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# Error estimates of a high order numerical method for solving linear fractional differential equations

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## Abstract

In this paper, we first introduce an alternative proof of the error estimates of the numerical methods for solving linear fractional differential equations proposed in Diethelm [6] where a first-degree compound quadrature formula was used to approximate the Hadamard finite-part integral and the convergence order of the proposed numerical method is  $O(\Delta t^{2-\alpha})$ ,  $0 < \alpha < 1$ , where  $\alpha$  is the order of the fractional derivative and  $\Delta t$  is the step size. We then use the similar idea to prove the error estimates of a high order numerical method for solving linear fractional differential equations proposed in Yan et al. [37], where a second-degree compound quadrature formula was used to approximate the Hadamard finite-part integral and we show that the convergence order of the numerical method is  $O(\Delta t^{3-\alpha})$ ,  $0 < \alpha < 1$ . The numerical examples are given to show that the numerical results are consistent with the theoretical results.

*Key words:*

Fractional differential equations, fractional derivative, error estimates

*AMS Subject Classification:* 65M12; 65M06; 65M70; 35S10

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## 1. Introduction

In this paper, we will consider the numerical methods for solving the following linear fractional differential equation

$${}^C_0 D_t^\alpha x(t) = \beta x(t) + f(t), \quad t \in [0, 1], \quad (1)$$

$$x(0) = x^0, \quad (2)$$

where  $0 < \alpha < 1$  and  $\beta < 0$ ,  $x^0 \in \mathbb{R}$  denotes the initial value,  $f$  is a given function on the interval  $[0, 1]$  and  ${}^C_0 D_t^\alpha x(t)$  denotes the Caputo fractional order derivative.

Diethelm [6] introduced a numerical method for solving (1)-(2) by approximating the Hadamard finite-part integral with the first-degree compound quadrature formula and proved that the convergence order is  $O(\Delta t^{2-\alpha})$ , where  $\Delta t$  is the step size. Ford et al. [15] used the similar method to consider the time discretization of the following time-fractional partial differential equation

$${}^C_0 D_t^\alpha u(t, x) - \Delta u(t, x) = f(t, x), \quad t \in [0, T], \quad x \in \Omega, \quad (3)$$

$$u(0, x) = 0, \quad x \in \Omega, \quad (4)$$

$$u(t, x) = 0, \quad t \in [0, T], \quad x \in \partial\Omega, \quad (5)$$

where  $0 < \alpha < 1$  and  $\Omega$  is the bounded open domain in  $\mathbb{R}^d$ ,  $d = 1, 2, 3$  and  $\partial\Omega$  is the boundary of  $\Omega$ . Here  $\Delta = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}$  denotes the Laplacian operator with respect to the  $x$  variable.

Define  $A = -\Delta$ ,  $\mathcal{D}(A) = H_0^1(\Omega) \cap H^2(\Omega)$ . Then the system (3)-(5) can be written in the abstract form

$${}^C_0 D_t^\alpha u(t) + Au(t) = f(t), \quad 0 < t < T, \quad 0 < \alpha < 1, \quad (6)$$

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$$u(0) = u_0, \quad (7)$$

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The time discretization problem of (6)-(7) is then the same as the discretization problem for solving (1)-(2). Ford et al. [15] used the similar numerical method as in Diethelm [6] to consider the time discretization of (6)-(7) and proved that the convergence order of the time discretization scheme is  $O(\Delta t^{2-\alpha})$ .

In [37], Yan et al. introduced a higher order numerical method for solving (1)-(2) by approximating the Hadamard finite-part integral with second-degree compound quadrature formula and proved that the error has the asymptotic expansion as in [8]. However the authors in [37] can not prove the error estimates of the higher order numerical method by using the argument in Diethelm [6]. It is not clear if it is possible to

stability condition. Sun and Wu [35] proposed a finite difference method for the fractional diffusion-wave equation. Langlands and Henry [22] considered an implicit numerical scheme for fractional diffusion equation. Lin and Xu [27] proposed a finite difference method in time and Legendre spectral method in space. Li and Xu [26] proposed a time-space spectral method for time-space fractional partial differential equation based on a weak formulation and a detailed error analysis was carried out. Ervin and Roop [10], [11] used finite element methods to find the variational solution of the fractional advection dispersion equation, in which the fractional derivative depends on the space, related to the nonlocal operator, but the time derivative term is of first order, related to the local operator. Adolfsson et al. [1], [2] considered an efficient numerical method to integrate the constitutive response of fractional order viscoelasticity based on the finite element method. Li et al. [25] considered a time fractional partial differential equation by using the finite element method and obtain the error estimates in both semidiscrete and fully discrete cases. Jiang et al. [21] considered a high-order finite element method for the time fractional partial differential equations and proved the optimal order error estimates. See other numerical methods for solving time-fractional differential equations, [22], [35], [27], [28], [16], [24], [17], etc.

Recently, Gao et al. [18] obtained a high order numerical differentiation formula with  $O(\Delta t^{3-\alpha}), 0 < \alpha < 1$  for the Caputo fractional derivative by discretizing fractional derivative directly and applied this formula for solving a time-fractional diffusion equation. But there are no error estimates in [18]. Li et al. [23] also introduced a high order  $O(\Delta t^{3-\alpha}), 0 < \alpha < 1$  numerical method to approximate the Caputo fractional derivative and applied this method for solving time-fractional advection-diffusion equation. The error estimates and stability analysis are considered only for  $\alpha \in (0, \alpha_1)$  with some positive  $\alpha_1 \in (0, 1)$  in [23]. In this paper, we will prove the error estimates of the high order numerical methods introduced by Yan et al. [37] and the convergence order is  $O(\Delta t^{3-\alpha}), 0 < \alpha < 1$ . We emphasize that our analysis works for all  $0 < \alpha < 1$ .

The paper is organized as follows. In Section 2, we consider the proof of the error estimates of the numerical methods for solving linear fractional differential equations proposed by Diethelm [6]. In Section 3, we consider the proof of the error estimates of the numerical methods for solving linear fractional differential equation proposed by Yan et al. [37]. The numerical examples are given in Section 4.

By  $C, c_0$  we denote some positive constants independent of the functions and parameters concerned, but not necessarily the same at different occurrences.

## 2. Linear interpolation

In this section, we will review Diethelm's method [6] where the Hadamard finite-part integral is approximated by using the piecewise linear interpolation polynomials.

Let us write (1)-(2) as the following form, [6], with  $0 < \alpha < 1$ ,

$${}_0^R D_t^\alpha [x(t) - x^0] = \beta x(t) + f(t), \quad 0 \leq t \leq 1, \quad (8)$$

where  ${}_0^R D_t^\alpha x(t)$  denotes the Riemann-Liouville fractional derivative defined by

$${}_0^R D_t^\alpha x(t) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_0^t (t-\tau)^{-\alpha} x(\tau) d\tau. \quad (9)$$

The Riemann-Liouville fractional derivative  ${}_0^R D_t^\alpha x(t)$  can be written as, with  $x \in C^2[0, 1]$ ,

$${}_0^R D_t^\alpha x(t) = \frac{1}{\Gamma(-\alpha)} \oint_0^t (t-\tau)^{-1-\alpha} x(\tau) d\tau, \quad (10)$$

where the integral must be interpreted as a Hadamard finite-part integral. [9, Theorem 2.1]

Let  $n$  be a fixed positive integer. Let  $0 = t_0 < t_1 < t_2 < \dots < t_j < \dots < t_n = 1$  be a partition of  $[0, 1]$  and  $\Delta t$  the step size. At the points  $t_j = \frac{j}{n}, j = 1, 2, \dots, n$ , we have

$${}_0^R D_t^\alpha [x(t_j) - x^0] = \beta x(t_j) + f(t_j), \quad j = 1, 2, \dots, n,$$

that is,

$$\frac{1}{\Gamma(-\alpha)} \oint_0^{t_j} (t_j - \tau)^{-1-\alpha} [x(\tau) - x^0] d\tau = \beta x(t_j) + f(t_j), \quad j = 1, 2, \dots, n. \quad (11)$$

Let us consider how to approximate the Hadamard integral in (11). By the change of variable, we have

$$\frac{1}{\Gamma(-\alpha)} \oint_0^{t_j} (t_j - \tau)^{-1-\alpha} x(\tau) d\tau = \frac{t_j^{-\alpha}}{\Gamma(-\alpha)} \oint_0^1 w^{-1-\alpha} x(t_j - t_j w) dw.$$

For every  $j$ , we approximate the integral by a piecewise linear interpolation polynomial with the equispaced nodes  $0, \frac{1}{j}, \frac{2}{j}, \dots, \frac{j}{j}$ . We then have, for some smooth function  $g(w)$ ,

$$\oint_0^1 w^{-1-\alpha} g(w) dw = \oint_0^1 w^{-1-\alpha} g_1(w) dw + E_j(g), \quad (12)$$

where  $g_1(w)$  is the piecewise linear interpolation polynomial of  $g(w)$  and  $E_j(g)$  is the remainder term.

We have

**Lemma 2.1.** [6] Let  $0 < \alpha < 1$ . Assume that  $g \in C^2[0, 1]$ . Then

$$\int_0^1 w^{-1-\alpha} g(w) dw = \sum_{k=0}^j \alpha_{kj} g\left(\frac{k}{j}\right) + E_j(g), \quad (13)$$

where

$$\alpha_{kj} = \begin{cases} -1, & \text{for } k = 0, \\ 2k^{1-\alpha} - (k-1)^{1-\alpha} - (k+1)^{1-\alpha}, & \text{for } k = 1, 2, \dots, j-1, \\ (\alpha-1)k^{-\alpha} - (k-1)^{1-\alpha} + k^{1-\alpha}, & \text{for } k = j. \end{cases}$$

By using (11)-(13), we obtain the following approximation of the Riemann-Liouville fractional derivative  ${}^R D_t^\alpha x(t)$  at  $t = t_j$

$${}^R D_t^\alpha x(t_j) = \Delta t^{-\alpha} \sum_{k=0}^j w_{k,j} x(t_{j-k}) + R_1^j,$$

where  $R_1^j = C \Delta t^{2-\alpha} (\max_{0 \leq s \leq 1} |x''(s)|) = O(\Delta t^{2-\alpha})$  [6] is the remainder term and the weights  $w_{k,j}, k = 0, 1, 2, \dots, j$  satisfy

$$\Gamma(2-\alpha) w_{k,j} = (-\alpha)(-\alpha+1)(j)^{-\alpha} \alpha_{k,j}, \quad (14)$$

For the Caputo fractional derivative  ${}^C D_t^\alpha x(t)$  at  $t = t_j$ , we have, noting that  ${}^R D_t^\alpha x(0) = x(0) {}^R D_t^\alpha(1) = \frac{x(0)}{\Gamma(1-\alpha)} t^{-\alpha}$ ,

$${}^C D_t^\alpha x(t_j) = {}^R D_t^\alpha (x(t_j) - x(0)) = \Delta t^{-\alpha} \sum_{k=0}^j \bar{w}_{k,j} x(t_{j-k}) + R_1^j, \quad (15)$$

where  $\bar{w}_{k,j} = w_{k,j}$  for  $k = 0, 1, 2, \dots, j-1, j \geq 1$  and  $\bar{w}_{j,j} = w_{j,j} - \frac{j^{-\alpha}}{\Gamma(1-\alpha)}$ .

The exact solution of (1)-(2) then satisfies

$$\bar{w}_{0,j} x(t_j) - \Delta t^\alpha \beta x(t_j) = - \sum_{k=1}^j \bar{w}_{k,j} x(t_{j-k}) + \Delta t^\alpha f(t_j) - \Delta t^\alpha R_1^j,$$

or

$$x(t_j) - (\bar{w}_{0,j})^{-1} (\Delta t^\alpha \beta) x(t_j) = \sum_{k=1}^j d_{j-k} x(t_{j-k}) + (\bar{w}_{0,j})^{-1} \Delta t^\alpha f(t_j) - (\bar{w}_{0,j})^{-1} \Delta t^\alpha R_1^j, \quad (16)$$

where  $d_{j-k} = -\bar{w}_{k,j}/\bar{w}_{0,j}$ ,  $k = 1, 2, \dots, j$ ,  $j \geq 1$ .

