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Research article

A high order numerical method for solving Caputo nonlinear fractional ordinary differential equations

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Abstract: In this paper, we construct a high order numerical scheme for Caputo nonlinear fractional ordinary differential equations. Firstly, we use the piecewise Quadratic Lagrange interpolation method to construct a high order numerical scheme for Caputo nonlinear fractional ordinary differential equations, and then analyze the local truncation error of the high order numerical scheme. Secondly, based on the local truncation error, the convergence order of $3-\theta$ order is obtained. And the convergence are strictly analyzed. Finally, the numerical simulation of the high order numerical scheme is carried out. Through the calculation of typical problems, the effectiveness of the numerical algorithm and the correctness of theoretical analysis are verified.

Keywords: nonlinear fractional ordinary differential equations; Caputo derivative; finite difference method; higher order numerical scheme; convergence analysis
Mathematics Subject Classification: 26A33, 65L12, 65M06, 65M12

1. Introduction

Fractional calculus is a branch of study that of any order integral or derivative. It is obtained by replacing the integer order of differential equations with the fractional order. Because fractional derivative has heredity or memory, the fractional differential equation is widely used in various fields. In the past few decades, fractional derivative has been studied by a large number of scholars. They firstly proved a $(3-\theta)$-order convergence and stability scheme for time-fractional derivative θ under the time step $k \geq 2$ in [1]. The similar $(3-\theta)$-order scheme to efficiently solve the time-fractional diffusion equation in time was first constructed in [2]. Based on the idea of block-by-block approach method, the reference [3] presented a general technique to construct high order schemes for the numerical solution of the fractional ordinary differential equations. The reference [4] established a fractional Gronwall inequality to prove some stability and convergence estimates of schemes for fractional reaction-subdiffusion problems. In [5], a space-time finite element method was used to solve the distributed-order time fractional reaction diffusion equations. The scheme with $(3-\theta)$ convergence order for time step $k \geq 2$ and $(2-\theta)$ convergence order for time step $k = 1$ was constructed for time-fractional derivative in [6]. They proved the $(2-\theta)$-order convergence and stability of the time scheme, where θ is the order of the time-fractional derivative in [7]. A series of high order numerical approximations to θ-Caputo derivatives $(0 < \theta < 2)$ and Riemann-Liouville derivatives were given in [8]. They investigated numerical solutions of coupled nonlinear time-fractional reaction-diffusion equations obtained by the Lie symmetry analysis in [9]. They built a robust finite difference scheme for a nonlinear Caputo fractional differential equation on an adaptive grid with first-order convergent result in [10]. Spectral methods was popularly used to solve fractional derivative in [11–13]. An implicit numerical method was constructed to solve the two-dimensional $\theta(1 < \theta < 2)$ time fractional diffusion-wave equation with the convergence order $3-\theta$ in [14]. They used the piecewise linear and quadratic Lagrange interpolation functions to construct a $(3-\theta)$-order numerical approximate method for the Caputo fractional derivative in [15]. In [16], a fast high order numerical method for nonlinear fractional-order differential equations with non-singular kernel was constructed. The numerical scheme for nonlinear fractional differential equations was constructed by the Galerkin finite element method in [17]. The reference [18] established a *hp*-version Chebyshev collocation method for nonlinear fractional differential equations. The Spectral collocation method for nonlinear Riemann-Liouville fractional differential equations was given in [19]. The above high order schemes are either implicit or low-order schemes are used in the first step or obtained by discretizing the equivalent form of the original equation. Therefore, we will give a high order numerical scheme with uniform convergence order in this paper using the direct numerical discretization of original equations based on the idea of [1–3].

This paper is arranged as follows: In Section 2 the higher order numerical scheme is proposed. And the local truncation error of the constructed higher order numerical scheme is given in Section 3. The convergence analysis is studied in Section 4. In Section 5 some numerical examples are given. Finally, some conclusion are given in Section 6.

2. A high order finite difference scheme for Caputo derivative

We consider the following initial value problem of nonlinear fractional ordinary differential equations

$$\begin{cases} {}_0D_t^{\theta}u(t) = f(t,u(t)), 0 \leq t \leq T, 0 < \theta < 1, & (2.1)\\ u(0) = u_0, & (2.2)\end{cases}$$

where θ is the order of the fractional derivative, ${}_0D_t^{\theta}u(t)$ in (2.1) is defined as the Caputo fractional derivatives of order θ given by

$${}_0D_t^{\theta}u(t) = \int_0^t \omega_{1-\theta}(t-\tau)u'(\tau)d\tau, \tag{2.3}$$

with $\omega_{1-\theta}$ is defined by $\omega_{1-\theta}(t) = \frac{1}{t^{\theta}\Gamma(1-\theta)}$, and $\Gamma(\cdot)$ denotes Gamma function [20].

First, the finite difference scheme is introduced to discretize the fractional derivative. Dividing the interval $[0,T]$ into K equal subintervals, set $t_k = k\Delta t, k = 0,1,\ldots,K$, with $\Delta t = \frac{T}{K}$, the numerical solution of (2.1) at t_k is u_k, and ${}_0D_t^{\theta}u(t_k) = {}_0D_t^{\theta}u_k$, $f_k = f(t_k,u_k)$.

Next, we start discretizing the fractional derivative (2.3). Firstly, the values of $u(t)$ on t_1 and t_2 are determined. Using Quadratic Lagrange interpolation, the approximation formula of $u(t)$ on the interval $[t_0, t_2]$ is

$$J_{[t_0,t_2]}u(t) = \varpi_{0,0}(t)u_0 + \varpi_{1,0}(t)u_1 + \varpi_{2,0}(t)u_2, \tag{2.4}$$

where $\varpi_{i,0}(t), i = 0, 1, 2$, are the Quadratic Lagrangian interpolation basis functions on point t_0, t_1 and t_2, are defined as following

$$\varpi_{0,0}(t) = \frac{(t-t_1)(t-t_2)}{2\Delta t^2},\ \varpi_{1,0}(t) = \frac{(t-t_0)(t-t_2)}{-\Delta t^2},\ \varpi_{2,0}(t) = \frac{(t-t_0)(t-t_1)}{2\Delta t^2}.$$

Let $\Delta u_k = u_k - u_{k-1}, \Delta u_0 = u_0, \forall k \geq 1$. when $k = 1, 2$, we use ${}_0D_t^\theta\left(J_{[t_0,t_2]}u\right)(t_1)$, ${}_0D_t^\theta\left(J_{[t_0,t_2]}u\right)(t_2)$ to approximate ${}_0D_t^\theta u(t_1)$, ${}_0D_t^\theta u(t_2)$, respectively, then we get

$$\begin{aligned}
{}_0D_t^\theta u(t_1) &= \int_0^{t_1} \omega_{1-\theta}(t_1-\tau)u'(\tau)d\tau \approx \int_0^{t_1} \omega_{1-\theta}(t_1-\tau)\left[J_{[t_0,t_2]}u(\tau)\right]' d\tau \\
&= \frac{1}{\Delta t^2}\int_0^{t_1} \omega_{1-\theta}(t_1-\tau)[(\tau - t_{\frac{1}{2}})\Delta u_2 - (\tau - t_{\frac{3}{2}})\Delta u_1]d\tau = B_1^1\Delta u_1 + B_1^2\Delta u_2 \doteq {}_0D_{\Delta t}^\theta u_1, \quad (2.5)\\
{}_0D_t^\theta u(t_2) &= \int_0^{t_2} \omega_{1-\theta}(t_2-\tau)u'(\tau)d\tau \approx \int_0^{t_2} \omega_{1-\theta}(t_2-\tau)\left[J_{[t_0,t_2]}u(\tau)\right]' d\tau \\
&= \frac{1}{\Delta t^2}\int_0^{t_2} \omega_{1-\theta}(t_2-\tau)[(\tau - t_{\frac{1}{2}})\Delta u_2 - (\tau - t_{\frac{3}{2}})\Delta u_1]d\tau = B_2^1\Delta u_1 + B_2^2\Delta u_2 \doteq {}_0D_{\Delta t}^\theta u_2, \quad (2.6)
\end{aligned}$$

where

$$B_j^1 = -\frac{1}{\Delta t^2}\int_0^{t_j} \omega_{1-\theta}(t_j-\tau)(\tau - t_{\frac{3}{2}})d\tau,\ \ B_j^2 = \frac{1}{\Delta t^2}\int_0^{t_j} \omega_{1-\theta}(t_j-\tau)(\tau - t_{\frac{1}{2}})d\tau, j = 1, 2. \tag{2.7}$$

When $k \geq 3$, we have

$$\begin{aligned}
{}_0D_t^\theta u(t_k) &= \int_0^{t_1} \omega_{1-\theta}(t_k-\tau)u'(\tau)d\tau + \sum_{j=1}^{k-1}\int_{t_j}^{t_{j+1}} \omega_{1-\theta}(t_k-\tau)u'(\tau)d\tau \\
&\approx \int_0^{t_1} \omega_{1-\theta}(t_k-\tau)\left[J_{[t_0,t_2]}u(\tau)\right]' d\tau + \sum_{j=1}^{k-1}\int_{t_j}^{t_{j+1}} \omega_{1-\theta}(t_k-\tau)\left[J_{[t_{j-1},t_{j+1}]}u(\tau)\right]' d\tau \\
&= \int_0^{t_1} \omega_{1-\theta}(t_k-\tau)\Big[\frac{2\tau - t_1 - t_2}{2\Delta t^2}u_0 + \frac{2\tau - t_0 - t_2}{-\Delta t^2}u_1 + \frac{2\tau - t_0 - t_1}{2\Delta t^2}u_2\Big]d\tau \\
&\quad + \sum_{j=1}^{k-1}\int_{t_j}^{t_{j+1}} \omega_{1-\theta}(t_k-\tau)\Big[\frac{2\tau - t_j - t_{j+1}}{2\Delta t^2}u_{j-1} + \frac{2\tau - t_{j-1} - t_{j+1}}{-\Delta t^2}u_j + \frac{2\tau - t_{j-1} - t_j}{2\Delta t^2}u_{j+1}\Big]d\tau \\
&= \frac{1}{\Delta t^2}\int_0^{t_1} \omega_{1-\theta}(t_k-\tau)[(\tau - t_{\frac{1}{2}})\Delta u_2 - (\tau - t_{\frac{3}{2}})\Delta u_1]d\tau \\
&\quad + \frac{1}{\Delta t^2}\sum_{j=1}^{k-1}\int_{t_j}^{t_{j+1}} \omega_{1-\theta}(t_k-\tau)[(\tau - t_{j-\frac{1}{2}})\Delta u_{j+1} - (\tau - t_{j+\frac{1}{2}})\Delta u_j]d\tau \\
&= -\frac{1}{\Delta t^2}\Big[\int_0^{t_2} \omega_{1-\theta}(t_k-\tau)(\tau - t_{\frac{3}{2}})d\tau\Big]\Delta u_1 + \frac{1}{\Delta t^2}\Big[\int_0^{t_2} \omega_{1-\theta}(t_k-\tau)(\tau - t_{\frac{1}{2}})d\tau\Big]\Delta u_2 \\
&\quad + \frac{1}{\Delta t^2}\sum_{j=2}^{k-1}\int_{t_j}^{t_{j+1}} \omega_{1-\theta}(t_k-\tau)[(\tau - t_{j-\frac{1}{2}})\Delta u_{j+1} - (\tau - t_{j+\frac{1}{2}})\Delta u_j]d\tau \doteq {}_0D_{\Delta t}^\theta u_k,
\end{aligned}$$

we can conclude that

$$ {}_0D^{\theta}_{\Delta t}u_k = A^k_{k-1}\Delta u_1 + A^k_{k-2}\Delta u_2 + \sum_{j=3}^{k-1} A^k_{k-j}\Delta u_j + A^k_0\Delta u_k, \quad 3 \le k \le K, \tag{2.8} $$

where

$$ \begin{aligned} A^k_0 &= \frac{1}{\Delta t^2}\int_{t_{k-1}}^{t_k} \omega_{1-\theta}(t_k-\tau)(\tau - t_{k-\frac{3}{2}})d\tau, \ \ A^k_{k-1} = -\frac{1}{\Delta t^2}\int_0^{t_2} \omega_{1-\theta}(t_k-\tau)(\tau - t_{\frac{3}{2}})d\tau, \\ A^k_{k-2} &= \frac{1}{\Delta t^2}\Big[\int_0^{t_2} \omega_{1-\theta}(t_k-\tau)(\tau - t_{\frac{1}{2}})d\tau - \int_{t_2}^{t_3} \omega_{1-\theta}(t_k-\tau)(\tau - t_{\frac{5}{2}})d\tau\Big], \\ A^k_{k-j} &= \frac{1}{\Delta t^2}\Big[\int_{t_{j-1}}^{t_j} \omega_{1-\theta}(t_k-\tau)(\tau - t_{j-\frac{3}{2}})d\tau - \int_{t_j}^{t_{j+1}} \omega_{1-\theta}(t_k-\tau)(\tau - t_{j+\frac{1}{2}})d\tau\Big], j = 3, \dots, k-1. \end{aligned} \tag{2.9} $$

