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Blow-up of error estimates in time-fractional initial-boundary value problems

Hu Chen
School of Mathematical Sciences, Ocean University of China, Qingdao 266100, China

and

Martin Stynes*
Applied and Computational Mathematics Division, Beijing Computational Science Research Center, Beijing 100193, China
*Corresponding author: m.stynes@csrc.ac.cn

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Time-fractional initial-boundary value problems of the form $D_t^\alpha u - p\Delta u + cu = f$ are considered, where $D_t^\alpha u$ is a Caputo fractional derivative of order $\alpha \in (0,1)$ and the spatial domain lies in $\mathbb{R}^d$ for some $d \in \{1,2,3\}$. As $\alpha \to 1^-$ we prove that the solution u converges, uniformly on the space-time domain, to the solution of the classical parabolic initial-boundary value problem where $D_t^\alpha u$ is replaced by $\partial u/\partial t$. Nevertheless, most of the rigorous analyses of numerical methods for this time-fractional problem have error bounds that blow up as $\alpha \to 1^-$, as we demonstrate. We show that in some cases these analyses can be modified to obtain robust error bounds that do not blow up as $\alpha \to 1^-$.

Keywords: time-fractional; initial-boundary value problem; error estimate blow-up.

1. Introduction and summary

The numerical analysis of differential equations containing fractional derivatives has attracted much attention in the past decade. In the current paper we discuss one of the most popular classes of these problems: time-fractional initial-boundary value problems (IBVP). Our aims are to draw the reader's attention to a glaring inadequacy that appears in the vast majority of published numerical error analyses for this widely studied class of problems, and to provide—in some cases—an alternative error analysis that remedies this flaw.

Let Ω be a bounded domain in $\mathbb{R}^d$, where $d \in \{1,2,3\}$. Its closure is denoted by $\bar{\Omega}$. We assume that Ω has smooth boundary $\partial\Omega$ or is convex. Consider the time-fractional IBVP

$$D_t^\alpha u - p\Delta u + c(x)u = f(x,t) \text{ for } (x,t) \in Q := \Omega \times (0,T], \tag{1.1a}$$

with

$$u(x,t) = 0 \text{ for } x \in \partial\Omega,\ t \in (0,T], \tag{1.1b}$$

$$u(x,0) = \phi(x) \text{ for } x \in \Omega, \tag{1.1c}$$

where $\alpha \in (0,1)$ is fixed, p is a positive constant, $c \in C(\bar{\Omega})$ with $c \geqslant 0, f \in C(\bar{Q})$ where $\bar{Q} = \bar{\Omega} \times [0,T]$ and $\phi \in C(\bar{\Omega})$. More regularity and compatibility of the data is needed in many of the papers that we cite later, but we shall not give the details of these additional conditions. In (1.1a) the *Caputo fractional derivative* D_t^α is defined by

$$D_t^\alpha g(x,t) := \frac{1}{\Gamma(1-\alpha)} \int_{s=0}^{t} (t-s)^{-\alpha} \frac{\partial g(x,s)}{\partial s}\, \mathrm{d}s \quad \text{for } (x,t) \in Q.$$

A technical comment: in the problems and papers that we consider the function $g(x,\cdot)$ is absolutely continuous on $[0,T]$ for each x, and, consequently, Diethelm (2010, Theorem 3.1) permits us to use the above definition of $D_t^\alpha g(x,t)$ instead of the more general definition given in Diethelm (2010, Definition 3.2).

The problem (1.1) and some of its variants are considered in many recent numerical analysis papers, see, e.g., Jin *et al.* (2019); Stynes *et al.* (2017) and their references. Existence, uniqueness and the regularity of a solution to (1.1) is discussed in Stynes *et al.* (2017) and Kopteva (2019). A fundamental attribute of (1.1) is that, even when the data of the problem are smooth and compatible, typical solutions exhibit a weak singularity at the initial time $t = 0$. That is, for each fixed x, the solution behaves like a multiple of t^α as $t \to 0^+$, so after making some regularity and compatibility hypotheses on the data, one has the bounds of Stynes *et al.* (2017, Theorem 2.1) and (Kopteva, 2019, Section 6):

$$\left|\frac{\partial^k u}{\partial x^k}(x,t)\right| \leqslant C \quad \text{for } k = 0,1,2,3,4, \tag{1.2a}$$

$$\left|\frac{\partial^\ell u}{\partial t^\ell}(x,t)\right| \leqslant C(1+t^{\alpha-\ell}) \quad \text{for } \ell = 0,1,2, \tag{1.2b}$$

for all $(x,t) \in \bar{\Omega} \times (0,T]$.

Consider now what happens to (1.1) if one (formally) takes the limit $\alpha \to 1^-$. Then the time-fractional IBVP reduces to a classical parabolic IBVP, whose solution (given sufficient smoothness and compatibility of the data) has no singularity at $t = 0$. As we shall demonstrate in Section 2, the weakly singular solution of (1.1) approaches the smoother solution of the parabolic problem without any unpleasant behaviour.

But when we examine the theoretical convergence results in those numerical analysis papers that consider (1.1) or a variant of (1.1) and take into account the weak singularity of its solution at $t = 0$, we find—surprisingly—that in most papers, the error bounds obtained *blow up as* $\alpha \to 1^-$, even though there is no 'blow-up' behaviour in the continuous problem (1.1) as $\alpha \to 1^-$. This happens for a variety of numerical methods and a variety of norms. In Jin *et al.* (2019, Remark 4.3) the authors write: 'This phenomenon does not fully agree with the results for the continuous model. Such a blowup phenomenon appears also in some existing error analysis...and it is of interest to further refine the estimates to fill in the gap.'

Our paper is the first to investigate systematically the above 'gap' in the research literature mentioned in Jin *et al.* (2019) by surveying the current situation and giving several new results that partly fill the gap. We begin by proving that there is no blow-up in the continuous problem (1.1) as $\alpha \to 1^-$. Then we describe many published analyses that exhibit blow-up in their error bounds and a few papers that avoid this flaw. Finally, we devote some time to explaining in detail how (in some cases) one can modify existing analyses to avoid blow-up in the final error estimate.

REMARK 1.1 A further reason for considering the analysis of numerical methods when $\alpha \to 1^-$ is provided by recent work (Wang & Zheng, 2019), where it is argued that one should consider time-fractional problems in which the order of the temporal derivative is $\alpha = \alpha(t) \in [0, 1)$, and the case where $\lim_{t\to 0} \alpha(t) = 1$ is of particular significance. While our discussion below is confined to constant α, it is nevertheless a stepping stone towards devising numerical methods that are robust for the situation where $\alpha = \alpha(t)$ with $\lim_{t\to 0} \alpha(t) = 1$.

The structure of the paper is as follows. Section 2 considers the solution of problem (1.1) as $\alpha \to 1^-$. It is established that this solution converges, uniformly on the space-time domain $\bar{Q}$, to the solution of the classical parabolic problem obtained by replacing D_t^α in (1.1a) by the partial derivative $\partial u/\partial t$. In Section 3 we give a detailed description of numerical analysis papers where blow-up occurs in error estimates for computed solutions. The short Section 4 lists a few numerical analysis papers whose theoretical error bounds do not exhibit blow-up as $\alpha \to 1^-$. Then in Section 5 we revisit some of the error analyses of Section 3 and give new improved error analyses for these methods that do not blow up as $\alpha \to 1^-$.

2. Behaviour of the continuous problem as $\alpha \to 1^-$

In this section we consider the exact solution u of the fractional IBVP (1.1), and we show that as $\alpha \to 1^-$, this solution converges, uniformly in the space-time domain $\bar{Q}$, to the solution v of the classical parabolic IBVP

$$\frac{\partial v}{\partial t} - p\Delta u + c(x)v = f(x,t) \text{ for } (x,t) \in Q, \tag{2.1a}$$

with

$$v(x,t) = 0 \text{ for } x \in \partial\Omega,\ t \in (0,T], \tag{2.1b}$$

$$v(x,0) = \phi(x) \text{ for } x \in \bar{\Omega}. \tag{2.1c}$$

We begin by stating an explicit formula for the exact solution of (1.1) that is discussed at length in Stynes *et al.* (2017, Section 2), based on earlier work of Luchko (2012) and Sakamoto & Yamamoto (2011). Let $\{(\lambda_i, \psi_i) : i = 1, 2, \dots\}$ be the eigenvalues and eigenfunctions for the Sturm–Liouville two-point boundary value problem

$$\mathscr{L}\psi_i := -p\Delta\psi_i + c\psi_i = \lambda_i\psi_i \text{ on } \Omega, \quad \psi_i|_{\partial\Omega} = 0,$$

with the eigenfunctions normalized by requiring $(\psi_i, \psi_i) = 1$ for all i; here $(\cdot,\cdot)$ denotes the inner product in $L^2(\Omega)$. It is well known that $\lambda_i > 0$ for all i. Under suitable regularity and compatibility assumptions on the data of (1.1), a standard separation of variables technique (Luchko, 2012, equation (4.29)), (Sakamoto & Yamamoto, 2011, equation (2.11)) yields (Stynes *et al.*, 2017, equation (2.2)), (Kopteva, 2019, Section 6):

$$u(x,t) = \sum_{i=1}^{\infty}\Big[(\phi, \psi_i)E_{\alpha,1}(-\lambda_i t^\alpha) + J_{i,\alpha}(E_{\alpha,\alpha}; t)\Big]\psi_i(x) \text{ for all } (x,t) \in \bar{Q}, \tag{2.2}$$

where

$$J_{i,\alpha}(g;t) := \int_{s=0}^{t} s^{\alpha-1} g(-\lambda_i s^{\alpha}) f_i(t-s)\,\mathrm{d}s \quad \text{with} \quad f_i(t) := (f(\cdot,t), \psi_i(\cdot)), \tag{2.3}$$

and the two-parameter Mittag–Leffler function (Podlubny, 1999, Section 1.2) is defined for $\alpha > 0, \beta > 0$ by

$$E_{\alpha,\beta}(z) := \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}.$$

In the framework of sectorial operators (Sakamoto & Yamamoto, 2011) for each $\gamma \in \mathbb{R}$, the fractional power $\mathscr{L}^{\gamma}$ of the operator $\mathscr{L}$ is defined with domain

$$D(\mathscr{L}^{\gamma}) := \left\{ g \in L^2(\Omega) : \sum_{i=1}^{\infty} \lambda_i^{2\gamma} |(g,\psi_i)|^2 < \infty \right\},$$

and for each $g \in D(\mathscr{L}^{\gamma})$ we set

$$\|g\|_{\mathscr{L}^{\gamma}} = \left[\sum_{i=1}^{\infty} \lambda_i^{2\gamma} |(g,\psi_i)|^2 \right]^{1/2}.$$

(Here we have used the variant $\|\cdot\|_{\mathscr{L}^{\gamma}}$ of the norm notation of Sakamoto & Yamamoto, 2011; one could instead use the equivalent notation $\|\cdot\|_{\dot{H}^{\gamma}}$—see, e.g., Thomée, 2006, Chapter 3.) Using these fractional powers in Sakamoto & Yamamoto (2011, Theorems 2.1 and 2.2), the existence and uniqueness of solutions to (1.1) in various Hilbert spaces is proved by representing the solution in the form (2.2).