Let  $x_j \approx x(t_j)$ ,  $j \geq 0$  denote the approximate solution of  $x(t_j)$ . We define the following numerical method for solving (16), with  $x_0 = x^0$ ,

$$x_j - (\bar{w}_{0,j})^{-1}(\Delta t^\alpha \beta)x_j = \sum_{k=1}^j d_{j-k}x_{j-k} + (\bar{w}_{0,j})^{-1}\Delta t^\alpha f(t_j), \quad j = 1, 2, \dots, n. \quad (17)$$

We have the following error estimates.

**Theorem 2.2.** [6] Let  $x(t)$  and  $x_j$  be the exact solution and the approximate solution of (16) and (17), respectively. Assume that  $x \in C^2[0, 1]$ . Then there exists a constant  $C = C(\alpha, f, \beta)$  such that

$$|x(t_j) - x_j| \leq C\Delta t^{2-\alpha}, \quad j = 1, 2, \dots, n.$$

**Remark 2.1.** Our proof of Theorem 2.2 is new and is different from the proof in [6]. We shall use the same idea to consider the proof of Theorem 3.4 for the higher order method in Section 3. Therefore it may be helpful to give the new proof of Theorem 2.2 in detail here in order to understand the idea of the proof of Theorem 3.4.

To prove Theorem 2.2, we need the following lemma.

**Lemma 2.3.** For  $0 < \alpha < 1$ , the coefficients in (17) satisfy, with  $j = 1, 2, \dots, n$ ,

$$\sum_{k=1}^j d_{j-k} = 1, \quad (18)$$

$$d_{j-k} > 0, \quad k = 1, 2, \dots, j, \quad (19)$$

$$d_0^{-1} \leq c_0 \Delta t^{-\alpha}, \quad \text{for some constant } c_0. \quad (20)$$

**Proof:** We first show (18). Choose  $x(t) = 1$  in (15), we have

$$\Delta t^{-\alpha} \sum_{k=0}^j \bar{w}_{k,j} = 0, \quad j = 1, 2, \dots, n,$$

which implies that

$$\bar{w}_{0,j} + \bar{w}_{1,j} + \bar{w}_{2,j} + \dots + \bar{w}_{j,j} = 0, \quad j = 1, 2, \dots, n,$$

or, noting that  $d_{j-k} = -w_{k,j}/w_{0,j}$ ,  $k = 1, 2, \dots, j$ ,  $j = 1, 2, \dots, n$ ,

$$d_{j-1} + d_{j-2} + \dots + d_1 + d_0 = 1,$$

which is (18).

We now consider (19). It is trivial for  $j = 1$ . Here we only consider the case for  $k = 1, 2, \dots, j-1$ ,  $j = 2, 3, \dots, n$ , we have

$$\begin{aligned} \Gamma(2-\alpha)w_{k,j} &= (-\alpha)(-\alpha+1)(j)^{-\alpha}\alpha_{k,j} = -2k^{1-\alpha} + (k-1)^{1-\alpha} + (k+1)^{1-\alpha} \\ &= k^{1-\alpha} \left( -2 + \left(1 - \frac{1}{k}\right)^{1-\alpha} + \left(1 + \frac{1}{k}\right)^{1-\alpha} \right) \\ &= k^{1-\alpha} \left[ -2 + \left(1 + (1-\alpha)\left(-\frac{1}{k}\right) + \frac{(1-\alpha)(-\alpha)}{2!}\left(-\frac{1}{k}\right)^2 + \frac{(1-\alpha)(-\alpha)(-\alpha-1)}{3!}\left(-\frac{1}{k}\right)^3 + \dots \right) \right. \\ &\quad \left. + \left(1 + (1-\alpha)\frac{1}{k} + \frac{(1-\alpha)(-\alpha)}{2!}\left(\frac{1}{k}\right)^2 + \frac{(1-\alpha)(-\alpha)(-\alpha-1)}{3!}\left(\frac{1}{k}\right)^3 + \dots \right) \right] \\ &= 2(1-\alpha)(-\alpha)k^{1-\alpha} \left( \frac{1}{2k^2} + \sum_{m=2}^{\infty} \frac{(\alpha+1)(\alpha+2)\dots(\alpha+2m-3)(\alpha+2m-2)}{(2m)!} \frac{1}{k^{2m}} \right), \end{aligned}$$

which implies that  $w_{k,j} < 0$  for  $k = 1, 2, \dots, j-1$ ,  $j = 2, 3, \dots, n$ . Thus, noting that  $\Gamma(2-\alpha)w_{0,j} = 1$ , we have

$$d_{j-k} = -\frac{\bar{w}_{k,j}}{\bar{w}_{0,j}} = -\frac{w_{k,j}}{w_{0,j}} > 0, \quad k = 1, 2, \dots, j-1, \quad j = 2, 3, \dots, n.$$

For  $k = j$ ,  $j = 2, 3, \dots, n$ , we have

$$\begin{aligned} \Gamma(2-\alpha)w_{j,j} &= -(\alpha-1)j^{-\alpha} + (j-1)^{1-\alpha} - j^{1-\alpha} \\ &= j^{1-\alpha} \left[ -(\alpha-1)\frac{1}{j} - 1 \right. \\ &\quad \left. + \left( 1 + (1-\alpha)\left(-\frac{1}{j}\right) + \frac{(1-\alpha)(-\alpha)}{2!}\left(-\frac{1}{j}\right)^2 + \frac{(1-\alpha)(-\alpha)(-\alpha-1)}{3!}\left(-\frac{1}{j}\right)^3 + \dots \right) \right] \\ &= (1-\alpha)(-\alpha)j^{1-\alpha} \left( \frac{1}{2j^2} + \sum_{m=3}^{\infty} \frac{(\alpha+1)(\alpha+2)\dots(\alpha+m-2)}{(m)!} \frac{1}{j^m} \right), \end{aligned}$$

which implies that  $w_{j,j} < 0$ ,  $j = 2, 3, \dots, n$ . Hence

$$d_0 = -\frac{\bar{w}_{j,j}}{\bar{w}_{0,j}} = -\frac{w_{j,j}}{w_{0,j}} + \frac{j^{-\alpha}}{\Gamma(1-\alpha)w_{0,j}} > 0, \quad j = 2, 3, \dots, n.$$

Finally we estimate (20). Note that, with  $j = 1, 2, \dots, n$ ,

$$d_0 = -\frac{\bar{w}_{j,j}}{\bar{w}_{0,j}} = -\frac{w_{j,j}}{w_{0,j}} + \frac{j^{-\alpha}}{\Gamma(1-\alpha)w_{0,j}} > \frac{j^{-\alpha}}{\Gamma(1-\alpha)w_{0,j}}.$$

Hence

$$d_0^{-1} \leq \Gamma(1-\alpha)w_{0,j}j^\alpha = \Gamma(1-\alpha)w_{0,j}t_j^\alpha \Delta t^{-\alpha} < c_0 \Delta t^{-\alpha},$$

for some constant  $c_0$ .

Together these estimates complete the proof of Lemma 2.3. ■

**Proof of Theorem 2.2:** Let  $e_j = x_j - x(t_j)$ ,  $j = 0, 1, \dots, n$ . Subtracting (16) from (17), we have

$$e_j - (\bar{w}_{0,j})^{-1}(\Delta t^\alpha \beta) e_j = \sum_{k=1}^j d_{j-k} e_{j-k} + (\bar{w}_{0,j})^{-1} \Delta t^\alpha R_1^j, \quad j = 1, 2, \dots, n, \quad (21)$$

where  $e_0 = 0$  and  $d_{j-k} = -\bar{w}_{k,j}/\bar{w}_{0,j}$ ,  $k = 1, 2, \dots, j$ .

Multiplying  $e_j$  in both sides of (21), we have, denoting  $(u, v) = u \cdot v$ ,  $\forall u, v \in \mathbb{R}$ , with  $j = 1, 2, \dots, n$ ,

$$(e_j, e_j) - (\bar{w}_{0,j})^{-1}(\Delta t^\alpha \beta)(e_j, e_j) = \sum_{k=1}^j d_{j-k}(e_{j-k}, e_j) + (\bar{w}_{0,j})^{-1} \Delta t^\alpha R_1^j(e_j).$$

Denote the norm, noting that  $\beta < 0$ ,

$$|e_j|_1^2 = (e_j, e_j) - (\bar{w}_{0,j})^{-1}(\Delta t^\alpha \beta)(e_j, e_j), \quad j \geq 1.$$

We have, by (19),

$$|e_j|_1^2 \leq \sum_{k=1}^j d_{j-k} |e_{j-k}| |e_j| + |(\bar{w}_{0,j})^{-1} \Delta t^\alpha R_1^j| |e_j|, \quad j = 1, 2, \dots, n.$$

Note that  $|e_j| \leq |e_j|_1$ , we have

$$|e_j|_1 \leq \sum_{k=1}^j d_{j-k} |e_{j-k}|_1 + d_0 |d_0^{-1} (\bar{w}_{0,j})^{-1} \Delta t^\alpha R_1^j|, \quad j = 1, 2, \dots, n. \quad (22)$$

We will use the mathematical induction to show that, with  $k = 1, 2, \dots, j$ ,  $j = 1, 2, \dots, n$ ,

$$|e_1|_1 \leq d_0 \max_{1 \leq l \leq j} |d_0^{-1} (\bar{w}_{0,j})^{-1} \Delta t^\alpha R_1^l|, \quad (23)$$

$$|e_k|_1 \leq \left(1 - d_{j-1} - \dots - d_{j-(k-1)}\right)^{-1} \left(d_0 \max_{1 \leq l \leq j} |d_0^{-1} (\bar{w}_{0,j})^{-1} \Delta t^\alpha R_1^l|\right), \quad (24)$$

It is easy to see (23) holds. In fact, we have, by (21), with  $j = 1$ ,

$$|e_1|_1 \leq |(\bar{w}_{0,1})^{-1} \Delta t^\alpha R_1^1| \leq d_0 \max_{1 \leq l \leq j} |d_0^{-1} (\bar{w}_{0,j})^{-1} \Delta t^\alpha R_1^l|.$$

Let  $j \geq 2$  and assume that (23) and (24) hold true for  $k = 1, 2, \dots, j-1$ , then for  $k = j$ , we have, by (22),

$$\begin{aligned} |e_j|_1 &\leq d_{j-1} (1 - d_{j-1} - \dots - d_2)^{-1} \left(d_0 \max_{1 \leq l \leq j} |d_0^{-1} (\bar{w}_{0,j})^{-1} \Delta t^\alpha R_1^l|\right) \\ &\quad + d_{j-2} (1 - d_{j-1} - \dots - d_3)^{-1} \left(d_0 \max_{1 \leq l \leq j} |d_0^{-1} (\bar{w}_{0,j})^{-1} \Delta t^\alpha R_1^l|\right) \\ &\quad + \dots \\ &\quad + d_2 (1 - d_{j-1})^{-1} \left(d_0 \max_{1 \leq l \leq j} |d_0^{-1} (\bar{w}_{0,j})^{-1} \Delta t^\alpha R_1^l|\right) \\ &\quad + d_1 (1)^{-1} \left(d_0 \max_{1 \leq l \leq j} |d_0^{-1} (\bar{w}_{0,j})^{-1} \Delta t^\alpha R_1^l|\right) \\ &\quad + (1 - d_{j-1} - \dots - d_1) (1 - d_{j-1} - \dots - d_1)^{-1} \left(d_0 \max_{1 \leq l \leq j} |d_0^{-1} (\bar{w}_{0,j})^{-1} \Delta t^\alpha R_1^l|\right). \end{aligned}$$