According to approximations (2.5), (2.6) and (2.8), the higher order numerical scheme of Eq (2.1) corresponding to the initial value (2.2) is as follows

$$ {}_0D^{\theta}_{\Delta t}u_k = f_k, k = 1, 2, \dots, K. \tag{2.10} $$

Remark 2.1. *The numerical algorithm in this paper is different from [15]. In [15], in order to obtain* $(3-\theta)$*-order numerical scheme for the linear form of (2.1), they changed (2.1) into the following equation*

$$ \frac{1}{\Gamma(1-\theta)}\int_0^t \frac{u(s)}{(t-s)^{\theta}}ds = \frac{u(0)t^{1-\theta}}{\Gamma(1-\theta)(1-\theta)} + \int_0^t f(s)ds. \tag{2.11} $$

And using the linear Lagrange interpolation in $[t_0, t_1]$ *to* $u(s)$*, they obtain a* $(3-\theta)$*-order numerical scheme. In this paper, we use the Quadratic Lagrange interpolation in* $[t_0, t_2]$ *to* $u(s)$ *in (2.1) and directly obtain the* $(3-\theta)$*-order numerical scheme (2.5) and (2.6).*

Next, we will introduce a lemma to prove the sign of A^k_{k-j} and judge its size relation.

Lemma 2.1. $A^k_0 > 0$*, the sign of* A^k_1 *is uncertain,* $A^k_2 > A^k_3 > \dots > A^k_{k-1} > 0$.

Proof. Through calculation, we can get the following results

$$ A^k_0 = \frac{-1}{\Delta t^2\Gamma(2-\theta)}\int_{t_{k-1}}^{t_k}(\tau - t_{k-\frac{3}{2}})d(t_k-\tau)^{1-\theta} = \frac{1}{\Delta t^{\theta}\Gamma(3-\theta)}(2-\frac{\theta}{2}) > 0, \tag{2.12} $$

$$ \begin{aligned} A^k_1 &= \frac{1}{\Delta t^2}\Big[\int_{t_{k-2}}^{t_{k-1}} \omega_{1-\theta}(t_k-\tau)(\tau - t_{k-\frac{5}{2}})d\tau - \int_{t_{k-1}}^{t_k} \omega_{1-\theta}(t_k-\tau)(\tau - t_{k-\frac{1}{2}})d\tau\Big] \\ &= \frac{1}{\Delta t^{\theta}\Gamma(3-\theta)}[(6-\theta)2^{-\theta} - 4 + \theta] \doteq \frac{1}{\Delta t^{\theta}\Gamma(3-\theta)}M(\theta). \end{aligned} \tag{2.13} $$

The sign of A^k_1 is determined by the sign of $M(\theta)$, which satisfies

$$ M''(\theta) = 2^{-\theta}(\log 2)[2 + (6-\theta)\log 2] > 0, \ \ M'(1) = \frac{1}{2}(1 - 5\log 2) < 0. $$

Therefore $M(\theta)$ is a decrease function on $\theta \in (0,1)$. By $M(0) = 2 > 0$ and $M(1) = -\frac{1}{2} < 0$, we know that $M(\theta)$ has only one zero θ_0 in $(0,1)$, and $M(\theta) > 0$ if $\theta \in (0,\theta_0)$ and $M(\theta) < 0$ if $\theta \in (\theta_0, 1)$, which agrees with the conclusion of Lemma 2.1.

For $j = 3, \ldots, k-2$, we have

$$\begin{aligned} A_{k-j}^{k} \;=\; & \frac{1}{\Delta t^{\theta}\Gamma(3-\theta)}\Big\{\frac{1}{2}(2-\theta)[(k-j-1)^{1-\theta} - 2(k-j)^{1-\theta} \\ & +(k-j+1)^{1-\theta}] + (k-j-1)^{2-\theta} - 2(k-j)^{2-\theta} + (k-j+1)^{2-\theta}\Big\}, \end{aligned} \tag{2.14}$$

let $\bar{j} = k - j$, $\bar{j} \geq 2$, then using Taylor expansion, we can get the following results

$$A_{k-j}^{k} = \frac{1}{\Delta t^{\theta}\Gamma(2-\theta)}\bar{j}^{-\theta}\sum_{i=0}^{+\infty} a_i \bar{j}^{-i}, \tag{2.15}$$

where $a_i = \Pi_{n=0}^{i}(1-\theta-n)\frac{1}{(i+2)!}[(-1)^i(\frac{-i}{2}) + \frac{i+4}{2}]$. Next, we will prove $\bar{j}^{-\theta}\sum_{i=0}^{+\infty} a_i\bar{j}^{-i}$ is decrease function on $\bar{j}$. Because $\sum_{i=0}^{+\infty} a_i\bar{j}^{-i}$ is a convergence series, and the radius of convergence exists, it can exchange the derivative and the sum.

$$\Big(\bar{j}^{-\theta}\sum_{i=0}^{+\infty} a_i\bar{j}^{-i}\Big)' = -\bar{j}^{-\theta}\Big[\theta\bar{j}^{-1}\sum_{i=0}^{+\infty} a_i\bar{j}^{-i} + \sum_{i=1}^{+\infty} i a_i\bar{j}^{-i-1}\Big] = -\bar{j}^{-\theta}\Big[\theta\bar{j}^{-1}a_0 + (1+\theta)\bar{j}^{-2}a_1 + \sum_{i=2}^{+\infty}(i+\theta)a_i\bar{j}^{-i-1}\Big].$$

We can find $\sum_{i=2}^{+\infty}(i+\theta)a_i\bar{j}^{-i-1}$ is an alternating series with positive first term. So $\sum_{i=2}^{+\infty}(i+\theta)a_i\bar{j}^{-i-1} > 0$, we have

$$\begin{aligned} & \theta\bar{j}^{-1}a_0 + (1+\theta)\bar{j}^{-2}a_1 + \sum_{i=2}^{+\infty}(i+\theta)a_i\bar{j}^{-i-1} > \theta\bar{j}^{-1}a_0 + (1+\theta)\bar{j}^{-2}a_1 \\ & = \theta\bar{j}^{-1}(1-\theta) + (1+\theta)\bar{j}^{-2}(-\frac{1}{2})(1-\theta)\theta = (1-\theta)\theta[\bar{j}^{-1} - \frac{1}{2}(1+\theta)\bar{j}^{-2}] > 0. \end{aligned}$$

Therefore, we have already proved $\bar{j}^{-\theta}\sum_{i=0}^{+\infty} a_i\bar{j}^{-i}$ is decrease function on $\bar{j}$. According to (2.15), we obtain

$$A_2^k > A_3^k > \ldots > A_{k-3}^k. \tag{2.16}$$

Next, let's prove $A_{k-3}^k > A_{k-2}^k > A_{k-1}^k > 0$. Through careful calculation, we can get

$$A_{k-2}^k - A_{k-1}^k = \frac{1}{\Gamma(3-\theta)\Delta t^{\theta}}F_1, \quad A_{k-3}^k - A_{k-2}^k = \frac{1}{\Gamma(3-\theta)\Delta t^{\theta}}F_2,$$

where

$$\begin{aligned} F_1 = & -\frac{3}{2}(2-\theta)(k-2)^{1-\theta} + \frac{1}{2}(2-\theta)(k-3)^{1-\theta} - 2(2-\theta)k^{1-\theta} + (k-3)^{2-\theta} - 3(k-2)^{2-\theta} + 2k^{2-\theta}, \\ F_2 = & \frac{1}{2}(2-\theta)k^{1-\theta} + \frac{3}{2}(2-\theta)(k-2)^{1-\theta} - \frac{3}{2}(2-\theta)(k-3)^{1-\theta} + \frac{1}{2}(2-\theta)(k-4)^{1-\theta} \\ & -k^{2-\theta} + 3(k-2)^{2-\theta} - 3(k-3)^{2-\theta} + (k-4)^{2-\theta}, \end{aligned}$$

According to (1) in Lemma A.1, we get $F_1 > 0, F_2 > 0$. Therefore, we have

$$A_{k-2}^k - A_{k-1}^k > 0, \quad A_{k-3}^k - A_{k-2}^k > 0. \tag{2.17}$$

The following step, we will prove $A_{k-1}^k > 0$. By carefully calculation, we have

$$A_{k-1}^k = \frac{1}{\Delta t^\theta \Gamma(3-\theta)} \Big\{ \frac{2-\theta}{2} [(k-2)^{1-\theta} + 3k^{1-\theta}] + (k-2)^{2-\theta} - k^{2-\theta} \Big\}, \tag{2.18}$$

According to (2.33), we have

$$A_{k-1}^k > 0. \tag{2.19}$$

Combining (2.12), (2.13), (2.16), (2.17) with (2.19), we already proved Lemma 2.1. □

We let $\Delta \bar{u}_j = \Delta(u_j - \rho u_{j-1})$, $\Delta \bar{u}_0 = \Delta u_0$. Let $\rho = \frac{1}{2}(1 - \frac{A_1^k}{A_0^k}) = \frac{1}{2}(3 + \frac{\theta-6}{4-\theta} \cdot 2^{1-\theta})$. Therefore, from (2.8), we can get that

$$\begin{aligned} {}_0D_{\Delta t}^\theta u_k &= A_0^k \Delta u_k + A_1^k \Delta u_{k-1} + A_2^k \Delta u_{k-2} + \ldots + A_{k-2}^k \Delta u_2 + A_{k-1}^k \Delta u_1 \\ &= A_0^k \Delta(u_k - \rho u_{k-1}) + (A_1^k + \rho A_0^k) \Delta(u_{k-1} - \rho u_{k-2}) + \ldots \\ &\quad + (A_{k-j}^k + \rho A_{k-j-1}^k + \ldots + \rho^{k-j} A_0^k) \Delta(u_j - \rho u_{j-1}) \\ &\quad + \ldots + (A_{k-1}^k + \rho A_{k-2}^k + \ldots + \rho^{k-1} A_0^k) \Delta(u_1 - \rho u_0) \\ &\quad + (\rho A_{k-1}^k + \rho^2 A_{k-2}^k + \ldots + \rho^k A_0^k) \Delta u_0 \\ &= \sum_{j=1}^k \bar{A}_{k-j}^k \Delta \bar{u}_j + \Delta u_0 \sum_{i=1}^n \rho^i A_{k-i}^k, \end{aligned} \tag{2.20}$$

where

$$\bar{A}_{k-j}^k = \sum_{i=j}^k \rho^{i-j} A_{k-i}^k. \tag{2.21}$$

Next, we discuss the relationship between the size of $\bar{A}_{k-j}^k$.

