



# Global-in-Time $H^1$ -Stability of $L_2-1_\sigma$ Method on General Nonuniform Meshes for Subdiffusion Equation

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## Abstract

In this work the  $L_2-1_\sigma$  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  $L_2-1_\sigma$  fractional-derivative operator is proved to be positive semidefinite and a new global-in-time  $H^1$ -stability of  $L_2-1_\sigma$  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 ·  $L_2-1_\sigma$  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  $L_2-1_\sigma$  scheme has second order accuracy [2] and the  $L_2$ -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  $L_1$ ,  $L_2-1_\sigma$ , and  $L_2$  methods on the graded meshes have been developed. Stynes-Riordan-Gracia [25] prove the sharp error analysis of  $L_1$  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  $H^1$ -stability of the L2-1 $\sigma$  method proposed initially in [2] on general nonuniform meshes for subdiffusion equation with homogeneous Dirichlet boundary condition:

$$\partial_t^\alpha u(t, x) = \Delta u(t, x) + f(t, x), \quad (t, x) \in (0, \infty) \times \Omega, \tag{1.1}$$

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

$$\mathcal{B}_n(v, w) = \sum_{k=1}^n \langle L_k^{\alpha,*} v, \delta_k w \rangle, \quad \delta_k w := w^k - w^{k-1}, \quad n \geq 1, \tag{1.2}$$

is positive semidefinite under the restrictions (3.2) on time step ratios  $\rho_k := \tau_k/\tau_{k-1}$  with  $\tau_k$  the  $k$ th time step and  $k \geq 2$ . 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*  $H^1$ -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  $H^1$ -stability can be ensured for all time.

Besides the global-in-time  $H^1$ -stability of the L2-1 $\sigma$  scheme in Theorem 2, we revisit the sharp convergence analysis in [15] 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 [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  $H^1$ -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 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

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

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. [2] for this setting of  $\sigma$ ). 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

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

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

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

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

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

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 (1.2).

### 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  $\rho_k, k \geq 2$ .

**Lemma 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

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



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

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

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 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 [23, 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  $\rho_k$ . We first provide two equivalent forms of  $a_j^{(k)}$  according to (2.2):  $\forall 1 \leq j \leq k-1$ ,

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

and

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

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

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

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

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

*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

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

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

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

Substituting (3.12) into (3.11) yields

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

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

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

*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

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

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

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

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  $\int_0^1 (1 - 3s)(1 - s) ds = 0$ , 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:

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

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

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

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  $\rho_n$ . From (3.6), (3.7) and (3.9), we can derive

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

$$\begin{aligned}
 & - \frac{\alpha \tau_{n-2}^3}{\tau_{n-1}(\tau_{n-2} + \tau_{n-1})} \int_0^1 s(1-s)(t_n^* - t_{n-2} + s\tau_{n-2})^{-\alpha-1} ds \\
 & - (\sigma \tau_n)^{-\alpha} + \frac{\alpha \tau_{n-1}}{\tau_{n-1} + \tau_n} \int_0^1 (\tau_{n-1} + \tau_n + s\tau_{n-1})(1-s)(t_n^* - t_{n-1} + s\tau_{n-1})^{-\alpha-1} ds \Big) \\
 & > \frac{1}{2} c_{n-1}^{(n)} + \frac{1}{2(1-\alpha)(\sigma \tau_n)^\alpha} (2\sigma - (1-\alpha)), \tag{3.17}
 \end{aligned}$$

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  $2 \leq k \leq n - 1$  and

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

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  $2 \leq k \leq n - 1$ ;

which ensure

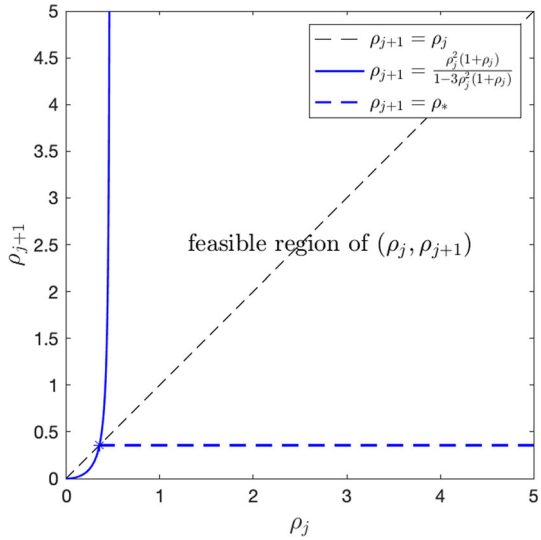
$$\mathbf{M} + \mathbf{M}^T = (\mathbf{A} + \mathbf{A}^T) + 2\mathbf{B} \geq 2\mathbf{B} \geq (1-\alpha)^{-1} \text{diag}(g_1(\alpha), g_2(\alpha), \dots, g_n(\alpha)) \geq 0,$$