One can apply the same separation of variables technique to (2.1) to show that

$$v(x,t) = \sum_{i=1}^{\infty} \Big[(\phi,\psi_i) E_{1,1}(-\lambda_i t) + J_{i,1}(E_{1,1};t) \Big] \psi_i(x) \text{ for all } (x,t) \in \bar{Q}; \tag{2.4}$$

note here that $E_{1,1}(z) = e^z$ for all z.

Our goal in this section is to use (2.2)–(2.4) to show that $u(x,t) \to v(x,t)$ uniformly on $\bar{Q}$ as $\alpha \to 1^-$. From these equations it is clear that we need to consider $E_{\alpha,\beta}(z)$, where $\beta \in [\alpha, 1]$ and $z \in \mathbb{R}$ with $z < 0$. Furthermore, since we are examining the limit as $\alpha \to 1^-$, for the rest of Section 2 we shall assume that

$$\frac{3}{4} \leqslant \alpha < 1 \quad \text{and} \quad \alpha \leqslant \beta \leqslant 1. \tag{2.5}$$

LEMMA 2.1 For all α, β satisfying (2.5) and all $z \in \mathbb{R}$ with $z < 0$, there exists a constant C_7, which is independent of α, β and z, such that

$$|E_{\alpha,\beta}(z) - E_{1,1}(z)| \leqslant \frac{C_7(1-\alpha)}{1+|z|}.$$

Proof. The Mittag–Leffler function can be represented as a complex contour integral, as described in Gorenflo *et al.* (2014, Section 4.7) and Podlubny (1999, Section 1.2.7). From Gorenflo *et al.* (2014, equation (4.7.13)) (where we choose $\varepsilon = 1$ and $\delta = 3\pi/4$ to facilitate our analysis), this contour integral can be expressed as

$$E_{\alpha,\beta}(z) = \int_1^{+\infty} K[\alpha,\beta,r,z]\,\mathrm{d}r + \int_{-3\pi/4}^{3\pi/4} P[\alpha,\beta,\varphi,z]\,\mathrm{d}\varphi, \tag{2.6}$$

where, after correcting a small error in the definition of ψ in Gorenflo *et al.* (2014, equation (4.7.12)), one has

$$\begin{aligned}
K[\alpha,\beta,r,z] &= \frac{1}{2\pi\alpha} r^{(1-\beta)/\alpha} \exp[r^{1/\alpha}\cos(3\pi/(4\alpha))]\,\frac{r\sin(\psi - 3\pi/4) - z\sin\psi}{r^2 + \sqrt{2}\,rz + z^2},\\
\psi(\alpha,\beta) &= r^{1/\alpha}\sin(3\pi/(4\alpha)) + (3\pi/4)[1 + (1-\beta)/\alpha],\\
P[\alpha,\beta,\varphi,z] &= \frac{\exp[\cos(\varphi/\alpha)]\,e^{i\omega}}{2\pi\alpha(e^{i\varphi} - z)},
\end{aligned} \tag{2.7}$$

$$\omega(\alpha,\beta) = \sin(\varphi/\alpha) + \varphi[1 + (1-\beta)/\alpha]. \tag{2.8}$$

We shall use (2.6) to bound $|E_{\alpha,\beta}(z) - E_{1,1}(z)|$.

In (2.8) one has $|\varphi| \leqslant 3\pi/4$ because of the integral of P in (2.6), so it is straightforward to use the mean value theorem (and $\alpha \leqslant \beta \leqslant 1$) to verify that $|\omega(\alpha,\beta) - \omega(1,1)| \leqslant C_1(1-\alpha)$ for some fixed constant C_1. Then in (2.7) one can verify in a similar manner that

$$|P[\alpha,\beta,\varphi,z] - P[1,1,\varphi,z]| \leqslant \frac{C_2(1-\alpha)}{1+|z|}$$

for some fixed constant C_2, since it is easily seen from a diagram that

$$|e^{i\varphi} - z| \geqslant \begin{cases} 1/\sqrt{2} & \text{for } -2 \leqslant z < 0,\\ |z|/2 & \text{for } z < -2,\end{cases}$$

so $|e^{i\varphi} - z| \geqslant (1+|z|)/5$ for all $z < 0$. Hence,

$$\left| \int_{-3\pi/4}^{3\pi/4} P[\alpha,\beta,\varphi,z]\,\mathrm{d}\varphi - \int_{-3\pi/4}^{3\pi/4} P[1,1,\varphi,z]\,\mathrm{d}\varphi \right| \leqslant \frac{C_3(1-\alpha)}{1+|z|} \tag{2.9}$$

for some fixed constant C_3.

To deal with the first integral in (2.6) write $K = K_1 K_2 K_3$, where

$$K_1(\alpha,\beta) := \frac{1}{2\pi\alpha} r^{(1-\beta)/\alpha},$$
$$K_2(\alpha) := \exp[r^{1/\alpha}\cos(3\pi/(4\alpha))],$$
$$K_3(\alpha,\beta) := \frac{r\sin(\psi - 3\pi/4) - z\sin\psi}{r^2 + \sqrt{2}\,rz + z^2}.$$

Note that $r \geqslant 1$ in (2.6). By the mean value theorem, for some θ_1 with $\alpha \leqslant \theta_1 \leqslant 1$ and ξ_1 with $\beta \leqslant \xi_1 \leqslant 1$ we have

$$\begin{aligned} 0 \leqslant K_1(\alpha,\beta) - K_1(1,1) &= \frac{1-\alpha}{2\pi\theta_1^2} r^{(1-\xi_1)/\theta_1}\left(1 + \frac{1-\xi_1}{\theta_1}\ln r\right) + \frac{1-\beta}{2\pi\theta_1^2} r^{(1-\xi_1)/\theta_1}\ln r \\ &\leqslant \frac{8(1-\alpha)}{9\pi} r^{1/3}\left(1 + \frac{4}{3}\ln r\right), \end{aligned} \tag{2.10}$$

by (2.5). Before estimating K_2 set $g(\alpha) = r^{1/\alpha}\cos(3\pi/(4\alpha))$. Then applying the mean value theorem, for some θ_2 with $\alpha \leqslant \theta_2 \leqslant 1$ one gets

$$\begin{aligned} \left|K_2(\alpha) - K_2(1)\right| &= \left|(1-\alpha)\, e^{g(\theta_2)} r^{1/\theta_2}\left[\frac{1}{\theta_2^2}(\ln r)\cos\left(\frac{3\pi}{4\theta_2}\right) + \frac{3\pi}{4\theta_2^2}\sin\left(\frac{3\pi}{4\theta_2}\right)\right]\right| \\ &\leqslant (1-\alpha)\, e^{-r/\sqrt{2}} r^{4/3}\left[\frac{16}{9}\ln r + \frac{4\pi}{3}\right] \\ &\leqslant C_4(1-\alpha)\, e^{-r/2}, \end{aligned} \tag{2.11}$$

for some fixed constant $C_4 > 0$, where we used (2.5) and $r \geqslant 1$. To handle K_3, first observe that for some θ_3 with $\alpha \leqslant \theta_3 \leqslant 1$ and ξ_3 with $\beta \leqslant \xi_3 \leqslant 1$, the mean value theorem gives

$$\begin{aligned} |\psi(\alpha,\beta) - \psi(1,1)| &= \Bigg|(\alpha - 1)\Bigg[-\frac{1}{\theta_3^2}(r^{1/\theta_3}\ln r)\sin\left(\frac{3\pi}{4\theta_3}\right) \\ &\qquad + r^{1/\theta_3}\left(-\frac{3\pi}{4\theta_3^2}\right)\cos\left(\frac{3\pi}{4\theta_3}\right) - \frac{3\pi(1-\xi_3)}{4\theta_3^2}\Bigg] - \frac{3\pi}{4\theta_3}(\beta - 1)\Bigg| \\ &\leqslant \frac{16(1-\alpha)}{9}\left[r^{4/3}\left(\ln r + \frac{3\pi}{4}\right) + \frac{21\pi}{16}\right] \\ &\leqslant C_5(1-\alpha) r^{4/3}(1 + \ln r) \end{aligned}$$

for some fixed constant $C_5 > 0$, where we used (2.5). Now $|\sin x - \sin y| \leqslant |x - y|$ for all $x, y \in \mathbb{R}$, so it follows that

$$|K_3(\alpha,\beta) - K_3(1,1)| \leqslant C_5(1-\alpha)r^{4/3}(1+\ln r)\,\frac{r+|z|}{r^2+\sqrt{2}\,rz+z^2}\,. \tag{2.12}$$

But

$$\frac{r+|z|}{r^2+\sqrt{2}\,rz+z^2} \leqslant \frac{r+|z|}{(r+|z|)^2/\sqrt{2}} = \frac{\sqrt{2}}{r+|z|} \leqslant \frac{\sqrt{2}}{1+|z|}\,. \tag{2.13}$$