Lemma 2.2. $\bar{A}_0^k > \bar{A}_1^k > \bar{A}_2^k > \ldots > \bar{A}_{k-1}^k > 0$.

Proof. When $k = 3$, we only need to prove $\bar{A}_0^3 > \bar{A}_1^3 > \bar{A}_2^3 > 0$. By careful calculation, we can get

$$\bar{A}_1^3 - \bar{A}_0^3 = -\frac{1}{2\Delta t^\theta \Gamma(3-\theta)} \Big[\frac{3}{2}(4-\theta) - (4+\theta)3^{1-\theta} + (6-\theta)2^{-\theta} \Big].$$

According to (2) in Lemma A.1, we get

$$\bar{A}_0^3 > \bar{A}_1^3. \tag{2.22}$$

By direct calculation, we have

$$\begin{aligned} &\bar{A}_2^3 - \bar{A}_1^3 = A_2^3 - A_1^3 + \rho(\bar{A}_1^3 - \bar{A}_0^3) \\ &= -\frac{4-\theta}{2\Delta t^\theta \Gamma(3-\theta)} \Big[-\frac{3}{4} + \frac{5\theta - 4}{2(4-\theta)} \cdot 3^{1-\theta} + \frac{(4+\theta)(6-\theta)}{(4-\theta)^2} \cdot 3^{1-\theta} \cdot 2^{-\theta} - \frac{(6-\theta)^2}{(4-\theta)^2} (2^{-\theta})^2 \Big]. \end{aligned}$$

According to (3) in Lemma A.1, we have

$$\bar{A}_1^3 > \bar{A}_2^3. \tag{2.23}$$

Next, we will prove $\bar{A}_2^3 = A_2^3 + \rho\bar{A}_1^3 > 0$. According to (2.41), we get $\bar{A}_1^3 > 0$. Hence, we just need to prove $A_2^3 > 0$. By calculation, we have $A_2^3 = \frac{1}{2\Delta t^\theta\Gamma(3-\theta)}[4 - \theta - \theta \cdot 3^{2-\theta}] > 0$, therefore,

$$\bar{A}_2^3 > 0. \tag{2.24}$$

Combining (2.22), (2.23) and (2.24), when $k = 3$, we know that Lemma 2.2 holds.

When $k \geq 4$, through careful calculation, we can draw the following conclusions

$$\bar{A}_1^k - \bar{A}_0^k = -\frac{2 - \frac{\theta}{2}}{\Delta t^\theta\Gamma(3-\theta)}\Big[\frac{3}{2} + \frac{(\theta-6)2^{-\theta}}{4-\theta}\Big] = -\frac{2 - \frac{\theta}{2}}{\Delta t^\theta\Gamma(3-\theta)}\rho. \tag{2.25}$$

According to (4) in Lemma A.1, we can get $\rho > 0$, we have $\bar{A}_0^k > \bar{A}_1^k$. Because

$$\bar{A}_2^k - \bar{A}_1^k = A_2^k - A_1^k + \rho(\bar{A}_1^k - \bar{A}_0^k) = -\frac{1}{8(4-\theta)\Delta t^\theta\Gamma(3-\theta)}\tilde{f}(\theta),$$

where $\tilde{f}(\theta) = -3(4-\theta)^2 + 6(4-\theta)(6-\theta)2^{1-\theta} - 4(4-\theta)(8-\theta)3^{1-\theta} + (6-\theta)^2 \cdot 4^{1-\theta}$. According to (5) in Lemma A.1, we can get $\tilde{f}(\theta) > 0$. It can be concluded that

$$\bar{A}_1^k > \bar{A}_2^k. \tag{2.26}$$

By careful calculation, we can get $\bar{A}_3^k - \bar{A}_2^k = A_3^k - A_2^k + \rho(\bar{A}_2^k - \bar{A}_1^k)$. According to $\rho > 0$, (2.26) and Lemma 2.1, we can get

$$\bar{A}_2^k > \bar{A}_3^k. \tag{2.27}$$

By mathematical induction, and Lemma 2.1 we can conclude that

$$\bar{A}_{k-1-j} - \bar{A}_{k-2-j} = A_{k-1-j}^k - A_{k-2-j}^k + \rho(\bar{A}_{k-2-j}^k - \bar{A}_{k-3-j}^k) > 0, \;\; j = 0, \dots, k-4.$$

So we have

$$\bar{A}_0^k > \bar{A}_1^k > \bar{A}_2^k > \dots > \bar{A}_{k-1}^k. \tag{2.28}$$

Next we prove that $\bar{A}_{k-1}^k > 0$. According to (2.21), we have

$$\bar{A}_{k-1}^k = A_{k-1}^k + \sum_{i=2}^{k-2} \rho^{i-j} A_{k-i}^k + \rho^{k-2}\bar{A}_1^k.$$

According to (2.37), we get $\bar{A}_1^k > 0$. Using Lemma 2.1, $\rho > 0$, we have

$$\bar{A}_{k-1}^k > 0. \tag{2.29}$$

Combining (2.28) with (2.29), we already proved Lemma 2.2. □

Lemma 2.3. *There is a constant $\pi_A \geq 6$ such that the discrete kernel satisfies the lower bound.*

$$\bar{A}_j^k \geq \frac{1}{\pi_A \Delta t}\int_{t_{k-j-1}}^{t_{k-j}} \omega_{1-\theta}(t_k-\tau)d\tau = \frac{1}{\pi_A \Delta t^{\theta}\Gamma(2-\theta)}[(j+1)^{1-\theta} - j^{1-\theta}]. \tag{2.30}$$

Proof. When $k \geq 4$, According to (2.21), Lemma 2.1 and Lemma 2.2, we can get

$$\bar{A}_{k-j}^k = A_{k-j}^k + \sum_{i=j+1}^{k-2} A_{k-i}^k \rho^{i-j} + \rho^{k-1-j}\bar{A}_1^k \geq A_{k-j}^k.$$

For $j = 1$, we have

$$\bar{A}_{k-1}^k \geq A_{k-1}^k = \frac{1}{\Delta t^{\theta}\Gamma(3-\theta)}\Big\{\frac{2-\theta}{2}[(k-2)^{1-\theta} + 3k^{1-\theta}] + (k-2)^{2-\theta} - k^{2-\theta}\Big\}, \tag{2.31}$$

let $\tilde{j} = k-1$, $\tilde{j} \geq 3$, using Taylor formula to expand the calculation, we can get the following results

$$A_{k-1}^k = \frac{\tilde{j}^{-\theta}}{\Delta t^{\theta}\Gamma(2-\theta)}\sum_{i=0}^{+\infty} a_i, \tag{2.32}$$

where $a_i = \Pi_{i=0}^{i}(1-\theta-i)\frac{1}{(i+2)!}(\frac{1}{\tilde{j}})^i[(-1)^{i+1}\frac{i}{2} + \frac{3i+4}{2}]$, $a_0 = (1-\theta)$, $a_1 = \frac{8(1-\theta)(-\theta)}{12\tilde{j}}$, $\sum_{i=2}^{+\infty} a_i$ is a convergent alternating series, and $a_2 > 0$, therefore, we have $0 \leq \sum_{i=2}^{+\infty} a_i \leq a_2$, so

$$A_{k-1}^k = \frac{\tilde{j}^{-\theta}}{\Delta t^{\theta}\Gamma(2-\theta)}\Big(a_0 + a_1 + \sum_{i=2}^{+\infty} a_i\Big) \geq \frac{\tilde{j}^{-\theta}}{\Delta t^{\theta}\Gamma(1-\theta)}\Big(1 - \frac{8}{36}\Big) = \frac{\tilde{j}^{-\theta}}{\Delta t^{\theta}\Gamma(1-\theta)\frac{9}{7}}. \tag{2.33}$$

We have

$$\pi_A \geq \frac{9}{7}. \tag{2.34}$$

For $j = 2$, we have

$$\bar{A}_{k-2}^k \geq A_{k-2}^k = \frac{1}{\Delta t^{\theta}\Gamma(3-\theta)}\Big\{\frac{2-\theta}{2}[(k-3)^{1-\theta} - 2(k-2)^{1-\theta} - k^{1-\theta}] + (k-3)^{2-\theta} - 2(k-2)^{2-\theta} + k^{2-\theta}\Big\},$$

let $\hat{j} = k-2$, $\hat{j} \geq 2$, and then using Taylor expansion, similar to $j = 1$, it can be obtained by calculation

$$A_{k-2}^k = \frac{\hat{j}^{-\theta}}{\Delta t^{\theta}\Gamma(3-\theta)}\sum_{i=0}^{+\infty} a_i,$$

where $a_i = \Pi_{n=0}^{i}(1-\theta-n)\frac{1}{(i+2)!}(\frac{1}{\hat{j}})^i[\frac{i}{-2}\cdot(-1)^i + \frac{2-i}{2}2^{i+1}]$, because $\sum_{i=3}^{+\infty} a_i$ is a convergent staggered series, and $a_3 > 0$, $0 < \sum_{i=3}^{+\infty} a_i < a_3$, we get

$$\bar{A}_{k-2}^k \geq \frac{\hat{j}^{-\theta}}{\Delta t^{\theta}\Gamma(2-\theta)}[a_0 + a_1 + a_2] \geq \frac{\hat{j}^{-\theta}}{\Delta t^{\theta}\Gamma(2-\theta)}\Big[1 - \frac{5}{12\cdot 2} - \frac{1}{24\cdot 2}\Big] = \frac{\hat{j}^{-\theta}}{\Delta t^{\theta}\Gamma(2-\theta)}\cdot\frac{37}{48},$$

therefore, we have

$$\pi_A \geq \frac{48}{37}. \tag{2.35}$$

For $j = 3, 4, \ldots, k-2$, we have

$$\begin{aligned}\bar{A}^k_{k-j} &\geq A^k_{k-j} = \frac{1}{\Delta t^\theta \Gamma(3-\theta)}\Big\{\frac{1}{2}(2-\theta)[(k-j-1)^{1-\theta} - 2(k-j)^{1-\theta} \\ &\quad +(k-j+1)^{1-\theta}] + (k-j-1)^{2-\theta} - 2(k-j)^{2-\theta} + (k-j+1)^{2-\theta}\Big\},\end{aligned}$$

let $\bar{j} = k - j$, $\bar{j} \geq 2$, we have

$$A^k_{k-j} = \frac{\bar{j}^{1-\theta}}{\Delta t^\theta \Gamma(3-\theta)}\Big\{\frac{1}{2}(2-\theta)\Big[\Big(1-\frac{1}{\bar{j}}\Big)^{1-\theta} - 2 + \Big(1+\frac{1}{\bar{j}}\Big)^{1-\theta}\Big] + \bar{j}\Big[\Big(1-\frac{1}{\bar{j}}\Big)^{2-\theta} - 2 + (1+\frac{1}{\bar{j}})^{2-\theta}\Big]\Big\},$$

then using Taylor expansion, we can get the following results

$$A^k_{k-j} = \frac{\bar{j}^{-\theta}}{\Delta t^\theta \Gamma(2-\theta)} \sum_{i=0}^{+\infty} a_i,$$

where $a_i = \Pi^i_{n=0}(1-\theta-n)\frac{1}{(i+2)!}(\frac{1}{\bar{j}})^i[(-1)^i(\frac{-i}{2}) + \frac{i+4}{2}]$. Because $\sum_{i=2}^{+\infty} a_i$ is a convergent alternating series and $a_2 > 0, 0 \leq \sum_{i=2}^{+\infty} a_i \leq a_2$, so

$$\bar{A}^k_{k-j} \geq \frac{\bar{j}^{-\theta}}{\Delta t^\theta \Gamma(1-\theta)} \cdot \frac{1}{1-\theta}\Big[1-\theta + \frac{3}{3!}(1-\theta)(-\theta)\frac{1}{\bar{j}}\Big] \geq \frac{\bar{j}^{-\theta}}{\Delta t^\theta \Gamma(1-\theta)}\Big(1-\frac{1}{4}\Big),$$

so we can get

$$\pi_A \geq \frac{4}{3}. \tag{2.36}$$

When $j = k-1$,

$$\begin{aligned}\bar{A}^k_1 &= \rho \bar{A}^k_0 + A^k_1 = \frac{1}{\Delta t^\theta \Gamma(3-\theta)}\Big[\frac{\theta}{4} - 1 + (3-\frac{\theta}{2})2^{-\theta}\Big] \\ &\geq \frac{1}{2\Delta t^\theta \Gamma(1-\theta)}\Big[\frac{\theta}{4} - 1 + (3-\frac{\theta}{2})2^{-\theta}\Big] \geq \frac{1}{4\Delta t^\theta \Gamma(1-\theta)}.\end{aligned} \tag{2.37}$$