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  $(\rho_j, \rho_{j+1})$  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  $\rho_* \geq \rho_j \geq \rho_{j+1} \geq \rho_{j+2} \geq \dots$  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  $j \geq 2$ ,

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

**Fig. 1** Feasible region of  $(\rho_j, \rho_{j+1})$ , 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  $(\rho_*, \rho_*)$



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 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:

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

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

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

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  $u^0 \in H_0^1(\Omega)$ . 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  $C_f = 2\|f\|_{L^\infty([0,\infty);L^2(\Omega))} + \|f\|_{BV([0,\infty);L^2(\Omega))}$ ,  $C_\Omega$  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

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

Applying the Cauchy–Schwarz inequality yields

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

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

$n \geq 1$ ,

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

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

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

The proof is completed. □

**Remark 2** 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

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

According to [26],

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

and moreover,

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

Thus we derive the  $H^1$ -stability at the continuous level

$$\|\nabla u(T, x)\|_{L^2(\Omega)} \leq \|\nabla u(0, x)\|_{L^2(\Omega)} + 2C_f^{\text{cont}} C_\Omega, \quad \forall T > 0,$$

which corresponds to our  $H^1$ -stability result in Theorem 2 for the  $L2-1_\sigma$  scheme of the subdiffusion equation (4.1).

**Remark 3** In the case of  $\alpha = 1$ , i.e., the standard diffusion equation, the energy stability (or  $H^1$ -stability) has been established for the second order BDF2 schemes in [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 $_{\sigma}$ Scheme for Subdiffusion Equation

We show the error estimate of the L2-1 $_{\sigma}$  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):

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

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

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

(Q1)

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

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

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

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

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),

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

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

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

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 trivial. In the case of  $k \geq 3$ , we have

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

$$\geq 0,$$

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 [12], 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 3** *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*

$$r_k := \frac{1}{\Gamma(1-\alpha)} \int_0^{t_k^*} (t_k^* - s)^{-\alpha} \partial_s [u(s) - I_2u(s)] ds, \quad k \geq 1, \tag{4.6}$$

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  $k \geq 1$ ,

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

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

$$|\partial_s I_2u(s)| \leq \max\{|\partial_s I_2u(t_0)|, |\partial_s I_2u(t_1)|\} \leq C_1 \frac{1 + \rho_2}{\tau_1\rho_2} (t_2 + t_2^\alpha/\alpha),$$



where we use the facts

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

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

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

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

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

from (Q2) in Lemma 2.

*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

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

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  $|\partial_t^m u(t)| \leq C_m(1 + t^{\alpha-m})$ , 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- $I_\sigma$  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  $\Omega$ .

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

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

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

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

According to [2, Lemma 1] as well as Lemma 2, 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

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

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

$$\mathbf{P}\mathbf{M} = \mathbf{E}_L$$

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 [14]. 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  $\forall 1 \leq k \leq n$ ,

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

where we use

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

$$= \sum_{j=1}^k \left( \|e^j\|_{L^2(\Omega)}^2 - \|e^{j-1}\|_{L^2(\Omega)}^2 \right) = \|e^k\|_{L^2(\Omega)}^2.$$

According to Lemma 3,

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

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  $[\mathbf{M}]_{j,1}$ :

$$\begin{aligned} \text{Mt} \quad j,j &= c_{j-1}^{(j)} + \frac{\sigma^{1-\alpha}}{(1 - \alpha) \tau_j^\alpha} \tag{4.15} \\ &= \int_0^1 \frac{\tau_{j-1}^2 (2\theta - 1)}{\tau_j (\tau_{j-1} + \tau_j) (t_j^* - (t_{j-2} + \theta \tau_{j-1}))^\alpha} d\theta + \frac{\sigma^{1-\alpha}}{(1 - \alpha) \tau_j^\alpha} \\ &\leq \frac{1}{\rho_j (1 + \rho_j) (\sigma \tau_j)^\alpha} + \frac{\sigma^{1-\alpha}}{(1 - \alpha) \tau_j^\alpha} \leq \frac{1}{\eta (1 + \eta) (\sigma \tau_j)^\alpha} + \frac{\sigma^{1-\alpha}}{(1 - \alpha) \tau_j^\alpha}, \\ [\mathbf{M}]_{j,1} &\geq \frac{\eta}{(1 + \eta) \tau_1} \int_0^{t_1^*} (t_j^* - s)^{-\alpha} ds \geq \frac{\eta}{(1 + \eta) (t_j^*)^\alpha}, \end{aligned}$$

where we use (Q1) in Lemma 2 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

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

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

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

The proof is completed. □

In the case of graded mesh with grading parameter  $r$ ,

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

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:

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

and

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

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  $r$ :

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

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  $\alpha = 0.3$

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

**Remark 4** When  $\alpha \rightarrow 1^-$ , 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  $\alpha \rightarrow 1^-$ .

