Higher order numerical methods for fractional order differential equations

Thesis submitted in accordance with the requirements of the University of Chester for the degree of Doctor in Philosophy by

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Abstract

This thesis explores higher order numerical methods for solving fractional differential equations.

Firstly, we consider two approaches to construct higher order numerical methods for solving fractional differential equations. Based on a direct discretization of the fractional differential operator we show that, the order of convergence of the linear fractional differential equation with $0 < \alpha < 1$ is $O(h^{3-\alpha})$, where α denotes the order of the fractional derivative. Based on discretization of the integral in the equivalent form of non-linear fractional differential equations the order of convergence of the numerical method is $O(h^3)$ for $\alpha \geq 1$ and $O(h^{1+2\alpha})$ for $0 < \alpha \leq 1$ for sufficiently smooth functions.

Secondly, we introduce extrapolation algorithms for accelerating the convergence order of the two considered numerical methods. Numerical experiments are given for each algorithm to show that the numerical results are consistent with the theoretical results.

Finally we introduce a higher order algorithm for solving two-sided space-fractional partial differential equations. The space-fractional derivatives we consider here are left-handed and right-handed Riemann-Liouville fractional derivatives which are expressed by using the Hadamard finite-part integrals. We approximate the Hadamard finite-part integrals by using piecewise quadratic interpolation polynomials and obtain a numerical approximation of the space-fractional derivative with convergence order $O(\Delta x^{3-\alpha})$, $1 < \alpha < 2$. A shifted implicit finite difference method is applied for solving the two-sided space-fractional partial differential equation and we prove that the order of convergence of the finite difference method is $O(\Delta t + \Delta x^{\min(3-\alpha, \beta)}), 1 < \alpha < 2$, $\beta > 0$, where $\Delta t, \Delta x$ denote the time and space stepsizes, respectively, and α is the order of the fractional derivative and β is the Lipschitz constant related to the exact solution. Numerical examples, where the solutions have varying degrees of smoothness, are presented and compared with the exact analytical solution to compare the practical performance of the method with the theoretical order of convergence.

Declaration

No part of the work referred to in this thesis has been submitted in support of an application for another degree or qualification of this or any other institution of learning. However some parts of the materials contained herein have been published previously.

Publications

- Y. Yan, K. Pal and N. J. Ford [93], Higher order numerical methods for solving fractional differential equations, BIT Numer. Math., 54 (2014), 555-584.
- K. Pal, F. Liu and Y. Yan [73], Numerical solutions for fractional differential equations by extrapolation, Lecture Notes in Computer Science, Springer series, Volume 9045 (2015), 299-306.
- K. Pal, F. Liu, Y. Yan and G. Roberts [74], Finite difference method for two-sided space-fractional partial differential equations, Lecture Notes in Computer Science, Springer series, Volume 9045 (2015), 307-314.
- N. J. Ford, K. Pal and Y. Yan [42], An algorithm for the numerical solution of two-sided space-fractional partial differential equations, Computational Methods in Applied Mathematics, 15 (2015), 497-514.

Conference presentations

- Finite difference methods for solving space-fractional partial differential equations; Faculty of Applied Sciences Post-graduate Research Conference, 27th June 2013, University of Chester.
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- A higher order numerical method for solving fractional differential equations (FDEs) (Predictor-corrector method); 6th International Conference on Computational Methods in Applied Mathematics, Sep 28- Oct 4, 2014, Strobl, Austria.

- Basic concepts of fractional differential equations (PDEs); SCI Early Career Research Meeting on 6th Nov, 2014, in Thornton Science Park, University of Chester.
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Chapter 1

Introduction

1.1 Fractional calculus

Fractional calculus deals with the study of so-called fractional order integral and derivative operators over real and complex domain and their applications. It does not mean the calculus of fractions [76]. Neither does it mean a fraction of any calculus - differential, integral or calculus of variations. The fractional calculus is a name for the theory of integrals and derivatives of arbitrary order, which unify and generalize the notions of integer-order differentiation and n-fold integration.

Fractional derivatives and fractional integrals are not new in the household subject area of mathematics. In recent years a huge interest in fractional calculus has arisen because of its applicability to vast areas of scientific interest. In 18th and 19th centuries many brilliant scientists motivated to focus their attention on fractional calculus [4]. For instance, we can mention Euler(1738), Laplace (1812), Fourier (1822), Abel (1823-1826), Liouville (1832-1873), Riemann (1847), Holmgren (1865-1867), Grünward (1867-1872), Letnikov (1868-1872), Laurent (1884), Nekrassov (1888), Krug (1890), Hadamard (1892), Heaviside (1892-1912), Pincherle (1902), Hardy and Littlewood (1917-1928), Weyl (1917), Lévy (1923), Marchaud (1927), Davis (1924-1936), Zygmund (1935-1945), Love (1938-1996), Erdelyi (1939-1965), Kober (1940), Widder (1941), Riesz (1949).

However the interest in the specific topic of fractional calculus surged only at the end of the last century. Fractional differential equations, that is, those involving real and complex order derivatives, have assumed an important role in modelling the anomalous dynamics of many processes related to complex systems in the most diverse areas of science and engineering [4]. During the last 25 years there has been a spectacular increase in the use of fractional differential models to simulate the dynamics of many different anomalous process, especially those involving ultra-slow diffusion. The following table is only based on the Scopus database, but it reflects this state of affairs clearly: [4]

Words in title or abstract	1960-1980	1981-1990	1991-2000	2001-2010
Fractional Brownian Motion	2	38	532	1295
Anomalous Diffusion	185	261	626	1205
Anomalous Relaxation	21	23	70	61
Superdiffusion or Subdiffusion	0	22	121	521
Fractional Models, Kinetics, Dynamics	11	24	128	443
Fractional Differential Equations	1	1	74	943

Table 1.1.1: Evolution in the number of publications on fractional differential equations and their applications.

1.2 Basic functions of fractional calculus

In fractional calculus, the gamma function and beta function are the basic mathematical tools to understand the origin of its computational challenges. The Gamma function generalizes the factorial $n!$ and allows n to take also non-integer and even complex values [76].

1.2.1 Gamma Function

The gamma function $\Gamma(z)$ is defined by the integral [51]

$$\Gamma(z) = \int_0^\infty e^{-t} t^{z-1} dt, \quad Re(z) > 0 \tag{1.2.1}$$

which is the Euler integral of the second kind and converges in the right half of the complex plane $Re(z) > 0$. If $z = x + iy$, indeed we have

$$\Gamma(x+iy) = \int_0^\infty e^{-t} t^{x-1+iy} dt = \int_0^\infty e^{-t} t^{x-1} e^{iy\log(\mathrm{t})} dt.$$
$$= \int_0^\infty e^{-t} t^{x-1} \big(\cos(y\log(\mathrm{t})) + i \sin(y\log(\mathrm{t}))\big)\, dt, \tag{1.2.2}$$

which is convergent for any $x > 0$. The reduction formula of the gamma function is

$$\Gamma(z+1) = z\Gamma(z), \quad Re(z) > 0 \tag{1.2.3}$$

which can be proved by integrating by parts [76], with $z > 0$, $z \in \mathbb{R}$

$$\Gamma(z+1) = \int_0^\infty e^{-t} t^z dt = [-e^{-t} t^z]_0^\infty + z \int_0^\infty e^{-t} t^{z-1} dt = z\Gamma(z).$$

Since, $\Gamma(1) = 1$, the recurrence shows that for any positive integer z [72],

$$\Gamma(z+1) = z\Gamma(z) = z(z-1)\Gamma(z-1) = \cdots = z(z-1)(z-2)\ldots 2.1.\Gamma(1) = z!$$

1.2.2 Beta Function

The beta function $\mathcal{B}(z, w)$ is defined by [76]

$$\mathcal{B}(z, w) = \int_0^1 t^{z-1} (1-t)^{w-1} dt, \quad Re(z) > 0, Re(w) > 0, \tag{1.2.4}$$

which is the Euler's integral of first kind. By using Laplace transform the beta function can be written in terms of gamma function.

$$\mathcal{B}(z, w) = \frac{\Gamma(z)\Gamma(w)}{\Gamma(z+w)}, \quad Re(z) > 0, Re(w) > 0. \tag{1.2.5}$$

1.2.3 Mittag-Leffler function

The Mittag-Leffler function also plays a very important role in the research of fractional calculus. The classical Mittag-Leffler function for one parameter is defined by [51],

$$E_\alpha(z) \;:=\; \sum_{k=0}^\infty \frac{z^k}{\Gamma(\alpha k + 1)}, \quad z \in \mathbb{C}, Re(\alpha) > 0, \tag{1.2.6}$$

In particular, when $\alpha = 1$ and $\alpha = 2$, we have, $E_1(z) = e^z$ and $E_2(z) = \cosh(\sqrt{z})$.

The Mittag-Leffler type function with two parameter α, β, is defined by the series expansion as follows [76],

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

1.3 Structure of the thesis

In Chapter 2, we will look into the basic preliminaries and fundamentals of fractional differential equations. Some of the important solution methods of fractional calculus are discussed in this chapter. Additionally we will present the existence and uniqueness theorems of the solution.

In Chapter 3, we will discuss Diethelm's numerical method for solving fractional ordinary differential equations (ODEs). In [26], Diethelm considered linear fractional differential equation and used a first-degree compound quadrature formula to approximate the Hadamard finite-part integral in the equivalent form of the considered equations and defined a numerical method for solving the equations. Here we approximate the Hadamard finite-part integral by using the second-degree compound quadrature formula and obtain a higher order numerical method for the considered fractional differential equations.

In Chapter 4, we will discuss another numerical method, the fractional Adams-type method (also called predictor-corrector method) for solving fractional differential equations (FDEs) which has been developed by three well-known mathematicians Kai Diethelm, Neville J. Ford and Alan D. Freed. In [29], the authors approximated the equivalent integral equation by using a piecewise linear interpolation polynomial and introduced a fractional Adams method for solving fractional ODEs. We will use piecewise quadratic interpolation polynomials to approximate the integral and introduce a high order fractional Adams method for solving the fractional ODEs.

In Chapter 5, we will consider the Richardson extrapolation technique for solving fractional differential equations. In this chapter we will also discuss the initial value and the initial integral approximation appeared in the numerical algorithm based on the piecewise quadratic interpolation polynomial approximations.

In Chapter 6, we will consider finite difference method for space-fractional partial differential equations. We will examine the stability, consistency and convergence of the proposed finite difference method. A shifted implicit finite difference method is introduced for solving two-sided space-fractional partial differential equation and we prove that the order of convergence of the finite difference method is $O(\Delta t + \Delta x^{\min(3-\alpha, \beta)}), 1 < \alpha < 2$, $\beta > 0$, where $\Delta t, \Delta x$ denote the time and space stepsizes, respectively.

In Chapter 7, we will outline the summary of the thesis and will indicate the further research plan.

Chapter 2

Fractional differential equations (FDEs)

2.1 Introduction

Fractional differential equations provide an excellent mathematical tool for the description of memory and hereditary properties of various materials and processes [10]. These operators are non-local which is the most significant advantage in the applications. The standard derivative of a function includes information about the value of the function at certain earlier time points only, while the fractional derivative encapsulates information about the function's behaviour from the earliest point in time up to the present.

The advantages of fractional differential equations become apparent in modelling mechanical and electrical properties of real materials, as well as in the description of rheological properties of rocks [10]. FDEs have been used successfully to model frequency dependent damping behaviour of many viscoelastic materials [52], cardiac electrophysiological model [8], electrochemical process [50], a radial flow problem [64]. Many papers have also been involved in illustrating the application of FDEs in dielectric polarization [87], control of viscoelastic structures [3].

Several analytical methods have been proposed to solve FDEs, for example Laplace transform, Mellin transform, Fourier transform, model synthesis, eigenvector expansion etc.. Most of these methods are only applicable to solve linear FDEs but cannot be applied in non-linear FDEs.

Recent developments have seen a tremendous interest in approximating numerical solution for FDEs which can be effectively applied to both linear and non-linear FDEs (see Diethelm [25, 31], Lubich [55]). As pointed out by Diethelm and Freed [31], most of the techniques of solving initial value problems (IVPs) of FDEs are equivalent to Volterra integral equations. Therefore the numerical schemes for Volterra integral equations can be applied to FDEs. Lubich [53, 54] took the advantage for the fact FDEs can be converted into Volterra integral equations. Diethelm and Walz [33] presented an extrapolation method for numerical solution of FDEs. This was based on the algorithm of [26] where the application of extrapolation was justified. The algorithm used the Hadamard finite-part integral stated in [24] to determine the weights of the numerical solution. Diethelm et al. [29] presented a predictor-corrector numerical method for solving FDEs. It was demonstrated that the Adam-Moulton predictor-corrector method of ODEs can be extended to predictor-corrector method of FDEs and a detailed error analysis for fractional Adams method was produced.

2.2 Definitions

In this section we will introduce some of the fundamental definitions of fractional derivatives and integrals, such as Riemann-Liouville integral, Riemann-Liouville fractional derivatives, Caputo derivative, Hadamard finite-part integral etc. We will also discuss some theorems and facts related to fractional calculus that we will apply in our research.

2.2.1 Riemann-Liouville (R-L) fractional integral

Let $n \in \mathbb{R}^+$. The operator J_a^n defined on $L^1(a, b)$ by [25]

$$J_a^n f(t) := \frac{1}{\Gamma(n)} \int_a^t (t-\tau)^{n-1} f(\tau) d\tau, \tag{2.2.1}$$

for $a \leq t \leq b$, is called the Riemann-Liouville fractional integral operator of order n.