Therefore, we have

$$\pi_A \geq 4. \tag{2.38}$$

When $j = k$, according to (2.30), we can get

$$\bar{A}^k_0 = A^k_0 = \frac{1}{\Delta t^\theta \Gamma(3-\theta)}\Big(2-\frac{\theta}{2}\Big) \geq \frac{1}{2\Delta t^\theta \Gamma(2-\theta)}\Big(2-\frac{\theta}{2}\Big) \geq \frac{1}{\Delta t^\theta \Gamma(2-\theta)}. \tag{2.39}$$

We have

$$\pi_A \geq 1. \tag{2.40}$$

When $k = 3$, $\bar{A}_0^3$ is in (2.39), so $\frac{1}{\pi_A} \le 1$. According to (2.30), we only need

$$\begin{aligned}
\bar{A}_1^3 &= \rho\bar{A}_0^3 + A_1^3 = \frac{1}{\Delta t^\theta\Gamma(3-\theta)}\Big[\frac{\theta}{4} - 1 + (\frac{\theta}{2} - 3)2^{-\theta} + (\frac{\theta}{2} + 2)3^{1-\theta}\Big] \\
&= \frac{2^{1-\theta} - 1}{\Delta t^\theta\Gamma(2-\theta)} \frac{\frac{\theta}{4} - 1 + (\frac{\theta}{2} - 3)2^{-\theta} + (\frac{\theta}{2} + 2)3^{1-\theta}}{(2^{1-\theta} - 1)(2-\theta)} \\
&\ge \frac{2^{1-\theta} - 1}{2\Delta t^\theta\Gamma(2-\theta)} \frac{1}{(2^{1-\theta} - 1)(2-\theta)} \ge \frac{2^{1-\theta} - 1}{4\Delta t^\theta\Gamma(2-\theta)}.
\end{aligned} \tag{2.41}$$

Therefore, we have

$$\pi_A \ge 4. \tag{2.42}$$

Next, we calculate $\bar{A}_2^3$,

$$\begin{aligned}
&\bar{A}_2^3 = A_2^3 + \rho\cdot\bar{A}_1^3 = \frac{1}{\Delta t^\theta\Gamma(3-\theta)}\cdot\frac{1}{8(4-\theta)}[(\theta-4)^2 + 4(4-\theta)(\theta-6)2^{-\theta} + 4(6-\theta)^2(2^{-\theta})^2 \\
&\quad +[6(4-\theta)^2 - 4(6-\theta)(4+\theta)2^{-\theta}]3^{1-\theta}] \ge \frac{3^{1-\theta} - 2^{1-\theta}}{\Delta t^\theta\Gamma(2-\theta)}\cdot\frac{1}{8(4-\theta)(3^{1-\theta} - 2^{1-\theta})(2-\theta)(2+\theta)} \\
&\quad \cdot[\theta^3 - 6\theta^2 + 32 + 4(-\theta^3 + 17\theta^2 - 76\theta + 96)2^{-\theta} + 4(\theta^3 - 4\theta^2 - 72)2^{-2\theta}] \\
&\ge \frac{3^{1-\theta} - 2^{1-\theta}}{\Delta t^\theta\Gamma(2-\theta)}\cdot\frac{1}{16(4-\theta)(2+\theta)}[\theta^3 - 6\theta^2 + 32 + 4(-\theta^3 + 17\theta^2 - 76\theta + 96)2^{-\theta} \\
&\quad +4(\theta^3 - 4\theta^2 - 72)2^{-2\theta}] \ge \frac{3^{1-\theta} - 2^{1-\theta}}{\Delta t^\theta\Gamma(2-\theta)}\cdot\frac{24}{16(4-\theta)(2+\theta)} \ge \frac{3^{1-\theta} - 2^{1-\theta}}{6\Delta t^\theta\Gamma(2-\theta)}.
\end{aligned}$$

Therefore, we have

$$\pi_A \ge 6. \tag{2.43}$$

Combining (2.34)–(2.38) with (2.40)–(2.43), we have already proved Lemma 2.3. □

3. Estimation of the truncation errors

Now we turn to derive an estimate for the truncation errors of the scheme (2.10). We start with deriving an error estimate for the finite difference operator ${}_0D^\theta_{\Delta_t}u_k$.

Theorem 3.1. *Assume $u(t) \in C^3[0, T]$. Let*

$$r_k(\Delta t) = {}_0D^\theta_t u(t_k) - {}_0D^\theta_{\Delta t}u_k, \quad \forall k \ge 1. \tag{3.1}$$

Then there exists a constant C_u depending only on the function u, such that for all $\Delta t > 0$,

$$|r_k(\Delta t)| \le C_u\Delta t^{3-\theta}. \tag{3.2}$$

Proof. Our error estimation will be established on the following Taylor theorem

$$u(t) - J_{[t_0,t_2]}u(t) = \frac{u^{(3)}(\xi(\tau))}{6}(\tau - t_0)(\tau - t_1)(\tau - t_2), \quad \forall\tau \in [t_0, t_2], \tag{3.3}$$

where $\xi(\tau)$ is a function defined on $[t_0, t_2]$ with range (t_0, t_2). We first estimate $r_1(\Delta t)$

$$
\begin{aligned}
|r_1(\Delta t)| &= \Big|\frac{1}{\Gamma(1-\theta)}\Big\{\int_0^{t_1} u'(\tau)(t_1-\tau)^{-\theta}d\tau - \int_0^{t_1}[J_{[t_0,t_2]}u(\tau)]'(t_1-\tau)^{-\theta}d\tau\Big\}\Big| \\
&= \frac{\theta}{\Gamma(1-\theta)}\Big|\int_0^{t_1}[u(\tau)-J_{[t_0,t_2]}u(\tau)](t_1-\tau)^{-\theta-1}d\tau\Big| \\
&= \frac{\theta}{\Gamma(1-\theta)}\Big|\int_0^{t_1}\frac{u^{(3)}(\xi(\tau))}{6}(\tau-t_0)(\tau-t_2)(t_1-\tau)^{-\theta}d\tau\Big| \\
&\le \frac{\theta}{\Gamma(1-\theta)}\frac{\max\limits_{t\in[0,T]}|u^{(3)}(t)|}{6}\int_0^{t_1}\tau(t_2-\tau)(t_1-\tau)^{-\theta}d\tau \\
&= \frac{\theta}{3(3-\theta)\Gamma(2-\theta)}\max_{t\in[0,T]}|u^{(3)}(t)|\Delta t^{3-\theta} \le C_u\Delta t^{3-\theta}.
\end{aligned}
$$

This proves (3.2) for $k = 1$. The case $k = 2$ can be similarly proven, and here we omit the details.

When $k \ge 3$, we have

$$
\begin{aligned}
|r_k(\Delta t)| &= |{}_0D_t^{\theta}u(t_k) - {}_0D_{\Delta t}^{\theta}u(t_k)| = \frac{1}{\Gamma(1-\theta)}\Big|\int_0^{t_1}(t_k-\tau)^{-\theta}[u(\tau)-J_{[t_0,t_2]}u(\tau)]'d\tau \\
&\quad + \sum_{j=1}^{k-1}\int_{t_j}^{t_{j+1}}(t_k-\tau)^{-\theta}[u(\tau)-J_{[t_{j-1},t_{j+1}]}u(\tau)]'d\tau\Big| \doteq |M+N|.
\end{aligned}
$$

Similar to the proof of $|r_1(\Delta t)|$, we have

$$
|M| \le C_u\Delta t^{3-\theta}. \tag{3.4}
$$

For N, we have

$$
\begin{aligned}
|N| &= \frac{1}{\Gamma(1-\theta)}\Big|\sum_{j=1}^{k-1}\int_{t_j}^{t_{j+1}}(t_k-\tau)^{-\theta}d[u(\tau)-J_{[t_{j-1},t_{j+1}]}u(\tau)]\Big| \\
&= \frac{1}{\Gamma(1-\theta)}\Big|\sum_{j=1}^{k-2}\int_{t_j}^{t_{j+1}}(t_k-\tau)^{-\theta}d[u(\tau)-J_{[t_{j-1},t_{j+1}]}u(\tau)] + \int_{t_{k-1}}^{t_k}(t_k-\tau)^{-\theta}d[u(\tau)-J_{[t_{j-1},t_{j+1}]}u(\tau)]\Big| \\
&= \frac{1}{\Gamma(1-\theta)}\Big\{\Big|-\sum_{j=1}^{k-2}\int_{t_j}^{t_{j+1}}\frac{u^{(3)}(\xi)}{6}(\tau-t_{j-1})(\tau-t_j)(\tau-t_{j+1})d(t_k-\tau)^{-\theta} \\
&\quad - \int_{t_{k-1}}^{t_k}\frac{u^{(3)}(\xi)}{6}(\tau-t_{k-2})(\tau-t_{k-1})(\tau-t_k)d(t_k-\tau)^{-\theta}\Big|\Big\} \\
&\le \frac{\sqrt{3}\theta}{27\Gamma(1-\theta)}\max_{t\in[0,T]}\Big|u^{(3)}(t)\Big|\Delta t^3\int_{t_j}^{t_{j+1}}(t_k-\tau)^{-\theta-1}d\tau \\
&\quad + \frac{\theta}{6\Gamma(1-\theta)}\max_{t\in[0,T]}|u^{(3)}(t)\Big|\Delta t^2\int_{t_{k-1}}^{t_k}(t_k-\tau)^{-\theta}d\tau \\
&\le \frac{\sqrt{3}\theta}{27\Gamma(1-\theta)}\max_{t\in[0,T]}\Big|u^{(3)}(t)\Big|\Delta t^{3-\theta} + \frac{\theta}{6\Gamma(1-\theta)}\max_{t\in[0,T]}\Big|u^{(3)}(t)\Big|\Delta t^{3-\theta}.
\end{aligned}
$$

In the above inequality, we use $|(\tau-t_{j-1})(\tau-t_j)(\tau-t_{j+1})| \leq \frac{2\sqrt{3}}{9}\Delta t^3$. We can get the following conclusions

$$|r_k(\Delta t)| = |M + N| \leq C_u \Delta t^{3-\theta}. \tag{3.5}$$

Complete the proof of Theorem 3.1.