Thus (2.12) implies that

$$|K_3(\alpha,\beta) - K_3(1,1)| \leqslant \frac{\sqrt{2}C_5(1-\alpha)r^{4/3}(1+\ln r)}{1+|z|}\,. \tag{2.14}$$

Our final inequalities for the K_i are (recall that α satisfies (2.5)):

$$0 \leqslant K_1(\alpha,\beta) \leqslant \frac{2}{3\pi}r^{1/3}, \quad 0 \leqslant K_2(\alpha) \leqslant e^{-r/\sqrt{2}} \text{ and } |K_3(\alpha,\beta)| \leqslant \frac{\sqrt{2}}{1+|z|} \text{ from (2.13).} \tag{2.15}$$

Now we can return to $\int_1^{+\infty} K[\alpha,\beta,r,z]\,\mathrm{d}r$ in (2.6). Using the identity

$$\begin{aligned}
&K_1(\alpha,\beta)K_2(\alpha)K_3(\alpha,\beta) - K_1(1,1)K_2(1)K_3(1,1)\\
&\quad= K_1(\alpha,\beta)K_2(\alpha)[K_3(\alpha,\beta) - K_3(1,1)] + K_1(\alpha,\beta)[K_2(\alpha) - K_2(1)]K_3(1,1)\\
&\qquad+ [K_1(\alpha,\beta) - K_1(1,1)]K_2(1)K_3(1,1)
\end{aligned}$$

and estimating the terms on the right-hand side by (2.10), (2.11), (2.14) and (2.15), we obtain

$$\begin{aligned}
&|K_1(\alpha,\beta)K_2(\alpha)K_3(\alpha,\beta) - K_1(1,1)K_2(1)K_3(1,1)|\\
&\quad\leqslant \frac{2\sqrt{2}C_5(1-\alpha)}{3\pi(1+|z|)}\,e^{-r/\sqrt{2}}r^{5/3}(1+\ln r) + \frac{2\sqrt{2}C_4(1-\alpha)}{3\pi(1+|z|)}\,e^{-r/2}r^{1/3}\\
&\qquad+ \frac{8\sqrt{2}(1-\alpha)}{9\pi(1+|z|)}\,e^{-r/\sqrt{2}}r^{1/3}\left(1+\frac{4}{3}\ln r\right)\\
&\quad\leqslant \frac{C_6(1-\alpha)e^{-r/4}}{1+|z|}
\end{aligned}$$

for some fixed constant C_6 and all $r \geqslant 1$. Hence,

$$\begin{aligned}
\left|\int_1^{+\infty} K[\alpha,\beta,r,z]\,\mathrm{d}r - \int_1^{+\infty} K[1,1,r,z]\,\mathrm{d}r\right| &\leqslant \frac{C_6(1-\alpha)}{1+|z|}\int_1^{+\infty} e^{-r/4}\,\mathrm{d}r\\
&= \frac{4C_6(1-\alpha)e^{-1/4}}{1+|z|}\,.
\end{aligned} \tag{2.16}$$

Finally, combine (2.6), (2.9) and (2.16) to get $|E_{\alpha,\beta}(z) - E_{1,1}(z)| \leqslant C_7(1-\alpha)/(1+|z|)$ for some fixed constant C_7. □

From (2.2) and (2.4) for all $(x,t) \in \bar{Q}$, one has

$$\begin{aligned}
&|u(x,t) - v(x,t)| \\
&\leqslant \left| \sum_{i=1}^{\infty} \left\{ (\phi, \psi_i) \left[E_{\alpha,1}(-\lambda_i t^\alpha) - E_{1,1}(-\lambda_i t^\alpha) \right] + \left[J_{i,\alpha}(E_{\alpha,\alpha}; t) - J_{i,\alpha}(E_{1,1}; t) \right] \right\} \psi_i(x) \right| \\
&\quad + \left| \sum_{i=1}^{\infty} \left\{ (\phi, \psi_i) \left[E_{1,1}(-\lambda_i t^\alpha) - E_{1,1}(-\lambda_i t) \right] + \left[J_{i,\alpha}(E_{1,1}; t) - J_{i,1}(E_{1,1}; t) \right] \right\} \psi_i(x) \right| \\
&= |S_1(x,t)| + |S_2(x,t)|, \text{ say.}
\end{aligned} \tag{2.17}$$

To estimate these sums we use the following idea from Kopteva (2019, Section 6.1). By a Sobolev imbedding theorem and our assumption that Ω is convex or has smooth boundary, there exist constants C such that

$$\|w\|_{L^\infty(\Omega)} \leqslant C\|w\|_{H^2(\Omega)} \leqslant C\|\mathscr{L}w\|_{L^2(\Omega)} \ \forall w \in H^2(\Omega); \tag{2.18}$$

see Grisvard (1985).

Lemma 2.2 There exists a constant C such that

$$|S_1(x,t)| \leqslant C(1-\alpha) \left[\|\phi\|_{\mathscr{L}^1} + \max_{0 \leqslant t \leqslant T} \|f(\cdot,t)\|_{\mathscr{L}^1} \right] \text{ for all } (x,t) \in \bar{Q}.$$

Proof. Appealing to (2.18) for each $t \in (0,T]$ we have

$$\begin{aligned}
&\|S_1(\cdot,t)\|^2_{L^\infty(\Omega)} \leqslant C\|\mathscr{L}S_1\|^2_{L^2(\Omega)} \\
&= C \left\| \sum_{i=1}^{\infty} \left\{ (\phi, \psi_i) \left[E_{\alpha,1}(-\lambda_i t^\alpha) - E_{1,1}(-\lambda_i t^\alpha) \right] + \left[J_{i,\alpha}(E_{\alpha,\alpha}; t) - J_{i,\alpha}(E_{1,1}; t) \right] \right\} \lambda_i \psi_i \right\|^2_{L^2(\Omega)} \\
&= C \sum_{i=1}^{\infty} \left\{ (\phi, \psi_i) \left[E_{\alpha,1}(-\lambda_i t^\alpha) - E_{1,1}(-\lambda_i t^\alpha) \right] + \left[J_{i,\alpha}(E_{\alpha,\alpha}; t) - J_{i,\alpha}(E_{1,1}; t) \right] \right\}^2 \lambda_i^2 \\
&\leqslant C \sum_{i=1}^{\infty} \left\{ (\phi, \psi_i)^2 \left[E_{\alpha,1}(-\lambda_i t^\alpha) - E_{1,1}(-\lambda_i t^\alpha) \right]^2 + \left[J_{i,\alpha}(E_{\alpha,\alpha}; t) - J_{i,\alpha}(E_{1,1}; t) \right]^2 \right\} \lambda_i^2.
\end{aligned} \tag{2.19}$$

Here Lemma 2.1, $\lambda_i \geqslant 0$ and $t \geqslant 0$ yield

$$\sum_{i=1}^{\infty} (\phi, \psi_i)^2 \left[E_{\alpha,1}(-\lambda_i t^\alpha) - E_{1,1}(-\lambda_i t^\alpha) \right]^2 \lambda_i^2 \leqslant C_7^2 (1-\alpha)^2 \sum_{i=1}^{\infty} \frac{(\phi, \psi_i)^2 \lambda_i^2}{(1+\lambda_i t^\alpha)^2} \leqslant C_7^2 (1-\alpha)^2 \|\phi\|^2_{\mathscr{L}^1}. \tag{2.20}$$

Similarly,

$$\begin{aligned}\sum_{i=1}^{\infty}\left[J_{i,\alpha}(E_{\alpha,\alpha};t)-J_{i,\alpha}(E_{1,1};t)\right]^2\lambda_i^2 &\leqslant \sum_{i=1}^{\infty} C_7^2(1-\alpha)^2\left[\int_{s=0}^{t} s^{\alpha-1}|f_i(t-s)|\,\mathrm{d}s\right]^2\lambda_i^2\\ &\leqslant C_7^2(1-\alpha)^2\sum_{i=1}^{\infty}\left[\int_{s=0}^{t} s^{2\alpha-2}\,\mathrm{d}s\right]\left[\int_{s=0}^{t}\lambda_i^2|f_i(t-s)|^2\,\mathrm{d}s\right]\\ &\leqslant C(1-\alpha)^2\int_{s=0}^{t}\sum_{i=1}^{\infty}\lambda_i^2|f_i(t-s)|^2\,\mathrm{d}s\\ &\leqslant CT(1-\alpha)^2\max_{0\leqslant t\leqslant T}\|f(\cdot,t)\|^2_{\mathscr{L}^1},\end{aligned} \tag{2.21}$$

where we used a Cauchy–Schwarz inequality and the boundedness of $\int_{s=0}^{t} s^{2\alpha-2}\,\mathrm{d}s$ because $\alpha \geqslant 3/4$.

The Lemma now follows from (2.19)–(2.21). □

To estimate $S_2(x,t)$ recall first that $E_{1,1}(z) = e^z$ for all z. In our calculations we shall assume for convenience that $T \geqslant 1$; if $T < 1$ then certain terms are obviously omitted and the bounds are simplified.