Thus, by (19),

$$|e_j|_1 \leq (1 - d_{j-1} - \dots - d_1)^{-1} \left(d_0 \max_{1 \leq l \leq j} |d_0^{-1} (\bar{w}_{0,j})^{-1} \Delta t^\alpha R_1^l|\right),$$

which is (24). By (18) and (20), we obtain, with  $j = 2, 3, \dots, n$ ,

$$\begin{aligned} |e_j|_1 &\leq \frac{d_0}{1 - d_{j-1} - \dots - d_1} \max_{1 \leq l \leq j} |d_0^{-1} (\bar{w}_{0,j})^{-1} \Delta t^\alpha R_1^l| \\ &\leq \max_{1 \leq l \leq j} |d_0^{-1} (\bar{w}_{0,j})^{-1} \Delta t^\alpha R_1^l| \leq \max_{1 \leq l \leq j} |R_1^l| \leq C \Delta t^{2-\alpha}. \end{aligned}$$

Together these estimates complete the proof of Theorem 2.2. ■

### 3. Quadratic interpolation polynomial

In this section, we will approximate the Hadamard finite-part integral in (10) by using piecewise quadratic interpolation polynomial. Let  $n = 2M$ , where  $M$  denotes a fixed positive integer. Let  $0 = t_0 < t_1 < t_2 < \dots < t_{2j} < t_{2j+1} < \dots < t_{2M} = 1$  be a partition of  $[0, 1]$  and  $\Delta t$  the step size. At the point  $t_{2j} = \frac{2j}{2M}$ , the equation (8) can be written as

$${}^R D_t^\alpha [x(t_{2j}) - x^0] = \beta x(t_{2j}) + f(t_{2j}), \quad j = 1, 2, \dots, M, \quad (25)$$

and at the point  $t_{2j+1} = \frac{2j+1}{2M}$ , the equation (8) can be written as

$${}_0^R D_t^\alpha [x(t_{2j+1}) - x^0] = \beta x(t_{2j+1}) + f(t_{2j+1}), \quad j = 1, 2, \dots, M-1. \quad (26)$$

Let us first consider the discretization of (25). Note that

$${}_0^R D_t^\alpha x(t_{2j}) = \frac{1}{\Gamma(-\alpha)} \oint_0^{t_{2j}} (t_{2j} - \tau)^{-1-\alpha} x(\tau) d\tau = \frac{t_{2j}^{-\alpha}}{\Gamma(-\alpha)} \oint_0^1 w^{-1-\alpha} x(t_{2j} - t_{2j}w) dw, \quad (27)$$

where the integral must be interpreted as a Hadamard finite-part integral.

We replace the integral by a piecewise quadratic interpolation polynomial with the equispaced nodes  $0, \frac{1}{2j}, \frac{2}{2j}, \dots, \frac{2j}{2j}$ ,  $j = 1, 2, \dots, M$ . We then have, for some smooth function  $g(w)$ ,

$$\oint_0^1 w^{-1-\alpha} g(w) dw = \oint_0^1 w^{-1-\alpha} g_2(w) dw + E_{2j}(g), \quad (28)$$

where  $g_2(w)$  is the piecewise quadratic interpolation polynomial of  $g(w)$  and  $E_{2j}(g)$  is the remainder term.

We have, [37]

**Lemma 3.1.** *Let  $0 < \alpha < 1$ . Assume that  $g \in C^3[0, 1]$ . Then, with  $j = 1, 2, \dots, M$ ,*

$$\oint_0^1 w^{-1-\alpha} g(w) dw = \sum_{k=0}^{2j} \alpha_{k,2j} g\left(\frac{k}{2j}\right) + R_{2j}(g), \quad (29)$$

where

$$(-\alpha)(-\alpha+1)(-\alpha+2)(2j)^{-\alpha} \alpha_{l,2j} = \begin{cases} 2^{-\alpha}(\alpha+2), & \text{for } l=0, \\ (-\alpha)2^{2-\alpha}, & \text{for } l=1, \\ (-\alpha)(-2^{-\alpha}\alpha) + \frac{1}{2}F_0(2), & \text{for } l=2, \\ -F_1(k), & \text{for } l=2k-1, \quad k=2,3,\dots,j, \\ \frac{1}{2}(F_2(k) + F_0(k+1)), & \text{for } l=2k, \quad k=2,3,\dots,j-1, \\ \frac{1}{2}F_2(j), & \text{for } l=2j, \end{cases}$$

where

$$\begin{aligned} F_0(k) &= (2k-1)(2k) \left( (2k)^{-\alpha} - (2(k-1))^{-\alpha} \right) (-\alpha+1)(-\alpha+2) \\ &\quad - \left( (2k-1) + 2k \right) \left( (2k)^{-\alpha+1} - (2(k-1))^{-\alpha+1} \right) (-\alpha)(-\alpha+2) \\ &\quad + \left( (2k)^{-\alpha+2} - (2(k-1))^{-\alpha+2} \right) (-\alpha)(-\alpha+1), \end{aligned} \quad (30)$$

$$\begin{aligned} F_1(k) &= (2k-2)(2k) \left( (2k)^{-\alpha} - (2k-2)^{-\alpha} \right) (-\alpha+1)(-\alpha+2) \\ &\quad - \left( (2k-2) + 2k \right) \left( (2k)^{-\alpha+1} - (2k-2)^{-\alpha+1} \right) (-\alpha)(-\alpha+2) \\ &\quad + \left( (2k)^{-\alpha+2} - (2k-2)^{-\alpha+2} \right) (-\alpha)(-\alpha+1), \end{aligned} \quad (31)$$

and

$$\begin{aligned} F_2(k) &= (2k-2)(2k-1) \left( (2k)^{-\alpha} - (2k-2)^{-\alpha} \right) (-\alpha+1)(-\alpha+2) \\ &\quad - \left( (2k-2) + (2k-1) \right) \left( (2k)^{-\alpha+1} - (2k-2)^{-\alpha+1} \right) (-\alpha)(-\alpha+2) \\ &\quad + \left( (2k)^{-\alpha+2} - (2k-2)^{-\alpha+2} \right) (-\alpha)(-\alpha+1). \end{aligned} \quad (32)$$

Next we consider the discretization of (26). At the points  $t_{2j+1} = \frac{2j+1}{2m}$ ,  $j = 1, 2, \dots, M-1$  we have

$$\begin{aligned} {}_0^R D_t^\alpha x(t_{2j+1}) &= \frac{1}{\Gamma(-\alpha)} \oint_0^{t_{2j+1}} (t_{2j+1} - \tau)^{-1-\alpha} x(\tau) d\tau \\ &= \frac{1}{\Gamma(-\alpha)} \int_0^{t_1} (t_{2j+1} - \tau)^{-1-\alpha} x(\tau) d\tau \\ &\quad + \frac{t_{2j+1}^{-\alpha}}{\Gamma(-\alpha)} \oint_0^{\frac{2j}{2j+1}} w^{-1-\alpha} x(t_{2j+1} - t_{2j+1}w) dw. \end{aligned}$$

**Remark 3.1.** Here we divided the integral  $\oint_0^{t_{2j+1}}$  into  $\int_0^{t_1}$  and  $\oint_0^{\frac{2j}{2j+1}}$ . Similarly one may divide the integral  $\oint_0^{t_{2j+1}}$  into  $\int_0^{t_{2j}}$  and  $\oint_{t_{2j}}^{t_{2j+1}}$  and obtain the similar weights.

**Remark 3.2.** In the expression of  ${}_0^R D_t^\alpha x(t_{2j+1})$  above, the first integral  $\int_0^{t_1} (t_{2j+1} - \tau)^{-1-\alpha} x(\tau) d\tau$ ,  $j \geq 1$  is the standard integral since the integrand has no singularity points on  $[0, t_1]$ . But the second integral  $\oint_0^{\frac{2j}{2j+1}} w^{-1-\alpha} x(t_{2j+1} - t_{2j+1}w) dw$  is the Hadamard finite-part integral since  $w^{-1-\alpha}$  has the strong singularity at  $w = 0$ .

We replace the integral by a piecewise quadratic interpolation polynomial with the equispaced nodes  $0, \frac{1}{2j+1}, \frac{2}{2j+1}, \dots, \frac{2j}{2j+1}$ ,  $j = 1, 2, \dots, M-1$ . More precisely, we have, for some smooth function  $g(w)$ ,

$$\oint_0^{\frac{2j}{2j+1}} w^{-1-\alpha} g(w) dw = \oint_0^{\frac{2j}{2j+1}} w^{-1-\alpha} g_2(w) dw + E_{2j+1}(g), \quad (33)$$

where  $g_2(w)$  is the piecewise quadratic interpolation polynomial of  $g(w)$  with the nodes  $0, \frac{1}{2j+1}, \frac{2}{2j+1}, \dots, \frac{2j}{2j+1}$ ,  $j = 1, 2, \dots, M-1$  and  $E_{2j+1}(g)$  is the remainder term.

We have, [37]

**Lemma 3.2.** Let  $0 < \alpha < 1$ . Assume that  $g \in C^3[0, 1]$ . Then

$$\oint_0^{\frac{2j}{2j+1}} w^{-1-\alpha} g(w) dw = \sum_{k=0}^{2j} \alpha_{k,2j+1} g\left(\frac{k}{2j}\right) + R_{2j+1}(g), \quad (34)$$

where  $\alpha_{k,2j+1} = \alpha_{k,2j}$ ,  $k = 1, 2, 3, \dots, 2j$ ,  $j = 1, 2, \dots, M-1$  and  $\alpha_{k,2j}$  are given in Lemma 3.1.

By using (27)-(29), we obtain the following approximation of the Riemann-Liouville fractional derivative  ${}_0^R D_t^\alpha x(t)$  at  $t = t_{2j}$ ,  $j = 1, 2, \dots, M$

$${}_0^R D_t^\alpha x(t_{2j}) = \Delta t^{-\alpha} \sum_{k=0}^{2j} w_{k,2j} x(t_{2j-k}) + R_2^{2j}, \quad (35)$$

where  $R_2^{2j} = C \Delta t^{3-\alpha} (\max_{0 \leq s \leq 1} |x'''(s)|) = O(\Delta t^{3-\alpha})$  [37] and the weights  $w_{k,2j}$ ,  $k = 0, 1, 2, \dots, 2j$ ,  $j = 1, 2, \dots, M$  satisfy

$$\Gamma(3-\alpha) w_{k,2j} = (-\alpha)(-\alpha+1)(-\alpha+2)(2j)^{-\alpha} \alpha_{k,2j}, \quad k = 0, 1, 2, \dots, 2j. \quad (36)$$

Similarly, we have at  $t = t_{2j+1}$ ,  $j = 1, 2, \dots, M-1$ ,

$${}_0^R D_t^\alpha x(t_{2j+1}) = \frac{1}{\Gamma(-\alpha)} \int_0^{t_1} (t_{2j+1} - s)^{-\alpha-1} x(s) ds + \Delta t^{-\alpha} \sum_{k=0}^{2j} w_{k,2j+1} x(t_{2j+1-k}) + R_2^{2j+1},$$

where  $w_{k,2j+1} = w_{k,2j}$ ,  $k = 0, 1, 2, \dots, 2j$  and  $R_2^{2j+1} = O(\Delta t^{3-\alpha})$ .