4. Convergence analysis

In order to obtain the convergence analysis, we now introduce an important tool: complementary discrete convolution kernel. Because of $\omega_\theta * \omega_\beta = \omega_{\theta+\beta}$, therefore

$$\int_s^t \omega_\theta(t-\mu)\omega_{1-\theta}(\mu - s)d\mu = \omega_1(t-s) = 1, \quad for \quad 0 < s < t < \infty. \tag{4.1}$$

A class of complementary discrete convolution kernels P^k_{k-i} with the same properties are given

$$\sum_{i=m}^{k} P^k_{k-i}\bar{A}^i_{i-m} \equiv 1, \quad for \quad 3 \leq m \leq k \leq K. \tag{4.2}$$

According to [3], we have

$$P^k_0 = \frac{1}{\bar{A}^k_0}, \quad P^k_i = \frac{1}{\bar{A}^{k-i}_0}\sum_{j=0}^{i-1}(\bar{A}^{k-j}_{i-j-1} - \bar{A}^{k-j}_{i-j})P^k_j, \quad for \ 1 \leq i \leq k-3, \tag{4.3}$$

where $P^k_i > 0, i = 0, 1, ..., k-3$ was obtained from Lemma 2.2. Next, we introduce Lemma 2.1 of [3], as follows.

Lemma 4.1. *In (4.3), the discrete kernel P^k_i has the property of (4.2) and satisfies the following conditions*

$$0 \leq P^k_{k-i} \leq \pi_A \Gamma(2-\theta)\Delta t^\theta, \quad 1 \leq i \leq k \leq N, \tag{4.4}$$

$$\sum_{j=1}^{k} P^k_{k-i}\omega_{1-\theta}(t_i) \leq \pi_A, \quad 1 \leq k \leq K. \tag{4.5}$$

Now we can analyze the convergence of ${}_0D^\theta_{\Delta t}u_j$. First, we consider $f(t,u)$ and assume that it satisfies the following differential mean value theorem and that there exists a constant L, such that

$$f(t_k, u(t_k)) - f(t_k, u_k) = L_k(u(t_k) - u_k) = L_k e_k, \quad \forall k = 1, 2, ..., K, \tag{4.6}$$

and $|L_k| \leq L, \forall k \geq 1$.

Theorem 4.1. *Assumes that u is the exact solution of (2.1) and (2.2), and $\{u_k\}^K_{k=1}$ is the numerical solution of (2.10). If $\theta \in (0,1)$ and step Δt satisfy*

$$\Delta t \leq \frac{1}{\sqrt[\theta]{2\pi_A\Gamma(2-\theta)\Lambda}}, \tag{4.7}$$

where $\pi_A \geq 6$, and $\Lambda = 12L$, then the following error estimates hold,

$$|u(t_k) - u_k| \leq C\Delta t^{3-\theta}, \tag{4.8}$$

here C is only dependent on the function u.

Proof. Because $\Delta u_1 = u_1 - u_0, \Delta u_2 = u_2 - u_1$, through calculation, we can get

$$\begin{cases} {}_0D_t^\theta u(t_1) = -B_1^1 u_0 + (B_1^1 - B_1^2)u_1 + B_1^2 u_2, \\ {}_0D_t^\theta u(t_2) = -B_2^1 u_0 + (B_2^1 - B_2^2)u_1 + B_2^2 u_2, \end{cases} \tag{4.9}$$

let $-B_1^1 = \Delta t^{-\theta}\bar{D}_0^1$, $B_1^1 - B_1^2 = \Delta t^{-\theta}\bar{D}_1^1$, $B_1^2 = \Delta t^{-\theta}\bar{D}_2^1$; $-B_2^1 = \Delta t^{-\theta}D_0^1$, $B_2^1 - B_2^2 = \Delta t^{-\theta}D_1^1$, $B_2^2 = \Delta t^{-\theta}D_2^1$. It is easy to obtain by calculation

$$\begin{cases} \Delta t^{-\theta}\bar{D}_1^1 e_1 + \Delta t^{-\theta}\bar{D}_2^1 e_2 = f(t_1, u(t_1)) - f(t_1, u_1) - r_1(\Delta t), \\ \Delta t^{-\theta}D_1^1 e_1 + \Delta t^{-\theta}D_2^1 e_2 = f(t_2, u(t_2)) - f(t_2, u_2) - r_2(\Delta t). \end{cases} \tag{4.10}$$

Among (4.6), then we can get

$$\begin{cases} \Delta t^{-\theta}\bar{D}_1^1 e_1 + \Delta t^{-\theta}\bar{D}_2^1 e_2 = L_1 e_1 - r_1(\Delta t), \\ \Delta t^{-\theta}D_1^1 e_1 + \Delta t^{-\theta}D_2^1 e_2 = L_2 e_2 - r_2(\Delta t). \end{cases}$$

That is

$$\begin{aligned} \left\| \begin{pmatrix} e_1 \\ e_2 \end{pmatrix} \right\|_\infty &= \left\| \Delta t^\theta D^{-1} \begin{pmatrix} L_1 e_1 - r_1(\Delta t) \\ L_2 e_2 - r_2(\Delta t) \end{pmatrix} \right\|_\infty \le \Delta t^\theta \left\| D^{-1} \right\|_\infty \left\| \begin{matrix} L_1 e_1 - r_1(\Delta t) \\ L_2 e_2 - r_2(\Delta t) \end{matrix} \right\|_\infty \\ &\le \Delta t^\theta \left\| D^{-1} \right\|_\infty \left(L \max\{|e_1|, |e_2|\} + \max\{|r_1(\Delta t)|, |r_2(\Delta t)|\} \right), \end{aligned} \tag{4.11}$$

where $D = \begin{pmatrix} \bar{D}_1^1 & \bar{D}_2^1 \\ D_1^1 & D_2^1 \end{pmatrix}$. Since $\bar{D}_1^1 D_2^1 - \bar{D}_2^1 D_1^1$ is bounded, then

$$\max\{|e_1|, |e_2|\} \le C_1 \Delta t^\theta \max\{|r_1(\Delta t)|, |r_2(\Delta t)|\}, \tag{4.12}$$

therefore,

$$\begin{cases} |e_1| \le C\Delta t^{3-\theta}, \\ |e_2| \le C\Delta t^{3-\theta}, \end{cases} \tag{4.13}$$

when $j = 1, 2$, (4.8) is proved.

When $i \ge 3$, let's set $\bar{e}_i = e_i - \rho e_{i-1}$, $i = 1, ..., j$, and $\bar{e}_0 = e_0$ for (4.13), we have

$$\begin{cases} |\bar{e}_1| = |e_1 - \rho e_0| \le C\Delta t^{3-\theta}, \\ |\bar{e}_2| = |e_2 - \rho e_1| \le \frac{5}{3} C\Delta t^{3-\theta}. \end{cases} \tag{4.14}$$

Combining with (2.20) and (4.6), $\bar{e}_j$, $j \ge 3$, satisfy

$$\sum_{j=1}^{k} \bar{A}_{k-j}^k \Delta\bar{e}_j = f(t_k, u(t_k)) - f(t_k, u_k) - r_k(\Delta t). \tag{4.15}$$

Because of $e_j = \sum_{n=1}^{j} \rho^{j-n}\bar{e}_n$, then

$$\sum_{j=3}^{k} \bar{A}_{k-j}^k \Delta\bar{e}_j = L_k \sum_{j=3}^{k} \rho^{k-j}\bar{e}_j - \bar{r}_k(\Delta t), \tag{4.16}$$

where

$$\bar{r}_k(\Delta t) = r_k(\Delta t) - L_k \sum_{j=1}^{2} \rho^{k-j}\bar{e}_j + \sum_{j=1}^{2} \bar{A}^k_{k-j}\Delta\bar{e}_j, \tag{4.17}$$

by multiplying $2\bar{e}_k$ on both sides of (4.16), from Lemma A.1 in Liao [3], we can obtain that

$$2\bar{e}_k \sum_{j=3}^{k} \bar{A}^k_{k-j}\Delta\bar{e}_j \geq \sum_{j=3}^{k} \bar{A}^k_{k-j}\Delta(|\bar{e}_j|^2),$$

$$2\bar{e}_k[L_k \sum_{j=3}^{k} \rho^{k-j}\bar{e}_j - \bar{r}_k(\Delta t)] \leq L\sum_{j=3}^{k} \rho^{k-j}(|\bar{e}_j|^2 + |\bar{e}_k|^2) + 2|\bar{e}_k||\bar{r}_k(\Delta t)| \leq 4L\sum_{j=3}^{k} \rho^{k-j}|\bar{e}_j|^2 + 2|\bar{e}_k||\bar{r}_k(\Delta t)|.$$

To sum up, we can get the following conclusions

$$\sum_{j=3}^{k} \bar{A}^k_{k-j}\Delta(|\bar{e}_j|^2) \leq 4L\sum_{j=3}^{k} \rho^{k-j}|\bar{e}_j|^2 + 2|\bar{e}_k| \cdot |\bar{r}_k(\Delta t)|. \tag{4.18}$$

We change k to i, and then multiply both sides of (4.18) by a $\sum_{i=3}^{k} P^k_{k-i}$, then

$$\sum_{i=3}^{k} P^k_{k-i} \sum_{j=3}^{i} \bar{A}^i_{i-j}\Delta(|\bar{e}_j|^2) \leq \sum_{i=3}^{k} P^k_{k-i} \sum_{j=3}^{i} 4L\rho^{i-j}|\bar{e}_j|^2 + 2\sum_{i=3}^{k} P^k_{k-i}|\bar{e}_i||\bar{r}_i(\Delta t)|. \tag{4.19}$$

From (4.2) and $\Delta u_j = u_j - u_{j-1}$, we can get the following results

$$\sum_{i=3}^{k} P^k_{k-i} \sum_{j=3}^{i} \bar{A}^i_{i-j}\Delta(|\bar{e}_j|^2) = \sum_{j=3}^{k} \Delta(|\bar{e}_j|^2) \sum_{i=j}^{k} P^k_{k-i}\bar{A}^i_{i-j} = \sum_{j=3}^{k} \Delta(|\bar{e}_j|^2) = |\bar{e}_k|^2 - |\bar{e}_2|^2, \tag{4.20}$$

substituting (4.20) into (4.19) yields

$$|\bar{e}_k|^2 \leq 4L\sum_{i=3}^{k} P^k_{k-i} \sum_{j=3}^{i} \rho^{i-j}|\bar{e}_j|^2 + |e_2|^2 + 2\sum_{i=3}^{k} P^k_{k-i}|\bar{e}_i||\bar{r}_i(\Delta t)|. \tag{4.21}$$

Next, we will prove it by mathematical induction

$$|\bar{e}_k| \leq 2E_\theta(2\pi_A \Lambda t_k^\theta)(|\bar{e}_2| + 2\max_{3\leq j\leq k} \sum_{i=3}^{k} p^j_{j-i}\,|\bar{r}_i(\Delta t)|) \doteq F_k G_k, \quad for\ k \geq 2, \tag{4.22}$$

where $\Lambda = 12L$, E_θ stands for the Mittag-Leffler function, we usually define it as: $E_\theta(z) = \sum_{j=0}^{\infty} \frac{Z^j}{\Gamma(1+j\theta)}$, and $E_\theta(0) = 1$, $\forall Z \in R$, and $Z > 0, E_\theta^{'}(Z) > 0$, so $F_k \geq F_{k-1} \geq 2$ for all $k \geq 2$. where $G_k = |\bar{e}_2| + 2\max_{3\leq j\leq k} \sum_{i=3}^{k} P^j_{j-i}\,|\bar{r}_i(\Delta t)|$.