For $n = 0$ we set $J_a^0 := I$, the identity operator and in this case the operator is quite convenient for further manipulations. In fact,

$$\begin{aligned}
\lim_{n\to 0} J_a^n f(t) &= \lim_{n\to 0} \frac{1}{\Gamma(n)} \int_a^t (t-\tau)^{n-1} f(\tau) d\tau, \\
&= \lim_{n\to 0} \frac{1}{\Gamma(n)} \int_a^t f(\tau) d\Big(-\frac{(t-\tau)^n}{n}\Big), \\
&= \lim_{n\to 0} \frac{1}{\Gamma(n+1)} \Big[f(a)(t-a)^n + \int_a^t f'(\tau)(t-\tau)^n d\tau\Big], \\
&= 1 \cdot [f(a) \cdot 1 + \int_a^t f'(\tau) \cdot 1 d\tau\Big], \\
&= f(a) + f(t) - f(a) = f(t).
\end{aligned}$$

Thus, $J_a^0 f(t) = f(t)$.
Moreover, in [25] the case of $n \geq 1$ it is obvious that the integral $J_a^n f(t)$ exists for every $t \in [a, b]$ because the integrand is the product of an integrable function f and the continuous function $(t - \cdot)^{n-1}$. One of the most important property of Riemman-Liouville integral is as follows.

Theorem 2.2.1. [25] Let $\alpha, \beta \geq 0$ and $f \in L^1(a, b)$.Then

$$J_a^\alpha J_a^\beta f = J_a^{\alpha+\beta} f. \tag{2.2.2}$$

holds almost everywhere on $[a, b]$. If additionally $f \in C[a, b]$ or $\alpha + \beta \geq 1$, then the identity holds everywhere on $[a, b]$. Theorem 2.2.1 gives the commutative property,

$$J_a^\alpha J_a^\beta = J_a^\beta J_a^\alpha. \tag{2.2.3}$$

2.2.2 Riemann-Liouville fractional derivative

Suppose $p > 0$ we define the following Riemann-Liouville fractional derivative as [76]

$${}_0^R D_t^p f(t) = D^n[{}_0^R D_t^{p-n} f(t)] = D^n \frac{1}{\Gamma(n-p)} \int_0^t (t-\tau)^{n-p-1} f(\tau) d\tau, \quad p > 0, \tag{2.2.4}$$

where $D^n = \frac{d^n}{dt^n}$ and $n - 1 < p < n$. Recall that $D^n = \frac{d^n}{dt^n}$ is the derivative part while $[{}_0^R D_t^{p-n} f(t)] = J_0^{n-p} f(t)$ is Riemann-Liouville integral part.

Example 1. *Suppose $f(t) = t^2$, find the value of ${}_0^R D_t^{\frac{1}{2}} f(t)$?*

Solution: *Here $p = \frac{1}{2}$ and lies on the interval $0 < p < 1$ such that $n = 1$. Using (2.2.4) gives*

$$ {}_0^R D_t^{\frac{1}{2}} f(t) = D^1[{}_0^R D_t^{-\frac{1}{2}} f(t)] = \frac{d}{dt}\left[\frac{1}{\Gamma(\frac{1}{2})}\int_0^t (t-\tau)^{-\frac{1}{2}}\tau^2 d\tau\right]. \tag{2.2.5} $$

2.2.3 Caputo fractional derivative

Suppose $n-1 < p < n$ and $p > 0$ we define the following Caputo's fractional derivative as [76]

$$ {}_0^C D_t^p f(t) = {}_0^R D_t^{p-n}[D^n f(t)] = \frac{1}{\Gamma(n-p)}\int_0^t (t-\tau)^{n-p-1}\left[D^n f(\tau)\right] d\tau, \tag{2.2.6} $$

Example 2. *Suppose $f(t) = t^2$, find the value of ${}_0^C D_t^{\frac{1}{2}} f(t)$?*

Solution: *Here $p = \frac{1}{2}$ and lies on the interval $0 < p < 1$ such that $n = 1$. Using (2.2.6) gives*

$$ {}_0^C D_t^{\frac{1}{2}} f(t) = {}_0^R D_t^{\frac{1}{2}-1}[D^1 f(t)] = \frac{1}{\Gamma(\frac{1}{2})}\int_0^t (t-\tau)^{-\frac{1}{2}}\left[\frac{d}{d\tau}f(\tau)\right] d\tau. \tag{2.2.7} $$

Remark 3. Suppose $p > 0$ and $n-1 < p < n$, then the relation between Riemman-Liouville and Caputo fractional derivative can be expressed by the theorem [25] below

Theorem 2.2.2. Let $p > 0$ and $n-1 < p < n$, we have,

$$ {}_0^R D_t^p f(t) = {}_0^C D_t^p f(t) + \sum_{k=0}^{n-1}\frac{f^{(k)}(0)}{\Gamma(-p+k+1)}t^{k-p}. \tag{2.2.8} $$

Proof. We only consider the case for $n = 1$ and $0 < p < 1$

$$ \begin{aligned} {}_0^R D_t^p f(t) &= D^1[{}_0^R D_t^{p-1} f(t)] = \frac{d}{dt}\left[\frac{1}{\Gamma(1-p)}\int_0^t (t-\tau)^{-p} f(\tau) d\tau\right] \\ &= \frac{d}{dt}\left(\frac{1}{\Gamma(1-p)}\left[-f(\tau)\frac{(t-\tau)^{-p+1}}{-p+1}\right]_{\tau=0}^{\tau=t} + \int_0^t \frac{(t-\tau)^{-p+1}}{-p+1} f'(\tau) d\tau\right) \\ &= \frac{d}{dt}\left(\frac{1}{\Gamma(1-p)}\left[f(0)\frac{t^{1-p}}{1-p} + \int_0^t \frac{(t-\tau)^{1-p}}{1-p} f'(\tau) d\tau\right]\right) \\ &= \frac{1}{\Gamma(1-p)} f(0) t^{-p} + \frac{d}{dt}\frac{1}{\Gamma(1-p)}\int_0^t \frac{(t-\tau)^{1-p}}{1-p} f'(\tau) d\tau \\ &= \frac{1}{\Gamma(1-p)} f(0) t^{-p} + \frac{1}{\Gamma(1-p)}\int_0^t \left[\frac{\partial}{\partial t}\left(\frac{(t-\tau)^{1-p}}{1-p} f'(\tau)\right)\right] d\tau \\ &= \frac{1}{\Gamma(1-p)} f(0) t^{-p} + \frac{1}{\Gamma(1-p)}\left[\int_0^t (t-\tau)^{-p} f'(\tau) d\tau\right] \\ &= {}_0^C D_t^p f(t) + \frac{1}{\Gamma(1-p)} f(0) t^{-p}. \end{aligned} $$

Similarly, we can prove the case for $n-1 < p < n$, $n > 1$, i.e;

$$ {}_0^R D_t^p f(t) = {}_0^C D_t^p f(t) + \sum_{k=0}^{n-1} \frac{f^{(k)}(0)}{\Gamma(-p+k+1)} t^{k-p}. \tag{2.2.9} $$

□

2.2.4 Hadamard finite -part integral

Hadamard finite-part integral is one of the most important mathematical tools in fractional derivatives, integral equations and partial differential equations. Let $\mathbb{N}$ denote the set of all natural numbers then, for $p \notin \mathbb{N}$, on a general interval $[a, b]$ Hadamard finite-part integral is defined in [24] as follows:

$$ \begin{aligned} &\oint_a^b (x-a)^{-p} f(x) dx \qquad (2.2.10)\\ &:= \sum_{k=0}^{\lfloor p \rfloor - 1} \frac{f^{(k)}(a)(b-a)^{k+1-p}}{(k+1-p)k!} + \int_a^b (x-a)^{-p} R_{\lfloor p \rfloor -1}(x, a) dx, \end{aligned} $$

where

$$ R_\mu(x, a) := \frac{1}{\mu!} \int_a^x (x-y)^\mu f^{(\mu+1)}(y) dy, \tag{2.2.11} $$

and $\oint$ denotes the Hadamard finite-part integral. $\lfloor p \rfloor$ denotes the largest integer not exceeding p, where $p \notin \mathbb{N}$.

Hadamard finite-part integral is the mathematical tool which reformulates a boundary value problem for a partial differential equation with integer-order singularities and also encountered the non-integer order singularities.

In particular, from [24] we can see that the Riemann-Liouville fractional derivatives ${}_a^R D_x^p f$ of order $p > 0$, $p \notin \mathbb{N}$ of the function f may be expressed as a finite-part integral according to

$$ {}_a^R D_x^p f(x) = \frac{1}{\Gamma(-p)} \oint_a^x (x-y)^{-p-1} f(y) dy. \tag{2.2.12} $$

2.2.5 Grünwald-Letnikov fractional derivative

Grünwald and Letnikov independently developed another non-integer derivative nearly the same time when Riemann and Liouville developed Riemann-Liouville fractional derivative to solve fractional differential equations. Later on many other authors use this Grünwald-Letnikov fractional derivative to construct numerical methods for fractional differential equations.

The Grünwald-Letnikov fractional derivative can be expressed as follows [51]. Let $\alpha \in \mathbb{R}^+$. The operator ${}^{GL}D_a^\alpha$ defined by,

$$
{}^{GL}D_a^\alpha f(t) = \lim_{h\to 0} \frac{(\Delta_h^\alpha f)(t)}{h^\alpha} = \lim_{mh=t-a,\, h\to 0} \frac{1}{h^\alpha} \sum_{k=0}^{m} (-1)^k \begin{pmatrix} \alpha \\ k \end{pmatrix} f(t-kh), \quad (2.2.13)
$$

for $a \leq t \leq b$, is called the Grünwald-Letnikov fractional derivative of order α. Here, $(\Delta_h^\alpha f)(t)$ is a fractional formulation of backward difference. This definition holds for arbitrary function $f(t)$, but the convergence of the infinite sum cannot be ensured for all functions.

2.3 Numerical methods for solving FDEs

In this section we will briefly review some numerical methods for fractional differential equations. There are a number of numerical and analytical methods developed for various types of FDEs, for example, variational iterative method, fractional differential transform method, a domain decomposition method, homotopy perturbation method and power series method [4].

Hadamard finite-part integral is used by Diethelm[1997] [24] to obtain an approximate algorithm for solving fractional differential equation. Podlubny [76] used the Grünwald-Letnikov method to solve FDEs. And very recently Diethelm, Ford and Freed [29] introduced a fractional Adams-type predictor-corrector method for solving FDEs. Lubich [53] wrote the fractional differential equation in the form of an Abel-Volterra integral equation and used the convolution quadrature method to approximate the fractional integral and obtained an approximate solution for fractional differential equations.

In our research we are aiming to use Diethelm's algorithm and Adams-type predictor-corrector algorithm for higher order numerical methods for solving fractional differential equations, the methods that are more accurate and cost effective in mathematical modelling. Diethelm [26] considered a linear fractional differential equation, with $0 < \alpha < 1$, and used a first-degree compound quadrature formula to approximate the Hadamard finite-part integral in the equivalent form of the considered equations and defined a numerical method with order of convergence of $O(h^{2-\alpha}), 0 < \alpha < 1$, see also [30]. Here we are aiming to use the second-degree compound quadrature formula to approximate the Hadamard finite-part integral for higher order convergence method. And in [29] Kai Diethelm, Neville J. Ford and Alan D. Freed introduced Adams-type predictor-corrector method for solving both linear and nonlinear fractional differential equations. In the numerical algorithm the authors converted the considered equations into the Volterra integral equation and then approximated the integral by using a piecewise linear interpolation polynomial and proved that the order of convergence of the numerical method is $O(h^2)$ for $1 < \alpha < 2$ and $O(h^{1+\alpha})$ for $0 < \alpha < 1$ if ${}_0^C D_t^\alpha y(t) \in C^2[0, T]$. We will use piecewise quadratic interpolation polynomials to approximate the integral and introduce a high order fractional Adams method for solving the fractional differential equations and prove that the order of convergence of our numerical method is higher than the order of the method in [29].

2.4 Existence and uniqueness of the solution of FDEs

Existence and uniqueness of the solution are very important mathematical elements for any differential equations. In this section we will discuss about the existence and uniqueness of FDEs in the Riemann-Liouville sense and the initial conditions are specified according to Caputo's suggestions [27], thus allowing for interpretation in a physically meaningful way.

Let us consider the initial-value problem, with $m - 1 < q < m$, $m \geq 1$

$$ {}_0^C D_x^q y(x) = f(x, y(x)), \tag{2.4.1} $$

$$ y^{(k)}(0) = y_0^k, \qquad k = 0, 1, 2, \ldots, m-1. \tag{2.4.2} $$

where ${}_0^C D_x^q y(x)$ represents the Caputo fractional derivative of order $q > 0$, with $m - 1 < q < m$,

$$ {}_0^C D_x^q y(x) := \frac{1}{\Gamma(m-q)} \int_0^x (x-u)^{m-1-q} y^{(m)}(u) du. \tag{2.4.3} $$

The existence and the uniqueness of the solution is described by Diethelm and Ford [27] in the following two theorems that are very similar to the corresponding classical theorems known in the case of first-order equation.

Theorem 2.4.1. (Existence) [27] Assume that $\mathbb{D} := [0, \mathcal{X}^*] \times [y_0^0 - \alpha, y_0^0 + \alpha]$ with some $\mathcal{X}^* > 0$ and some $\alpha > 0$, and let the function $f : \mathbb{D} \to \mathbb{R}$ be continuous. Furthermore, define $\mathcal{X} := \min\{\mathcal{X}^*, (\frac{\alpha\Gamma(q+1)}{||f||_\infty})^{\frac{1}{q}}\}$. Then there exists a function $y : [0, \mathcal{X}] \to \mathbb{R}$ solving the initial value problem (2.4.1)-(2.4.2).

Theorem 2.4.2. (Uniqueness) [27] Assume that $\mathbb{D} := [0, \mathcal{X}^*] \times [y_0^0 - \alpha, y_0^0 + \alpha]$ with some $\mathcal{X}^* > 0$ and some $\alpha > 0$. Furthermore, let the function $f : \mathbb{D} \to \mathbb{R}$ be bounded on $\mathbb{D}$ and fulfil a Lipschitz condition with respect to the second variable, i.e.

$$|f(x, y) - f(x, z)| \leq L|y - z|.$$

with some constant $L > 0$ independent of x, y, and z. Then, denoting $\mathcal{X}$ as in Theorem 2.4.1 there exists at most one function $y : [0, \mathcal{X}] \to \mathbb{R}$ solving the initial value problem (2.4.1)-(2.4.2).