For the Caputo fractional derivative  ${}^C_0 D_t^\alpha x(t)$  at  $t = t_{2j}$ ,  $j = 1, 2, \dots, M$ , we have, noting that  ${}^R_0 D_t^\alpha x(0) = x(0) {}^R_0 D_t^\alpha (1) = \frac{x(0)}{\Gamma(1-\alpha)} t^{-\alpha}$ ,

$${}^C_0 D_t^\alpha x(t_{2j}) = {}^R_0 D_t^\alpha (x(t_{2j}) - x(0)) = \Delta t^{-\alpha} \sum_{k=0}^{2j} \bar{w}_{k,2j} x(t_{2j-k}) + R_2^{2j},$$

where the weights, with  $k = 0, 1, 2, \dots, 2j - 1$ ,  $j = 1, 2, \dots, M$ ,

$$\bar{w}_{k,2j} = w_{k,2j}, \quad \bar{w}_{2j,2j} = w_{2j,2j} - \frac{(2j)^{-\alpha}}{\Gamma(1-\alpha)}. \quad (37)$$

Similarly, we have at  $t = t_{2j+1}$ ,  $j = 1, 2, \dots, M-1$

$${}^C_0 D_t^\alpha x(t_{2j+1}) = \frac{1}{\Gamma(-\alpha)} \int_0^{t_1} (t_{2j+1} - s)^{-\alpha-1} x(s) ds + \Delta t^{-\alpha} \sum_{k=0}^{2j+1} \bar{w}_{k,2j+1} x(t_{2j+1-k}) + R_2^{2j+1},$$

where, with  $k = 0, 1, 2, \dots, 2j$ ,  $j = 1, 2, \dots, M-1$ ,

$$\bar{w}_{k,2j+1} = w_{k,2j}, \quad \bar{w}_{2j+1,2j+1} = -\frac{(2j+1)^{-\alpha}}{\Gamma(1-\alpha)}. \quad (38)$$

The exact solution of (1)- (2) then satisfies, with  $l = 2, 3, \dots, 2M$ ,

$$\bar{w}_{0,l} x(t_l) - \Delta t^\alpha \beta x(t_l) = I_l - \sum_{k=1}^l \bar{w}_{k,l} x(t_{l-k}) + \Delta t^\alpha f(t_l) - \Delta t^\alpha R_2^l,$$

or

$$x(t_l) - (\bar{w}_{0,l})^{-1} (\Delta t^\alpha \beta) x(t_l) = (\bar{w}_{0,l})^{-1} I_l + \sum_{k=1}^l d_{k,l} x(t_{l-k}) + (\bar{w}_{0,l})^{-1} \Delta t^\alpha f(t_l) - (\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^l, \quad (39)$$

where  $d_{k,l} = -\bar{w}_{k,l}/\bar{w}_{0,l}$ ,  $k = 1, 2, \dots, l$ ,  $l = 2, 3, \dots, 2M$ , where  $I_l$  is defined by

$$I_l = \begin{cases} 0, & l = 2j, j = 1, 2, \dots, M, \\ -\frac{1}{\Gamma(-\alpha)} \int_0^{t_1} (t_{2j+1} - s)^{-\alpha-1} x(s) ds, & l = 2j + 1, j = 1, 2, \dots, M-1, \end{cases}$$

Let  $x_l \approx x(t_l)$ ,  $l = 0, 1, 2, \dots, 2M$  denote the approximate solution of  $x(t_l)$ . We define the following numerical method to approximate the exact solutions in (39), with  $l = 2, 3, \dots, 2M$ ,

$$x_l - (\bar{w}_{0,l})^{-1} (\Delta t^\alpha \beta) x_l = (\bar{w}_{0,l})^{-1} \tilde{I}_l + \sum_{k=1}^l d_{k,l} x_{l-k} + (\bar{w}_{0,l})^{-1} \Delta t^\alpha f(t_l). \quad (40)$$

where  $\tilde{I}_l$  is some approximation of  $I_l$  discussed below in (42). Here we assume that  $x_0 = x^0$  and  $x_1$  will be approximated below in (41).

To approximate  $x(t_1)$  with the required accuracy  $O(\Delta t^{3-\alpha})$  which will be the convergence order of our numerical method (40), we divide the interval  $[0, t_1]$  by the equispaced nodes  $0 = t_1^{(0)} < t_1^{(1)} < \dots < t_1^{(n_1)} = t_1$  with step size  $\tilde{\Delta t}$  such that  $\tilde{\Delta t}^{2-\alpha} \approx \Delta t^{3-\alpha}$ , where  $n_1$  is some positive integer. We then apply the numerical method with the convergence order  $O(\Delta t_1^{2-\alpha})$  in [6] to get the approximate value  $x_1 \approx x(t_1)$  such that

$$|x_1 - x(t_1)| = O(\tilde{\Delta t}^{2-\alpha}) = O(\Delta t^{3-\alpha}). \quad (41)$$

**Remark 3.3.** The computation of the approximate solution at the first grid point  $x_1$  is analogy to a classical technique for multistep methods for first-order differential equations where the starting values are also computed via a lower order (one-step or multistep with a smaller number of steps) method with a sufficiently small step size.

We also need to approximate the integral  $I_l$  in (39) with the required accuracy  $O(\Delta t^3)$  which we shall use in (43). Let  $n_2$  be some positive integer, we divide the interval  $[0, t_1]$  by the equispaced nodes  $0 = t_1^{(0)} < t_1^{(1)} < \dots < t_1^{(n_2)} = t_1$  with step size  $\overline{\Delta t}$  such that  $\overline{\Delta t}^2 \approx \Delta t^{4+\alpha}$ . We then apply the composite trapezoidal quadrature rule on  $[0, t_1]$  which has the convergence order  $O(\overline{\Delta t}^2)$ . More precisely, we have, noting that  $(t_{2j+1} - s)^{-\alpha-1} \leq (t_3 - t_1)^{-\alpha-1} = (2\Delta t)^{-\alpha-1}, j = 1, 2, \dots, M-1$ ,

$$\begin{aligned} |I_l - \tilde{I}_l| &= \left| \frac{1}{\Gamma(-\alpha)} \int_0^{t_1} (t_{2j+1} - s)^{-\alpha-1} x(s) ds - \frac{1}{\Gamma(-\alpha)} \int_0^{t_1} (t_{2j+1} - s)^{-\alpha-1} \tilde{x}(s) ds \right| \\ &= (\Delta t)^{-\alpha-1} O(\overline{\Delta t}^2) = O(\Delta t^3), \quad l = 2j + 1, j = 1, 2, \dots, M-1, \end{aligned} \quad (42)$$

where  $\tilde{x}(s)$  is the piecewise linear interpolation polynomial of  $x(s)$  on  $[0, t_1]$ , which implies that  $I_l - \tilde{I}_l = O(\Delta t^3)$ . We need this approximation below in (43).

Let  $e_l = x_l - x(t_l), l = 0, 1, \dots, 2M$ . Subtracting (39) from (40), we have, by (42),

$$e_l - (\bar{w}_{0,l})^{-1} (\Delta t^\alpha \beta) e_l = \sum_{k=1}^l d_{k,l} e_{l-k} + (\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^l, \quad l = 2, 3, \dots, 2M, \quad (43)$$

where  $e_0 = 0$  and  $e_1$  is approximated in (41) and  $d_{k,l} = -\bar{w}_{k,l}/\bar{w}_{0,l}, k = 1, 2, \dots, l, l = 2, 3, \dots, 2M$  are defined as in (37) and (38).

Denote

$$\bar{e}_l = e_l - \eta e_{l-1}, \quad \eta = \frac{d_{1,l}}{2}, \quad l = 1, 2, 3, \dots, 2M.$$

We have, with  $l = 2, 3, \dots, 2M$ ,

$$\begin{aligned} \bar{e}_l - (\bar{w}_{0,l})^{-1} (\Delta t^\alpha \beta) e_l &= e_l - \eta e_{l-1} - (\bar{w}_{0,l})^{-1} (\Delta t^\alpha \beta) e_l \\ &= \sum_{k=1}^{l-1} d_{k,l} e_{l-k} + (\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^l - \eta e_{l-1} \\ &= \eta (e_{l-1} - \eta e_{l-2}) + (\eta^2 + d_{2,l}) e_{l-2} + d_{3,l} e_{l-3} + \dots + d_{l-1,l} e_1 + d_{l,l} e_0 + (\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^l \\ &= \eta (e_{l-1} - \eta e_{l-2}) + (\eta^2 + d_{2,l}) (e_{l-2} - \eta e_{l-3}) \\ &\quad + (\eta^3 + d_{2,l} \eta + d_{3,l}) e_{l-3} + d_{4,l} e_{l-4} + \dots + d_{l-1,l} e_1 + d_{l,l} e_0 + (\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^l \\ &= \dots \\ &= \eta (e_{l-1} - \eta e_{l-2}) + (\eta^2 + d_{2,l}) (e_{l-2} - \eta e_{l-3}) \\ &\quad + (\eta^3 + d_{2,l} \eta + d_{3,l}) (e_{l-3} - \eta e_{l-4}) \\ &\quad + \dots \\ &\quad + (\eta^{l-2} + d_{2,l} \eta^{l-4} + \dots + d_{l-3,l} \eta + d_{l-2,l}) (e_2 - \eta e_1) \\ &\quad + (\eta^{l-1} + d_{2,l} \eta^{l-3} + \dots + d_{l-2,l} \eta + d_{l-1,l}) (e_1 - \eta e_0) \\ &\quad + (\eta^l + d_{2,l} \eta^{l-2} + \dots + d_{l-1,l} \eta + d_{l,l}) e_0 + (\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^l. \end{aligned}$$

Denote

$$\bar{d}_{i,l} := \eta^i + \sum_{j=2}^i \eta^{i-j} d_{j,l}, \quad i = 2, 3, \dots, l, \quad l = 2, 3, \dots, 2M,$$

we have, with  $\bar{d}_{1,l} = \eta$ ,

$$\bar{e}_l - (\bar{w}_{0,l})^{-1}(\Delta t^\alpha \beta) e_l = \sum_{k=1}^{l-1} \bar{d}_{k,l} \bar{e}_{l-k} + (\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^l, \quad l = 2, 3, \dots, 2M. \quad (44)$$

**Lemma 3.3.** For  $0 < \alpha < 1$ , the coefficients in (44) satisfy, with  $l = 2, 3, \dots, 2M$ ,

$$0 < \eta = \frac{d_{1,l}}{2} < \frac{2}{3}, \quad (45)$$

$$\bar{d}_{k,l} > 0, \quad k = 1, 2, \dots, l, \quad (46)$$

$$\eta + \sum_{k=2}^l \bar{d}_{k,l} \leq 1, \quad (47)$$

$$\bar{d}_{l,l}^{-1} \leq c_0 \Delta t^{-\alpha}, \quad \text{for some constant } c_0. \quad (48)$$

**Proof:** We only consider the case with  $l = 2j, j = 1, 2, \dots, M$ . Similarly we may consider the case  $l = 2j + 1, j = 1, 2, \dots, M - 1$

We first estimate (45). By (67), we have

$$0 < \eta = \frac{d_{1,l}}{2} < \frac{2}{3}.$$

The estimate (46) follows from

$$\bar{d}_{1,l} = \eta > 0,$$

and, by (70),

$$\bar{d}_{2,l} = \eta^2 + d_{2,l} = \frac{1}{4}(d_{1,l})^2 + d_{2,l} > 0,$$

and, by (69)

$$\bar{d}_{k,l} = \bar{d}_{k-1,l} \eta + d_{l-k} > 0, \quad k = 3, 4, \dots, l, \text{ for } l = 3, 4, \dots, 2M.$$

We next estimate (47). Let  $S_l = \eta + \sum_{k=2}^l \bar{d}_{k,l}$ , we have

$$\begin{aligned} S_l &= \eta(1 + \eta + \eta^2 + \dots + \eta^{l-1}) + d_{2,l}(1 + \eta + \eta^2 + \dots + \eta^{l-2}) \\ &\quad + \dots + d_{l-2,l}(1 + \eta + \eta^2) + d_{l-1,l}(1 + \eta) + d_{l,l} \\ &= \eta \frac{1 - \eta^l}{1 - \eta} + d_{2,l} \frac{1 - \eta^{l-1}}{1 - \eta} + \dots + d_{l-2,l} \frac{1 - \eta^3}{1 - \eta} + d_{l-1,l} \frac{1 - \eta^2}{1 - \eta} + d_{l,l}. \end{aligned}$$

i.e.

$$\begin{aligned} (1 - \eta)S_l &= \eta(1 - \eta^l) + d_{2,l}(1 - \eta^{l-1}) + d_{3,l} + \dots + d_{l-1,l} + d_{l,l} \\ &\quad - d_{3,l}\eta^{l-2} - \dots - d_{l-2,l}\eta^3 - d_{l-1,l}\eta^2 - d_{l,l}\eta. \end{aligned}$$

By (70) and (71), we have

$$\begin{aligned} (1 - \eta)S_l &\leq \eta(1 - \eta^l) + d_{2,l}(1 - \eta^{l-1}) + d_{3,l} + \dots + d_{l-1,l} + d_{l,l} \\ &= (\eta + d_{2,l} + d_{3,l} + \dots + d_{l-1,l} + d_{l,l}) - \eta^{l-1}(\eta^2 + d_{2,l}) \\ &\leq (1 - \eta) - \eta^{l-1}(\eta^2 + d_{2,l}) \\ &= (1 - \eta) - \eta^{l-1}(\frac{1}{4}(d_{1,l})^2 + d_{2,l}) < (1 - \eta), \end{aligned}$$

which implies (47).