Lemma 2.3 There exists a constant C such that for all $(x,t) \in \bar{Q}$, one has

$$|S_2(x,t)| \leqslant C\left[(1-\alpha)+(T-T^{\alpha})\right]\|\phi\|_{\mathscr{L}^2} + CT^{1/2}[\rho(\alpha,T)]^{1/2}\max_{0\leqslant t\leqslant T}\|f(\cdot,t)\|_{\mathscr{L}^1},$$

where

$$\rho(\alpha,T) := 2\int_0^T (s^{\alpha-1}-1)^2\,\mathrm{d}s + 2e^{-2}\int_0^1 (s^{\alpha-1}-1)^2\,\mathrm{d}s + 2e^{-2}\int_1^T (T^{1-\alpha}-1)^2\,\mathrm{d}s.$$

Proof. For $0 \leqslant t \leqslant 1$ one has $t^\alpha \geqslant t$ and from calculus one sees easily that $\max_{t\in[0,1]}(t^\alpha - t)$ occurs at the point $t = t_* \in (0,1)$ satisfying $t_*^{\alpha-1} = 1/\alpha$. Thus,

$$\max_{t\in[0,1]}(t^\alpha - t) = t_*^\alpha - t_* = t_*^\alpha(1-t_*^{1-\alpha}) = t_*^\alpha(1-\alpha) \leqslant 1-\alpha. \tag{2.22}$$

It is easy to check that $1-e^{-y} \leqslant y$ and $ye^{-y} \leqslant e^{-1}$ for all $y \geqslant 0$. Hence, for $0 \leqslant t \leqslant 1$ and each i, one has

$$0 \leqslant e^{-\lambda_i t} - e^{-\lambda_i t^\alpha} = e^{-\lambda_i t}\left(1-e^{-\lambda_i(t^\alpha - t)}\right) \leqslant e^{-\lambda_i t}\lambda_i(t^\alpha - t) \leqslant \min\{\lambda_i(1-\alpha), e^{-1}(t^{\alpha-1}-1)\}, \tag{2.23}$$

where (2.22) yields the first term. For $1 < t \leqslant T$ we get likewise

$$0 \leqslant e^{-\lambda_i t^\alpha} - e^{-\lambda_i t} \leqslant e^{-\lambda_i t^\alpha}\lambda_i(t-t^\alpha) \leqslant \min\{\lambda_i(T-T^\alpha), e^{-1}(T^{1-\alpha}-1)\}. \tag{2.24}$$

Similarly to the derivation of (2.19)–(2.21) by using (2.23) and (2.24) one gets

$$
\begin{aligned}
\|S_2(\cdot,t)\|^2_{L^\infty(\Omega)} &\leqslant C\sum_{i=1}^{\infty}\left\{(\phi,\psi_i)^2\left[E_{1,1}(-\lambda_i t^\alpha)-E_{1,1}(-\lambda_i t)\right]^2+\left[J_{i,\alpha}(E_{1,1};t)-J_{i,1}(E_{1,1};t)\right]^2\right\}\lambda_i^2\\
&\leqslant C\left[(1-\alpha)+(T-T^\alpha)\right]^2\sum_{i=1}^{\infty}\lambda_i^4(\phi,\psi_i)^2\\
&\quad + C\sum_{i=1}^{\infty}\left[\int_{s=0}^{t}\left|\left(s^{\alpha-1}e^{-\lambda_i s^\alpha}-e^{-\lambda_i s}\right)f_i(t-s)\right|\,\mathrm{d}s\right]^2\lambda_i^2\\
&\leqslant C\left[(1-\alpha)+(T-T^\alpha)\right]^2\|\phi\|^2_{\mathscr{L}^2}\\
&\quad + C\sum_{i=1}^{\infty}\left[\int_{s=0}^{t}\left(s^{\alpha-1}e^{-\lambda_i s^\alpha}-e^{-\lambda_i s}\right)^2\mathrm{d}s\right]\left[\int_{s=0}^{t}\lambda_i^2 f_i^2(t-s)\,\mathrm{d}s\right]
\end{aligned}
$$

for each $t\in(0,T]$. But

$$
\begin{aligned}
&\int_0^t\left(s^{\alpha-1}e^{-\lambda_i s^\alpha}-e^{-\lambda_i s}\right)^2\mathrm{d}s\\
&\qquad=\int_0^t\left[(s^{\alpha-1}-1)e^{-\lambda_i s^\alpha}+(e^{-\lambda_i s^\alpha}-e^{-\lambda_i s})\right]^2\mathrm{d}s\\
&\qquad\le 2\int_0^t\left[(s^{\alpha-1}-1)^2e^{-2\lambda_i s^\alpha}+(e^{-\lambda_i s^\alpha}-e^{-\lambda_i s})^2\right]\mathrm{d}s\\
&\qquad\le 2\int_0^T(s^{\alpha-1}-1)^2\,\mathrm{d}s+2e^{-2}\int_0^1(s^{\alpha-1}-1)^2\,\mathrm{d}s+2e^{-2}\int_1^T(T^{1-\alpha}-1)^2\,\mathrm{d}s
\end{aligned}
$$

by (2.23) and (2.24) and we are done. □

REMARK 2.4 In the case $d=1$ one can replace the proofs of Lemmas 2.2 and 2.3 by arguments similar to those of Stynes *et al.* (2017, Section 2), which require less regularity of ϕ and f, obtaining

$$
|S_1(x,t)\leqslant C(1-\alpha)\left[\|\phi\|_{\mathscr{L}^{1/2}}+\max_{0\leqslant t\leqslant T}\|f(\cdot,t)\|_{\mathscr{L}^{1/2}}\right]
$$

and

$$
|S_2(x,t)\leqslant C\left[(1-\alpha)+(T-T^\alpha)\right]\|\phi\|_{\mathscr{L}^{3/2}}+C[\rho(\alpha,T)]^{1/2}\max_{0\leqslant t\leqslant T}\|f(\cdot,t)\|_{\mathscr{L}^{1/2}}.
$$

Now we can derive the main result of this section, which shows that the solution u of the time-fractional problem (1.1) converges uniformly on $\bar{Q}$ to the solution v of the classical parabolic problem (2.1) as $\alpha\to 1^-$.

Theorem 2.5 One has

$$\lim_{\alpha\to 1^-}\left[\max_{(x,t)\in\bar{Q}} |u(x,t)-v(x,t)|\right]=0.$$

Proof. This follows from (2.17) by invoking Lemmas 2.2 and 2.3. □

3. Numerical methods with α-nonrobust error bounds

Only numerical methods for solving (1.1) (or some variant of (1.1)) that take into account the weak singularity of the solution at $t=0$ are considered here, as any assumption of extra regularity in the solution imposes an implicit unnatural constraint on the data of the problem (Stynes, 2016, 2019).

Given a numerical method for solving (1.1), we say that an error bound for this method that blows up as $\alpha\to 1^-$ is α*-nonrobust*. If the error bound does not blow up as $\alpha\to 1^-$, then it is α*-robust*.

In this section we present brief descriptions of the methods and error bounds from several papers with α-nonrobust results. Our list is not exhaustive, but it is representative.

Note: for each paper in this section we exhibit one place where the paper's analysis produces a bound that blows up as $\alpha\to 1^-$, but similar α-nonrobust behaviour may also appear elsewhere in the same paper.

Our first example of an α-nonrobust result comes from Stynes *et al.* (2017), where $d=1$ and the authors consider a finite difference method on a mesh $\{(x_m,t_n)\}$ that is uniform in space (with M mesh intervals) and graded in time (with N mesh intervals), so that mesh points are clustered near $t=0$. A standard classical finite difference method is used in space, and the L1 scheme is used for the time discretization of D_t^α. Write $\|w^n\|_\infty$ for the maximum of each mesh function $\{w_m^n\}$ at each time level t_n, i.e., $\|w^n\|_\infty := \max_{m=0,1,\dots,M}|w_m^n|$. Then for the general discrete problem $L_{M,N}v_m^n=g_m^n$, one has the following stability result:

Lemma 3.1 (Stynes *et al.*, 2017, Lemma 4.2) The solution of the discrete problem satisfies

$$\|v^n\|_\infty \leqslant \|v^0\|_\infty + \tau_n^\alpha\,\Gamma(2-\alpha)\sum_{j=1}^{n}\theta_{n,j}\|g^j\|_\infty$$

for $n=1,2,\dots,N$, where $\tau_n=t_n-t_{n-1}$ and the $\theta_{n,j}$ are certain positive stability multipliers.

This lemma is useful only if one has some bound on the $\theta_{n,j}$. Such a bound is provided by the next result:

Lemma 3.2 (Stynes *et al.*, 2017, Lemma 4.3) Let the parameter β satisfy $\beta\leqslant r\alpha$, where $r\geqslant 1$ is the user-chosen mesh grading parameter. Then for $n=1,2,\dots,N$, one has

$$\tau_n^\alpha\sum_{j=1}^{n} j^{-\beta}\theta_{n,j}\le \frac{T^\alpha N^{-\beta}}{1-\alpha}\,. \tag{3.1}$$

It is clear that the bound (3.1) blows up as $\alpha\to 1^-$, and, consequently, the subsequent analysis leading to the final error bound of Stynes *et al.* (2017, Theorem 5.3) is α-nonrobust.

In Liao *et al.* (2018b) a numerical method similar to Stynes *et al.* (2017) is used, but on a more general family of meshes, and without requiring $c\geqslant 0$ in (1.1a). The error analysis uses stability multipliers similar to Stynes *et al.* (2017), and (like Lemma 3.2 above) we find that Liao *et al.* (2018b, equation (3.4)) contains a factor $1-\alpha$ in its denominator, so the analysis is α-nonrobust.

Kopteva (2019) gives an alternative (shorter) analysis of the numerical method of Stynes *et al.* (2017). An inspection of the proof of Kopteva (2019, Lemma 2.1) shows that the bound obtained there relies on the inequality $\kappa_{n,1} \geqslant t_n^{-\alpha}/\Gamma(1-\alpha)$, where $\kappa_{n,1}$ is defined in Kopteva (2019, equation (2.2)) but the right-hand side of this inequality collapses to zero as $\alpha \to 1^-$. It follows that the error analysis of Kopteva (2019) is α-nonrobust.

Gracia *et al.* (2018b) prove that in the special case of Stynes *et al.* (2017), where the temporal mesh is uniform one obtains (Gracia *et al.*, 2018b, Theorem 4), a higher order of accuracy away from the initial time $t = 0$ than is predicted by the global error estimate of Stynes *et al.* (2017, Theorem 5.2). But the bound of Gracia *et al.* (2018b, Lemma 3) contains a factor $\Gamma(1-\alpha)$ hidden in the constant multiplier, so the result is α-nonrobust. Nevertheless, we shall show in Section 5.2 that a modification of the proof of Gracia *et al.* (2018b, Lemma 3) will yield an α-robust final error estimate.