To prove the existence and uniqueness theorems we need to know the following results:

Lemma 2.4.3. [27] If the function f is continuous, then the initial value problem (2.4.1)-(2.4.2) is equivalent to the non-linear Volterra integral equation of the second kind

$$y(x) = \sum_{k=0}^{m-1} \frac{x^k}{k!} y^{(k)}(0) + \frac{1}{\Gamma(q)} \int_0^x (x - z)^{q-1} f(z, y(z)) dz. \tag{2.4.4}$$

with $m - 1 < q \leq m$. In other words, every solution of the Volterra equation (2.4.4) is also a solution of our initial value problem (2.4.1)-(2.4.2), and vice-versa.

Theorem 2.4.4. [27] Let U be a nonempty closed subset of a Banach space E, and let $\alpha_n \geq 0$ for every n and such that $\sum_{n=0}^{\infty} \alpha_n$ converges. Moreover, let the mapping $A : U \to U$ satisfy the inequality

$$||A^n u - A^n v|| \leq \alpha_n ||u - v||, \tag{2.4.5}$$

for every $n \in \mathbb{N}$ and every $u, v \in U$. Then, A has a unique defined fixed point u^*. Furthermore, for any $u_0 \in U$, the sequence $(A^n u_0)_{n=1}^{\infty}$ converges to this point u^*.

Proof. of Theorem 2.4.2 (Uniqueness): [27] As we identified previously, we need only discuss the case $0 < q < 1$. In this situation, the Volterra equation (2.4.4) reduces to

$$y(x) = y_0^0 + \frac{1}{\Gamma(q)} \int_0^x (x-z)^{q-1} f(z, y(z)) dz. \tag{2.4.6}$$

we thus introduce the set $U = \{y \in C[0, \mathcal{X}] : \| y - y_0^0 \|_\infty \leq \alpha\}$. Obviously, this is a closed subset of the Banach space of all continuous functions on $[0, \mathcal{X}]$, equipped with the Chebyshev norm. Since the constant function $y \equiv y_0^0$ is in U, we also see that U is not empty. On U we define the operator A by

$$(Ay)(x) = y_0^0 + \frac{1}{\Gamma(q)} \int_0^x (x-z)^{q-1} f(z, y(z)) dz. \tag{2.4.7}$$

Using this operator, the equation under consideration can be rewritten as

$$y = Ay.$$

and in order to prove our desired uniqueness result, we have to show that A has a unique fixed point. Let us therefore investigate the properties of the operator A. First we note that, for $0 \leq x_1 \leq x_2 \leq \mathcal{X}$,

$$\begin{aligned}
&\Big|(Ay)(x_1) - (Ay)(x_2)\Big| \\
&= \frac{1}{\Gamma(q)} \Big| \int_0^{x_1} (x_1 - z)^{q-1} f(z, y(z)) dz - \int_0^{x_2} (x_2 - z)^{q-1} f(z, y(z)) dz \Big| && (2.4.8) \\
&= \frac{1}{\Gamma(q)} \Big| \int_0^{x_1} \Big((x_1 - z)^{q-1} - (x_2 - z)^{q-1} \Big) f(z, y(z) dz + \int_{x_1}^{x_2} (x_2 - z)^{q-1} f(z, y(z)) dz \Big| \\
&\leq \frac{\| f \|_\infty}{\Gamma(q)} \Big[\int_0^{x_1} \Big((x_2 - z)^{q-1} - (x_1 - z)^{q-1} \Big) dz + \int_{x_1}^{x_2} (x_2 - z)^{q-1} dz \Big] \\
&= \frac{\| f \|_\infty}{\Gamma(q+1)} \Big(2(x_2 - x_1)^q + x_1^q - x_2^q \Big). && (2.4.9)
\end{aligned}$$

proving that Ay is a continuous function. Moreover, for $y \in U$ and $x \in [0, \mathcal{X}]$, we find

$$\begin{aligned}
\Big|(Ay)(x) - y_0^0\Big| &= \frac{1}{\Gamma(q)} \Big| \int_0^x (x-z)^{q-1} f(z, y(z)) dz \Big| \leq \frac{1}{\Gamma(q+1)} \| f \|_\infty x^q \\
&\leq \frac{1}{\Gamma(q+1)} \| f \|_\infty \mathcal{X}^q \leq \frac{1}{\Gamma(q+1)} \| f \|_\infty \frac{\alpha \Gamma(q+1)}{\| f \|_\infty} = \alpha.
\end{aligned}$$

Thus, we have shown that $Ay \in U$ if $y \in U$; i.e., A maps the set U to itself. Then next step is to prove that, for every $n \in \mathbb{N}_0$ and every $x \in [0, \mathcal{X}]$, we have

$$\| A^n y - A^n \bar{y} \|_{L_\infty[0,x]} \leq \frac{(Lx^q)^n}{\Gamma(1+qn)} \| y - \bar{y} \|_{L_\infty[0,x]} . \tag{2.4.10}$$

This can be seen by induction. In the case $n = 0$, the statement is trivially true. For the induction step $n-1 \to n$, we write

$$\begin{aligned}
\| A^n y - A^n \bar{y} \|_{L_\infty[0,x]} &= \| A(A^{n-1}y) - A(A^{n-1}\bar{y}) \|_{L_\infty[0,x]} \\
&= \frac{1}{\Gamma(q)} \sup_{0\leq w \leq x} \Big| \int_0^w (w-z)^{q-1}[f(z, A^{n-1}y(z)) - f(z, A^{n-1}\bar{y}(z))]dz \Big|.
\end{aligned}$$

In the next steps, we use the Lipschitz assumption on f and the induction hypothesis and find

$$\begin{aligned}
\| A^n y - A^n \bar{y} \|_{L_\infty[0,x]} &\leq \frac{L}{\Gamma(q)} \sup_{0\leq w \leq x} \int_0^w (w-z)^{q-1} \Big| A^{n-1}y(z) - A^{n-1}\bar{y}(z) \Big| dz \\
&\leq \frac{L}{\Gamma(q)} \int_0^x (x-z)^{q-1} \sup_{0\leq w \leq z} \Big| A^{n-1}y(w) - A^{n-1}\bar{y}(w) \Big| dz \\
&\leq \frac{L^n}{\Gamma(q)\Gamma(1+q(n-1))} \int_0^x (x-z)^{q-1} z^{q(n-1)} \sup_{0\leq w \leq z} \Big| y(w) - \bar{y}(w) \Big| dz \\
&\leq \frac{L^n}{\Gamma(q)\Gamma(1+q(n-1))} \sup_{0\leq w \leq x} \Big| y(w) - \bar{y}(w) \Big| \int_0^x (x-z)^{q-1} z^{q(n-1)} dz \\
&= \frac{L^n}{\Gamma(q)\Gamma(1+q(n-1))} \| y - \bar{y} \|_{L_\infty[0,x]} \frac{\Gamma(q)\Gamma\Big(1+q(n-1)\Big)}{\Gamma(1+qn)} x^{qn}.
\end{aligned}$$

which is our desired result (2.4.10). As a consequence, we find, taking Chebyshev norms on our fundamental interval $[0, x]$,

$$\| A^n y - A^n \bar{y} \|_\infty \leq \frac{(Lx^q)^n}{\Gamma(1+qn)} \| y - \bar{y} \|_\infty .$$

We have now shown that the operator A fulfills the assumptions of Theorem 2.4.4 with $\alpha_n = (Lx^q)^n/\Gamma(1+qn)$. In order to apply that theorem, we only need to verify that the series $\sum_{n=0}^\infty \alpha_n$ converges. This, however, is a well known result; the limit

$$\sum_{n=0}^\infty \frac{(Lx^q)^n}{\Gamma(1+qn)} = E_q(Lx^q).$$

is the Mittag-Leffler function of order q, evaluated at Lx^q (see[36, Chapter 18] for general results on Mittag-Leffler functions or [49] for details on the role of these functions in fractional calculus). Therefore, we may apply the fixed point theorem and deduce the uniqueness of the solution of our differential equation.

Remark 1. Note that Theorem 2.4.4 not only asserts that the solution is unique; it actually gives us (at least theoretically) a means of determining this solution by Picard-type iteration process.

Remark 2. Without the Lipschitz assumption on f the solution needs not be unique. To see this, look at the simple one-dimensional example
${}_{0}^{C}D_{x}^{q}y = y^{k}, \qquad 0 < q < 1,$
with initial condition $y(0) = 0$. Consider $0 < k < 1$, so that the function on the right-hand side of the differential equation is continuous, but the Lipschitz condition is violated. Obviously, the zero function is a solution of the initial value problem. However, setting $p_j(x) = x^j$, we recall that

$${}_{0}^{C}D_{x}^{q}p_j(x) = \frac{\Gamma(j+1)}{\Gamma(j+1-q)}p_{j-q}(x).$$

Thus, the function $y(x) = \sqrt[k]{\Gamma(j+1)/\Gamma(j+1-q)}x^j$ with $j = q/(1-k)$ also solves the problem, proving that the solution is not unique.

Proof. of Theorem 2.4.1 [27]: We begin by argument similar to those of the previous proof. In particular, we use the same operator A defined in (2.4.7) and recall that it maps the nonempty, convex, and closed set $U = \{y \in C[0,x] : \| y - y_0^0 \|_\infty \leq \alpha\}$ to itself.

We shall now prove that A is a continuous operator. A stronger result, (2.4.10), has been derived above, but in that derivation we used the Lipschitz property of f which we do not assume to hold here. Therefore, we proved differently and note that, since f is continuous on the compact set D, it is uniformly continuous there. Thus, given an arbitrary $\epsilon > 0$, we can find $\delta > 0$ such that

$$|f(x,y) - f(x,z)| < \frac{\epsilon}{x^q}\Gamma(q+1) \qquad \text{whenever} \qquad |y - z| < \delta. \tag{2.4.11}$$

Now let $y, \bar{y} \in U$ such that $\| y - \bar{y} \| < \delta$. Then, in view of (2.4.11),

$$|f(x, y(x)) - f(x, \bar{y}(x))| < \frac{\epsilon}{x^q}\Gamma(q+1), \tag{2.4.12}$$

for all $x \in [0, \mathcal{X}]$. Hence,

$$\begin{aligned} |(Ay)(x) - (A\bar{y})(x)| &= \frac{1}{\Gamma(q)}\Big|\int_0^x (x-z)^{q-1}(f(z,y(z)) - f(z,\bar{y}(z)))dz\Big| \\ &\leq \frac{\Gamma(q+1)\epsilon}{x^q\Gamma(q)}\int_0^x (x-z)^{q-1}dz = \frac{\epsilon x^q}{x^q} \leq \epsilon, \end{aligned}$$

proving the continuity of the operator A.

Next we look at the set of functions

$$A(U) := \{Ay : y \in U\}.$$

For $z \in A(U)$ we find that, for all $x \in [0, \mathcal{X}]$,

$$\begin{aligned} |z(x)| &= |(Ay)(x)| \leq |y_0^0| + \frac{1}{\Gamma(q)}\int_0^x (x-z)^{q-1}\big|f\big(z, y(z)\big)\big|dz \\ &\leq |y_0^0| + \frac{1}{\Gamma(q+1)} \parallel f \parallel_\infty \mathcal{X}^q, \end{aligned}$$

which means that $A(U)$ is bounded in a pointwise sense. Moreover, for $0 \leq x_1 \leq x_2 \leq \mathcal{X}$, we have found in the proof of Theorem 2.4.2 that

$$|(Ay)(x_1) - (Ay)(x_2)| \leq \frac{\parallel f \parallel_\infty}{\Gamma(q+1)}(x_1^q - x_2^q + 2(x_2 - x_1)^q) \leq 2\frac{\parallel f \parallel_\infty}{\Gamma(q+1)}(x_2 - x_1)^q.$$

Thus, if $|x_2 - x_1| < \delta$, then

$$|(Ay)(x_1) - (Ay)(x_2)| \leq 2\frac{\parallel f \parallel_\infty}{\Gamma(q+1)}\delta^q.$$

Noting that the expression on the right-hand side is independent of y, we see that the set $A(U)$ is equicontinuous. Then, the *Arzelà*-Ascoli theorem yields that every sequence of functions from $A(U)$ has got a uniformly convergent subsequence, and therefore $A(U)$ is relatively compact. Then, Schauder's fixed point theorem asserts that A has a unique fixed point. By construction, a fixed point of A is a solution of our initial value problem.

2.5 Applications of fractional differential equations

Applications come from a very wide range of science and engineering. Fractional differential equations are becoming increasingly used as a modelling tool for understanding the many aspects of nonlocality, for example;

- Fractional-order viscoelasticity models in blood flow [14] : The integer-order stress-strain relation models (such as; Hook's law for elastic solids and Newton's law for viscous liquids , Voigt and standard liner or Kelvin-Zener) for heterogeneous soft tissue with complex bio-mechanical properties in blood flow, provide a reasonable qualitative description; however, they do not satisfactorily describe the real situation in the real world [75, 17]. On the other hand for the cell and tissue biomechanics the fractional-order models proposed by Craiem and Armentano [16], Craiem et al [15], and Doehring et al. [23], seem to be more adequate from both quantitative and qualitative view points.

- Fractional-order model of neurons in biology [17]: In 1981, the neurodynamics of the vestibulo-ocular reflex (VOR) model have been described by Robinson [78]. This model is based on direct and integrated parallel pathways to the motoneurons. The first-order transfer functions approximate time and frequency domain data from canal afferents, vestibular and prepositus nuclei neurons, and motoneurons. Anastasio [1] recognized some difficulties in the classical integer-order models to describe the behaviour of premotor neurons in the vestibulo–ocular relax system. To overcome this problem he proposed a fractional-order model in terms of the Laplace transform of the premotor neuron discharge rate and proved that fractional differentiation and integrations can effectively be used to describe various aspects of vestibulo-oculomotor dynamics.

- Fractional calculus in physics : Fractional derivatives are involved in the modelling of electrical circuits and generalized voltage divider [17]. Le Mehaute and Crepy [59] suggested electrical circuits may have the fractance which represents an electrical element with fractional-order impedance.