Finally we estimate (48). For  $l = 2j$ ,  $j = 1, 2, \dots, M$ , we have

$$d_{l,l} = -\frac{\bar{w}_{l,l}}{\bar{w}_{0,l}} = -\frac{w_{l,l}}{\bar{w}_{0,l}} + \frac{l^{-\alpha}}{\Gamma(1-\alpha)\bar{w}_{0,l}} > \frac{t_l^{-\alpha}}{\Gamma(1-\alpha)\bar{w}_{0,l}} \Delta t^\alpha,$$

which implies that  $d_{l,l}^{-1} < c_0 \Delta t^{-\alpha}$  for some positive constant  $c_0$ . Thus, by (70)

$$\bar{d}_{l,l} = \eta^l + \sum_{j=2}^l \eta^{l-j} d_{j,l} = \eta^{l-2}(\eta^2 + d_{2,l}) + d_{3,l}\eta^{l-3} + \dots + d_{l-1,l}\eta + d_{l,l} > d_{l,l}, \quad (49)$$

which implies that  $\bar{d}_{l,l}^{-1} < d_{l,l}^{-1} < c_0 \Delta t^{-\alpha}$  for some constant  $c_0$ .

For  $l = 2j + 1$ ,  $j = 1, 2, \dots, M - 1$ , we have

$$d_{l,l} = -\frac{\bar{w}_{l,l}}{\bar{w}_{0,l}} = \frac{l^{-\alpha}}{\Gamma(1-\alpha)\bar{w}_{0,l}} = \frac{t_l^{-\alpha}}{\Gamma(1-\alpha)\bar{w}_{0,l}} \Delta t^\alpha,$$

which implies that  $d_{l,l}^{-1} < c_0 \Delta t^{-\alpha}$  for some positive constant  $c_0$ . Thus (49) also holds in this case and  $\bar{d}_{l,l}^{-1} < d_{l,l}^{-1} < c_0 \Delta t^{-\alpha}$  for some constant  $c_0$ . The proof of Lemma 3.3 is now complete. ■

We are now in the position to prove the following error estimates.

**Theorem 3.4.** *Let  $x(t)$  and  $x_l, l = 0, 1, \dots, 2M$  be the exact solution and the approximate solution of (39) and (40), respectively. Assume that  $x \in C^3[0, 1]$ . Further assume that  $x_0 = x^0$  and there exists a constant  $C$  such that*

$$|x_1 - x(t_1)| \leq C \Delta t^{3-\alpha}. \quad (50)$$

Then there exists a constant  $C = C(\alpha, f, \beta)$  such that

$$|x_l - x(t_l)| \leq C \Delta t^{3-\alpha}, \quad l = 2, 3, \dots, 2M.$$

**Proof:**

Multiplying  $2\bar{e}_l$  in both sides of (44), we have, denoting  $(u, v) = u \cdot v, \forall u, v \in \mathbb{R}$ , with  $l = 2, 3, \dots, 2M$ ,

$$(\bar{e}_l, 2\bar{e}_l) - (\bar{w}_{0,l})^{-1}(\Delta t^\alpha \beta)(e_l, 2\bar{e}_l) = \sum_{k=1}^{l-1} \bar{d}_{k,l}(\bar{e}_{l-k}, 2\bar{e}_l) + ((\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^l, 2\bar{e}_l), \quad (51)$$

Note that

$$2(e_l, \bar{e}_l) = (e_l, e_l) + (\bar{e}_l, \bar{e}_l) - \eta^2(e_{l-1}, e_{l-1}), \text{ for } l = 1, 2, \dots, 2M.$$

We have, with  $l = 2, 3, \dots, 2M$ ,

$$\begin{aligned} & 2|\bar{e}_l|^2 - (\bar{w}_{0,l})^{-1}(\Delta t^\alpha \beta)(e_l, e_l) - (\bar{w}_{0,l})^{-1}(\Delta t^\alpha \beta)(\bar{e}_l, \bar{e}_l) + (\bar{w}_{0,l})^{-1}(\Delta t^\alpha \beta)\eta^2(e_{l-1}, e_{l-1}) \\ &= \sum_{k=1}^{l-1} \bar{d}_{k,l}(\bar{e}_{l-k}, 2\bar{e}_l) + ((\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^l, 2\bar{e}_l). \end{aligned}$$

We write, with  $l = 2, 3, \dots, 2M$ ,

$$((\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^l, 2\bar{e}_l) = \bar{d}_{l,l}(\bar{d}_{l,l}^{-1}(\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^l, 2\bar{e}_l).$$

By Cauchy-Schwarz inequality, we have, with  $l = 2, 3, \dots, 2M$ ,

$$\begin{aligned}
& 2|\bar{e}_l|^2 - (\bar{w}_{0,l})^{-1}(\Delta t^\alpha \beta)|e_l|^2 - (\bar{w}_{0,l})^{-1}(\Delta t^\alpha \beta)|\bar{e}_l|^2 + (\bar{w}_{0,l})^{-1}(\Delta t^\alpha \beta)\eta^2|e_{l-1}|^2 \\
& \leq \sum_{k=1}^{l-1} \bar{d}_{k,l}(|\bar{e}_{l-k}|^2 + |\bar{e}_l|^2) + \bar{d}_{l,l}(|\bar{d}_{l,l}^{-1}(\bar{w}_{0,l})^{-1}\Delta t^\alpha R_2^l|^2 + |\bar{e}_l|^2). \\
& = \sum_{k=1}^{l-1} \bar{d}_{k,l}|\bar{e}_{l-k}|^2 + \bar{d}_{l,l}|\bar{d}_{l,l}^{-1}(\bar{w}_{0,l})^{-1}\Delta t^\alpha R_2^l|^2 + \sum_{k=1}^l \bar{d}_{k,l}|\bar{e}_l|^2.
\end{aligned}$$

By (47) and noting that  $\bar{d}_{1,l} = \eta$  and  $\beta < 0$ , we have

$$\begin{aligned}
|\bar{e}_l|^2 - (\bar{w}_{0,l})^{-1}(\Delta t^\alpha \beta)|e_l|^2 & \leq \bar{d}_{1,l}|\bar{e}_{l-1}|^2 - (\bar{w}_{0,l})^{-1}(\Delta t^\alpha \beta)\eta^2|e_{l-1}|^2 + \bar{d}_{2,l}|\bar{e}_{l-2}|^2 \\
& \quad + \dots + \bar{d}_{l-1,l}|\bar{e}_1|^2 + \bar{d}_{l,l}|\bar{d}_{l,l}^{-1}(\bar{w}_{0,l})^{-1}\Delta t^\alpha R_2^l|^2.
\end{aligned}$$

By (45), we have, noting that  $\beta < 0$  and  $\bar{d}_{1,l} = \eta$ ,

$$\begin{aligned}
& |\bar{e}_l|^2 - (\bar{w}_{0,l})^{-1}(\Delta t^\alpha \beta)|e_l|^2 \\
& \leq \bar{d}_{1,l}(|\bar{e}_{l-1}|^2 - (\bar{w}_{0,l})^{-1}(\Delta t^\alpha \beta)\eta|e_{l-1}|^2) \\
& \quad + \bar{d}_{2,l}|\bar{e}_{l-2}|^2 + \dots + \bar{d}_{l-1,l}|\bar{e}_1|^2 + \bar{d}_{l,l}|\bar{d}_{l,l}^{-1}(\bar{w}_{0,l})^{-1}\Delta t^\alpha R_2^l|^2. \\
& \leq \bar{d}_{1,l}(|\bar{e}_{l-1}|^2 - (\bar{w}_{0,l})^{-1}(\Delta t^\alpha \beta)|e_{l-1}|^2) \\
& \quad + \bar{d}_{2,l}(|\bar{e}_{l-2}|^2 - (\bar{w}_{0,l})^{-1}(\Delta t^\alpha \beta)|e_{l-2}|^2) \\
& \quad + \dots + \bar{d}_{l-1,l}(|\bar{e}_1|^2 - (\bar{w}_{0,l})^{-1}(\Delta t^\alpha \beta)|e_1|^2) + \bar{d}_{l,l}|\bar{d}_{l,l}^{-1}(\bar{w}_{0,l})^{-1}\Delta t^\alpha R_2^l|^2.
\end{aligned}$$

Denote the norm, with  $l = 1, 2, \dots, 2M$ ,

$$|\bar{e}_l|_1^2 = |\bar{e}_l|^2 - (\bar{w}_{0,l})^{-1}(\Delta t^\alpha \beta)|e_l|^2.$$

We then have, with  $l = 2, 3, \dots, 2M$ ,

$$|\bar{e}_l|_1^2 \leq \bar{d}_{1,l}|\bar{e}_{l-1}|_1^2 + \bar{d}_{2,l}|\bar{e}_{l-2}|_1^2 + \dots + \bar{d}_{l-1,l}|\bar{e}_1|_1^2 + \bar{d}_{l,l}|\bar{d}_{l,l}^{-1}(\bar{w}_{0,l})^{-1}\Delta t^\alpha R_2^l|^2.$$

For  $l = 2, 3, \dots, 2M$ , we first show that

$$|\bar{e}_1|_1^2 \leq \bar{d}_{l,l} \max_{2 \leq s \leq l} |\bar{d}_{l,l}^{-1}(\bar{w}_{0,l})^{-1}\Delta t^\alpha R_2^s|^2. \quad (52)$$

In fact, noting that  $\bar{w}_{0,l} = \frac{1}{\Gamma(3-\alpha)}2^{-\alpha}(\alpha+2)$ ,  $l = 2, 3, \dots, 2M$  which is a constant independent on  $l = 2, 3, \dots, 2M$ , we have, by (50), with  $\bar{e}_1 = e_1 - \eta e_0 = e_1$ ,

$$(\bar{e}_1, 2\bar{e}_1) - (\bar{w}_{0,l})^{-1}(\Delta t^\alpha \beta)(e_1, 2e_1) = (e_1, 2e_1) - (\bar{w}_{0,l})^{-1}(\Delta t^\alpha \beta)(e_1, 2e_1) = O(\Delta t^{3-\alpha}). \quad (53)$$

Note that  $\bar{d}_{l,l} < 1$  by (47), we have, by (48) and (50),

$$|\bar{e}_1|_1^2 = O(\Delta t^{3-\alpha}) \leq \bar{d}_{l,l} \max_{2 \leq s \leq l} |\bar{d}_{l,l}^{-1}(\bar{w}_{0,l})^{-1}\Delta t^\alpha R_2^s|^2,$$

which is (52).