In Chen & Stynes (2019) the method of Stynes *et al.* (2017) is modified by replacing the L1 scheme by the higher-order 'L2-1_σ' discretization $\delta^\alpha_{t_{j+\sigma}}$ of D^α_t of Alikhanov (2015). Then the techniques of Kopteva (2019) are used to carry out the error analysis. But this analysis depends on the following result, which is analogous to Kopteva (2019, Lemma 2.1):

Lemma 3.3 (Chen & Stynes (2019) Lemma 5) Assume certain conditions on the temporal mesh. Then for any mesh function $\{V^j\}_{j=0}^M$, one has

$$|V^{k+1}| \le |V^0| + \Gamma(1-\alpha) \max_{j=0,\dots,k} \left\{ t^\alpha_{j+\sigma} \delta^\alpha_{t_{j+\sigma}} |V| \right\} \text{ for } k = 0, \dots, M-1.$$

Here we see immediately that as $\alpha \to 1^-$ one has $\Gamma(1-\alpha) \to \infty$, and, consequently, the error analysis in Chen & Stynes (2019) is α-nonrobust.

A more general analysis is developed by Liao *et al.* (2018a); it includes the method of Chen & Stynes (2019) as a special case and permits the coefficient c in (1.1a) to take negative values. But the error bounds of the main convergence result (Liao *et al.*, 2018a, Theorem 3.8) (see also (Liao *et al.*, 2018a, Lemma 3.6)) have a factor $1-\alpha$ in their denominators, so this analysis is nonrobust as $\alpha \to 1^-$.

In Gracia *et al.* (2018a) the authors use a fitted scheme for the time discretization, which enables the use of a less severe mesh grading than in Stynes *et al.* (2017). But Gracia *et al.* (2018a) relies on the following result, with D^α_N the discretization of D^α_t:

Lemma 3.4 (Gracia *et al.*, 2018a, Lemma 5) If a grid function $b(x_m, t_n)$ satisfies

$$b(x_m, 0) = 0 \quad \text{and} \quad b(x_m, t_i) \leqslant b(x_m, t_j) \text{ if } i \leqslant j,$$

then

$$b(x_m, t_n) \leqslant \Gamma(1-\alpha)\, t_n^\alpha D^\alpha_N b(x_m, t_n). \tag{3.2}$$

The right-hand side of (3.2) obviously blows up as $\alpha \to 1^-$. Consequently, the subsequent analysis, which uses this lemma, yields a final bound (Gracia *et al.*, 2018a, Theorem 4) that is α-nonrobust.

In Jin *et al.* (2019) the error analysis is carried out using Laplace transforms and operator theory; we do not give any of its details here and merely draw the reader's attention to Jin *et al.* (2019, Remark 4.3), where the authors point out that the constant multipliers in their error estimates (which of course depend on α) will blow up as $\alpha \to 1^-$.

In Le *et al.* (2016) a time-fractional Fokker–Planck problem is considered:

$$\begin{cases} u_t(x,t) - \kappa_\alpha \partial_t^{1-\alpha} u_{xx} + \mu_\alpha^{-1} \left(F \partial_t^{1-\alpha} u \right)_x = g \text{ for } (x,t) \in (0,l) \times (0,T), \\ u(x,0) = u_0(x) \text{ for } x \in (0,l), \\ u(x,t) = 0 \text{ for } x \in \{0,l\} \text{ and } 0 < t < T, \end{cases} \tag{3.3}$$

where κ_α and μ_α are positive constants and $u_0(x) \in H^2(\Omega) \cap H_0^1(\Omega)$. Here $\partial_t^{1-\alpha}$ is the standard Riemann–Liouville fractional derivative operator defined by $\partial_t^{1-\alpha} u = (J^\alpha u)_t$, where J^α is the temporal Riemann–Liouville integral operator of order α, viz.,

$$J^\alpha u(x,t) = \int_0^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)} u(x,s)\, \mathrm{d}s.$$

The authors take $F = F(x,t)$ in (3.3); if instead one has the simpler case $F = F(x)$, then the differential equation of (3.3) can be reduced to (1.1a) (with an extra convection term) by the change of variable $v := \partial_t^{1-\alpha} u$. A fundamental result in the analysis of Le *et al.* (2016) is

Lemma 3.5 (simplified form of Le *et al.*, 2016, Lemma 2.2) For real-valued functions $v \in C[0,T]$, one has

$$\int_{t=0}^T \left(J^\alpha v(t)\right) v(t)\, \mathrm{d}t \geqslant \cos\left(\frac{\alpha\pi}{2}\right) \int_{t=0}^T \left(J^{\alpha/2} v(t)\right)^2 \mathrm{d}t. \tag{3.4}$$

Clearly, the factor $\cos(\alpha\pi/2)$ in the right-hand side here will collapse to zero as $\alpha \to 1^-$. As a consequence the error analysis of Le *et al.* (2016) is α-nonrobust.

Remark 3.6 Inequalities similar to Lemma 3.5 and leading to α-nonrobust error estimates appear in several papers: Karaa (2018, equation (2.3)), Karaa *et al.* (2018, equation. (6)), Le *et al.* (2016, Lemma 2.2), Mustapha *et al.* (2016, Lemma 2), Mustapha (2018, equation (2.2)), and Mustapha & Schötzau (2014, Lemma 3.1) where the inequality of Lemma 3.5 first appeared. Some of these papers deal with the problem (1.1), some with related problems.

4. α-Robust error bounds

Compared with Section 3 a much smaller number of published papers that consider temporal discretizations of (1.1a) have error bounds that are α-robust. These include Gunzburger & Wang (2019), some papers of Jin *et al*. (e.g., Jin *et al.*, 2017) and some papers of McLean and Mustapha (e.g., Mustapha & McLean, 2013). In each of these papers an inspection of the analysis does not reveal any blow-up in the error estimates, but it is unclear whether this α-robustness is fortuitous or is due to some subtle mechanism.

The only paper where the authors set out explicitly to devise an α-robust analysis is Huang *et al.* (2020), who investigate the time-fractional Fokker–Planck IBVP (3.3). This problem was previously considered by Le *et al.* (2016), who solve it numerically by a semidiscrete method where a piecewise-linear Galerkin finite element method is used for the spatial discretization. Unfortunately (recall Lemma 3.5 above, which is used in Le *et al.*, 2016), the constant multipliers in their error bounds are α-nonrobust; see for example Le *et al.* (2016, Theorems 3.2 and 3.3). In Huang *et al.* (2020) the authors consider the same semidiscrete method for solving this Fokker–Planck problem, but to avoid blow-up in their error estimates, they make the crucial replacement of Lemma 3.5 by the following α-robust result.

LEMMA 4.1 (Huang *et al.*, 2020, Lemma 2.2) Let α satisfy $1/2 < \alpha < 1$. Assume that $v \in L^2(0,T)$. Then for $t \in [0,T]$, one has

$$J^{\alpha}\left(vJ^{\alpha}v\right)(t) \geq \frac{1}{2}\left(J^{\alpha}v(t)\right)^2 \text{ and } \int_0^t \left(vJ^{\alpha}v\right)(s)\,\mathrm{d}s \geq \frac{1}{2}J^{1-\alpha}\left(J^{\alpha}v(t)\right)^2.$$

The consequent final error bound of Huang *et al.* (2020, Theorem 3.5) is α-robust.

REMARK 4.2 Some α-robust error estimates for a simplified version of (1.1), where it is assumed that the solution has no singularity at time $t = 0$, appear in Deng (2008/2009, Theorem 3.3) and Lin & Xu (2007, Theorem 4.2) for the L1 scheme and in Chen *et al.* (2016, Theorem 4.2) for the $L2\text{-}1_{\sigma}$ scheme.

5. Improved analyses of α-nonrobust error bounds

In this section we show that it is possible to improve some α-nonrobust inequalities in the literature to make them α-robust without sacrificing any sharpness in the subsequent error analysis.

5.1 *Improvement of analysis in Stynes et al. (2017)*

In Lemma 3.2 above, which is identical to Stynes *et al.* (2017, Lemma 4.3), we stated a bound that is evidently α-nonrobust. We shall now present an α-robust bound on the left-hand side of this lemma.

To begin, recall the notation of Stynes *et al.* (2017): the temporal mesh points are $t_n := T(n/N)^r$ for $n = 0, 1, \ldots, N$, where $r \geqslant 1$ is the user-chosen mesh grading parameter. Set $\tau_n = t_n - t_{n-1}$ for $n = 1, 2, \ldots, N$. For $1 \leqslant k \leqslant n$, let

$$d_{n,k} := \frac{(t_n - t_{n-k})^{1-\alpha} - (t_n - t_{n-k+1})^{1-\alpha}}{\tau_{n-k+1}}.$$

Hence, $d_{n,1} = \tau_n^{-\alpha}$.

Define the real numbers $\theta_{n,j}$, for $n = 1, 2, \ldots, N$ and $j = 1, 2, \ldots, n-1$, by

$$\theta_{n,n} = 1, \quad \theta_{n,j} = \sum_{k=1}^{n-j} \tau_{n-k}^{\alpha}(d_{n,k} - d_{n,k+1})\theta_{n-k,j}. \tag{5.1}$$

These quantities are related by the following result, which appeared in a preprint of Stynes *et al.* (2017) (see Gracia *et al.*, 2015, Proof of Lemma 3), but was removed from the final published paper. The same formula (modulo some scaling) is fundamental for the more general analyses of Liao *et al.* (2018b, Lemma 2.1(i)) and Liao *et al.* (2019, equation (2.5)).

LEMMA 5.1 For $n = 1, 2, \ldots, N$ and $1 \leq k \leq n$, one has

$$\sum_{j=k}^{n} d_{j,j+1-k}\theta_{n,j} = \tau_n^{-\alpha}. \tag{5.2}$$

Proof. If $n = 1$, then $k = 1$ and $d_{1,1}\theta_{1,1} = d_{1,1} = \tau_1^{-\alpha}$ as desired.

Now assume that $i \geq 2$. Suppose that (5.2) holds for $n = 1, 2, \ldots, i-1$ and $1 \leq k \leq n$. We want to prove (5.2) for $n = i$ and $1 \leqslant k \leqslant i$.