- Fractional calculus in electrochemistry and tracer fluid flows: The fractional advection-dispersion equation (FADE) is used in groundwater hydrology to model the transport of passive tracers carried by fluid flow in a porous medium. Dispersion (or spreading) of tracers depends strong on the scale of observation. In general, there are three different mechanisms of dispersion [17]: molecular diffusion, variations in the permeability field (microdispersion), and variations of the fluid velocity in a porous medium (microdispersion). These mechanisms take place at different scales. At large scale, dispersion is essentially controlled by permeability heterogenetic. A fractal structure model for heterogeneous media has been developed by Maloy et al for details see [69].

- Continuous time random walk (CTRW) model: The CTRW models impose a random waiting time between particle jumps [67] and the non-local CTRW model is a good phenomenological description of the tick-by-tick dynamics, which can take into account the pathological time evolution of financial markets. This non-local CTRW model is very much related to the fractional calculus. For details see [63, 68].

- Cardiac electrical propagation model [8] : Fractional diffusion model in electrical propagation with heterogeneous media describe their application to cardiac muscle as a representative case of composite biological tissue. It describes the propagation of electrical excitation in the cable equation; for details see [8].

- Fractional order dynamical systems in control theory [17] : This is the generalization of the classical PID-controller, the concept of the $PI^{\lambda}D^{\mu}$-controller, involving fractional-order integrator and fractional order differentiator [76], which has been found to be a more efficient control of fractional order dynamic systems.

Chapter 3

Higher order numerical method for fractional ODEs (Diethelm's method)

3.1 Introduction

We consider numerical methods for solving the fractional differential equation

$$
{}_0^C D_t^{\alpha} y(t) = f(t, y(t)), \quad 0 < t < T, \tag{3.1.1}
$$

$$
y^{(k)}(0) = y_0^k, \quad k = 0, 1, 2, \ldots, \lceil \alpha \rceil - 1, \tag{3.1.2}
$$

where the y_0^k may be arbitrary real numbers and $\alpha > 0$. Here ${}_0^C D_t^{\alpha}$ denotes the differential operator in the sense of Caputo, $n - 1 < \alpha < n$,

$$
{}_0^C D_t^{\alpha} y(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t (t-u)^{n-\alpha-1} y^{(n)}(u)\, du,
$$

where $n = \lceil \alpha \rceil$ is the smallest integer $\geq \alpha$.

Existence and uniqueness of solutions for (3.1.1) -(3.1.2) have been studied, for example, in Podlubny [76], Diethelm and Ford [27]. Numerical methods for solving fractional differential equations have been considered by many authors and we mention here a few key contributions. Lubich [53] wrote the fractional differential equation in the form of an Abel-Volterra integral equation and used the convolution quadrature method to approximate the fractional integral and obtained approximate solutions of the fractional differential equation. Diethelm [26] wrote the fractional Riemann-Liouville derivative by using the Hadamard finite-part integral and approximated the integral by using a quadrature formula and obtained an implicit numerical algorithm for solving a linear fractional differential equation. Diethelm and Luchko [32] used the observation that a fractional differential equation has an exact solution, which can be expressed as a Mittag-Leffler type function. Then they used convolution quadrature and discretised operational calculus to produce an approximation to this Mittag-Leffler function. Blank [5] applied a collocation method to approximate the fractional differential equation. Podlubny [76] used the Grünwald and Letnikov method to approximate the fractional derivative and defined an implicit finite difference method for solving (3.1.1)-(3.1.2) and proved that the order of convergence is $O(h)$, where h is the stepsize. Gorenflo [47] introduced a second order $O(h^2)$ difference method for solving (3.1.1)-(3.1.2), but the conditions to achieve the desired accuracy are restrictive. In [28], the authors converted the equations (3.1.1)-(3.1.2) into a Volterra integral equation and then approximated the integral by using a piecewise linear interpolation polynomial and introduced a fractional Adams-type predictor-corrector method for solving (3.1.1)-(3.1.2), proving that the order of convergence of the numerical method is $\min\{2, 1+\alpha\}$ for $0 < \alpha \leq 2$ if ${}_0^C D_t^\alpha y \in C^2[0, T]$. Deng [18] modified the method in [28] and introduced a new predictor-corrector method for solving (3.1.1)-(3.1.2) and the convergence order is proved to be $\min\{2, 1 + 2\alpha\}$ for $\alpha \in (0, 1]$. In [95], the authors introduced a so-called Jacobi-predictor-corrector approach to solve (3.1.1)-(3.1.2) which is based on the polynomial interpolation and the Gauss-Lobatto quadrature with respect to some Jacobi-weight function and the computational cost is $O(N), N = 1/h$ and any desired convergence order can be obtained. In [9], a higher order numerical method for solving (3.1.1)-(3.1.2) is obtained where a quadratic interpolation polynomial was used to approximate the integral. Ford, Morgado and Rebelo recently (see [41]) used a non-polynomial collocation method to achieve good convergence properties without assuming any smoothness of the solution. There are also several works that are related to the fixed memory principle and the nested memory concept for solving (3.1.1)-(3.1.2), see, e.g., [44, 29, 18, 19, 22].

In [26], Diethelm considered the following linear fractional differential equation, with

$0 < \alpha < 1$,

$$ {}_0^C D_t^{\alpha} y(t) = \beta y(t) + f(t), \quad 0 \le t \le 1, \tag{3.1.3} $$

$$ y(0) = y_0, \tag{3.1.4} $$

where $\beta < 0$, f is a given function on the interval $[0, 1]$. Diethelm [26] used a first-degree compound quadrature formula to approximate the Hadamard finite-part integral in the equivalent form of (3.1.3)-(3.1.4) and defined a numerical method for solving (3.1.3)-(3.1.4) and proved that the order of convergence of the numerical method is $O(h^{2-\alpha}), 0 < \alpha < 1$. Here we approximate the Hadamard finite-part integral by using the second-degree compound quadrature formula and obtain an asymptotic expansion of the error for solving (3.1.3)-(3.1.4), which implies that the order of convergence of the numerical method is $O(h^{3-\alpha}), 0 < \alpha < 1$. Moreover, a high order finite difference method ($O(h^{3-\alpha}), 0 < \alpha < 2$) for approximating the Riemann-Liouville fractional derivative is given, which may be applied to construct high order numerical methods for solving time-space-fractional partial differential equations.

3.2 Diethelm's method

In this section we review Diethelm's method for solving fractional differential equations where the Hadamard finite-part integral is approximated by piecewise linear interpolation polynomials.

Consider, with $0 < \alpha < 1$,

$$ {}_0^C D_t^{\alpha} y(t) = \beta y(t) + f(t), \tag{3.2.1} $$

$$ y(0) = y_0. \tag{3.2.2} $$

It is well-known that (3.2.1)- (3.2.2) is equivalent to, with $0 < \alpha < 1$,

$$ {}_0^R D_t^{\alpha} \left[y(t) - y_0 \right] = \beta y(t) + f(t), \quad 0 \le t \le 1, \tag{3.2.3} $$

where α is the order of the derivative, f is a given function on the interval [0,1], $\beta \le 0$ and y is the unknown function. From the definition of Riemann-Liouville fractional derivative in Chapter 2, for $0 < \alpha < 1$ we get

$$ {}_0^R D_t^\alpha y(t) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_0^t (t-\tau)^{-\alpha} y(\tau) d\tau. \tag{3.2.4} $$

Let us recall the Diethelm's numerical algorithm for piecewise linear interpolation polynomial with the equispaced nodes. The Lemmas below will help the reader to understand the algorithm of the numerical method for solving fractional differential equations.

Lemma 3.2.1. [35] The Hadamard finite-part integral for the Riemann-Liouville derivative (3.2.4) can be written as

$$ {}_0^R D_t^\alpha y(t) = \frac{1}{\Gamma(-\alpha)} \oint_0^t (t-\tau)^{-1-\alpha} y(\tau) d\tau. $$

where $0 < \alpha \leq 1$, $\oint$ represents the symbol of Hadamard finite-part integral.

Lemma 3.2.2. [26] Assume that $0 = t_0 < t_1 < t_2 < \cdots < t_k < \cdots < t_n = 1$ is the partition on the interval $[0, 1]$ and $0 < \alpha < 1$, then at $t = t_j$,

$$ {}_0^R D_t^\alpha [y(t_j)] = h^{-\alpha} \sum_{k=0}^{j} \omega_{kj} y(t_j - t_k) + \frac{t_j^{-\alpha}}{\Gamma(\alpha)} R_j, \quad j = 1, 2, 3, \ldots, n. $$

where ω_{kj} are called the weights and R_j is the remainder term given by

$$ |R_j| \leq C j^{\alpha-2} \|y''(t_j - t_j\omega)\|_\infty, \quad 0 < \omega \leq 1, $$

where ω is the new variable $[y(\tau) = y(t_j - t_j\omega)]$ introduce in the proof, h is the time-step size and the weights ω_{kj} satisfy

$$ \Gamma(2-\alpha)\omega_{kj} = \begin{cases} 1, & k = 0 \\ -2k^{1-\alpha} + (k-1)^{1-\alpha} + (k+1)^{1-\alpha}, & k = 1, 2, \ldots, j-1 \\ -(\alpha-1)k^{-\alpha} + (k-1)^{1-\alpha} - k^{1-\alpha}, & k = j \end{cases} $$

The proof for this Lemma 3.2.2 is straightforward and requires a piecewise linear Lagrange interpolation polynomial.

Proof. We have

$$ {}_0^R D_t^\alpha y(t_j) = \frac{1}{\Gamma(-\alpha)} \oint_0^{t_j} \frac{y(\tau)}{(t_j - \tau)^{\alpha+1}} d\tau. $$

Suppose $t_j - \tau = t_j\omega$, then

$$ {}_0^R D_t^\alpha y(t_j) = \frac{t_j^{-\alpha}}{\Gamma(-\alpha)} \oint_0^1 \frac{y(t_j - t_j\omega)}{\omega^{\alpha+1}} d\omega. $$

Performing another substitution such that $g(\omega) = y(t_j - t_j\omega)$, we have

$$ {}_0^R D_t^\alpha y(t_j) = \frac{t_j^{-\alpha}}{\Gamma(-\alpha)} \oint_0^1 g(\omega)\omega^{-(\alpha+1)} d\omega. $$

For every j, we replace the integral by a piecewise interpolation polynomial with equispaced nodes $0, 1/j, 2/j, 3/j, \ldots, j/j$. That is,

$$ \oint_0^1 g(\omega)\omega^{-\alpha-1} d\omega = \oint_0^1 g_1(\omega)\omega^{-\alpha-1} d\omega + R_j, $$

where $g_1(\omega)$ is the piecewise linear interpolation polynomial of $g(\omega)$ with the equispaced nodes and R_j is the remainder term.

Note that,

$$ g_1(\omega) = \frac{\omega - \frac{k}{j}}{\frac{k-1}{j} - \frac{k}{j}} g\left(\frac{k-1}{j}\right) + \frac{\omega - \frac{k-1}{j}}{\frac{k}{j} - \frac{k-1}{j}} g\left(\frac{k}{j}\right), \quad \text{on } \left[\frac{k-1}{j}, \frac{k}{j}\right]. $$

Thus,

$$ \oint_0^1 g(\omega)\omega^{-(1+\alpha)} d\omega \approx \oint_0^1 g_1(\omega)\omega^{-(1+\alpha)} d\omega = Q_j(g). \tag{3.2.5} $$

Here we observe generally that

$$ Q_j(g) = \oint_0^1 g_1(\omega)\omega^{-(1+\alpha)} d\omega = \oint_0^{\frac{1}{j}} g_1(\omega)\omega^{-(1+\alpha)} d\omega + \sum_{k=2}^{j} \oint_{\frac{k-1}{j}}^{\frac{k}{j}} g_1(\omega)\omega^{-(1+\alpha)} d\omega \tag{3.2.6} $$

Applying the Lagrange interpolation polynomial on each integral on the right hand side of (3.2.5) gives

$$ \begin{aligned} \oint_0^{\frac{1}{j}} g_1(\omega)\omega^{-(1+\alpha)} d\omega &= \oint_0^{\frac{1}{j}} \left[\frac{\omega - \frac{1}{j}}{0 - \frac{1}{j}} g(0) + \frac{\omega - 0}{\frac{1}{j} - 0} g\left(\frac{1}{j}\right)\right] \omega^{-(\alpha+1)}\, d\omega \\ \oint_{\frac{1}{j}}^{\frac{2}{j}} g_1(\omega)\omega^{-(1+\alpha)} d\omega &= \oint_{\frac{1}{j}}^{\frac{2}{j}} \left[\frac{\omega - \frac{2}{j}}{\frac{1}{j} - \frac{2}{j}} g\left(\frac{1}{j}\right) + \frac{\omega - \frac{1}{j}}{\frac{2}{j} - \frac{1}{j}} g\left(\frac{2}{j}\right)\right] \omega^{-(\alpha+1)}\, d\omega \\ &\cdots \\ \oint_{\frac{j}{j}}^{\frac{j-1}{j}} g_1(\omega)\omega^{-(1+\alpha)} d\omega &= \oint_{\frac{j}{j}}^{\frac{j-1}{j}} \left[\frac{\omega - \frac{j}{j}}{\frac{j-1}{j} - \frac{j}{j}} g\left(\frac{j-1}{j}\right) + \frac{\omega - \frac{j-1}{j}}{\frac{j}{j} - \frac{j-1}{j}} g\left(\frac{j}{j}\right)\right] \omega^{-(\alpha+1)}\, d\omega. \end{aligned} $$

