + t_{l-1}^{\alpha-2}) \tau_l^2)^2 \right) \\ & \leq C \left(\frac{1}{[\mathbf{M}]_{1,1}} (\tau_1^\alpha/\alpha + \tau_1)^2 + \max_{2 \leq l \leq k} \frac{1}{[\mathbf{M}]_{l,2}} ((1 + t_{l-1}^{\alpha-2}) \tau_l^2)^2 \right) \\ & \leq C \left((1 - \alpha) \tau_1^\alpha (\tau_1^\alpha/\alpha + \tau_1)^2 + \max_{2 \leq l \leq k} (t_l^*)^\alpha ((1 + t_{l-1}^{\alpha-2}) \tau_l^2)^2 \right), \end{aligned}$$

where we use $[\mathbf{M}]_{l,2} \geq [\mathbf{M}]_{l,1}$ and (4.15).

Taking the max for $1 \leq k \leq n$ on both sides of (4.14), we can derive

$$\begin{aligned} \max_{1 \leq k \leq n} \|e_k\|_{L^2(\Omega)} & \leq C \left((t_2^\alpha/\alpha + t_2) + \frac{1}{1 - \alpha} \max_{2 \leq k \leq n} (1 + \rho_{k+1}) (1 + t_{k-1}^{\alpha-3}) (t_{k-1}^*)^\alpha \tau_k^3 \tau_{k-1}^{-\alpha} \right. \\ & \quad \left. + (\tau_1^\alpha/\alpha + \tau_1) \tau_1^{\alpha/2} + \sqrt{\Gamma(1 - \alpha)} \max_{2 \leq k \leq n} (t_k^*)^{\alpha/2} (1 + t_{k-1}^{\alpha-2}) \tau_k^2 \right). \end{aligned} \quad (4.16)$$

The proof is completed.

In the case of graded mesh with grading parameter r ,

$$t_j = \left(\frac{j}{K} \right)^r T, \quad \tau_j = t_j - t_{j-1} = \left[\left(\frac{j}{K} \right)^r - \left(\frac{j-1}{K} \right)^r \right] T, \quad (4.17)$$

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:

$$\begin{aligned} & (1 + \rho_{k+1}) (1 + t_{k-1}^{\alpha-3}) (t_{k-1}^*)^\alpha \tau_k^3 \tau_{k-1}^{-\alpha} \leq C t_{k-1}^{2\alpha-3} \tau_k^{3-\alpha} \\ & = C t_{k-1}^{2\alpha-3} (t_k - t_{k-1})^{3-\alpha} = C (t_{k-1})^\alpha (t_k/t_{k-1} - 1)^{3-\alpha} \\ & = C t_{k-1}^\alpha ((1 + 1/(k-1))^r - 1)^{3-\alpha} \\ & \leq C r^{3-\alpha} T^\alpha \frac{(k-1)^{r\alpha-(3-\alpha)}}{K^{r\alpha}} = \frac{C_{T,1}}{K^{\min\{r\alpha, 3-\alpha\}}} \end{aligned} \quad (4.18)$$

and

$$\begin{aligned} (t_k^*)^{\alpha/2}(1+t_{k-1}^{\alpha-2})\tau_k^2 &\leq Ct_{k-1}^{\alpha-2}\tau_k^2 = Ct_{k-1}^{\alpha-2}(t_k-t_{k-1})^2 = Ct_{k-1}^\alpha(t_k/t_{k-1}-1)^2 \\ &= CT^\alpha \left(\frac{k-1}{K}\right)^{r\alpha} ((1+1/(k-1))^r - 1)^2 \leq Cr^2T^\alpha \frac{(k-1)^{r\alpha-2}}{K^{r\alpha}} = \frac{C_{T,2}}{K^{\min\{r\alpha,2\}}}. \end{aligned} \quad (4.19)$$

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 4.2, then we have the following error estimate of numerical solutions of the L2-1 σ scheme on the graded mesh with grading parameter r :

$$\max_{1 \leq k \leq K} \|u(t_k) - u^k\|_{L^2(\Omega)} \leq \frac{\tilde{C}}{K^{\min\{r\alpha,2\}}}. \quad (4.20)$$

where \tilde{C} depends on C_m with $m = 1, 2, 3$, α and Ω .

Remark 4.3 When $\alpha \rightarrow 1^-$, the constant \tilde{C} in (4.20) will tend to infinity. However, using the technique by Chen-Stynes in [6], one can obtain α -robust error estimate in the sense that \tilde{C} won't tend to infinity when $\alpha \rightarrow 1^-$.