We next prove the following by the mathematical induction, with  $k = 2, 3, \dots, l$ ,  $l = 2, 3, \dots, 2M$ ,

$$|\bar{e}_k|_1^2 \leq \left(1 - \bar{d}_{1,l} - \dots - \bar{d}_{k-1,l}\right)^{-1} \left(\bar{d}_{l,l} \max_{2 \leq s \leq l} |\bar{d}_{l,l}^{-1}(\bar{w}_{0,l})^{-1}\Delta t^\alpha R_2^s|^2\right). \quad (54)$$

Assume that (54) holds true for  $k = 1, 2, \dots, l-1$ ,  $l = 2, 3, \dots, 2M$ , we have, for  $k = l$ , by (46),

$$\begin{aligned}
|\bar{e}_l|_1^2 &\leq \bar{d}_{1,l}(1 - \bar{d}_{1,l} - \dots - \bar{d}_{l-2,l})^{-1} \left( \bar{d}_{l,l} \max_{2 \leq s \leq l} |\bar{d}_{l,l}^{-1}(\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^s|^2 \right) \\
&\quad + \bar{d}_{2,l}(1 - \bar{d}_{1,l} - \dots - \bar{d}_{l-3,l})^{-1} \left( \bar{d}_{l,l} \max_{2 \leq s \leq l} |\bar{d}_{l,l}^{-1}(\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^s|^2 \right) \\
&\quad + \dots \\
&\quad + \bar{d}_{l-2,l}(1 - \bar{d}_{1,l})^{-1} \left( \bar{d}_{l,l} \max_{2 \leq s \leq l} |\bar{d}_{l,l}^{-1}(\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^s|^2 \right) \\
&\quad + \bar{d}_{l-1,l}(1)^{-1} \left( \bar{d}_{l,l} \max_{2 \leq s \leq l} |\bar{d}_{l,l}^{-1}(\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^s|^2 \right) \\
&\quad + (1 - \bar{d}_{1,l} - \dots - \bar{d}_{l-1,l})(1 - \bar{d}_{1,l} - \dots - \bar{d}_{l-1,l})^{-1} \left( \bar{d}_{l,l} \max_{2 \leq s \leq l} |\bar{d}_{l,l}^{-1}(\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^s|^2 \right) \\
&\leq (1 - \bar{d}_{1,l} - \dots - \bar{d}_{l-1,l})^{-1} \left( \bar{d}_{l,l} \max_{2 \leq s \leq l} |\bar{d}_{l,l}^{-1}(\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^s|^2 \right).
\end{aligned}$$

By (46), we have, with  $l = 2, 3, \dots, 2M$ ,

$$|\bar{e}_l|_1^2 \leq (1 - \bar{d}_{1,l} - \dots - \bar{d}_{l-1,l})^{-1} \left( \bar{d}_{l,l} \max_{2 \leq s \leq l} |\bar{d}_{l,l}^{-1}(\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^s|^2 \right),$$

which is (54).

By (47), we have, with  $l = 2, 3, \dots, 2M$ ,

$$\begin{aligned}
|\bar{e}_l|_1^2 &\leq \frac{\bar{d}_{l,l}}{1 - \bar{d}_{1,l} - \dots - \bar{d}_{l-1,l}} \max_{2 \leq s \leq l} |\bar{d}_{l,l}^{-1}(\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^s|^2 \\
&\leq \max_{2 \leq s \leq l} |\bar{d}_{l,l}^{-1}(\bar{w}_{0,l})^{-1} \Delta t^\alpha R_2^s|^2 \leq C \max_{2 \leq s \leq l} |R_2^s|^2 \leq C(\Delta t^{3-\alpha})^2,
\end{aligned}$$

which implies that

$$|\bar{e}_l|_1 \leq C\Delta t^{3-\alpha}, \quad l = 2, 3, \dots, 2M.$$

Further we have, by (45), with  $l = 2, 3, \dots, 2M$ ,

$$\begin{aligned}
|e_l| &= |\bar{e}_l + \eta e_{l-1}| \leq |\bar{e}_l| + |\eta e_{l-1}| \leq C\Delta t^{3-\alpha} + |\eta e_{l-1}| \\
&\leq C\Delta t^{3-\alpha} + \eta(C\Delta t^{3-\alpha} + \eta e_{l-2}) \leq (1 + \eta)C\Delta t^{3-\alpha} + \eta^2 |e_{l-2}| \\
&\leq \dots \\
&\leq (1 + \eta + \eta^2 + \dots + \eta^l)C\Delta t^{3-\alpha} \leq \frac{1}{1 - \eta} C\Delta t^{3-\alpha} \leq C\Delta t^{3-\alpha}
\end{aligned} \tag{55}$$

The proof of Theorem 3.4 is now complete. ■

#### 4. Numerical simulations

In this section, we will consider two examples.

**Example 4.1.** *Consider*

$${}_0^C D_t^\alpha x(t) = \beta x(t) + f(t), \quad t \in [0, 1], \tag{56}$$

$$x(0) = x^0, \tag{57}$$

where  $x^0 = 0$ ,  $0 < \alpha < 1$ ,  $\beta = -1$  and  $f(t) = \frac{\Gamma(4+\gamma)}{\Gamma(4+\gamma-\alpha)}t^{3+\gamma-\alpha} - \beta t^{3+\gamma}$ ,  $\gamma > 0$ . The exact solution is  $x(t) = t^{3+\gamma}$ .

The main purpose is to check the order of convergence of the numerical method with respect to the fractional order  $\alpha$ . For various choices of  $\alpha \in (0, 1)$ , we computed the errors at  $t = 1$ . We choose the step size  $h = 1/(5 \times 2^l)$ ,  $l = 1, 2, \dots, 7$ , i.e, we divided the interval  $[0, 1]$  into  $n = 1/h$  small intervals with nodes  $0 = t_0 < t_1 < \dots < t_n = 1$ . Then we compute the error  $e(t_n) = |x(t_n) - x_n|$ . By Theorem 3.4, we have

$$|e(t_n)| = |x(t_n) - x_n| \leq Ch^{3-\alpha}, \quad (58)$$

To observe the order of convergence we shall compute the error  $|e(t_n)|$  at  $t_n = 1$  for the different values of  $h$ . Denote  $|e_h(t_n)|$  the error at  $t_n = 1$  for the step size  $h$ . Let  $h_l = h = 1/(5 \times 2^l)$  for a fixed  $l = 1, 2, \dots, 7$ . We then have

$$\frac{|e_{h_l}(t_n)|}{|e_{h_{l+1}}(t_n)|} \approx \frac{Ch_l^{3-\alpha}}{Ch_{l+1}^{3-\alpha}} = 2^{3-\alpha},$$

which implies that the order of convergence satisfies  $3 - \alpha \approx \log_2 \left( \frac{|e_{h_l}(t_n)|}{|e_{h_{l+1}}(t_n)|} \right)$ . In Table 1, we compute the orders of convergence for the different values of  $\alpha$ . The numerical results are consistent with the theoretical results.

$n$	ERC ( $\alpha = 0.5$ )	ERC ( $\alpha = 0.75$ )	ERC ( $\alpha = 0.25$ )
10			
20	2.6676	2.4010	2.9229
40	2.6038	2.3313	2.8701
80	2.5664	2.2947	2.8395
160	2.5435	2.2748	2.8199
320	2.5291	2.2639	2.8064
640	2.5198	2.2578	2.7963

Table 1: Results at  $t = 1$  for  $\beta = -1$  and  $\gamma = 0.6$

In Figure 1, we will plot the order of the convergence for  $\alpha = 0.25$ . We have from (58)

$$\log_2(|e(t_n)|) \leq \log_2(C) + (3 - \alpha)\log_2(h).$$

Let  $y = \log_2(|e(t_n)|)$  and  $x = \log_2(h)$ . In Figure 1, we plot the function  $y = y(x)$  for the different values of  $x = \log_2(h)$  where  $h = 1/(5 \times 2^l)$ ,  $l = 1, 2, \dots, 7$ . To observe the order of convergence, we also plot the straight line  $y = (3 - \alpha)x$ . We see that these two lines are almost parallel which means that the order of convergence of the numerical method indeed is  $O(h^{3-\alpha})$ .

**Example 4.2.** Consider

$${}_0^C D_t^\alpha x(t) = \beta x(t) + f(t), \quad t \in [0, 1], \quad (59)$$

$$x(0) = x^0, \quad (60)$$

where  $x^0 = 0$ ,  $0 < \alpha < 1$ ,  $\beta = -1$  and  $f(t) = (t^2 + 2t^{2-\alpha}/\Gamma(3 - \alpha)) + (t^3 + 3t^{3-\alpha}/\Gamma(4 - \alpha))$ . The exact solution is  $x(t) = t^2 + t^3$ .

We use the same notation as in Example 4.1.

For various choices of  $\alpha \in (0, 1)$ , we computed the errors at  $t = 1$ . We choose the step size  $h = 1/(5 \times 2^l)$ ,  $l = 1, 2, \dots, 7$ , i.e, we divided the interval  $[0, 1]$  into  $n = 1/h$  small intervals with nodes  $0 = t_0 < t_1 < \dots < t_n = 1$ . Then we compute the error  $e(t_n) = |x(t_n) - x_n|$ . In Table 2, we compute the orders of convergence for the different values of  $\alpha$ . The numerical results are consistent with the theoretical results.

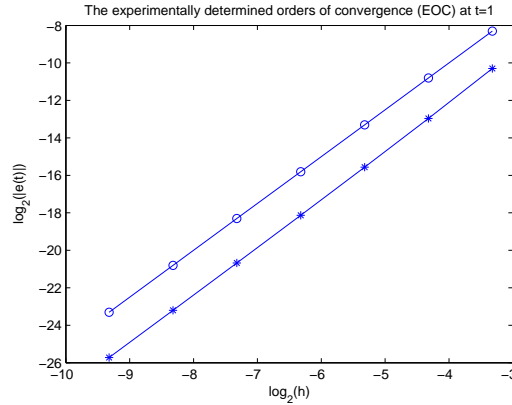


Figure 1: The experimentally determined orders of convergence (“EOC ”) at  $t = 1$  in Example 4.1

$n$	ERC ( $\alpha = 0.5$ )	ERC ( $\alpha = 0.75$ )	ERC ( $\alpha = 0.25$ )
10			
20	1.8035	1.7855	3.1098
40	2.2424	2.0737	1.5696
80	2.3758	2.1694	2.3199
160	2.4324	2.2102	2.5172
320	2.4604	2.2296	2.6017
640	2.4756	2.2393	2.6467

Table 2: Results at  $t = 1$  for  $\beta = -1$   
and  $f(t) = (t^2 + 2t(2 - \alpha)/\Gamma(3 - \alpha)) + (t^3 + 3!t^{3-\alpha}/\Gamma(4 - \alpha))$

Let  $y = \log_2(|e(t_n)|)$  and  $x = \log_2(h)$ . In Figure 2, we consider  $\alpha = 0.75$  and we plot the function  $y = y(x)$  for the different values of  $x = \log_2(h)$  where  $h = 1/(5 \times 2^l)$ ,  $l = 1, 2, \dots, 7$ . To observe the order of convergence, we also plot the straight line  $y = (3 - \alpha)x$ . We see that these two lines are almost parallel which means that the order of convergence of the numerical method indeed is  $O(h^{3-\alpha})$ .

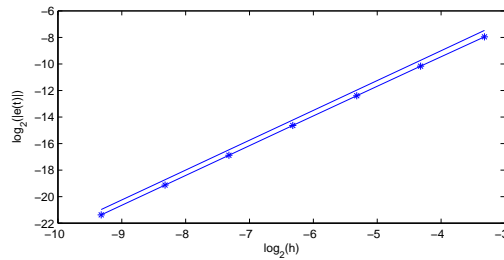


Figure 2: The experimentally determined orders of convergence (“EOC ”) at  $t = 1$  in Example 4.2

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## 5. Appendix

In this Appendix, we will give two lemmas.