When $k = 3$, (i) if $|\bar{e}_3| \leq |e_2|, G_3 = |e_2| + 2P^3_0|\bar{r}_3(\Delta t)| \geq |\bar{e}_2|$, we have $|\bar{e}_3| \leq |\bar{e}_2| \leq G_3 \leq F_3G_3$,

(ii) if $|\bar{e}_3| > |e_2|$, from (4.21), it can be concluded that

$$|\bar{e}_3|^2 \leq 4LP^3_0|\bar{e}_3|^2 + |\bar{e}_2|^2 + 2P^3_0|\bar{e}_3||\bar{r}_3(\Delta t)|.$$

According to (4.4), it can be concluded that

$$4LP_0^3 \le \pi_A\Gamma(2-\theta)\Delta t^\theta\Lambda \le \frac{1}{2} \quad \Longrightarrow \Delta t \le \frac{1}{\sqrt[\theta]{2\pi_A\Gamma(2-\theta)\Lambda}},$$

so $|\bar{e}_3| \le 2(|\bar{e}_2| + 2P_0^3|\bar{r}_3(\Delta t)|) \le 2G_3 \le F_3G_3$.

When $4 \le k \le K$, we assume that: $|\bar{e}_j| \le F_jG_j$, for $3 \le j \le k-1$, let $|\bar{e}_{j(k)}| = \max_{2\le i\le k-1}|\bar{e}_i|$.

(i) When $|\bar{e}_k| \le |\bar{e}_{j(k)}|$, because F_j and G_j monotonically increase with j, so

$$|\bar{e}_k| \le |\bar{e}_{j(k)}| \le F_{j(k)}G_{j(k)} \le F_kG_k.$$

(ii) When $|\bar{e}_k| \ge |\bar{e}_{j(k)}|$, from (4.21) we can obtain that

$$|\bar{e}_k|^2 \le |\bar{e}_k|\sum_{i=3}^{k-1}P_{k-i}^k\sum_{j=3}^{i}4L\rho^{i-j}|\bar{e}_j| + |\bar{e}_k|^2P_0^k\sum_{j=3}^{k}4L\rho^{i-j} + |\bar{e}_k||\bar{e}_2| + 2|\bar{e}_k|\sum_{i=3}^{k}P_{k-i}^k|\bar{r}_i(\Delta t)|.$$

From (4.4), we give the limit of the maximum step size, which means that

$$P_0^k\sum_{j=3}^{k}4L\rho^{i-j} \le \pi_A\Gamma(2-\theta)\Delta t^\theta\Lambda < \frac{1}{2} \Longrightarrow \Delta t \le \frac{1}{\sqrt[\theta]{2\pi_A\Gamma(2-\theta)\Lambda}}.$$

Using of Lemma 2.3 in [3] for any real $\mu > 0$,

$$\sum_{i=3}^{k-1}P_{k-i}^kE_\theta(\mu t_i^\theta) \le \pi_A\frac{E_\theta(\mu t_k^\theta)-1}{\mu}, \quad for\ \ 3 \le k \le K.$$

We have

$$\begin{aligned}
|\bar{e}_k| &\le 2\sum_{i=3}^{k-1}P_{k-i}^k\sum_{j=3}^{i}4L\rho^{i-j}|\bar{e}_j| + 2|\bar{e}_2| + 4\sum_{i=3}^{k}P_{k-i}^k|\bar{r}_i(\Delta t)| \le 2\Lambda\sum_{i=3}^{k-1}P_{k-i}^kF_iG_k + 2G_k \\
&\le 2\sum_{i=3}^{k-1}P_{k-i}^k\sum_{j=3}^{i}4L\theta^{i-j}F_jG_j + 2G_k \le [4\Lambda\sum_{i=3}^{k-1}P_{k-i}^kE_\theta(2\pi_A\Lambda t_i^\theta) + 2]G_k \\
&\le \{4\Lambda\cdot\frac{\pi_A}{2\pi_A\Lambda}[E_\theta(2\pi_At_k^\theta) - 1] + 2\}G_k = 2E_\theta(2\pi_A\Lambda t_k^\theta)G_k = F_kG_k.
\end{aligned}$$

To sum up, the proof of (4.22) is complete.

Next, we carefully estimate $|\bar{r}_i(\Delta t)|$. According to (4.17), we have

$$|\bar{r}_k(\Delta t)| \le |r_k(\Delta t)| + L\sum_{j=1}^{2}\rho^{k-j}|\bar{e}_j| + (\bar{A}_{k-1}^k + \bar{A}_{k-2}^k)|\bar{e}_1| + \bar{A}_{k-2}^k|\bar{e}_2|. \tag{4.23}$$

Next, we estimate the upper bounds of $\bar{A}_{k-1}^{(k)}$ and $\bar{A}_{k-2}^{(k)}$. According to (2.37), Lemma 2.1 and (4) in Lemma A.1, we can obtain

$$\bar{A}_{k-2}^k = \sum_{j=2}^{k-2}A_{k-j}^k\rho^{j-2} + \rho^{k-3}\bar{A}_1^k \le A_2^k\sum_{j=2}^{k-2}\rho^{j-2} + \rho^{k-3}\bar{A}_1^k \le 3A_2^k + \frac{1}{\Delta t^\theta\Gamma(3-\theta)}[\frac{\theta}{4} - 1 + (3-\frac{\theta}{2})2^{-\theta}]$$

$$
\begin{aligned}
&= \frac{1}{\Delta t^{\theta}\Gamma(3-\theta)}\Big[\frac{5}{4}(4-\theta)+\frac{9}{2}(8-\theta)3^{-\theta}+\frac{11}{2}(-6+\theta)\cdot 2^{-\theta}\Big] \\
&\leq \frac{1}{\Delta t^{\theta}\Gamma(3-\theta)}\Big[5+\frac{9}{2}\cdot 8+\frac{11}{2}(-6+1)\cdot\frac{1}{2}\Big] = \frac{1}{\Delta t^{\theta}\Gamma(3-\theta)}\frac{109}{4}.
\end{aligned}
$$

Therefore, $\bar{A}^k_{k-2} \leq \frac{109}{4\Delta t^{\theta}\Gamma(3-\theta)}$. According to Lemma 2.2, we can get $\bar{A}^k_{k-1} < \bar{A}^k_{k-2} \leq \frac{109}{4\Delta t^{\theta}\Gamma(3-\theta)}$. Therefore, we can obtain from (4.23),

$$
\begin{aligned}
|\bar{r}_i(\Delta t)| &\leq C\Delta t^{3-\theta}+5LC\Delta t^3+\frac{109}{2\Gamma(3-\theta)}\Delta t^{3-\theta}+\frac{545}{12\Gamma(3-\theta)}C\Delta t^{3-\theta} \\
&\leq \Big[C+5LC\Delta t^{\theta}+\frac{100}{\Gamma(3-\theta)}C\Big]\Delta t^{3-\theta}.
\end{aligned}
$$

In the expression on the right side of (4.22),

$$
\sum_{i=3}^{k} P^j_{j-i}|\bar{r}_i(\Delta t)| = \sum_{i=3}^{k} P^j_{j-i}\omega_{1-\theta}(t_i)\cdot \max_{3\leq i\leq k}\frac{|\bar{r}_i(\Delta t)|}{\omega_{1-\theta}(t_i)}, \tag{4.24}
$$

according to (4.5) in Lemma 4.1, we can obtain that

$$
\sum_{i=3}^{k} P^j_{j-i}\omega_{1-\theta}(t_i) \leq \sum_{i=1}^{k} P^j_{j-i}\omega_{1-\theta}(t_i) \leq \pi_A, \quad 1\leq k\leq K.
$$

Because of $\frac{1}{\omega_{1-\theta}(t_i)} = \Gamma(1-\theta)t_i^{\theta}$, therefore (4.24) becomes

$$
\sum_{i=3}^{k} P^j_{j-i}|\bar{r}_i(\Delta t)| \leq \pi_A \max_{3\leq i\leq k}\frac{|\bar{r}_i(\Delta t)}{\omega_{1-\theta}(t_i)} \leq \pi_A\Big[C+5LC\Delta t^{\theta}+\frac{100}{\Gamma(3-\theta)}C\Big]\Delta t^{3-\theta}\max_{3\leq i\leq k}\Gamma(1-\theta)t_i^{\theta}. \tag{4.25}
$$

Based on (4.13), (4.25) and (4.22), we obtain

$$
|\bar{e}_k| \leq 2E_{\theta}(2\pi_A\Lambda t_k^{\theta})\Big\{\frac{5}{3}C\Delta t^{\theta}+2\pi_A\Big[C+5LC\Delta t^{\theta}+\frac{100}{\Gamma(3-\theta)}C\Big]\Gamma(1-\theta)t_k^{\theta}\Big\}\Delta t^{3-\theta}.
$$

According to $e_k = \bar{e}_k - \rho e_{k-1} = \sum_{n=0}^{k}\rho^{k-n}\bar{e}_n$, we have $|e_k| \leq 3\max_{0\leq n\leq k}|\bar{e}_n|$. Then the proof is completed. □

5. Numerical results

In this section, two examples are presented to verify the effectiveness of our numerical method (2.10).

Example 5.1. *we consider the problem (2.1) with* $u(0) = 0$*, and*

$$
f(t,u(t)) = \frac{\Gamma(4+\theta)}{6}t^3 + t^{3+\theta} - u(t), \tag{5.1}
$$

$$
f(t,u(t)) = \frac{\Gamma(4+\theta)}{6}t^3 + t^{6+2\theta} - u^2(t). \tag{5.2}
$$

The exact solution of Eq (2.1) is $u(t) = t^{3+\theta}$*. We take* $T = 1$ *and choose the step size to be* $\Delta t = 2^{-l}, l = 7, 8, \ldots, 11$*. The error we will display is defined by* $e_{\Delta t} = \max_{k=1,2,\cdots,K} |u(t_k) - u_k|, K = T/\Delta t$*.*

In (5.1), f *is a linear case of* u*. From Table 1, the convergence order is computed by* $\log_2(e_{2\Delta t}/e_{\Delta t})$*. it is observed that for* $\theta = 0.3, 0.6$ *and* 0.9*, the convergence rates are close to* $2.7, 2.4$ *and* 2.1*, respectively. This is in a good agreement with the theoretical prediction. In Table 2, we can take* $\theta = 0.01$ *and* 0.99 *and obtain that the convergence rates are close to* 2.99 *and* 2.01*. That tells us that as* $\theta \to 0$ *or* 1*, the convergence rate still* $3-\theta$*. In (5.2),* f *is the nonlinear case of* u*. From Tables 3 and 4, once again these results confirm that the convergence of the numerical solution is close to of order* $3 - \theta$ *for* $0 < \theta < 1$*.*

Table 1. Maximum errors $e_{\Delta t}$ and decay rate as functions of Δt with the right hand side (5.1).

Δt	$\theta = 0.3$	Rate	$\theta = 0.6$	Rate	$\theta = 0.9$	Rate
$\frac{1}{128}$	5.1545E-6	-	5.3113E-5	-	3.8546E-4	-
$\frac{1}{256}$	8.1757E-7	2.6564	1.0192E-5	2.3815	9.0841E-5	2.0851
$\frac{1}{512}$	1.2874E-7	2.6668	1.9457E-6	2.3891	2.1297E-5	2.0926
$\frac{1}{1024}$	2.0164E-8	2.6746	3.7032E-7	2.3934	4.9804E-6	2.0963
$\frac{1}{2048}$	3.1714E-9	2.6686	7.0366E-8	2.3958	1.1632E-6	2.0981

Table 2. Maximum errors $e_{\Delta t}$ and decay rate as $\Delta t = 0.01, 0.99$ with the right hand side (5.1).