If $n=i$ and $k=i$, then $d_{i,1}\theta_{i,i}=d_{i,1}=\tau_i^{-\alpha}$ so (5.2) holds. Next, consider $n=i$ and $1\leqslant k\leqslant i-1$. We have, by (5.1) and the inductive hypothesis,

$$\begin{aligned}
\sum_{j=k}^{i} d_{j,j+1-k}\theta_{i,j} &= \sum_{j=k}^{i-1} d_{j,j+1-k}\left[\sum_{\xi=1}^{i-j}\tau_{i-\xi}^{\alpha}(d_{i,\xi}-d_{i,\xi+1})\theta_{i-\xi,j}\right]+d_{i,i+1-k}\\
&= \sum_{\xi=1}^{i-k}\tau_{i-\xi}^{\alpha}(d_{i,\xi}-d_{i,\xi+1})\left[\sum_{j=k}^{i-\xi} d_{j,j+1-k}\theta_{i-\xi,j}\right]+d_{i,i+1-k}\\
&= \sum_{\xi=1}^{i-k}\tau_{i-\xi}^{-\alpha}\tau_{i-\xi}^{\alpha}(d_{i,\xi}-d_{i,\xi+1})+d_{i,i+1-k}\\
&= d_{i,1}=\tau_i^{-\alpha}.
\end{aligned}$$

This completes the proof of (5.2) for $n=i$ and $1\leqslant k\leqslant i$. By the principle of induction we are done. □

LEMMA 5.2 (Chebyshev's integral inequality). (Hardy *et al.*, 1988, Theorem 43) Let f and g be integrable over the interval $[a,b]$ with f monotonically decreasing and g monotonically increasing. Then

$$\frac{1}{b-a}\int_a^b f(x)g(x)\,\mathrm{d}x\leq\left[\frac{1}{b-a}\int_a^b f(x)\,\mathrm{d}x\right]\left[\frac{1}{b-a}\int_a^b g(x)\,\mathrm{d}x\right].$$

Now we can derive a bound on a weighted sum of the $\theta_{n,j}$ that improves the result of Stynes *et al.* (2017, Lemma 4.3) because it is α-robust. This result and its proof are essentially a special case of Liao *et al.* (2019, equation (2.8)); we give the details here for ease of reading.

LEMMA 5.3 Let $\gamma\in(0,1)$ be a constant. Then for $n=1,2,\dots,N$, one has

$$\tau_n^{\alpha}\sum_{j=1}^{n} j^{r(\gamma-\alpha)}\theta_{n,j}\leq\frac{\Gamma(1+\gamma-\alpha)}{\Gamma(1+\gamma)\Gamma(2-\alpha)}\,T^{\alpha}\left(\frac{t_n}{T}\right)^{\gamma}N^{r(\gamma-\alpha)}. \tag{5.3}$$

Proof. First, $D_t^{\alpha}(t^{\gamma})=t^{\gamma-\alpha}\Gamma(1+\gamma)/\Gamma(1+\gamma-\alpha)$. Hence, for $j\geq 1$ we have

$$\begin{aligned}
&\frac{\Gamma(1+\gamma)}{\Gamma(1+\gamma-\alpha)}(t_j)^{\gamma-\alpha}\\
&\quad=\frac{1}{\Gamma(1-\alpha)}\int_0^{t_j}(t_j-s)^{-\alpha}\gamma s^{\gamma-1}\mathrm{d}s=\frac{1}{\Gamma(1-\alpha)}\sum_{k=1}^{j}\int_{t_{k-1}}^{t_k}(t_j-s)^{-\alpha}\gamma s^{\gamma-1}\mathrm{d}s\\
&\quad\leq\frac{1}{\Gamma(1-\alpha)}\sum_{k=1}^{j}\int_{t_{k-1}}^{t_k}(t_j-s)^{-\alpha}\left[\frac{(t_k)^{\gamma}-(t_{k-1})^{\gamma}}{\tau_k}\right]\mathrm{d}s\\
&\quad=\frac{1}{\Gamma(2-\alpha)}\sum_{k=1}^{j}\left[(t_j-t_{k-1})^{1-\alpha}-(t_j-t_k)^{1-\alpha}\right]\left[\frac{(t_k)^{\gamma}-(t_{k-1})^{\gamma}}{\tau_k}\right]\\
&\quad=\frac{1}{\Gamma(2-\alpha)}\sum_{k=1}^{j}d_{j,j+1-k}\left[(t_k)^{\gamma}-(t_{k-1})^{\gamma}\right],
\end{aligned}$$

where we used Chebyshev's integral inequality (Lemma 5.2) in the calculation. Multiply this inequality by $\theta_{n,j}$ then sum from $j = 1$ to n. This yields

$$\begin{aligned}
\frac{\Gamma(1+\gamma)}{\Gamma(1+\gamma-\alpha)}\sum_{j=1}^{n}(t_j)^{\gamma-\alpha}\theta_{n,j} &\le \frac{1}{\Gamma(2-\alpha)}\sum_{j=1}^{n}\theta_{n,j}\sum_{k=1}^{j}d_{j,j+1-k}\left[(t_k)^{\gamma}-(t_{k-1})^{\gamma}\right]\\
&= \frac{1}{\Gamma(2-\alpha)}\sum_{k=1}^{n}\left[(t_k)^{\gamma}-(t_{k-1})^{\gamma}\right]\left(\sum_{j=k}^{n}\theta_{n,j}d_{j,j+1-k}\right)\\
&= \frac{1}{\tau_n^{\alpha}\Gamma(2-\alpha)}\sum_{k=1}^{n}\left[(t_k)^{\gamma}-(t_{k-1})^{\gamma}\right]\\
&= \frac{1}{\tau_n^{\alpha}\Gamma(2-\alpha)}(t_n)^{\gamma},
\end{aligned}$$

by changing the order of summation then invoking Lemma 5.1. But $t_j = T(j/N)^r$, so we can rewrite this inequality as (5.3). □

Note that the only values of the parameter β of Stynes *et al.* (2017, Lemma 4.3) (i.e., Lemma 3.2 above) that are used in the error analysis of Stynes *et al.* (2017, Theorem 5.3) are $\beta = 0$ and $\beta = \min\{2-\alpha, r\alpha\}$. Thus, in our analysis here we shall consider only these values. Our next result corresponds to $\beta = 0$ in Lemma 3.2.

Corollary 5.4

$$\tau_n^{\alpha}\sum_{j=1}^{n}\theta_{n,j} \le \frac{(t_n)^{\alpha}}{\Gamma(1+\alpha)\Gamma(2-\alpha)}.$$

Proof. Take $\gamma = \alpha$ in Lemma 5.3. □

The bound of Corollary 5.4 is clearly α-robust, unlike the bound $T^{\alpha}/(1-\alpha)$ of Lemma 3.2 for $\beta = 0$. Moreover, Corollary 5.4 shows that $\tau_n^{\alpha}\sum_{j=1}^{n}\theta_{n,j}$ is small when n is small, which Lemma 3.2 fails to do.

To improve the bound for $\beta = \min\{2-\alpha, r\alpha\}$ in Lemma 3.2 is more complicated. For notational convenience set $m^* = \min\{2-\alpha, r\alpha\}$. Assume that $N \geqslant 2$, which is not a restriction. Then choose

$$\gamma = \frac{1}{\ln N} + \alpha - \frac{m^*}{r}. \tag{5.4}$$

To use this value of γ in Lemma 5.3 we must check that $\gamma \in (0,1)$. First, $\gamma > 0$ because $-m^*/r \geqslant -r\alpha/r = -\alpha$. To show that $\gamma < 1$ we assume that the user-chosen mesh grading parameter r satisfies $r \leqslant 2(2-\alpha)/\alpha$. This assumption is not a practical restriction since our analysis will show that the optimal value of r is $r = (2-\alpha)/\alpha$. Consider now the value of γ in (5.4). If $m^* = r\alpha$, then $\gamma = 1/(\ln N)$, so $\gamma < 1$ if $N > e$. If $m^* = 2-\alpha$, then

$$\gamma \leqslant \frac{1}{\ln N} + \alpha - \frac{2-\alpha}{2(2-\alpha)/\alpha} = \frac{1}{\ln N} + \frac{\alpha}{2}.$$

Hence, $\gamma < 1$ will follow (since $\alpha < 1$) if $1/(\ln N) < 1/2$, i.e., if $N > e^2 \approx 7.34$. Thus, we are guaranteed $\gamma < 1$ if $N \geqslant 8$, which is not a practical restriction.

COROLLARY 5.5 Assume that $r \leqslant 2(2-\alpha)/\alpha$ and $N \geqslant 8$. Set $\ell_N = 1/(\ln N)$. Then

$$\tau_n^\alpha \sum_{j=1}^{n} j^{-m^*}\theta_{n,j} \le \frac{e^r\,\Gamma(1+\ell_N-m^*/r)}{\Gamma(1+\ell_N+\alpha-m^*/r)\Gamma(2-\alpha)}\, T^\alpha \left(\frac{t_n}{T}\right)^{\ell_N+\alpha-m^*/r} N^{-m^*}. \tag{5.5}$$

Proof. In Lemma 5.3 choose γ according to (5.4). (Our earlier calculation shows that $\gamma \in (0,1)$, so this choice of γ is permitted in Lemma 5.3.) This yields

$$\begin{aligned}\tau_n^\alpha &\sum_{j=1}^{n} j^{r\ell_N-m^*}\theta_{n,j}\\ &\le \frac{\Gamma(1+\ell_N-m^*/r)}{\Gamma(1+\ell_N+\alpha-m^*/r)\Gamma(2-\alpha)}\, T^\alpha \left(\frac{t_n}{T}\right)^{\ell_N+\alpha-m^*/r} N^{-(m^*-r\ell_N)}.\end{aligned}$$

Using $1 \leqslant j^{r\ell_N} \leqslant N^{r\ell_N} = e^r$ the result follows. □

The bound of Corollary 5.5 has as its main factor $T^\alpha N^{-m^*}$, which is exactly the same as Lemma 3.2 when $\beta = m^*$. Note that $(t_n/T)^\gamma \leqslant 1$ in the bound. Thus, using Corollaries 5.4 and 5.5 in the error analysis of Stynes *et al.* (2017, Theorem 5.3) instead of Stynes *et al.* (2017, Lemma 4.3) we will conclude as in Stynes *et al.* (2017) that the optimal value of r is $r = (2-\alpha)/\alpha$.