**Lemma 5.1.** *Let  $0 < \alpha < 1$ . Let  $M$  be a positive integer defined before and let  $w_{k,2j}, k = 0, 1, 2, \dots, 2j, j = 1, 2, \dots, M$  be defined as in (35), we have*

$$\frac{\alpha^2 2^{-\alpha}}{\Gamma(3-\alpha)} + \frac{5-6\ln 2}{4^\alpha \Gamma(-\alpha)} < w_{2,2j} < \frac{\alpha^2 2^{-\alpha}}{\Gamma(3-\alpha)} + \frac{-4+10\ln 2}{4^\alpha \Gamma(-\alpha)}, \quad (61)$$

$$w_{2l-1,2j} < 0, \quad w_{2l,2j} < 0, \quad l = 1, 2, \dots, j. \quad (62)$$

**Proof:** We first show (61). The case  $j = 1$  is trivial. We only consider the case for  $j = 2, 3, \dots, M$ . We have, by (30),

$$F_0(k) = -(-\alpha+2)(2k)^{-\alpha+1} + 2(2k)^{-\alpha+2} - 2(-\alpha+1)(-\alpha+2)(2k-2)^{-\alpha} \\ - 3(-\alpha+2)(2k-2)^{-\alpha+1} - 2(2k-2)^{-\alpha+2}, \quad k = 2, 3, \dots, j.$$

Denote

$$I(m) = -(-\alpha+2)(m)^{-\alpha+1} + 2(m)^{-\alpha+2} - 2(-\alpha+1)(-\alpha+2)(m-2)^{-\alpha} \\ - 3(-\alpha+2)(m-2)^{-\alpha+1} - 2(m-2)^{-\alpha+2}.$$

We see that  $F_0(k) = I(m)$  with  $m = 2k, k = 2, 3, \dots, j$ . We now estimate  $I(m)$ . After some tedious but direct calculation, we have

$$I(m) = m^{-\alpha+2} \left( -(-\alpha+2) \frac{1}{m} + 2 - 2(-\alpha+1)(-\alpha+2) \left(1 - \frac{2}{m}\right)^{-\alpha} \frac{1}{m^2} \right. \\ \left. - 3(-\alpha+2) \left(1 - \frac{2}{m}\right)^{-\alpha+1} \frac{1}{m} - 2 \left(1 - \frac{2}{m}\right)^{-\alpha+2} \right) \\ = m^{-\alpha+2} \left[ -(-\alpha+2) \frac{1}{m} + 2 - 2(-\alpha+1)(-\alpha+2) \frac{1}{m^2} \left(1 + (-\alpha) \left(-\frac{2}{m}\right) + \frac{(-\alpha)(-\alpha-1)}{2!} \left(-\frac{2}{m}\right)^2 \right. \right. \\ \left. \left. + \frac{(-\alpha)(-\alpha-1)(-\alpha-2)}{3!} \left(-\frac{2}{m}\right)^3 + \dots \right) - 3(-\alpha+2) \frac{1}{m} \left(1 + (-\alpha+1) \left(-\frac{2}{m}\right) + \frac{(-\alpha+1)(-\alpha)}{2!} \left(-\frac{2}{m}\right)^2 \right. \right. \\ \left. \left. + \frac{(-\alpha+1)(-\alpha)(-\alpha-1)}{3!} \left(-\frac{2}{m}\right)^3 + \dots \right) - 2 \left(1 + (-\alpha+2) \left(-\frac{2}{m}\right) + \frac{(-\alpha+2)(-\alpha+1)}{2!} \left(-\frac{2}{m}\right)^2 \right. \right. \\ \left. \left. + \frac{(-\alpha+2)(-\alpha+1)(-\alpha)}{3!} \left(-\frac{2}{m}\right)^3 + \frac{(-\alpha+2)(-\alpha+1)(-\alpha)(-\alpha-1)}{4!} \left(-\frac{2}{m}\right)^4 + \dots \right) \right] \\ = \frac{(-\alpha+2)(-\alpha+1)(-\alpha)}{m^{\alpha+1}} \sum_{k=1}^{\infty} \frac{k^2 \cdot 2^{k+1}}{(k+2)!} \frac{(\alpha+1)(\alpha+2) \dots (\alpha+k-1)}{m^{k-1}},$$

which implies that  $I(m) < 0$  and therefore

$$F_0(k) < 0, \quad k = 2, 3, \dots, j, \quad j = 2, 3, \dots, M. \quad (63)$$

In particular, for  $k = 2$ , we have

$$\frac{5 - 6 \ln 2}{4^\alpha \Gamma(-\alpha)} < \frac{\frac{1}{2} F_0(2)}{\Gamma(3 - \alpha)} < \frac{-4 + 10 \ln 2}{4^\alpha \Gamma(-\alpha)},$$

which implies that, noting that  $w_{2,2j} = \frac{\alpha^2 2^{-\alpha}}{\Gamma(3-\alpha)} + \frac{\frac{1}{2} F_0(2)}{\Gamma(3-\alpha)}$ ,  $j = 2, 3, \dots, M$ ,

$$\frac{\alpha^2 2^{-\alpha}}{\Gamma(3 - \alpha)} + \frac{5 - 6 \ln 2}{4^\alpha \Gamma(-\alpha)} < w_{2,2j} < \frac{\alpha^2 2^{-\alpha}}{\Gamma(3 - \alpha)} + \frac{-4 + 10 \ln 2}{4^\alpha \Gamma(-\alpha)},$$

which is (61).

We next prove (62). For the weights  $w_{2l-1,2j}$ ,  $l = 2, 3, \dots, j$ , we have, by (31),

$$\Gamma(3 - \alpha) w_{2l-1,2j} = 2 \left( (2l - 2)^{-\alpha+2} - (2l)^{-\alpha+2} \right) + 2(-\alpha + 2) \left( (2l - 2)^{-\alpha+1} + (2l)^{-\alpha+1} \right).$$

Denote

$$I(m) = \left( (m - 2)^{-\alpha+2} - (m)^{-\alpha+2} \right) + (-\alpha + 2) \left( (m - 2)^{-\alpha+1} + (m)^{-\alpha+1} \right).$$

We see that  $\Gamma(3 - \alpha) w_{2l-1,2j} = 2I(m)$  with  $m = 2l$ . We now estimate  $I(m)$ . After some tedious but direct calculation, we have

$$\begin{aligned} I(m) &= m^{-\alpha+2} \left( -1 + (-\alpha + 2) \frac{1}{m} + \left( 1 - \frac{2}{m} \right)^{-\alpha+2} + (-\alpha + 2) \left( 1 - \frac{2}{m} \right)^{-\alpha+1} \frac{1}{m} \right) \\ &= m^{-\alpha+2} \left( \frac{(-\alpha + 2)(-\alpha + 1)(-\alpha)}{m^3} \left( -\frac{2^3}{3!} + \frac{2^2}{2!} \right) + \frac{(-\alpha + 2)(-\alpha + 1)(-\alpha)(-\alpha - 1)}{m^4} \left( \frac{2^4}{4!} - \frac{2^3}{3!} \right) \right. \\ &\quad + \frac{(-\alpha + 2)(-\alpha + 1)(-\alpha)(-\alpha - 1)(-\alpha - 2)}{m^5} \left( -\frac{2^5}{5!} + \frac{2^4}{4!} \right) + \dots \\ &\quad \left. + \frac{(-\alpha + 2)(-\alpha + 1) \dots (-\alpha - k + 3)}{m^k} \left( (-1)^k \frac{2^k}{k!} + (-1)^{k-1} \frac{2^{k-1}}{(k-1)!} \right) + \dots \right) \\ &= \frac{(-\alpha + 2)(-\alpha + 1)(-\alpha)}{m^{1+\alpha}} \left( \frac{2}{3} + \sum_{k=1}^{\infty} \frac{(\alpha + 1)(\alpha + 2) \dots (\alpha + k)}{m^k} \frac{k + 1}{(k + 3)!} 2^{k+2} \right), \end{aligned}$$

which implies that  $w_{2l-1,2j} < 0$ ,  $l = 1, 2, \dots, j$ ,  $j = 2, 3, \dots, M$ .

We now consider the weights  $w_{2l,2j}$ ,  $l = 1, 2, \dots, j - 1$ ,  $j = 2, 3, \dots, M$ . Here we only consider the case for  $l \geq 2$ . The case  $l = 1$  can be considered similarly.

we have, by (30) and (32),

$$\begin{aligned} \Gamma(3 - \alpha) w_{2l,2j} &= -3(-\alpha + 2)(2l)^{-\alpha+1} + \left( (2l + 2)^{-\alpha+2} - (2l - 2)^{-\alpha+2} \right) \\ &\quad - \frac{1}{2}(-\alpha + 2) \left( (2l + 2)^{-\alpha+1} + (2l - 2)^{-\alpha+1} \right) \end{aligned}$$

Denote

$$\begin{aligned} I(m) &= -3(-\alpha + 2)(m)^{-\alpha+1} - (m - 2)^{-\alpha+2} - \frac{1}{2}(-\alpha + 2)(m - 2)^{-\alpha+1} \\ &\quad + (m + 2)^{-\alpha+2} - \frac{1}{2}(-\alpha + 2)(m + 2)^{-\alpha+1} \end{aligned}$$

(64)

We see that  $\Gamma(3 - \alpha) w_{2l,2j} = I(m)$  with  $m = 2l$ ,  $l \geq 2$ . We now estimate  $I(m)$ . After some tedious but direct calculation, we have

$$\begin{aligned}
I(m) &= m^{-\alpha+2} \left( -3(-\alpha+2) \frac{1}{m} - \left(1 - \frac{2}{m}\right)^{-\alpha+2} - \frac{1}{2}(-\alpha+2) \left(1 - \frac{2}{m}\right)^{-\alpha+1} \frac{1}{m} \right. \\
&\quad \left. + \left(1 + \frac{2}{m}\right)^{-\alpha+2} - \frac{1}{2}(-\alpha+2) \left(1 + \frac{2}{m}\right)^{-\alpha+1} \frac{1}{m} \right) \\
&= m^{-\alpha+2} \left( \frac{(-\alpha+2)(-\alpha+1)(-\alpha)}{m^3} \left( \frac{2^3 \cdot 2}{3!} - \frac{2^2}{2!} \right) \right. \\
&\quad + \frac{(-\alpha+2)(-\alpha+1)(-\alpha)(-\alpha-1)(-\alpha-2)}{m^5} \left( \frac{2^5 \cdot 2}{5!} - \frac{2^4}{4!} \right) \\
&\quad \left. + \frac{(-\alpha+2)(-\alpha+1)(-\alpha)(-\alpha-1)(-\alpha-2)(-\alpha-3)(-\alpha-4)}{m^7} \left( \frac{2^7 \cdot 2}{7!} - \frac{2^6}{6!} \right) + \dots \right) \\
&= \frac{(-\alpha+2)(-\alpha+1)(-\alpha)}{m^{1+\alpha}} \left( \frac{2}{3} - \sum_{k=1}^{\infty} \frac{(\alpha+1)(\alpha+2) \dots (\alpha+2k)}{m^{2k}(2k+1)!} \frac{2k-1}{(2k+2)(2k+3)} 2^{2k+2} \right)
\end{aligned}$$

Note that, with  $m \geq 4$ ,

$$\begin{aligned}
&\sum_{k=1}^{\infty} \frac{(\alpha+1)(\alpha+2) \dots (\alpha+2k)}{m^{2k}(2k+1)!} \frac{2k-1}{(2k+2)(2k+3)} 2^{2k+2} \\
&\leq \sum_{k=1}^{\infty} \frac{(1+1)(\alpha+2) \dots (1+2k)}{m^{2k}(2k+1)!} \frac{2k-1}{(2k+2)(2k+3)} 2^{2k+2} \leq \sum_{k=1}^{\infty} \left(\frac{2}{m}\right)^{2k} \frac{4(2k-1)}{(2k+2)(2k+3)} \\
&\leq \sum_{k=1}^{\infty} \left(\frac{2}{m}\right)^{2k} \cdot 1 = \frac{\left(\frac{2}{m}\right)^2}{1 - \left(\frac{2}{m}\right)^2} = \frac{4}{m^2 - 4} \leq \frac{4}{4^2 - 4} = \frac{1}{3} < \frac{2}{3}.
\end{aligned} \tag{65}$$

We have  $I(m) < 0$  for  $m \geq 4$  which implies that  $w_{2l,2j} < 0$ ,  $l = 2, 3, \dots, j-1$ .