We can deduce that

$$\begin{aligned}
\oint_{0}^{\frac{1}{j}} g_1(\omega)\omega^{-(1+\alpha)}d\omega &= \frac{g_1(0)\left(\frac{1}{j}\right)^{1-(1+\alpha)}}{(0+1-(1+\alpha))0!} + \int_0^{\frac{1}{j}} \omega^{-(1+\alpha)}\frac{1}{0!}\left[\int_0^{\omega}(\omega-y)^0 g_1^{(1)}(y)dy\right]d\omega \\
&= \frac{1}{(-\alpha)j^{-\alpha}}g(0) + \int_0^{\frac{1}{j}} \omega^{-(1+\alpha)}\left[\int_0^{\omega}\left(jg\left(\frac{1}{j}\right)-jg(0)\right)dy\right]d\omega \\
&= \frac{1}{(-\alpha)j^{-\alpha}}g(0) + \left[jg\left(\frac{1}{j}\right)-jg(0)\right].\int_0^{\frac{1}{j}}\omega^{-\alpha}d\omega \\
&= \left[\frac{1}{(-\alpha)j^{-\alpha}} - \frac{1}{(1-\alpha)j^{-\alpha}}\right]g(0) + \frac{1}{(1-\alpha)j^{-\alpha}}g\left(\frac{1}{j}\right) \\
&= \frac{1}{(1-\alpha)j^{-\alpha}}g\left(\frac{1}{j}\right) - \frac{1}{\alpha(1-\alpha)j^{-\alpha}}g(0).
\end{aligned}$$

Now we consider in general:

$$\begin{aligned}
\int_{\frac{k-1}{j}}^{\frac{k}{j}} g_1(\omega)\omega^{-(1+\alpha)}\,d\omega &= \int_{\frac{k-1}{j}}^{\frac{k}{j}}\left[\frac{\omega-\frac{k}{j}}{-\frac{1}{j}}g\left(\frac{k-1}{j}\right) + \frac{\omega-\frac{k-1}{j}}{\frac{1}{j}}g\left(\frac{k}{j}\right)\right]\omega^{-(1+\alpha)}d\omega \\
&= g\left(\frac{k-1}{j}\right)\int_{\frac{k-1}{j}}^{\frac{k}{j}} j\left(\frac{k}{j}-\omega\right)\omega^{-(1+\alpha)}\,d\omega \\
&+ g\left(\frac{k}{j}\right)\int_{\frac{k-1}{j}}^{\frac{k}{j}} j\left(\omega-\frac{k-1}{j}\right)\omega^{-(1+\alpha)}\,d\omega \\
&= g\left(\frac{k-1}{j}\right)\int_{\frac{k-1}{j}}^{\frac{k}{j}}\left(k\omega^{-(1+\alpha)}d\omega - j\omega^{-\alpha}\right)d\omega \\
&+ g\left(\frac{k}{j}\right)\int_{\frac{k-1}{j}}^{\frac{k}{j}}\left(j\omega^{-\alpha}-(k-1)\omega^{-(1+\alpha)}\right)\,d\omega \\
&= g\left(\frac{k-1}{j}\right)\left[\frac{k}{-\alpha}\left(\frac{k}{j}\right)^{-\alpha} - \frac{j}{1-\alpha}\left(\frac{k}{j}\right)^{1-\alpha}\right. \\
&\left. - \frac{k}{-\alpha}\left(\frac{k-1}{j}\right)^{-\alpha} + \frac{j}{1-\alpha}\left(\frac{k-1}{j}\right)^{-\alpha}\right] \\
&+ g\left(\frac{k}{j}\right)\left[\frac{j}{1-\alpha}\left(\frac{k}{j}\right)^{1-\alpha} - \frac{k-1}{-\alpha}\left(\frac{k}{j}\right)^{-\alpha}\right. \\
&\left. - \frac{j}{1-\alpha}\left(\frac{k-1}{j}\right)^{1-\alpha} + \frac{k-1}{-\alpha}\left(\frac{k-1}{j}\right)^{-\alpha}\right].
\end{aligned}$$

Therefore

$$\begin{aligned}
Q_j(g) &= \frac{1}{(1-\alpha)j^{-\alpha}} g\left(\frac{1}{j}\right) - \frac{1}{\alpha(1-\alpha)j^{-\alpha}} g(0) \\
&+ \sum_{k=2}^{j} \left(\frac{k-1}{j}\right) \left[\frac{k}{-\alpha}\left(\frac{k}{j}\right)^{-\alpha} - \frac{j}{1-\alpha}\left(\frac{k}{j}\right)^{1-\alpha}\right. \\
&- \left. \frac{k}{-\alpha}\left(\frac{k-1}{j}\right)^{-\alpha} + \frac{j}{1-\alpha}\left(\frac{k-1}{j}\right)^{-\alpha}\right] \\
&+ g\left(\frac{k}{j}\right)\left[\frac{j}{1-\alpha}\left(\frac{k}{j}\right)^{1-\alpha} - \frac{k-1}{-\alpha}\left(\frac{k}{j}\right)^{-\alpha}\right. \\
&- \left. \frac{j}{1-\alpha}\left(\frac{k-1}{j}\right)^{1-\alpha} + \frac{k-1}{-\alpha}\left(\frac{k-1}{j}\right)^{-\alpha}\right] \\
&= \sum_{k=0}^{j} \alpha_{kj} g\left(\frac{k}{j}\right) = \sum_{k=0}^{j} \alpha_{kj} y(t_j - t_k),
\end{aligned}$$

where α_{kj} satisfy the following:

when $k = 0$,

$$\alpha_{0j} = \frac{-1}{\alpha(1-\alpha)j^{-\alpha}},$$

and when $k = j$,

$$\begin{aligned}
\alpha_{jj} &= \left[\frac{j}{1-\alpha}\left(\frac{j}{j}\right)^{1-\alpha} - \frac{j-1}{-\alpha}\left(\frac{j}{j}\right)^{-\alpha}\right. \\
&- \left. \frac{j}{1-\alpha}\left(\frac{j-1}{j}\right)^{1-\alpha} + \frac{j-1}{-\alpha}\left(\frac{j-1}{j}\right)^{-\alpha}\right] \\
&= \frac{j}{1-\alpha} - \frac{j-1}{-\alpha} - \frac{(j-1)^{1-\alpha}}{(1-\alpha)j^{-\alpha}} + \frac{(j-1)^{1-\alpha}}{(-\alpha)j^{-\alpha}} \\
&= \frac{\alpha j^{1-\alpha} + (1-\alpha)(j-1)j^{-\alpha} - \alpha(j-1)^{1-\alpha} + (\alpha-1)(j-1)^{1-\alpha}}{\alpha(1-\alpha)j^{-\alpha}} \\
&= \frac{\alpha j^{1-\alpha} + (1-\alpha)j^{1-\alpha} - (1-\alpha)^{-\alpha} - (j-1)^{1-\alpha}}{\alpha(1-\alpha)j^{-\alpha}} \\
&= \frac{(\alpha-1)j^{-\alpha} - (j-1)^{1-\alpha} + j^{1-\alpha}}{\alpha(1-\alpha)j^{-\alpha}}.
\end{aligned}$$

For $k = 1, 2, 3, 4, \ldots, j-1$, we have

$$\begin{aligned}
\alpha_{kj} &= \frac{k+1}{-\alpha}\left(\frac{k+1}{j}\right)^{-\alpha} - \frac{j}{1-\alpha}\left(\frac{k+1}{j}\right)^{-\alpha} - \frac{k+1}{-\alpha}\left(\frac{k}{j}\right)^{-\alpha} \\
&+ \frac{j}{1-\alpha}\left(\frac{k}{j}\right)^{1-\alpha} + \frac{j}{1-\alpha}\left(\frac{k}{j}\right)^{1-\alpha} - \frac{k-1}{-\alpha}\left(\frac{k}{j}\right)^{-\alpha} - \frac{j}{1-\alpha}\left(\frac{k-1}{j}\right)^{1-\alpha} \\
&+ \frac{k-1}{-\alpha}\left(\frac{k-1}{j}\right)^{-\alpha} \\
&= \left[\frac{1}{-\alpha j^{-\alpha}} - \frac{1}{(1-\alpha)j^{-\alpha}}\right](k+1)^{1-\alpha} + \left[-\frac{1}{(1-\alpha)j^{-\alpha}} + \frac{1}{(-\alpha)j^{-\alpha}}\right](k-1)^{1-\alpha} \\
&+ \left[-\frac{k+1}{-\alpha}\left(\frac{k}{j}\right)^{-\alpha} - \frac{k-1}{-\alpha}\left(\frac{k}{j}\right)^{-\alpha}\right] + \left[\frac{1}{(1-\alpha)j^{-\alpha}} + \frac{1}{(1-\alpha)j^{-\alpha}}\right]k^{1-\alpha} \\
&= \frac{\alpha-1-\alpha}{\alpha(1-\alpha)j^{-\alpha}}(k+1)^{1-\alpha} + \frac{-\alpha+(\alpha-1)}{\alpha(1-\alpha)j^{-\alpha}}(k-1)^{1-\alpha} \\
&+ \frac{2k}{\alpha}\left(\frac{k}{j}\right)^{-\alpha} + \frac{2}{(1-\alpha)j^{-\alpha}}k^{1-\alpha} \\
&= \frac{(k+1)^{1-\alpha}}{\alpha(1-\alpha)j^{-\alpha}} - \frac{(k-1)^{1-\alpha}}{\alpha(1-\alpha)j^{-\alpha}} + \frac{2k^{1-\alpha}}{\alpha(1-\alpha)j^{-\alpha}} \\
&= \frac{1}{\alpha(1-\alpha)j^{-\alpha}}\Big[2k^{1-\alpha} - (k-1)^{1-\alpha} - (k+1)^{1-\alpha}\Big].
\end{aligned}$$

Thus, we get

$$\begin{aligned}
{}_0^R D_t^\alpha y(t_j) &= \frac{t_j^{-\alpha}}{\Gamma(-\alpha)} \oint_0^1 g(\omega)\omega^{-(\alpha+1)} d\omega = \frac{t_j^{-\alpha}}{\Gamma(-\alpha)}\Big[\sum_{k=0}^{j} \alpha_{kj} y(t_j - t_k) + R_j(g)\Big] \\
&= h^\alpha \sum_{k=0}^{j} w_{kj} y(t_j - t_k) + \frac{t_j^{-\alpha}}{\Gamma(-\alpha)} R_j(g),
\end{aligned}$$

where

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

Together these estimates complete the proof of Lemma 3.2.2. □

Thus the solution of (3.2.3) has the form

$$\begin{aligned}
y(t_j) = \frac{1}{\alpha_{0j} - t_j^\alpha \Gamma(-\alpha)\beta}\Big[& t_j^\alpha \Gamma(-\alpha) f(t_j) - \sum_{k=1}^{j} \alpha_{kj} y(t_{j-k}) \\
& + y_0 \sum_{k=0}^{j} \alpha_{kj} - R_j(g)\Big],
\end{aligned} \tag{3.2.7}$$

where

$$|R_j(g)| \;\leq\; Cj^{\alpha-2}t_j^2||y''||_\infty.$$

Let $y_j \approx y(t_j)$ denote the approximate solution of $y(t_j)$, $j = 1, 2, 3, \dots, n$, then based on (3.2.7) we can define the following numerical method for solving (3.2.3) as

$$y_j \;=\; \frac{1}{\alpha_{0j} - t_j^\alpha \Gamma(-\alpha)\beta}\left[t_j^\alpha \Gamma(-\alpha) f(t_j) - \sum_{k=1}^{j} \alpha_{kj} y_{j-k} + y_0 \sum_{k=0}^{j} \alpha_{kj}\right]. \qquad (3.2.8)$$

We remark that Lemma 3.2.2 for $0 < \alpha < 1$ can be extended to the case for $1 < \alpha < 2$ to yield the following weights,

$$\alpha(1-\alpha)j^{-\alpha}\alpha_{kj} = \begin{cases} -1, & k = 0 \\ \alpha, & k = 1, j = 0 \\ 2 - 2^{1-\alpha}, & k = 1, j > 1 \\ 2k^{1-\alpha} - (k-1)^{1-\alpha} - (k+1)^{1-\alpha}, & k = 1, 2, \dots, j-1, j \geq 3 \\ (\alpha-1)k^{-\alpha} - (k-1)^{1-\alpha} + k^{1-\alpha}, & k = j, j \geq 2. \end{cases}$$

These weights are obtained by following the same process from Lemmas 3.2.1 and 3.2.2. The only difference lies from the Hadamard finite-part integral.

3.2.1 Error analysis

Theorem 3.2.3. [26] Let $0 < \alpha < 1$. Assume $y(t_j)$ and y_j are the exact and approximate solutions of (3.2.7) and (3.2.8), respectively. Also, assume that the function involved is sufficiently smooth, then there exists a constant $C = C(\alpha, g, \beta)$, such that

$$|y(t_j) - y_j| \;\leq\; Ch^{2-\alpha}||y''||_\infty. \quad j = 1, 2, \dots, n.$$

To prove the Theorem 3.2.3, we need the following Lemma.

Lemma 3.2.4. Let $0 < \alpha < 1$ be the order of derivative and the sequence (d_j) satisfy

$$\begin{cases} d_1 = 1 \\ d_j = 1 + \alpha(1-\alpha)j^{-\alpha}\sum_{k=1}^{j} \alpha_{kj} d_{j-k}. \end{cases}$$

Then, we have

$$1 \;\leq\; d_j \leq C_\alpha j^\alpha, \quad j = 1, 2, \dots, n.$$

where the positive constant $C_\alpha = \frac{1}{[(-\alpha)(-\alpha+1)\Gamma(-\alpha)\Gamma(\alpha+1)]}$

Proof. of Theorem 3.2.3:

Assume

$$e_j = y(t_j) - y_j.$$

then we have the error equation, subtracting (3.2.7) from (3.2.8),

$$e_j = \frac{1}{\alpha_{0j} - t_j^\alpha \Gamma(-\alpha)\beta}\left[-\sum_{k=1}^{j}\alpha_{kj}e_{j-k} - R_j\right].$$

Note that

$$\alpha_{0j} = \frac{1}{-\alpha(1-\alpha)j^{-\alpha}} < 0, \quad \Gamma(-\alpha) < 0, \quad \beta < 0, \quad \alpha_{kj} > 0.$$

then we have

$$\begin{aligned} |e_j| &\leq \frac{1}{-\alpha_{0j}}\left(\sum_{k=1}^{j}\alpha_{kj}\,|e_{j-k}| + |R_j|\right) \\ &\leq \alpha(1-\alpha)j^{-\alpha}\left(\sum_{k=1}^{j}\alpha_{kj}\,|e_{j-k}| + j^{\alpha-2}t_j^2||y''||_\infty\right) \\ &\leq \alpha(1-\alpha)h^2||y''||_\infty + \alpha(1-\alpha)j^{-\alpha}\sum_{k=1}^{j}\alpha_{kj}\,|e_{j-k}|. \end{aligned}$$

By denoting $a = \alpha(1-\alpha)h^2||y''||_\infty$ and assume for simplicity that $e_0 = 0$ then we get

$$|e_j| \leq a + \alpha(1-\alpha)j^{-\alpha}\sum_{k=1}^{j}\alpha_{kj}\,|e_{j-k}|, \quad j = 1, 2, \ldots, n,$$

which implies that

$$|e_j| \leq ad_j, \quad j = 1, 2, \ldots, n,$$

where

$$\begin{cases} d_1 = 1 \\ d_j = 1 + \alpha(1-\alpha)j^{-\alpha}\sum_{k=1}^{j}\alpha_{kj}d_{j-k} \end{cases}$$

Hence, the proof of Theorem 3.2.3 is complete.