### 5 Numerical Tests

In this section, we provide some numerical tests on the  $L_2$ - $1_\sigma$  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

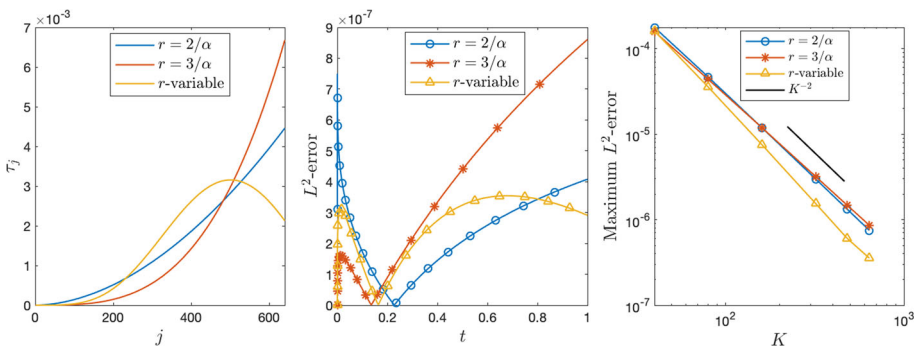
$$\begin{aligned}
 r_j &= 2/\alpha + 1.5 - \frac{3(j-1)}{K-1}, \\
 t_j &= \left(\frac{j}{K}\right)^{r_j} T, \quad \tau_j = t_j - t_{j-1} = \left[\left(\frac{j}{K}\right)^{r_j} - \left(\frac{j-1}{K}\right)^{r_{j-1}}\right] T.
 \end{aligned}
 \tag{5.1}$$

**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  $\alpha = 0.5$

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

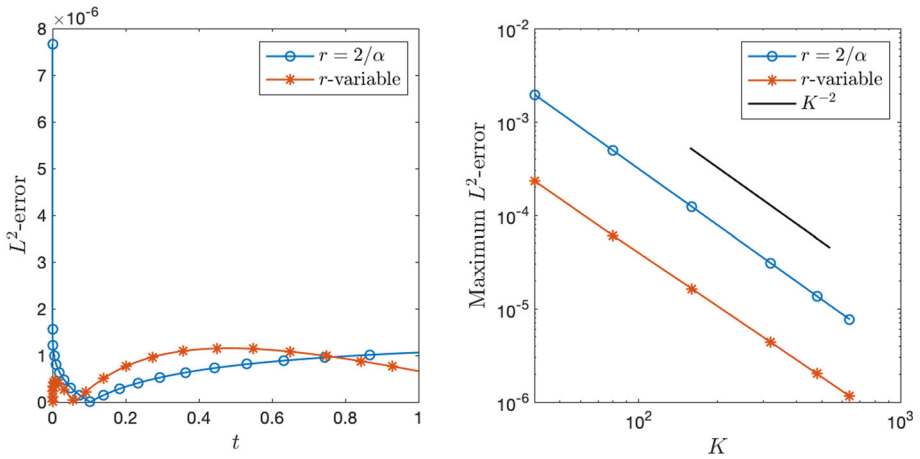
**Table 3**  $\max_{1 \leq k \leq K} \|u(t_k) - u^k\|_{L^2(\Omega)}$  for the graded meshes with different grading parameters and time step numbers where  $\alpha = 0.7$

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



**Fig. 2** Time steps (left), pointwise  $L^2$ -errors (middle), and maximum  $L^2$ -errors (right) of the  $L_2$ - $1_\sigma$  scheme in 1D on the  $r$ -variable graded mesh (5.1) and the graded meshes (4.17) with  $r = 2/\alpha, 3/\alpha$  ( $\alpha = 0.7$ )

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  $L_2-1_\sigma$  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  $L_2-1_\sigma$  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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**Data Availability** Enquiries about data availability should be directed to the authors.

### Declarations

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

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