Δt	$\theta = 0.01$	Rate	$\theta = 0.99$	Rate
$\frac{1}{128}$	3.7469E-8	-	6.6342E-4	-
$\frac{1}{256}$	5.1473E-9	2.8638	1.6645E-4	1.9947
$\frac{1}{512}$	7.0275E-10	2.8727	4.1540E-5	2.0025
$\frac{1}{1024}$	8.9656E-11	2.9705	1.0339E-5	2.0063
$\frac{1}{2048}$	1.1231E-11	2.9968	2.5703E-6	2.0081

Table 3. Maximum errors $e_{\Delta t}$ and decay rate as functions of Δt with the right hand side (5.2).

Δt	$\theta = 0.3$	Rate	$\theta = 0.6$	Rate	$\theta = 0.9$	Rate
$\frac{1}{128}$	1.0154E-6	-	1.0167E-5	-	9.1822E-5	-
$\frac{1}{256}$	1.4941E-7	2.7647	1.9494E-6	2.3828	2.1549E-5	2.0911
$\frac{1}{512}$	2.3628E-8	2.6607	3.7176E-7	2.3906	5.0416E-6	2.0957
$\frac{1}{1024}$	3.7049E-9	2.6729	7.0707E-8	2.3944	1.1777E-6	2.0978
$\frac{1}{2048}$	5.6279E-10	2.7187	1.3497E-8	2.3891	2.7492E-7	2.0989

Table 4. Maximum errors $e_{\Delta t}$ and decay rate as $\Delta t = 0.01, 0.99$ with the right hand side (5.2).

Δt	$\theta = 0.01$	Rate	$\theta = 0.99$	Rate
$\frac{1}{128}$	3.2116E-6	-	1.7072E-4	-
$\frac{1}{256}$	3.9867E-7	3.0099	4.2645E-5	2.0012
$\frac{1}{512}$	4.9490E-8	3.0099	1.0618E-5	2.0058
$\frac{1}{1024}$	6.1435E-9	3.0099	2.6400E-6	2.0079
$\frac{1}{2048}$	7.6264E-10	3.0099	6.5589E-7	2.0090

Example 5.2. *we consider the problem (2.1) and (2.2) with the following right hand side function*

$$f(t, u(t)) = t^{-\theta} Sin_{1,1-\alpha}(t) + \sin(t) - u(t), \tag{5.3}$$

$$f(t, u(t)) = t^{-\theta} Sin_{1,1-\alpha}(t) + \sin^2(t) - u^2(t). \tag{5.4}$$

The corresponding exact solution is $u(t) = \sin(t)$*, and* $Sin_{\alpha,\beta}(t) = \sum_{k=1}^{\infty}(-1)^{k+1}\frac{t^{2k-1}}{\Gamma(\alpha(2k-1)+\beta)}$*.* f *is a linear and nonlinear case of* u *in (5.3) and (5.4), respectively.*

We repeat the same calculation as in Example 5.1 using the proposed numerical scheme. Tables 5 and 6 show the maximum errors and decay rates of the step size for several a ranging from 0.3 to 0.9. This is consistent with the theoretical prediction. The convergence rate is close to $3 - \theta$ *for* $0 < \theta < 1$.

Table 5. Maximum errors $e_{\Delta t}$ and decay rate as functions of Δt with the right hand side (5.3).

Δt	$\theta = 0.3$	Rate	$\theta = 0.6$	Rate	$\theta = 0.9$	Rate
$\frac{1}{128}$	4.4720E-7	-	3.3763E-6	-	2.1961E-5	-
$\frac{1}{256}$	7.1175E-8	2.6515	6.4755E-7	2.3823	5.1721E-6	2.0861
$\frac{1}{512}$	1.1232E-8	2.6636	1.2353E-7	2.3901	1.2121E-6	2.0931
$\frac{1}{1024}$	1.7643E-9	2.6704	2.3497E-8	2.3942	2.8338E-7	2.0967
$\frac{1}{2048}$	2.6806E-10	2.7185	4.4390E-9	2.4041	6.6105E-8	2.0999

Table 6. Maximum errors $e_{\Delta t}$ and decay rate as functions of Δt with the right hand side (5.4).

Δt	$\theta = 0.3$	Rate	$\theta = 0.6$	Rate	$\theta = 0.9$	Rate
$\frac{1}{128}$	5.2408E-7	-	3.5338E-6	-	2.0939E-5	-
$\frac{1}{256}$	8.5515E-8	2.6155	6.8794E-7	2.3608	4.9822E-6	2.0713
$\frac{1}{512}$	1.3708E-8	2.6411	1.3230E-7	2.3784	1.1738E-6	2.0855
$\frac{1}{1024}$	2.1730E-9	2.6573	2.5279E-8	2.3878	2.7517E-7	2.0928
$\frac{1}{2048}$	3.4105E-10	2.6716	4.8110E-9	2.3935	6.4316E-8	2.0970

6. Conclusions

In this paper, we presented a high order numerical method for solving Caputo nonlinear fractional ordinary differential equations. The numerical method was constructed by using the Quadratic Lagrange interpolation. By careful error estimation, the proposed scheme is of order $3-\theta$ for $0 < \theta < 1$. Finally, numerical experiments are carried out to verify the theoretical prediction. In the future, we plan to apply this kind of methods to 3D fractional partial differential equations with time derivatives based the idea of [21] and [22].

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Conflict of interest

The authors declare that there is no conflict of interests regarding the publication of this article.

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A. Proof of some inequalities

Lemma A.1.

(1) $F_1 = -\frac{3}{2}(2-\theta)(k-2)^{1-\theta} + \frac{1}{2}(2-\theta)(k-3)^{1-\theta} - 2(2-\theta)k^{1-\theta} + (k-3)^{2-\theta} - 3(k-2)^{2-\theta} + 2k^{2-\theta} > 0,$

$$F_2 = \frac{1}{2}(2-\theta)k^{1-\theta} + \frac{3}{2}(2-\theta)(k-2)^{1-\theta} - \frac{3}{2}(2-\theta)(k-3)^{1-\theta} + \frac{1}{2}(2-\theta)(k-4)^{1-\theta} - k^{2-\theta} + 3(k-2)^{2-\theta} - 3(k-3)^{2-\theta} + (k-4)^{2-\theta} > 0,$$

(2) $\frac{3}{2}(4-\theta) - (4+\theta)3^{1-\theta} + (6-\theta)2^{-\theta} > 0,$

(3) $-\frac{3}{4} + \frac{5\theta-4}{2(4-\theta)} \cdot 3^{1-\theta} + \frac{(4+\theta)(6-\theta)}{(4-\theta)^2} \cdot 3^{1-\theta} \cdot 2^{-\theta} - \frac{(6-\theta)^2}{(4-\theta)^2}(2^{-\theta})^2 > 0,$

(4) $0 < \rho = \frac{1}{2}(3 + \frac{\theta - 6}{4 - \theta} \cdot 2^{1-\theta}) < \frac{2}{3}$,
(5) $\tilde{f}(\theta) = -3(4-\theta)^2 + 6(4-\theta)(6-\theta)2^{1-\theta} - 4(4-\theta)(8-\theta)3^{1-\theta} + (6-\theta)^2 \cdot 4^{1-\theta} > 0$,

Proof. (1) Firstly, we will prove $F_1 > 0$. let $k - 2 = x$, Taylor formula is used to obtain the following results

$$F_1 = (2-\theta)(1-\theta)x^{-\theta-1} \sum_{n=0}^{+\infty} \prod_{i=0}^{n} (-\theta - i)(\frac{1}{x})^n \cdot a_n,$$

where $a_n = \frac{\frac{1}{2}(n+1)\cdot(-1)^n - 8(n+1)\cdot 2^n}{(n+3)!} = \frac{\frac{1}{2}(n+1)[(-1)^n - 16\cdot 2^n]}{(n+3)!} < 0$, so $\sum_{n=0}^{+\infty} \prod_{i=0}^{n}(-\theta - i)(\frac{1}{x})^n \cdot a_n$ is an alternating series with positive first term, so satisfies $\sum_{n=0}^{+\infty} \prod_{i=0}^{n}(-\theta - i)(\frac{1}{x})^n \cdot a_n > 0$, so $F_1 > 0$.

Next, we will prove $F_2 > 0$. Let $k - 2 = \bar{x}$, Taylor formula is used to obtain the following results

$$F_2 = (2-\theta)(1-\theta)\bar{x}^{-\theta-1} \sum_{n=0}^{+\infty} \prod_{i=0}^{n} (-\theta - i)(\frac{1}{\bar{x}})^n \frac{1}{(n+3)!} b_n,$$

where $b_n = \frac{3}{2}(n+1)(-1)^{n+1} + 2(n-1)\cdot 2^n[1 + (-1)^n], b_0 = -\frac{11}{2}, b_1 = 3$, when $n \geq 2$, n is odd, $b_n > 0$; n is even, $b_n = (n-1)[4 \cdot 2^n - \frac{3}{2}] - 3 > [8 - \frac{3}{2}] - 3 > 0$, so $\sum_{n=1}^{+\infty} \prod_{i=0}^{n}(-\theta - i)(\frac{1}{\bar{x}})^n \frac{1}{(n+3)!} b_n$ is an alternating series with positive first term. So $\sum_{n=0}^{+\infty} \prod_{i=0}^{n}(-\theta - i)(\frac{1}{\bar{x}})^n \frac{1}{(n+3)!} b_n > (-\theta)\frac{1}{3!} b_0 + 0 > 0$. We get $F_2 > 0$.

(2) Let $f(\theta) = \frac{3}{2}(4-\theta) - (4+\theta)3^{1-\theta} + (6-\theta)2^{-\theta}$, through careful calculation, we get

$$f'(\theta) = -\frac{3}{2} - 3^{1-\theta}[1 + (4+\theta)(-\ln 3)] + 2^{-\theta}[-1 + (6-\theta)(-\ln 2)],$$

$f''(\theta) = 3^{-\theta} \cdot g(\theta)$, where $g(\theta) = 3(\ln 3)[2 - (4+\theta)\ln 3] + (\frac{3}{2})^\theta (\ln 2)[2 + (6-\theta)\ln 2]$, because

$$\begin{aligned} g'(\theta) &= -3(\ln 3)^2 + (\frac{3}{2})^\theta (\ln 2)\{[2 + (6-\theta)(\ln 2)]\ln(\frac{3}{2}) - \ln 2\}, \\ g''(\theta) &= (\frac{3}{2})^\theta (\ln 2)\ln(\frac{3}{2})\{[2 + (6-\theta)(\ln 2)]\ln(\frac{3}{2}) - 2\ln 2\} \doteq \{\frac{3}{2}\}^\theta (\ln 2)\ln(\frac{3}{2}) H(\theta), \end{aligned}$$

We can get $H'(\theta) = -\ln 2 \cdot \ln(\frac{3}{2}) < 0$, so we get $H(\theta) > H(1) > 0$, therefore $g'(\theta) < g'(1) < 0$, $g(\theta)$ monotone decreasing, $g(1) < g(\theta) < g(0) = -3.6227 < 0$, that is $f'(\theta)$ monotone decreasing, $0 < f'(1) < f'(\theta) < f'(0)$, where $f'(1) = -3 + 5\ln 3 - \frac{5}{2}\ln 2 > 0$, that is $f(\theta)$ monotone increasing, $f(0) < f(\theta) < f(1)$, where $f(0) = 0$, to sum up, we can get $f(\theta) > 0$.