Next we will show that $y_n - y(t_n)$ has an asymptotic expansion. We have the following Theorem.

Theorem 3.2.5. [33] Let $t_n = 1$ be fixed. Let y_n and $y(t_n)$ be the solutions of (3.2.8) and (3.2.7), respectively. Then there exist coefficients $C_\mu(\alpha)$ and $C^*_\mu(\alpha)$ such that the sequence $\{y_n\}$possesses an asymptotic expansion of the form.

$$y(t_n) = y_n + \sum_{\mu=2}^{M_1} C_\mu(\alpha) n^{\alpha-\mu} + \sum_{\mu=1}^{M_2} C^*_\mu(\alpha) n^{-2\mu} + O(n^{-M_3}) \quad for \quad n \to \infty,$$

where M_1 and M_2 depend on the smoothness of y, and $M_3 = \min\{M_1 - \alpha, 2M_2\}$.

To prove Theorem 3.2.5, we need the following

Lemma 3.2.6. [Theorem 1.3 in [33]]

Let $0 < \alpha < 1$ and let $g \in C^{m+2}[0,1], \quad m \geq 2$

Then

$$\begin{aligned} R_j(g) &= \oint_0^1 t^{-1-\alpha} g(t)dt - \oint_0^1 t^{-1-\alpha} g_1(t)dt \\ &= \sum_{k=0}^{j-1} \int_{\frac{k}{j}}^{\frac{k+1}{j}} t^{-1-\alpha}[g(t) - g_1(t)]dt = \sum_{\mu=2}^{m+1} d_\mu j^{\alpha-\mu} + \sum_{\mu=1}^{\mu^*} d^*_\mu j^{-2\mu} + O(j^{\alpha-m-1}), \end{aligned}$$

where μ^* is the integer satisfying $2\mu^* < m + 1 - \alpha < 2(\mu^* + 1)$, d_μ and d^*_μ are certain coefficients that depend on g. Here $g_1(t)$ is the linear interpolation polynomial of $g(t)$ on $[0,1]$.

For example, assume that $g \in C^{m+2}[0,1], \quad m = 4$. Then we have

$$R_j(g) = d_2 j^{\alpha-2} + d^*_1 j^{-2} + d_3 j^{\alpha-3} + d_4 j^{\alpha-4} + d_5 j^{\alpha-5} + d^*_2 j^{-4} + O(j^{\alpha-5}),$$

Here $\mu^* = 2$, and $2 \times 2 < 5 - \alpha < 2(2 + 1)$.

Proof of Theorem 3.2.5. To understand the idea of the proof. We assume, e.g, that $y \in C^{m+2}[0,1], \quad m = 4$. Then we shall prove that, there exist $\tilde{C}_2, \tilde{C}^*_1, \tilde{C}_3, \tilde{C}_4, \tilde{C}^*_2$, such that

$$\begin{aligned} y(t_n) - y_n &= \tilde{C}_2 n^{\alpha-2} + C^*_1 n^{-2} + \tilde{C}_3 n^{\alpha-3} + \tilde{C}_4 n^{\alpha-4} + \tilde{C}_5 n^{\alpha-5} \\ &\quad + \tilde{C}^*_2 n^{-4} + O(n^{\alpha-5}), \quad n \to \infty, \end{aligned} \tag{3.2.9}$$

To prove (3.2.9), we will consider $y_j - y(t_j), \quad j \to \infty$, for fixed t_j such that $\frac{t_j}{t_n} = \frac{j}{n} = c_0, \quad c_0$ is a constant, that is n depends on j. Here $t_n = 1, t_j = c_0$.

For example, choose $c_0 = \frac{1}{2}$, then when $j = 1$ we have $n = 2$ and when $j = 2$, we have $n = 4, \ldots$. We will prove that

$$\begin{aligned}\varepsilon_j = y(t_j) - y_j = \tilde{C}_2 n^{\alpha-2} + C_1^* n^{-2} + \tilde{C}_3 n^{\alpha-3} + \tilde{C}_4 n^{\alpha-4} \\ + \tilde{C}_5 n^{\alpha-5} + \tilde{C}_2^* n^{-4} + O(n^{\alpha-5}), \quad j \to \infty,\end{aligned} \tag{3.2.10}$$

Then let $j = n$. We get (3.2.9)

By Lemma 3.2.6, we see that, for $g \in C^{m+2}[0,1], m \geq 2, (m = 4)$, we have

$$\begin{aligned}R_j(g) &= \oint_0^1 t^{-1-\alpha} g(t)dt - \oint_0^1 t^{-1-\alpha} g_1(t)dt = \sum_{k=0}^{j-1} \oint_{\frac{k}{j}}^{\frac{k+1}{j}} t^{-1-\alpha}[g(t) - g_1(t)]dt \\ &= d_2 j^{\alpha-2} + d_1^* j^{-2} + d_3 j^{\alpha-3} + d_4 j^{\alpha-4} + d_5 j^{\alpha-5} + d_2^* j^{-4} + O(j^{\alpha-5}).\end{aligned} \tag{3.2.11}$$

Note that $j = c_0 n$, we can write (3.2.11) into

$$R_j(g) = \tilde{d}_2 n^{\alpha-2} + \tilde{d}_1^* n^{-2} + \tilde{d}_3 n^{\alpha-3} + \tilde{d}_4 n^{\alpha-4} + \tilde{d}_5 n^{\alpha-5} + \tilde{d}_2^* n^{-4} + O(n^{\alpha-5}). \tag{3.2.12}$$

Next we will prove that

$$\begin{aligned}\varepsilon_j = y(t_j) - y_j \;&=\; \tilde{C}_2 n^{\alpha-2} + \tilde{C}_1^* n^{-2} + \tilde{C}_3 n^{\alpha-3} + \tilde{C}_4 n^{\alpha-4} + \tilde{C}_5 n^{\alpha-5} \\ &\quad + \tilde{C}_2^* n^{-4} + O(n^{\alpha-5}), \quad j \to \infty,\end{aligned} \tag{3.2.13}$$

where

$$\tilde{C}_\ell = \frac{1}{-c_0^\alpha \Gamma(-\alpha)\beta - \frac{1}{\alpha}} \tilde{d}_\ell, \quad \ell = 2, 3, 4, 5.$$

$$\tilde{C}_\ell^* = \frac{1}{-c_0^\alpha \Gamma(-\alpha)\beta - \frac{1}{\alpha}} \tilde{d}_\ell^*, \quad \ell = 1, 2.$$

Suppose that (3.2.13) holds, then (3.2.9) follows by replacing j by n since $j = 1, 2, \ldots, n$.

We shall use mathematical induction to prove (3.2.13).

Step 1: When $j = 0$, we have $\varepsilon_0 = 0$, therefore (3.2.13) is true.

Step 2: When $j = 1$, we have, by (3.2.7) and (3.2.8),

$$\varepsilon_1 = y(t_1) - y_1 = \frac{1}{c_0^\alpha \Gamma(-\alpha)\beta - \frac{(nc_0)^\alpha}{\alpha(\alpha-1)}}\Big(\varepsilon_0\Big[\sum_{k=0}^{1}\alpha_{k1} - \alpha_{01}\Big] + R_1[g]\Big).$$

That is, noting that $\sum_{k=0}^{1}\alpha_{k1} = -\frac{1}{\alpha}$, by (3.2.10),

$$\begin{aligned}
&\Big[\frac{1}{\alpha(\alpha-1)}(nc_0)^\alpha - c_0^\alpha\Gamma(-\alpha)\beta\Big]\varepsilon_1\\
&= \frac{1}{\alpha}\Big[\tilde{C}_2 n^{\alpha-2} + \tilde{C}_1^* n^{-2} + \tilde{C}_3 n^{\alpha-3} + \tilde{C}_4 n^{\alpha-4} + \tilde{C}_5 n^{\alpha-5} + \tilde{C}_2^* n^{-4} + O(n^{\alpha-5})\Big]\\
&+ \frac{1}{\alpha(\alpha-1)}(nc_0)^\alpha\Big[\tilde{C}_2 n^{\alpha-2} + \tilde{C}_1^* n^{-2} + \tilde{C}_3 n^{\alpha-3} + \tilde{C}_4 n^{\alpha-4} + \tilde{C}_5 n^{\alpha-5} + \tilde{C}_2^* n^{-4} + O(n^{\alpha-5})\Big]\\
&+ \Big[\tilde{d}_2 n^{\alpha-2} + \tilde{d}_1^* n^{-2} + \tilde{d}_3 n^{\alpha-3} + \tilde{d}_4 n^{\alpha-4} + \tilde{d}_5 n^{\alpha-5} + \tilde{d}_2^* n^{-4} + O(n^{\alpha-5})\Big].
\end{aligned}$$

This shows that ε_1 possesses an asymptotic expansion w.r.t powers of n, and we can check indeed by comparing the coefficients of powers of n,

$$\varepsilon_1 = \tilde{C}_2 n^{\alpha-2} + \tilde{C}_1^* n^{-2} + \tilde{C}_3 n^{\alpha-3} + \tilde{C}_4 n^{\alpha-4} + \tilde{C}_5 n^{\alpha-5} + \tilde{C}_2^* n^{-4} + O(n^{\alpha-5}).$$

Step 3: Assume that

$$\varepsilon_\ell = \tilde{C}_2 n^{\alpha-2} + \tilde{C}_1^* n^{-2} + \tilde{C}_3 n^{\alpha-3} + \tilde{C}_4 n^{\alpha-4} + \tilde{C}_5 n^{\alpha-5} + \tilde{C}_2^* n^{-4} + O(n^{\alpha-5}), \quad \ell = 0, 1, 2, \dots, j-1.$$

Then we have, same as in Step 2,

$$\begin{aligned}
&\Big[\frac{1}{\alpha(\alpha-1)}(nc_0)^\alpha - c_0^\alpha\Gamma(-\alpha)\beta\Big]\varepsilon_j = \Big(\sum_{k=1}^{j}\alpha_{kj}\varepsilon_{j-k} + R_j[g]\Big)\\
&+ \Big[\Big(\tilde{C}_2 n^{\alpha-2} + \tilde{C}_1^* n^{-2} + \tilde{C}_3 n^{\alpha-3} + \tilde{C}_4 n^{\alpha-4} + \tilde{C}_5 n^{\alpha-5} + \tilde{C}_2^* n^{-4} + O(n^{\alpha-5})\Big)\\
&\qquad \Big(\sum_{k=0}^{j}\alpha_{kj} - \alpha_{0j}\Big) + R_j[g]\Big].
\end{aligned}$$

Note that $\sum_{k=0}^{j}\alpha_{kj} = -\frac{1}{\alpha}$, we have, by (3.2.12)

$$\begin{aligned}
&\Big[\frac{1}{\alpha(\alpha-1)}(nc_0)^\alpha - c_0^\alpha\Gamma(-\alpha)\beta\Big]\varepsilon_j\\
&= \frac{1}{\alpha}\Big[\tilde{C}_2 n^{\alpha-2} + \tilde{C}_1^* n^{-2} + \tilde{C}_3 n^{\alpha-3} + \tilde{C}_4 n^{\alpha-4} + \tilde{C}_5 n^{\alpha-5} + \tilde{C}_2^* n^{-4} + O(n^{\alpha-5})\Big]\\
&+ \frac{1}{\alpha(\alpha-1)}(nc_0)^\alpha\Big[\tilde{C}_2 n^{\alpha-2} + \tilde{C}_1^* n^{-2} + \tilde{C}_3 n^{\alpha-3} + \tilde{C}_4 n^{\alpha-4} + \tilde{C}_5 n^{\alpha-5} + \tilde{C}_2^* n^{-4} + O(n^{\alpha-5})\Big]\\
&+ \Big[\tilde{d}_2 n^{\alpha-2} + \tilde{d}_1^* n^{-2} + \tilde{d}_3 n^{\alpha-3} + \tilde{d}_4 n^{\alpha-4} + \tilde{d}_5 n^{\alpha-5} + \tilde{d}_2^* n^{-4} + O(n^{\alpha-5})\Big].
\end{aligned}$$

This shows that ε_j possesses an asymptotic expansion w.r.t powers of n, and we can check indeed, comparing with the coefficients of powers of n,

$$\varepsilon_j = \tilde{C}_2 n^{\alpha-2} + \tilde{C}_1^* n^{-2} + \tilde{C}_3 n^{\alpha-3} + \tilde{C}_4 n^{\alpha-4} + \tilde{C}_5 n^{\alpha-5} + \tilde{C}_2^* n^{-4} + O(n^{\alpha-5}), \quad j \to \infty.$$

Thus (3.2.13) holds.

Together these estimates complete the proof of Theorem 3.2.5.