What happens to the bound of Corollary 5.5 as $\alpha \to 1^-$? The factors $\Gamma(1+\ell_N+\alpha-m^*/r)$ and $\Gamma(2-\alpha)$ cause no problems. In $\Gamma(1+\ell_N-m^*/r)$ one has $m^* \to 1$ and, consequently, there is no risk of blow-up unless $r \to 1$ (which is the optimal choice when $\alpha \to 1^-$), but even in this worst case we obtain $\Gamma(1+\ell_N-m^*/r) \to \Gamma(\ell_N) \approx \ln N$ since $x\Gamma(x) = \Gamma(x+1) \to \Gamma(1) = 1$ as $x \to 0^+$, i.e., there is no blow-up, but there is a slight deterioration in the theoretical bound on the rate of convergence.

In summary, by using Corollaries 5.4 and 5.5 in the analysis of Stynes *et al.* (2017), one obtains again the final error bound of Stynes *et al.* (2017, Theorem 5.3), but now with a constant factor that is α-robust.

REMARK 5.6 Suppose that the *a priori* bound (1.2b) is replaced by the more general assumption that

$$\left|\frac{\partial^\ell u}{\partial t^\ell}(x,t)\right| \leqslant C(1+t^{\sigma-\ell}) \text{ for } \ell = 0,1,2, \quad \text{where } \sigma \in (0,\alpha] \text{ is fixed.} \tag{5.6}$$

This modification is discussed in Stynes *et al.* (2017, Remark 5.5), where it is shown that the temporal truncation error is now

$$\left|D_N^\alpha u(x_m,t_n) - D_t^\alpha u(x_m,t_n)\right| \leqslant CT^{\sigma-\alpha}N^{r(\alpha-\sigma)}n^{-\min\{2-\alpha+r(\alpha-\sigma),\, r\alpha\}}.$$

In our analysis above one should now choose $m^* = \min\{2-\alpha+r(\alpha-\sigma), r\alpha\}$. This will lead to the α-robust final error bound

$$\max_{(x_m,t_n)\in\bar{Q}} |u(x_m,t_n) - u_m^n| \leqslant C\left(T^\alpha h^2 + T^\sigma N^{-\min\{2-\alpha,\, r\sigma\}}\right).$$

Hence, the optimal choice of mesh grading is now $r = (2 - \alpha)/\sigma$.

5.2 *Improvement of analysis in Gracia et al. (2018b)*

Section 3 described how the convergence result of Gracia *et al.* (2018b, Theorem 4) is α-nonrobust because a constant multiplier in the bound of Gracia *et al.* (2018b, Lemma 3) blows up as $\alpha \to 1^-$. We shall now derive a modified version of Gracia *et al.* (2018b, Lemma 3) that avoids this pitfall.

We use a uniform temporal mesh with $N + 1$ mesh points $t_n := n\tau := n(T/N)$ for $n = 0, 1, \ldots, N$. Set $d_k = k^{1-\alpha} - (k-1)^{1-\alpha}$ for $k = 1, 2, \ldots$ Then define real numbers $\theta_0, \theta_1, \theta_2, \ldots$ by

$$\theta_0 := 1, \quad \theta_i := \sum_{k=1}^{i} (d_k - d_{k+1})\theta_{i-k} \text{ for } i = 1, 2, \ldots$$

Lemma 5.7 (Gracia *et al.*, 2018b, Lemma 2) The coefficients θ_i satisfy

$$\theta_i < (i+1)^{\alpha-1} \quad \text{for } i = 0, 1, 2, \ldots$$

Lemma 5.8 (Gracia *et al.*, 2018b, Lemma 3) Let $\beta > 1$ be constant. Then for $n = 1, 2, \ldots, N$, one has

$$\tau^{\alpha} \sum_{j=1}^{n} j^{-\beta}\theta_{n-j} \le CTN^{-1} t_n^{\alpha-1},$$

where the constant $C = C(\alpha)$ blows up as $\alpha \to 1^-$.

Proof. This result is obtained in Gracia *et al.* (2018b, Lemma 3) without any comment on the behaviour of C as $\alpha \to 1^-$. But an inspection of its proof shows readily that C contains a factor $\Gamma(1-\alpha)$. □

Let $\beta \geqslant 0$ be constant. Let n be a positive integer. Define

$$K_{\beta,n} := \begin{cases} 1 + \frac{1-n^{1-\beta}}{\beta-1} & \text{if } \beta \neq 1, \\ 1 + \ln n & \text{if } \beta = 1. \end{cases}$$

Lemma 5.9 Let $\beta \geqslant 0$ be constant. Then for $n = 1, 2, \ldots$ one has $\sum_{j=1}^{n} j^{-\beta} \leqslant K_{\beta,n}$. Moreover, for each n one has $\lim_{\beta\to 1} K_{\beta,n} = K_{1,n}$ and $K_{\beta,n}$ is a strictly decreasing function of β.

Proof. It is easy to see that

$$\sum_{j=1}^{n} j^{-\beta} = 1 + \sum_{j=2}^{n} j^{-\beta} \leqslant 1 + \int_{x=1}^{n} x^{-\beta}\,\mathrm{d}x = \begin{cases} 1 + \frac{1-n^{1-\beta}}{\beta-1} & \text{if } \beta \neq 1, \\ 1 + \ln n & \text{if } \beta = 1. \end{cases}$$

Furthermore, L'Hôpital's rule gives

$$\lim_{\beta\to 1} \frac{1-n^{1-\beta}}{\beta-1} = \lim_{\beta\to 1} \frac{n^{1-\beta}\ln n}{1} = \ln n.$$

For the final part recall that $K_{\beta,n} = 1 + \int_{x=1}^{n} x^{-\beta}\,\mathrm{d}x$. This is clearly a strictly decreasing function of β. □

In the next inequality the left-hand side is a rescaled variant of Lemma 5.8 (i.e., Gracia *et al.*, 2018b, Lemma 3), but the right-hand side is α-robust.

LEMMA 5.10 Let $\beta \geqslant 0$ be constant. Then for $n = 1, 2, \ldots,$ one has

$$\sum_{j=1}^{n} j^{-\beta}\theta_{n-j} \le K_{\beta,n}\left(\frac{n}{2}\right)^{\alpha-1} + \frac{2^{\beta-\alpha}}{\alpha}\, n^{-\beta+\alpha}.$$

Proof. From Lemma 5.7 we have

$$\begin{aligned}
\sum_{j=1}^{n} j^{-\beta}\theta_{n-j} &\le \sum_{j=1}^{n} j^{-\beta}(n+1-j)^{\alpha-1} \\
&\le \left(\frac{n}{2}\right)^{\alpha-1}\sum_{j=1}^{\lceil n/2\rceil} j^{-\beta} + \left(\frac{n}{2}\right)^{-\beta}\sum_{j=\lceil n/2\rceil+1}^{n}(n+1-j)^{\alpha-1}.
\end{aligned} \tag{5.7}$$

But $(n+1-j)^{\alpha-1} \le (n-s)^{\alpha-1}$ for $j-1 \le s \le j \le n$. Thus,

$$\begin{aligned}
\sum_{j=\lceil n/2\rceil+1}^{n}(n+1-j)^{\alpha-1} &\le \sum_{j=\lceil n/2\rceil+1}^{n}\int_{s=j-1}^{j}(n-s)^{\alpha-1}\,\mathrm{d}s \\
&\le \int_{s=n/2}^{n}(n-s)^{\alpha-1}\,\mathrm{d}s \\
&= \left(\frac{n}{2}\right)^{\alpha}\frac{1}{\alpha}.
\end{aligned}$$

Substituting this inequality into (5.7) and invoking Lemma 5.9 gives the desired result. □

The next result involves two special cases of Lemma 5.10. In it we assume that α is bounded away from zero as it will be used to investigate what happens when $\alpha \to 1^{-}$.

COROLLARY 5.11 Assume that $0 < \underline{\alpha} \leqslant \alpha < 1$ for some constant $\underline{\alpha}$. For $n = 1, 2, \ldots, N$, one has

$$\left(\frac{T}{N}\right)^{\alpha}\sum_{j=1}^{n} j^{-\beta}\theta_{n-j} \le \begin{cases} \hat{C} & \text{if } \beta = 0, \\ \hat{C}K_{\beta,n}N^{-1}t_n^{\alpha-1} & \text{if } \beta > 1, \end{cases}$$

where the constant $\hat{C} = \hat{C}(\underline{\alpha}, T)$.

Proof. If $\beta = 0$ then Lemma 5.10 and $K_{0,n} = n$ yield

$$\begin{aligned}\left(\frac{T}{N}\right)^{\alpha}\sum_{j=1}^{n}\theta_{n-j} &\leqslant \left(\frac{T}{N}\right)^{\alpha}\left[n\left(\frac{n}{2}\right)^{\alpha-1}+\frac{2^{-\alpha}}{\alpha}n^{\alpha}\right]\\ &= \left[2^{1-\alpha}+\frac{2^{-\alpha}}{\alpha}\right]\left(\frac{n}{N}\right)^{\alpha}T^{\alpha}\\ &\leqslant \hat{C},\end{aligned}$$

since $0 < \underline{\alpha} \leqslant \alpha < 1$ and $n \leqslant N$.