5 Numerical tests

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

As in [20,5], 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 $\max_{1 \leq k \leq K} \|u(t_k) - u^k\|_{L^2(\Omega)}$. Table 5.1–5.3 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 4.2.

In [35, 13], 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 5.1–5.3. 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

Table 5.1 $\max_{1 \leq k \leq K} \|u(t_k) - u^k\|_{L^2(\Omega)}$ for the graded meshes with different grading parameters and time step numbers where $\alpha = 0.3$.

	$K = 40$	$K = 80$	$K = 160$	$K = 320$	$K = 480$	$K = 640$
$r = 1$	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	4.4967e-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	1.3655e-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 5.2 $\max_{1 \leq k \leq K} \|u(t_k) - u^k\|_{L^2(\Omega)}$ for the graded meshes with different grading parameters and time step numbers where $\alpha = 0.5$.

	$K = 40$	$K = 80$	$K = 160$	$K = 320$	$K = 480$	$K = 640$
$r = 1$	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 5.3 $\max_{1 \leq k \leq K} \|u(t_k) - u^k\|_{L^2(\Omega)}$ for the graded meshes with different grading parameters and time step numbers where $\alpha = 0.7$.

	$K = 40$	$K = 80$	$K = 160$	$K = 320$	$K = 480$	$K = 640$
$r = 1$	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	0.6836
$r = 2$	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

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

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

$$t_j = \left(\frac{j}{K}\right)^{r_j} T, \quad \tau_j = t_j - t_{j-1} = \left[\left(\frac{j}{K}\right)^{r_j} - \left(\frac{j-1}{K}\right)^{r_{j-1}}\right] T. \quad (5.1)$$

In Figure 5.1, 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 Figure 5.1, the maximum L^2 -error for the r -variable graded mesh is smaller than the standard graded meshes with $r = 2/\alpha, 3/\alpha$.

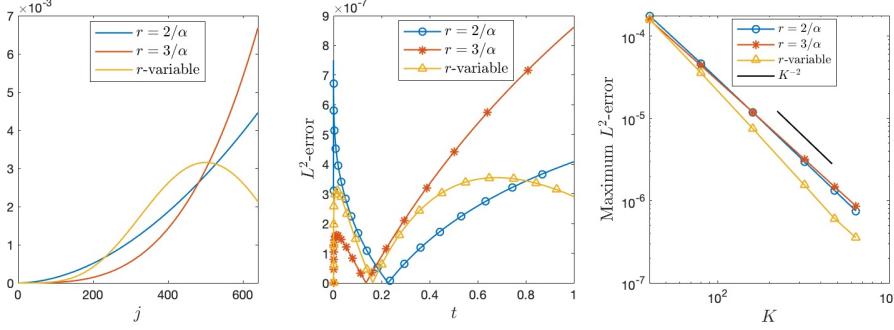


Fig. 5.1 Time steps (left), pointwise L^2 -errors (middle), and maximum L^2 -errors (right) of the L2- 1_σ scheme in 1D on the r -variable graded mesh (5.1) and the graded meshes (4.17) with $r = 2/\alpha, 3/\alpha$ ($\alpha = 0.7$).

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 256×256 Fourier modes. In Figure 5.2, we show the pointwise L^2 -errors (with $K = 640$) and the maximum L^2 -errors of the L2- 1_σ 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.

Declarations

Conflicts of interest The authors declared that they have no conflicts of interest to this work.

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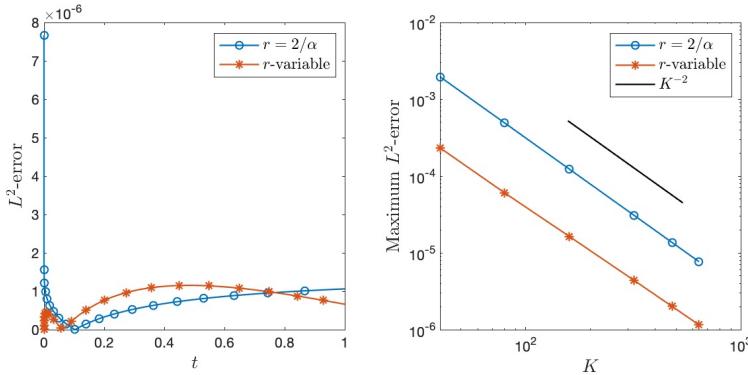


Fig. 5.2 Pointwise L^2 -errors (left) with $K = 640$ and maximum L^2 -errors (right) of L2-1 σ scheme in 2D on the r -variable graded mesh (5.1) and the graded mesh (4.17) with $r = 2/\alpha$ ($\alpha = 0.7$).

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