3.3 Extending Diethelm's method

In this section we will consider a higher order numerical method for solving (3.1.3)-(3.1.4). It is well-known that (3.1.3)-(3.1.4) is equivalent, with $0 < \alpha < 1$, to the following problem:

$$ {}_0^R D_t^{\alpha} [y(t) - y_0] = \beta y(t) + f(t), \quad 0 \le t \le 1, \tag{3.3.1}$$

where ${}_0^R D_t^{\alpha} y(t)$ denotes the Riemann-Liouville fractional derivative defined by, with $0 < \alpha < 1$,

$$ {}_0^R D_t^{\alpha} y(t) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_0^t (t-\tau)^{-\alpha} y(\tau)\, d\tau. \tag{3.3.2}$$

The Riemann-Liouville fractional derivative ${}_0^R D_t^{\alpha} y(t)$ can be written as [26]

$$ {}_0^R D_t^{\alpha} y(t) = \frac{1}{\Gamma(-\alpha)} \oint_0^t (t-\tau)^{-1-\alpha} y(\tau)\, d\tau, \tag{3.3.3}$$

where the integral $\oint$ denotes the Hadamard finite-part integral.

In [26], Diethelm approximated the Hadamard finite-part integral in (3.3.3) by piecewise linear interpolation polynomials and defined a numerical method for solving (3.3.1). In this section, we will approximate the Hadamard finite-part integral by using piecewise quadratic interpolation polynomials.

Let M be a fixed positive integer and let $0 = t_0 < t_1 < t_2 < \cdots < t_{2j} < t_{2j+1} < \cdots < t_{2M} = 1$ be a partition of $[0, 1]$ and h the stepsize. At node $t_{2j} = \frac{2j}{2M}$, the equation (3.3.1) satisfies

$$ {}_0^R D_t^{\alpha} [y(t_{2j}) - y_0] = \beta y(t_{2j}) + f(t_{2j}), \quad j = 1, 2, \dots, M, \tag{3.3.4}$$

and at node $t_{2j+1} = \frac{2j+1}{2M}$, the equation (3.3.1) satisfies

$$ {}_0^R D_t^\alpha [y(t_{2j+1}) - y_0] = \beta y(t_{2j+1}) + f(t_{2j+1}), \quad j = 0, 1, 2, \ldots, M-1. \tag{3.3.5}$$

Let us first consider the discretization of (3.3.4). Note that

$$ {}_0^R D_t^\alpha y(t_{2j}) = \frac{1}{\Gamma(-\alpha)} \oint_0^{t_{2j}} (t_{2j}-\tau)^{-1-\alpha} y(\tau)\, d\tau = \frac{t_{2j}^{-\alpha}}{\Gamma(-\alpha)} \oint_0^1 w^{-1-\alpha} y(t_{2j}-t_{2j}w)\, dw. \tag{3.3.6}$$

For every j, we replace $g(w) = y(t_{2j} - t_{2j}w)$ in the integral in (3.3.6) by a piecewise quadratic interpolation polynomial with equispaced nodes $0, \frac{1}{2j}, \frac{2}{2j}, \ldots, \frac{2j}{2j}$. We then have

$$\oint_0^1 w^{-1-\alpha} g(w)\, dw = \oint_0^1 w^{-1-\alpha} g_2(w)\, dw + R_{2j}(g), \tag{3.3.7}$$

where $g_2(w)$, defined by (3.3.9), is the piecewise quadratic interpolation polynomial of $g(w)$ with equispaced nodes $0, \frac{1}{2j}, \frac{2}{2j}, \ldots, \frac{2j}{2j}$ and $R_{2j}(g)$ is the remainder term.

Lemma 3.3.1. Let $0 < \alpha < 1$. We have

$$\oint_0^1 w^{-1-\alpha} g_2(w)\, dw = \sum_{k=0}^{2j} \alpha_{k,2j}\, g\Big(\frac{k}{2j}\Big), \tag{3.3.8}$$

where

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

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

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

and

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

Proof. For fixed $2j$, let $0<\frac{1}{2j}<\frac{2}{2j}<\cdots<\frac{2j}{2j}=1$ be a partition of $[0,1]$. Denote $w_l=\frac{l}{2j}$, $l=0,1,2,\ldots,2j$. We then have, for $k=1,2,\ldots,j$,

$$
\begin{aligned}
g_2(w) =& \frac{(w-w_{2k-1})(w-w_{2k})}{(w_{2k-2}-w_{2k-1})(w_{2k-2}-w_{2k})}g(w_{2k-2})\\
&+\frac{(w-w_{2k-2})(w-w_{2k})}{(w_{2k-1}-w_{2k-2})(w_{2k-1}-w_{2k})}g(w_{2k-1})\\
&+\frac{(w-w_{2k-2})(w-w_{2k-1})}{(w_{2k}-w_{2k-2})(w_{2k}-w_{2k-1})}g(w_{2k}), \quad \text{for } w\in\Big[w_{2k-2},w_{2k}\Big].
\end{aligned}
\tag{3.3.9}
$$

Let us now consider

$$
\oint_0^1 w^{-1-\alpha}g_2(w)\,dw=\Big[\oint_0^{w_2}+\int_{w_2}^{w_4}+\cdots+\int_{w_{2j-2}}^{w_{2j}}\Big]w^{-1-\alpha}g_2(w)\,dw.
$$

By the definition of the Hadamard finite-part integral [24], we obtain

$$
\begin{aligned}
\oint_0^{w_2} w^{-1-\alpha}g_2(w)\,dw &= \frac{g_2(0)(w_2)^{-\alpha}}{-\alpha}+\int_0^{w_2} w^{-1-\alpha}\Big[\int_0^{w} g_2'(y)\,dy\Big]\,dw\\
&=\frac{2^{-\alpha}}{(-\alpha)(2j)^{-\alpha}}g_2(0)+\int_0^{w_2} w^{-1-\alpha}(g_2(w)-g_2(0))\,dw.
\end{aligned}
\tag{3.3.10}
$$

By using (3.3.9), we have

$$
\begin{aligned}
&\oint_0^{w_2} g_2(w) w^{-1-\alpha}\, dw \\
&= \frac{2^{-\alpha}}{(-\alpha)(2j)^{-\alpha}} g(0) + \int_0^{w_2} w^{-1-\alpha} \Big[\frac{(2j)^2}{2} \Big(w^2 - (w_1 + w_2) w \Big) g(0) \\
&\quad + \frac{(2j)^2}{-1} \Big(w^2 - (0 + w_2) w \Big) g(w_1) + \frac{(2j)^2}{2} \Big(w^2 - (0 + w_1) w \Big) g(w_2) \Big]\, dw \\
&= \frac{2^{-\alpha}(\alpha+2)}{(-\alpha)(-\alpha+1)(-\alpha+2)(2j)^{-\alpha}} g(0) + \frac{2^{2-\alpha}}{(-\alpha+1)(-\alpha+2)(2j)^{-\alpha}} g(w_1) \\
&\quad + \frac{-2^{-\alpha}\alpha}{(-\alpha+1)(-\alpha+2)(2j)^{-\alpha}} g(w_2).
\end{aligned}
$$

Similarly, we have, after a simple calculation,

$$
\begin{aligned}
&(-\alpha)(-\alpha+1)(-\alpha+2)(2j)^{-\alpha} \int_{w_{2k}}^{w_{2k+2}} g_2(w) w^{-1-\alpha}\, dw \\
&\qquad = \frac{1}{2} F_0(k) g(w_{2k-2}) + (-1) F_1(k) g(w_{2k-1}) + \frac{1}{2} F_2(k) g(w_{2k}),
\end{aligned}
$$

where $F_i(k), i = 0, 1, 2$ and $k = 2, 3, ..., j$ are defined as above.

Together these estimates lead to (3.3.8) and the proof of Lemma 3.3.1 is complete.

□

Next we consider the discretization of (3.3.5). At the node $t_{2j+1} = \frac{2j+1}{2M}$, $j = 1, 2, \ldots, M-1$. We have

$$
\begin{aligned}
{}_0^R D_t^\alpha y(t_{2j+1}) &= \frac{1}{\Gamma(-\alpha)} \oint_0^{t_{2j+1}} (t_{2j+1} - \tau)^{-1-\alpha} y(\tau)\, d\tau \\
&= \frac{1}{\Gamma(-\alpha)} \int_0^{t_1} (t_{2j+1} - \tau)^{-1-\alpha} y(\tau)\, d\tau + \frac{t_{2j+1}^{-\alpha}}{\Gamma(-\alpha)} \oint_0^{\frac{2j}{2j+1}} w^{-1-\alpha} y(t_{2j+1} - t_{2j+1} w)\, dw.
\end{aligned}
\tag{3.3.11}
$$

For $j = 1, 2, \ldots, M-1$, we replace $g(w) = y(t_{2j+1} - t_{2j+1} w)$ in the integral in (3.3.11) by a piecewise quadratic interpolation polynomial with equispaced nodes $0, \frac{1}{2j+1}, \frac{2}{2j+1}, \ldots, \frac{2j}{2j+1}$. We then have, for a sufficient smooth function $g(w)$,

$$
\oint_0^{\frac{2j}{2j+1}} w^{-1-\alpha} g(w)\, dw = \oint_0^{\frac{2j}{2j+1}} w^{-1-\alpha} g_2(w)\, dw + R_{2j+1}(g), \tag{3.3.12}
$$

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

Similarly, we can prove the following lemma.

Lemma 3.3.2. Let $0 < \alpha < 1$. We have

$$\oint_0^{\frac{2j}{2j+1}} w^{-1-\alpha} g_2(w)\, dw = \sum_{k=0}^{2j} \alpha_{k,2j+1} g\Big(\frac{k}{2j+1}\Big), \tag{3.3.13}$$

where $\alpha_{k,2j+1} = \alpha_{k,2j}$, $k = 0, 1, 2, \dots, 2j$ and $\alpha_{k,2j}$ are given in Lemma 3.3.1.

Remark 4. By direct calculation, we can show that, with $0 < \alpha < 1$,

$$\alpha_{0,2j} = \frac{2^{-\alpha}(\alpha+2)}{(-\alpha)(-\alpha+1)(-\alpha+2)(2j)^{-\alpha}} < 0, \tag{3.3.14}$$

and $\alpha_{k,2j} > 0$ for $k > 0,\ k \neq 2$. For $k = 2$, there exists $\alpha_1 \in (0,1)$ such that $\alpha_{2,2j} \geq 0$ for $0 < \alpha < \alpha_1$ and $\alpha_{2,2j} \leq 0$ for $\alpha_1 < \alpha < 1$.

Now solutions of (3.3.1) satisfy, with $j = 1, 2, \dots, M$,

$$y(t_{2j}) = \frac{1}{\alpha_{0,2j} - t_{2j}^{\alpha}\Gamma(-\alpha)\beta}\Big[t_{2j}^{\alpha}\Gamma(-\alpha)f(t_{2j}) - \sum_{k=1}^{2j}\alpha_{k,2j}y(t_{2j-k}) + y_0\sum_{k=0}^{2j}\alpha_{k,2j} - R_{2j}(g)\Big], \tag{3.3.15}$$

and, with $j = 1, 2, \dots, M-1$,

$$\begin{aligned} y(t_{2j+1}) = {} & \frac{1}{\alpha_{0,2j+1} - t_{2j+1}^{\alpha}\Gamma(-\alpha)\beta}\Big[t_{2j+1}^{\alpha}\Gamma(-\alpha)f(t_{2j+1}) - \sum_{k=1}^{2j}\alpha_{k,2j+1}y(t_{2j+1-k}) \\ & + y_0\sum_{k=0}^{2j}\alpha_{k,2j+1} - R_{2j+1}(g) - t_{2j+1}^{\alpha}\int_0^{t_1}(t_{2j+1}-\tau)^{-1-\alpha}y(\tau)\, d\tau\Big]. \end{aligned} \tag{3.3.16}$$

Here $\alpha_{0,l} - t_l^{\alpha}\Gamma(-\alpha)\beta < 0,\ l = 2j, 2j+1$, which follow from (3.3.14) and $\Gamma(-\alpha) < 0$, $\beta < 0$ and $\alpha_{0,2j+1} = \alpha_{0,2j}$.

Let $y_{2j} \approx y(t_{2j})$ and $y_{2j+1} \approx y(t_{2j+1})$ denote the approximations of the exact solutions $y(t_{2j})$ and $y(t_{2j+1})$, respectively. Assume that the starting values y_0 and y_1 are given. We define the following numerical methods for solving (3.3.1), with $j = 1, 2, \dots, M$,

$$y_{2j} = \frac{1}{\alpha_{0,2j} - t_{2j}^{\alpha}\Gamma(-\alpha)\beta}\Big[t_{2j}^{\alpha}\Gamma(-\alpha)f(t_{2j}) - \sum_{k=1}^{2j}\alpha_{k,2j}y_{2j-k} + y_0\sum_{k=0}^{2j}\alpha_{k,2j}\Big], \tag{3.3.17}$$

and, with $j = 1, 2, \dots, M-1$,

$$\begin{aligned} y_{2j+1} = {} & \frac{1}{\alpha_{0,2j+1} - t_{2j+1}^{\alpha}\Gamma(-\alpha)\beta}\Big[t_{2j+1}^{\alpha}\Gamma(-\alpha)f(t_{2j+1}) - \sum_{k=1}^{2j}\alpha_{k,2j+1}y_{2j+1-k} \\ & + y_0\sum_{k=0}^{2j}\alpha_{k,2j+1} - t_{2j+1}^{\alpha}\int_0^{t_1}(t_{2j+1}-\tau)^{-1-\alpha}y(\tau)\, d\tau\Big]. \end{aligned} \tag{3.3.18}$$

Remark 5. In practice, we need to approximate $\int_0^{t_1}(t_{2j+1}-\tau)^{-1-\alpha}y(\tau)\,d\tau$. One way is to divide the integral $[0,t_1]$ into small intervals $0 \le t_1^1 \le t_1^2 \le \cdots \le t_1^N = t_1$ with stepsize $\tilde{h} \ll h$. We first obtain $y_{1p} \approx y(t_1^p)$, $p = 1,2,\ldots,N$ by using some numerical method for solving fractional differential equation. Then we apply a quadrature formula to approximate the integral.

3.3.1 Error analysis

We have the following asymptotic expansion theorem.