(3) Let $f_1(\theta) = -\frac{3}{4} + \frac{5\theta-4}{2(4-\theta)} \cdot 3^{1-\theta} + \frac{(4+\theta)(6-\theta)}{(4-\theta)^2} \cdot 3^{1-\theta} \cdot 2^{-\theta} - \frac{(6-\theta)^2}{(4-\theta)^2}(2^{-\theta})^2 \doteq -\frac{3}{4} + a_1 \cdot 3^{1-\theta} + a_2 \cdot 3^{1-\theta} 2^{-\theta} + a_3 \cdot (2^{-\theta})^2$, where

$$a_1 = \frac{5\theta - 4}{2(4-\theta)}, a_2 = \frac{(4+\theta)(6-\theta)}{(4-\theta)^2}, a_3 = -\frac{(6-\theta)^2}{(4-\theta)^2}.$$

Next, we just need to prove that $f_1(\theta) > 0$, using a Taylor expansion yields

$$\begin{aligned} f_1(\theta) &= -\frac{3}{4} + [a_1 \cdot 2^{1-\theta} + a_2 \cdot 2^{1-2\theta}](1 + \frac{1}{2})^{1-\theta} + a_3 \cdot (2^{-\theta})^2 = -\frac{3}{4} + a_1 \cdot 2^{1-\theta} + a_2 \cdot 2^{1-2\theta} + a_3 \cdot 2^{-2\theta} \\ &\quad + [a_1 \cdot 2^{1-\theta} + a_2 \cdot 2^{1-2\theta}][\frac{1-\theta}{1!}\frac{1}{2} + \frac{(1-\theta)(-\theta)}{2!}(\frac{1}{2})^2 + \frac{(1-\theta)(-\theta)(-\theta-1)}{3!}(\frac{1}{2})^3 + \cdots], \end{aligned}$$

where

$$a_1 2^{1-\theta} + a_2 2^{1-2\theta} = 2^{-\theta} \cdot \frac{1}{(4-\theta)^2}[(5\theta-4)(4-\theta) + 2(4+\theta)(6-\theta)2^{-\theta}]$$
$$\geq 2^{-\theta} \cdot \frac{1}{(4-\theta)^2}[(5\theta-4)(4-\theta) + (4+\theta)(6-\theta)] \geq 0.$$

Because of $\frac{1-\theta}{1!} \cdot \frac{1}{2} + \frac{(1-\theta)(-\theta)}{2!} \cdot (\frac{1}{2})^2 + \frac{(1-\theta)(-\theta)(-\theta-1)}{3!}(\frac{1}{2})^3 + \ldots \doteq \sum_{k=0}^{+\infty} a_k$ is an alternating series with positive first term, and $\sum_{k=0}^{+\infty} a_k = a_0 + a_1 + \sum_{k=2}^{+\infty} a_k$, where $\sum_{k=2}^{+\infty} a_k$ is an alternating series with positive first term, so $0 < \sum_{k=2}^{+\infty} a_k < a_2$, we have

$$f_1(\theta) > -\frac{3}{4} + a_3 \cdot 2^{-2\theta} + [a_1 \cdot 2^{1-\theta} + a_2 \cdot 2^{1-2\theta}][1 + \frac{1-\theta}{1!} \cdot \frac{1}{2} + \frac{(1-\theta)(-\theta)}{2!}(\frac{1}{2})^2]$$
$$= -\frac{3}{4} + \frac{2^{-\theta}}{8(4-\theta)^2}[-5\theta^4 + 49\theta^3 - 196\theta^2 + 368\theta - 192 + (-\theta^4 + 7\theta^3 - 2\theta^2 - 48\theta + 144)2^{1-\theta}]$$
$$\doteq -\frac{3}{4} + \frac{2^{-\theta}}{8(4-\theta)^2}[f_2(\theta) + f_3(\theta)].$$

We wish prove $f_1(\theta) > 0$, only need $-\frac{3}{4} + \frac{2^{-\theta}}{8(4-\theta)^2}[f_2(\theta) + f_3(\theta)] > 0 \Longleftrightarrow f_2(\theta) + f_3(\theta) > \frac{3}{4} \cdot 8(4-\theta)^2 2^\theta = 6(4-\theta)^2 2^\theta$, that is $f_2(\theta) + f_3(\theta) > 6(4-\theta)^2 2^\theta \doteq 6 f_4(\theta)$, so to prove $f_1(\theta) > 0$, just prove $f_2(\theta) + f_3(\theta) - 6f_4(\theta) > 0$, let's remember $\bar{f}(\theta) = f_2(\theta) + f_3(\theta) - 6f_4(\theta)$, since $\bar{f}(\theta)$ first increases and then decreases, and the two endpoints are $\bar{f}(0) = 0, \bar{f}(1) = 16 > 0$, $\bar{f}(\theta) > 0$ is always true, so $f_1(\theta) > 0$.

(4) Firstly, we will prove $\rho > 0$. Because $\rho = \frac{3(4-\theta)+(\theta-6)2^{1-\theta}}{2(4-\theta)}$, let $\bar{g}(\theta) = 3(4-\theta) + (\theta-6)2^{1-\theta}$, by calculation, we can get $\bar{g}(\theta)$ is monotonically increasing function on θ, that is $\bar{g}(\theta) > \bar{g}(0) = 0$. therefore, we have $\rho > 0$.

In addition, $\rho - \frac{2}{3} = \frac{5(4-\theta)+3(\theta-6)2^{1-\theta}}{6(4-\theta)} \doteq \frac{\bar{g}_1(\theta)}{6(4-\theta)}$. we can directly find $\bar{g}_1(\theta) < \bar{g}_1(1) = 0$, so $0 < \rho < \frac{2}{3}$.

(5) We use Lagrange's mean value theorem $4^{1-\theta} > \frac{4}{3+\theta} \cdot 3^{1-\theta}$, and we have

$$\tilde{f}(\theta) > -3(4-\theta)^2 + 6(4-\theta)(6-\theta)2^{1-\theta} + [-4(4-\theta)(8-\theta) + \frac{4(6-\theta)^2}{3+\theta}]3^{1-\theta}. \tag{A.1}$$

Let $a_1 = -3(4-\theta)^2, a_2 = 6(4-\theta)(6-\theta), a_3 = \frac{4}{3+\theta}[-(4-\theta)(8-\theta)(3+\theta)+(6-\theta)^2], a_4 = 1+\frac{1-\theta}{1!}\frac{1}{2}+\frac{(1-\theta)(-\theta)}{2}(\frac{1}{2})^2$. (A.1) is becomes

$$\tilde{f}(\theta) > a_1 + a_2 \cdot 2^{1-\theta} + a_3 \cdot 3^{1-\theta} = a_1 + 2^{1-\theta}[a_2 + a_3(1+\frac{1}{2})^{1-\theta}]$$
$$= a_1 + 2^{1-\theta}\{a_2 + a_3[1 + \frac{1-\theta}{1!}\frac{1}{2} + \frac{(1-\theta)(-\theta)}{2}(\frac{1}{2})^2]$$
$$+ a_3 \cdot [\frac{(1-\theta)(-\theta)(-\theta-1)}{3!}(\frac{1}{2})^3 + \frac{(1-\theta)(-\theta)(-\theta-1)(-\theta-2)}{4!}(\frac{1}{2})^4 + \ldots]\}$$
$$= a_1 + 2^{1-\theta}\{a_2 + a_3 \cdot a_4 + a_3(1-\theta)\theta \sum_{k=0}^{+\infty} \Pi_{i=0}^{k}(-\theta-1-i) \cdot \frac{-1}{(k+3)!}(\frac{1}{2})^{k+3}\}$$
$$\doteq a_1 + 2^{1-\theta}\{a_2 + a_3 \cdot a_4 + a_3(1-\theta)\theta \sum_{k=0}^{+\infty} b_k\},$$

where $b_k = \Pi_{i=0}^{k}(-\theta-1-i)\cdot\frac{-1}{(k+3)!}(\frac{1}{2})^{k+3}$, and $b_0 = \frac{-(-\theta-1)}{3!}(\frac{1}{2})^3 > 0$, $|\frac{b_{k+1}}{b_k}| = \frac{\theta+2+k}{2(k+4)} < 1$, so $\sum_{k=0}^{+\infty} b_k$ is a convergent alternating series, that is $0 < \sum_{k=0}^{+\infty} b_k < b_0$. Because of $a_3 < 0$, so we get

$$\begin{aligned}\tilde{f}(\theta) &> a_1 + 2^{1-\theta}\{a_2 + a_3\cdot a_4 + a_3(1-\theta)\theta b_0\} = a_1 + 2^{1-\theta}\{a_2 + a_3[a_4 + (1-\theta)\theta\cdot\frac{-(-\theta-1)}{3!}(\frac{1}{2})^3]\}\\ &\doteq a_1 + 2^{1-\theta}\{a_2 + a_3\cdot a_5\} \doteq \tilde{f}_1(\theta),\end{aligned}$$

where $a_5 = a_4 + (1-\theta)\theta\cdot\frac{-(-\theta-1)}{3!}(\frac{1}{2})^3 = \frac{48+24(1-\theta)-6(\theta-\theta^2)+(\theta-\theta^3)}{48}$, by careful calculation, we can get

$$\begin{aligned}&\tilde{f}_1(\theta) = \frac{-36}{12(3+\theta)}[\theta^3-5\theta^2-8\theta+48]\\ &+2^{1-\theta}\frac{1}{12(3+\theta)}[\theta^6-16\theta^5+97\theta^4-278\theta^3+88\theta^2+732\theta+864]\\ &= \frac{1}{12(3+\theta)}\{-36(\theta^3-5\theta^2-8\theta+48)+2^{1-\theta}(\theta^6-16\theta^5+97\theta^4-278\theta^3+88\theta^2+732\theta+864)\}\\ &\doteq \frac{1}{12(3+\theta)}\tilde{f}_2(\theta),\end{aligned}$$

because $\theta\in(0,1)$, so $\theta^3<\theta^2, \theta^6>0$.

$$\begin{aligned}&\tilde{f}_2(\theta) > -36(\theta^2-5\theta^2-8\theta+48)+2^{1-\theta}(0-16\theta^5+97\theta^4-278\theta^3+88\theta^2+732\theta+864)\\ &= 144(\theta^2+2\theta-12)+2^{1-\theta}(-16\theta^5+97\theta^4-278\theta^3+88\theta^2+732\theta+864)\\ &= 144(\theta^2+2\theta-12)+2^{1-\theta}\tilde{f}_4(\theta) \doteq \tilde{f}_3(\theta),\end{aligned}$$

where $\tilde{f}_4(\theta) = -16\theta^5+97\theta^4-278\theta^3+88\theta^2+732\theta+864$, by careful calculation, we can get $\tilde{f}_3''(\theta) < 0$, that is $\tilde{f}_3'(\theta)$ monotone decreasing, so $\tilde{f}_3'(1) < \tilde{f}_3'(\theta) < \tilde{f}_3'(0)$, by direct calculation, we can get $\tilde{f}_3'(\theta) = 144(2\theta+2)+2^{1-\theta}[\tilde{f}_4(\theta)(-\ln 2)+\tilde{f}_4'(\theta)]$, $\tilde{f}_3'(0) > 0$, $\tilde{f}_3'(0) < 0$, so $\tilde{f}_3'(0)$ changes from positive to negative, $\tilde{f}_3(0)$ increases first and then decreases, $\tilde{f}_3(0) = 0$, $\tilde{f}_3(1) = 223 > 0$, that is $\tilde{f}_3(\theta) > 0$ established, so $\tilde{f}(\theta) > 0$. □