If $\beta > 1$ then Lemma 5.10 yields

$$\begin{aligned}\left(\frac{T}{N}\right)^{\alpha}\sum_{j=1}^{n}j^{-\beta}\theta_{n-j} &\leqslant \left(\frac{T}{N}\right)^{\alpha}\left[K_{\beta,n}\left(\frac{n}{2}\right)^{\alpha-1}+\frac{2^{\beta-\alpha}}{\alpha}n^{\alpha-\beta}\right]\\ &\leqslant \hat{C}K_{\beta,n}N^{-1}\left(\frac{nT}{N}\right)^{\alpha-1}\\ &= \hat{C}K_{\beta,n}N^{-1}t_n^{\alpha-1}.\end{aligned}$$

□

We can now derive our final error bound.

Theorem 5.12 Assume that u satisfies the regularity bounds of Gracia *et al.* (2018b, equation (2.3)). Let u_m^n denote the computed solution at each mesh point (x_m, t_n). Let h denote the spatial mesh width. Assume that $0 < \underline{\alpha} \leqslant \alpha < 1$ for some constant $\underline{\alpha}$. Set $\sigma = \min\{2-\alpha, 1+\alpha\}$. Then there exists a constant $\hat{C} = \hat{C}(\underline{\alpha}, T)$ such that

$$\max_{0\leqslant m\leqslant M}|u(x_m,t_n)-u_m^n| \leqslant \hat{C}\left(h^2+K_{\sigma,n}N^{-1}t_n^{\alpha-1}\right) \text{ for } n = 1,2,\ldots,N. \tag{5.8}$$

Proof. Clearly $\sigma > 1$. Imitate the proof of Gracia *et al.* (2018b, Theorem 4), but invoke Corollary 5.11 instead of Gracia *et al.* (2018b, Lemma 3) (note that in this argument only the values $\beta = 0$ and $\beta = \sigma$ are required); this yields the error bound (5.8). □

In Gracia *et al.* (2018b, Theorem 4) an error bound $C\left(h^2+N^{-1}t_n^{\alpha-1}\right)$ is proved for the same method, but this bound is α-nonrobust since the constant C blows up as $\alpha \to 1^-$. Thus, Theorem 5.12 is an improvement because it obtains the same order of convergence, but is α-robust since by Lemma 5.9 we have $\lim_{\alpha\to 1^-} K_{\sigma,n} = K_{1,n} = 1 + \ln n$.

Remark 5.13 If we simplify (1.1) by assuming that its solution u is 'smooth', i.e., that the low-order temporal derivatives of u are bounded as $t \to 0^+$, then (Sun & Wu, 2006) the truncation error on a uniform temporal mesh of diameter τ is $O(\tau^{2-\alpha})$. One can now use the $\beta = 0$ parts of the above analysis to prove an α-robust $O(h^2 + \tau^{2-\alpha})$ final error bound.

Remark 5.14 In Chen *et al.* (2019) the authors consider the Grünwald–Letnikov discretization of a one-dimensional initial-value problem on a uniform mesh $\{t_m\}_{m=0}^{M}$ of diameter τ. Their final error bound is

α-nonrobust because its proof (when $\alpha \geqslant 1/2$) uses the integral $\int_{s=0}^{m} s^{-\alpha}(m-s)^{\alpha-1}\mathrm{d}s$. Our α-robust error analysis of Section 5.2 can be transferred to the setting of Chen *et al.* (2019), yielding the α-robust error bound $|u(t_m) - U_m| \leqslant \hat{C}K_{2-\alpha,m}\tau t_m^{\alpha-1}$ for all m, where $\hat{C}$ is independent of α.

5.3 *Improvement of analysis in Liao et al. (2018a)*

In Liao *et al.* (2018a) the authors consider Alikhanov's 'L2-1_σ' discretization on a general family of meshes that includes as a special case the mesh from Stynes *et al.* (2017) (uniform in space, graded in time) that was described in Section 3. As we stated in that section the theoretical error bound (Liao *et al.*, 2018a, Theorem 3.8) is α-nonrobust. This can be remedied by an analysis along the lines of Section 5.1, combining results from Chen & Stynes (2019) and Liao *et al.* (2018a), which we now outline.

In this subsection we use several generic constants $C = C(\alpha)$ that remain bounded when $\alpha \to 1^-$, as can be verified by inspecting the source material for each constant (e.g., in the first inequality below, one verifies this property by checking the proof of Chen & Stynes, 2019, Lemma 1).

For simplicity we present the argument only for the case of the graded temporal mesh of Section 5.1. By Chen & Stynes (2019, Lemma 1) the temporal truncation error of the L2-1_σ discretization δ_t^α at the specially chosen point $t_{j+\sigma} \in [t_j, t_{j+1}]$ satisfies

$$|\delta_t^\alpha v(t_{j+\sigma}) - D_t^\alpha v(t_{j+\sigma})| \leq Ct_{j+\sigma}^{-\alpha}\left(\psi_v^{j+\sigma} + \max_{s=1,\dots,j}\{\psi_v^{j,s}\}\right).$$

Now Chen & Stynes (2019, Lemma 7) gives

$$\psi_v^{j+\sigma} \leq CN^{-\min\{r\alpha,3-\alpha\}} \quad \text{and} \quad \psi_v^{j,s} \leq CN^{-\min\{r\alpha,3-\alpha\}}.$$

In Liao *et al.* (2018a, 2019) this temporal truncation error (at the point $t_{j-1+\sigma}$) is denoted by $\Upsilon^{j-\theta}$. Thus, the above inequalities and the definition of the mesh give

$$\left|\Upsilon^{j-\theta}\right| \leq Ct_{j-\theta}^{-\alpha}N^{-\min\{r\alpha,3-\alpha\}} \leq Cj^{-r\alpha}N^{r\alpha}N^{-\min\{r\alpha,3-\alpha\}} \text{ for } j = 1,\dots N. \tag{5.9}$$

From Liao *et al.* (2018a, equations (1.3) and (1.4)) we have

$$(D_\tau^\alpha v)^{n-\theta} := \sum_{k=1}^{n} A_{n-k}^{(n)}(v^k - v^{k-1}) \text{ for } n = 1,\dots,N,$$

with $\sum_{j=m}^{n} P_{n-j}^{(n)} A_{j-m}^{(j)} = 1$ for $1 \leq m \leq n \leq N$; the latter identity is analogous to Lemma 5.1.

Let $\gamma \in (0,1)$ be a constant. Set $v(t) = t^\gamma$ in Liao *et al.* (2019, equation (2.8)). This yields

$$\frac{\Gamma(1+\gamma)}{\Gamma(1+\gamma-\alpha)}\sum_{j=1}^{n} P_{n-j}^{(n)}(t_j)^{\gamma-\alpha} \leq \pi_A(t_n)^\gamma = \frac{11}{4}(t_n)^\gamma$$

as $\pi_A = 11/4$ follows from Liao *et al.* (2018a, Criterion A2 and Theorem 2.2(I)). Using the definition of the mesh $\{t_j\}$ and rearranging this inequality gives

$$\sum_{j=1}^{n} P_{n-j}^{(n)} j^{r(\gamma-\alpha)} \leq \frac{11\,\Gamma(1+\gamma-\alpha)}{4\,\Gamma(1+\gamma)} T^{\alpha} \left(\frac{t_n}{T}\right)^{\gamma} N^{r(\gamma-\alpha)}. \tag{5.10}$$

Note how (5.10) resembles Lemma 5.3. Using (5.9) and (5.10) and choosing $\gamma = 1/\ln N$, we get the following α-robust analogue of Corollary 5.5.

Lemma 5.15 Assume that $N \geqslant 3$. Set $\ell_N = 1/(\ln N)$. Then

$$\sum_{j=1}^{n} P_{n-j}^{(n)} |\Upsilon^{j-\theta}| \leq C \frac{11 e^{r}\,\Gamma(1+\ell_N-\alpha)}{4\,\Gamma(1+\ell_N)} T^{\alpha} \left(\frac{t_n}{T}\right)^{\ell_N} N^{-\min\{r\alpha,3-\alpha\}}. \tag{5.11}$$

Now one can replace the α-nonrobust bound of Liao *et al.* (2018a, Lemma 3.6) by Lemma 5.15 in the proof of Liao *et al.* (2018a, Theorem 3.8), thereby obtaining a final error estimate in Liao *et al.* (2018a) that is α-robust.

Remark 5.16 One can similarly replace the α-nonrobust bound of Liao *et al.* (2018b, Theorem 3.1) by an α-robust bound.

6. Conclusion

We have seen that, although the continuous problem (1.1) does not behave badly as $\alpha \to 1^-$, nevertheless most rigorous error analyses of numerical methods for solving (1.1) contain factors that blow up as this limit is taken. Sometimes this unnatural behaviour can be corrected, as was illustrated in Section 5 for several analyses, but we close with a warning example showing that it is not always possible to improve α-nonrobust bounds to α-robust bounds by changing the argument used to derive them.

Example 6.1 When $\alpha = 1$, the left-hand side of (3.4) becomes

$$I := \int_{t=0}^{T} \left(\int_{s=0}^{t} v(s)\,\mathrm{d}s \right) v(t)\,\mathrm{d}t.$$

Suppose that $v(t) = r'(t)$ where $r(t) := t(T-t)$. Then

$$I = \int_{t=0}^{T} r(t) r'(t)\,\mathrm{d}t = \frac{1}{2}\left[r(T)^2 - r(0)^2 \right] = 0,$$

but the right-hand side of (3.4) has the factor $\int_{t=0}^{T} \left(J^{1/2} v(t)\right)^2 \mathrm{d}t$, which is positive since v is not identically zero. Consequently, it is impossible to prove an inequality of the form

$$\int_{t=0}^{T} \left(J^{\alpha} v(t)\right) v(t)\,\mathrm{d}t \geqslant C_{\alpha} \int_{t=0}^{T} \left(J^{\alpha/2} v(t)\right)^2 \mathrm{d}t \text{ with } \lim_{\alpha \to 1^-} C_{\alpha} > 0.$$

Thus, the α-nonrobustness of Lemma 3.5 is intrinsic—it cannot be removed simply by sharpening the proof to replace $\cos(\alpha\pi/2)$ by a better constant. Instead, to achieve α-robustness one needs to modify Lemma 3.5 in a fundamental way, and this is exactly what Lemma 4.1 does.

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