Finally for the weights  $w_{2j,2j}$ ,  $j = 1, 2, \dots, M$ , we have

$$\begin{aligned}
\Gamma(3-\alpha)w_{2j,2j} &= F_2(j) = 2(-\alpha+1)(-\alpha+2)(2j)^{-\alpha} - 3(-\alpha+2)(2j)^{-\alpha+1} + 2(2j)^{-\alpha+2} \\
&\quad - (-\alpha+2)(2j-2)^{-\alpha+1} - 2(2j-2)^{-\alpha+2}
\end{aligned}$$

Denote

$$\begin{aligned}
I(m) &= 2(-\alpha+1)(-\alpha+2)(m)^{-\alpha} - 3(-\alpha+2)(m)^{-\alpha+1} + 2(m)^{-\alpha+2} \\
&\quad - (-\alpha+2)(m-2)^{-\alpha+1} - 2(m-2)^{-\alpha+2}
\end{aligned} \tag{66}$$

We see that  $2\Gamma(3-\alpha)w_{2j,2j} = I(m)$  with  $m = 2j$ ,  $j = 1, 2, \dots, M$ . We now estimate  $I(m)$  for  $m \geq 4$ . Similarly we can consider the case for  $m = 2$ . After some tedious but direct calculation, we have

$$\begin{aligned}
I(m) &= m^{-\alpha+2} \left( 2(-\alpha+1)(-\alpha+2) \frac{1}{m^2} - 3(-\alpha+2) \frac{1}{m} + 2 \right. \\
&\quad \left. - (-\alpha+2) \left( 1 - \frac{2}{m} \right)^{-\alpha+1} \frac{1}{m} - 2 \left( 1 - \frac{2}{m} \right)^{-\alpha+2} \right) \\
&= m^{-\alpha+2} \left[ 2(-\alpha+1)(-\alpha+2) \frac{1}{m^2} - 3(-\alpha+2) \frac{1}{m} + 2 \right. \\
&\quad \left. - \left( -\alpha+2 \right) \frac{1}{m} \left( 1 + (-\alpha+1) \left( -\frac{2}{m} \right) + \frac{(-\alpha+1)(-\alpha)}{2!} \left( -\frac{2}{m} \right)^2 \right. \right. \\
&\quad \left. \left. + \frac{(-\alpha+1)(-\alpha)(-\alpha-1)}{3!} \left( -\frac{2}{m} \right)^3 + \dots \right) \right. \\
&\quad \left. - 2 \left( 1 + (-\alpha+2) \left( -\frac{2}{m} \right) + \frac{(-\alpha+2)(-\alpha+1)}{2!} \left( -\frac{2}{m} \right)^2 \right. \right. \\
&\quad \left. \left. + \frac{(-\alpha+2)(-\alpha+1)(-\alpha)}{3!} \left( -\frac{2}{m} \right)^3 + \dots \right) \right] \\
&= \frac{(-\alpha+2)(-\alpha+1)(-\alpha)}{m^{1+\alpha}} \left( \frac{2}{3} - \sum_{k=1}^{\infty} \frac{(\alpha+1)(\alpha+2) \dots (\alpha+k+1)}{m^{k+1}} \frac{k \cdot 2^{k+3}}{(k+4)!} \right)
\end{aligned}$$

Following the arguments in (65), we may show that, with  $m \geq 4$ ,

$$\sum_{k=1}^{\infty} \frac{(\alpha+1)(\alpha+2) \dots (\alpha+k+1)}{m^{k+1}} \frac{k \cdot 2^{k+3}}{(k+4)!} \leq \frac{2}{3}.$$

Thus we proved  $w_{2j,2j} < 0, j = 2, 3, \dots, M$ . The proof of Lemma 5.1 is complete. ■

**Lemma 5.2.** *Let  $0 < \alpha < 1$ , Let  $d_{k,l}, k = 1, 2, \dots, l, l = 2, 3, \dots, 2M$  be defined as in (43), we have*

$$0 < d_{1,l} < \frac{4}{3}, \tag{67}$$

$$-\frac{1}{3} < d_{2,l} < \frac{5}{2} - 3 \ln 2, \tag{68}$$

$$d_{k,l} > 0, \quad \text{for } k = 3, 4, \dots, l, \text{ with } l = 3, 4, \dots, 2M, \tag{69}$$

$$\frac{1}{4} (d_{1,l})^2 + d_{2,l} > 0, \tag{70}$$

$$\sum_{k=1}^l d_{k,l} \leq 1. \tag{71}$$

**Proof:** We only consider the case for  $l = 2j, j = 1, 2, \dots, M$ . We can consider the case for  $l = 2j+1, j = 1, 2, \dots, M-1$  similarly.

For (67), we have, with  $l = 2, 3, \dots, 2M$ ,

$$d_{1,l} = -\frac{\bar{w}_{1,l}}{\bar{w}_{0,l}} = -\frac{\Gamma(3-\alpha)\bar{w}_{1,l}}{\Gamma(3-\alpha)\bar{w}_{0,l}} = -\frac{(-\alpha)2^{2-\alpha}}{2^{-\alpha}(2+\alpha)} = \frac{4\alpha}{2+\alpha} = 4 - \frac{8}{2+\alpha},$$

which implies that  $0 < d_{1,l} < \frac{4}{3}$  since  $0 < \alpha < 1$ .

We now prove (68). The case  $l = 2$  or  $l = 3$  is trivial. Here we only consider the case for  $l = 4, 5, \dots, 2M$ . Note that  $\bar{w}_{0,l} = \frac{2^{-\alpha}(\alpha+2)}{\Gamma(3-\alpha)}$ . We have, by (61),

$$\frac{\alpha^2 2^{-\alpha}}{\Gamma(3-\alpha)} + \frac{5-6 \ln 2}{4^\alpha \Gamma(-\alpha)} < \bar{w}_{2,l} < \frac{\alpha^2 2^{-\alpha}}{\Gamma(3-\alpha)} + \frac{-4+10 \ln 2}{4^\alpha \Gamma(-\alpha)}, \text{ for } l = 4, 5, \dots, 2M.$$

Thus, noting that  $d_{2,l} = -\frac{\bar{w}_{2,l}}{\bar{w}_{0,l}}$ , with  $l = 4, 5, \dots, 2M$ ,

$$-\frac{\alpha^2}{\alpha+2} - \frac{(-4+10\ln 2)\Gamma(3-\alpha)}{4^\alpha\Gamma(-\alpha)(\alpha+2)} < d_{2,l} < -\frac{\alpha^2}{\alpha+2} - \frac{(5-6\ln 2)\Gamma(3-\alpha)}{4^\alpha\Gamma(-\alpha)(\alpha+2)},$$

or

$$-\frac{\alpha^2}{\alpha+2} + \frac{(-4+10\ln 2)(2-\alpha)(1-\alpha)\alpha}{2^\alpha(\alpha+2)} < d_{2,l} < -\frac{\alpha^2}{\alpha+2} + \frac{(5-6\ln 2)(2-\alpha)(1-\alpha)\alpha}{2^\alpha(\alpha+2)}.$$

Noting that, for  $0 < \alpha < 1$ ,

$$-\frac{1}{3} < -\frac{\alpha^2}{\alpha+2} < 0, \quad \frac{(-4+10\ln 2)(2-\alpha)(1-\alpha)\alpha}{2^\alpha(\alpha+2)} > 0, \quad \frac{(2-\alpha)(1-\alpha)\alpha}{2^\alpha(\alpha+2)} < \frac{1}{2},$$

we get

$$-\frac{1}{3} < d_{2,l} < \frac{5}{2} - 3\ln 2, \text{ for } l = 4, 5, \dots, 2M,$$

which is (68).

We now consider (69). The case for  $l = 3$  is trivial. We here only consider the case for  $l = 4, 5, \dots, 2M$ . By (62), we have, noting that  $\Gamma(3-\alpha)\bar{w}_{0,l} = 2^{-\alpha}(2+\alpha) > 0$ ,

$$d_{k,l} = -\frac{\bar{w}_{k,l}}{\bar{w}_{0,l}} = -\frac{\Gamma(3-\alpha)\bar{w}_{k,l}}{\Gamma(3-\alpha)\bar{w}_{0,l}} > 0, \quad \text{for } k = 3, 4, \dots, l, \quad l = 4, 5, \dots, 2M.$$

For (70), we have, by (63), with  $l = 2, 3, \dots, 2M$ ,

$$\begin{aligned} \frac{1}{4}(d_{1,l})^2 + d_{2,l} &= \frac{1}{4} \left( \frac{4\alpha}{2+\alpha} \right)^2 - \frac{\alpha^2}{2+\alpha} - \frac{\frac{1}{2}F_0(2)}{2^{-\alpha}(2+\alpha)} \\ &= \frac{4\alpha^3 + 7\alpha^2}{(2+\alpha)^2} + \left( -\frac{\frac{1}{2}F_0(2)}{2^{-\alpha}(2+\alpha)} \right) > 0. \end{aligned}$$

Finally we estimate (71). For  $l = 2j, j = 1, 2, \dots, M$ , we have

$${}_0^C D_t^\alpha(x(t_{2j})) = {}_0^R D_t^\alpha(x(t_{2j}) - x(0)) = \Delta t^{-\alpha} \sum_{k=0}^{2j} \bar{w}_{k,2j} x(t_{2j-k}) + C \Delta t^{3-\alpha} \left( \max_{0 \leq s \leq 1} |f'''(s)| \right).$$

Let  $x(t) = 1$ , we get

$$\Delta t^{-\alpha} \sum_{k=0}^{2j} \bar{w}_{k,2j} = 0,$$

which implies that

$$\bar{w}_{0,2j} + \bar{w}_{1,2j} + \dots + \bar{w}_{2j,2j} = 0,$$

or

$$d_{1,2j} + d_{2,2j} + \dots + d_{2j-1,2j} + d_{2j,2j} = 1.$$

Similarly in the case  $l = 2j+1, j = 1, 2, \dots, M-1$ , we have, by (37) and (38),

$$\begin{aligned} &\bar{w}_{0,2j+1} + \bar{w}_{1,2j+1} + \dots + \bar{w}_{2j+1,2j+1} \\ &= \bar{w}_{0,2j} + \bar{w}_{1,2j} + \dots + \bar{w}_{2j,2j} + \left( \frac{(2j)^{-\alpha}}{\Gamma(1-\alpha)} - \frac{(2j+1)^{-\alpha}}{\Gamma(1-\alpha)} \right) \\ &\geq \bar{w}_{0,2j} + \bar{w}_{1,2j} + \dots + \bar{w}_{2j,2j} = 0, \end{aligned}$$

which implies that, with  $l = 2j+1, j = 1, 2, \dots, M-1$ ,

$$d_{1,l} + d_{2,l} + \dots + d_{l-1,l} + d_{l,l} < 1.$$

Together these estimates complete the proof of Lemma 5.2. ■