Theorem 3.3.3. Let $0 < \alpha < 1$ and M be a positive integer. Let $0 = t_0 < t_1 < t_2 < \cdots < t_{2j} < t_{2j+1} < \cdots < t_{2M} = 1$ be a partition of $[0,1]$ and h the stepsize. Let $y(t_{2j}), y(t_{2j+1}), y_{2j}$ and y_{2j+1} be the exact solutions and the approximate solutions of (3.3.15) - (3.3.18), respectively. Assume that the function $y \in C^{m+2}[0,1]$, $m \ge 3$. Further assume that we obtain the exact starting values $y_0 = y(0)$ and $y_1 = y(t_1)$. Then there exist coefficients $c_\mu = c_\mu(\alpha)$ and $c_\mu^* = c_\mu^*(\alpha)$ such that the sequence $\{y_l\}, l = 0,1,2,\ldots,2M$ possesses an asymptotic expansion of the form

$$y(t_{2M}) - y_{2M} = \sum_{\mu=3}^{m+1} c_\mu (2M)^{\alpha-\mu} + \sum_{\mu=2}^{\mu^*} c_\mu^* (2M)^{-2\mu} + o((2M)^{\alpha-m-1}), \quad \text{for } M \to \infty,$$

that is,

$$y(t_{2M}) - y_{2M} = \sum_{\mu=3}^{m+1} c_\mu h^{\mu-\alpha} + \sum_{\mu=2}^{\mu^*} c_\mu^* h^{2\mu} + o(h^{m+1-\alpha}), \quad \text{for } h \to 0,$$

where μ^* is the integer satisfying $2\mu^* < m+1-\alpha < 2(\mu^*+1)$, and c_μ and c_μ^* are certain coefficients that depend on y.

To prove Theorem 3.3.3, we need the following lemma for the asymptotic expansions for the remainder terms $R_{2j}(g)$ and $R_{2j+1}(g)$ in (3.3.7) and (3.3.12).

Lemma 3.3.4. Let $0 < \alpha < 1$ and $g \in C^{m+2}[0,1]$, $m \ge 3$. Let $R_{2j}(g)$ and $R_{2j+1}(g)$ be the remainder terms in (3.3.7) and (3.3.12), respectively. Then we have, with $l = 2,3,\ldots,2j,2j+1,\ldots,2M$,

$$R_l(g) = \sum_{\mu=3}^{m+1} d_\mu l^{\alpha-\mu} + \sum_{\mu=2}^{\mu^*} d_\mu^* l^{-2\mu} + o(l^{\alpha-m-1}), \tag{3.3.19}$$

where μ^* is the integer satisfying $2\mu^* < m+1-\alpha < 2(\mu^*+1)$, and d_μ and d_μ^* are certain coefficients that depend on g.

Proof. We follow the proof of Theorem 1.3 in [33] where the piecewise linear Lagrange interpolation polynomials are used.

We first consider the case $l = 2j$ for $j = 1, 2, \ldots, M$. Let $0 = w_0 < w_1 < w_2 < \cdots < w_{2j} = 1, w_k = \frac{k}{2j}, k = 0, 1, 2, \ldots, 2j$ be a partition of $[0, 1]$. Let $h_1 = \frac{1}{2j}$ be the stepsize. Let $g_2(w)$ denote the piecewise quadratic Lagrange interpolation polynomial defined by (3.3.9) on $[w_{2l}, w_{2l+2}], l = 0, 1, 2, \ldots, j-1$. Then we have

$$\begin{aligned}
R_{2j}(g) &= \oint_0^1 w^{-1-\alpha} g(w)\, dw - \oint_0^1 w^{-1-\alpha} g_2(w)\, dw \\
&= \sum_{l=0}^{j-1} \int_{w_{2l}}^{w_{2l+2}} w^{-1-\alpha} \Big(g(w) - g_2(w)\Big)\, dw = \sum_{l=0}^{j-1} \int_0^1 (w_{2l} + 2h_1 s)^{-1-\alpha} \Big[g(w_{2l} + 2h_1 s) \\
&- \Big(\frac{1}{2}(2s-1)(2s-2) g(w_{2l}) - (2s)(2s-2) g(w_{2l+1}) + \frac{1}{2}(2s)(2s-1) g(w_{2l+2})\Big)\Big] (2h_1)\, ds.
\end{aligned}$$

By using the Taylor formula, we have

$$\begin{aligned}
g(w_{2l}) &= g(w_{2l} + 2h_1 s) + \frac{g'(w_{2l} + 2h_1 s)}{1!}(-2h_1 s) + \frac{g''(w_{2l} + 2h_1 s)}{2!}(-2h_1 s)^2 \\
&+ \frac{g'''(w_{2l} + 2h_1 s)}{3!}(-2h_1 s)^3 + \cdots + \frac{g^{(M)}(w_{2l} + 2h_1 s)}{m!}(-2h_1 s)^m + R^{(1)}_{m+1}, \\
g(w_{2l+1}) &= g(w_{2l} + 2h_1 s) + \frac{g'(w_{2l} + 2h_1 s)}{1!}(h_1 - 2h_1 s) + \frac{g''(w_{2l} + 2h_1 s)}{2!}(h_1 - 2h_1 s)^2 \\
&+ \frac{g'''(w_{2l} + 2h_1 s)}{3!}(h_1 - 2h_1 s)^3 + \cdots + \frac{g^{(m)}(w_{2l} + 2h_1 s)}{m!}(h_1 - 2h_1 s)^m + R^{(2)}_{m+1}, \\
g(w_{2l+2}) &= g(w_{2l} + 2h_1 s) + \frac{g'(w_{2l} + 2h_1 s)}{1!}(2h_1 - 2h_1 s) + \frac{g''(w_{2l} + 2h_1 s)}{2!}(2h_1 - 2h_1 s)^2 \\
&+ \frac{g'''(w_{2l} + 2h_1 s)}{3!}(2h_1 - 2h_1 s)^3 + \cdots + \frac{g^{(m)}(w_{2l} + 2h_1 s)}{m!}(2h_1 - 2h_1 s)^m + R^{(3)}_{m+1},
\end{aligned} \tag{3.3.20}$$

where $R^{(i)}_{m+1}, i = 1, 2, 3$ denote the remainder terms. Thus we obtain

$$\begin{aligned}
R_{2j}(g) =&(2h_1) \sum_{l=0}^{j-1} \int_0^1 (w_{2l} + 2h_1 s)^{-1-\alpha} \Big[\sum_{r=0}^{m-3} h_1^{r+3} g^{(r+3)}(w_{2l} + 2h_1 s) \pi_r(s) \Big]\, ds \\
&+ (2h_1) \sum_{l=0}^{j-1} \int_0^1 (w_{2l} + 2h_1 s)^{-1-\alpha} \epsilon_{m+1}(s)\, ds = I + II,
\end{aligned}$$

where $\epsilon_{m+1}(s)$ depends on the remainder terms $R^{(i)}_{m+1}, i = 1, 2, 3$ and $\pi_r(s)$ are some functions of s.

For I, we have

$$I = \sum_{r=0}^{m-3} h_1^{r+3} \int_0^1 \Big[2h_1 \sum_{l=0}^{j-1} (w_{2l} + 2h_1 s)^{-1-\alpha} g^{(r+3)}(w_{2l} + 2h_1 s)\Big] \pi_r(s)\, ds.$$

Applying Theorem 3.2 in [56], we have, with $\bar{w}_l = w_{2l}, \bar{h}_1 = 2h_1$,

$$\begin{aligned}
&2h_1 \sum_{l=0}^{j-1} (w_{2l} + 2h_1 s)^{-1-\alpha} g^{(r+3)}(w_{2l} + 2h_1 s) \\
&= \bar{h}_1 \sum_{l=0}^{j-1} (\bar{w}_l + \bar{h}_1 s)^{-1-\alpha} g^{(r+3)}(\bar{w}_l + \bar{h}_1 s) \\
&= \sum_{j=0}^{m-r-3} a_j(s) h_1^j + \sum_{j=0}^{m-r-2} a_{0,j}(s) h_1^{j-\alpha} + o(h_1^{m-r-2}),
\end{aligned}$$

with some suitable functions $a_j(s), j = 0, 1, \ldots, m-r-3$ and $a_{0,j}(s),\ j = 0, 1, \ldots, m-r-2$, with $r = 0, 1, 2, \ldots, m-3,\ m \geq 3$.

Hence we have, noting that $h_1 = (2j)^{-1}$,

$$\begin{aligned}
I &= \sum_{r=0}^{m-3} h_1^{3+r} \Big[\int_0^1 \sum_{j=0}^{m-r-3} a_j(s) h_1^j \pi_r(s)\, ds\Big] \\
&+ \sum_{r=0}^{m-3} h_1^{3+r} \Big[\int_0^1 \sum_{j=0}^{m-r-2} a_{0,j}(s) h_1^{j-\alpha} \pi_r(s)\, ds)\Big] + o(h_1^{m+1}) \\
&= \sum_{r=0}^{m-3} \sum_{j=0}^{m-r-3} \Big[\int_0^1 a_j(s) \pi_r(s)\, ds\Big] h_1^{3+r+j} \\
&+ \sum_{r=0}^{m-3} \sum_{j=0}^{m-r-2} \Big[\int_0^1 a_{0,j}(s) \pi_r(s)\, ds\Big] h_1^{3+r+j-\alpha} + o(h_1^{m+1}) \\
&= \sum_{\mu=3}^{m+1} d_\mu (2j)^{\alpha-\mu} + \sum_{\mu=2}^{\mu^*} d_\mu^* (2j)^{-2\mu} + o((2j)^{-m-1}), \qquad (3.3.21)
\end{aligned}$$

where μ^* is the integer satisfying $2\mu^* < m + 1 - \alpha < 2(\mu^* + 1)$, and d_μ and d_μ^* are certain coefficients that depend on g. We remark that the expansion does not contain any odd integer of powers of $(2j)$ which follows from the argument in the proof of Theorem 1.3 in [33].

For II, we have, following the argument of the proof for Theorem 1.3 in [33],

$$II = 2h_1 \sum_{l=0}^{j-1} \int_0^1 (w_{2l} + 2h_1 s)^{-1-\alpha} \epsilon_{m+1}(s)\, ds = o((2j)^{\alpha-m-1}).$$

Thus (3.3.19) holds for $l = 2j$.

Next we consider the case $l = 2j+1$. Denote $w_{2l} = \frac{2l}{2j+1}$, $w_{2l+2} = \frac{2l+2}{2j+1}$ and $h_1 = \frac{1}{2j+1}$, we have

$$
\begin{aligned}
R_{2j+1}(g) &= \oint_0^{\frac{2j}{2j+1}} w^{-1-\alpha} g(w)\, dw - \oint_0^{\frac{2j}{2j+1}} w^{-1-\alpha} g_2(w)\, dw \\
&= \sum_{l=0}^{j-1} \int_{w_{2l}}^{w_{2l+2}} w^{-1-\alpha} \Big(g(w) - g_2(w) \Big)\, dw = \sum_{l=0}^{j-1} \int_0^1 (w_{2l} + 2h_1 s)^{-1-\alpha} \Big[g(w_{2l} + 2h_1 s) \\
&- \Big(\frac{1}{2}(2s-1)(2s-2) g(w_{2l}) - (2s)(2s-2) g(w_{2l+1}) + \frac{1}{2}(2s)(2s-1) g(w_{2l+2}) \Big) \Big] (2h_1)\, ds.
\end{aligned}
$$

Following the same argument as for the case $l = 2j$, we show that (3.3.19) also holds for $l = 2j+1$. Together these estimates complete the proof of Lemma 3.3.4.

□

Proof of Theorem 3.3.3. We follow the proof of Theorem 2.1 in [33] where the piecewise linear Lagrange interpolation polynomials are used to approximate the Hadamard finite-part integral.

Let us fix $t_l = c$ to be a constant for $l = 1, 2, \ldots, 2M$. Let $t_{2M} = 1$ be fixed. We will investigate the difference

$$
e_l = y(t_l) - y_l, \quad \text{for } l \to \infty, \quad \text{with } t_l = lh = \frac{l}{2M} = c,
$$

where $h = 1/(2M)$ is the stepsize. In other words, there is a constant c, independent of M, such that

$$
l = c \cdot (2M), \quad \text{or } M = l/(2c),
$$

and consequently, we see that if e_l possesses an asymptotic expansion with respect to l, then e_{2M} possesses at the same time one with respect to M, and vice versa.

We shall prove

$$
e_l = y(t_l) - y_l = \sum_{\mu=3}^{m+1} c_\mu (2M)^{\alpha-\mu} + \sum_{\mu=2}^{\mu^*} c^*_\mu (2M)^{-2\mu} + o((2M)^{\alpha-m-1}), \quad \text{for } l \to \infty, \tag{3.3.22}
$$

for some suitable constants c_μ, c^*_μ which we will determine later.

Let us first consider the case $l = 2j$. Subtracting (3.3.17) from (3.3.15), we have, noting $t_{2j} = (2j)h = \frac{2j}{2M} = c$,

$$e_{2j} = \frac{1}{\alpha_{0,2j} - (\frac{2j}{2M})^{\alpha}\Gamma(-\alpha)\beta}\Big[- \sum_{k=1}^{2j} \alpha_{k,2j}(y(t_{2j-k}) - y_{2j-k}) - R_{2j}(g)\Big]$$
$$= \frac{1}{c^{\alpha}\Gamma(-\alpha)\beta - \alpha_{0,2j}}\Big(\sum_{k=1}^{2j} \alpha_{k,2j} e_{2j-k} + R_{2j}(g)\Big). \tag{3.3.23}$$

Note that $g(\cdot) = y(t_{2j} - t_{2j}\cdot) \in C^{m+2}[0,1],\ m \geq 3$, we have, by Lemma 3.3.4,

$$R_{2j}(g) = \sum_{\mu=3}^{m+1} d_{\mu}(2j)^{\alpha-\mu} + \sum_{\mu=2}^{\mu^*} d_{\mu}^*(2j)^{-2\mu} + o((2j)^{\alpha-m-1}), \quad \text{for } j \to \infty, \tag{3.3.24}$$

where μ^* is the integer satisfying $2\mu^* < m + 1 - \alpha < 2(\mu^* + 1)$, and d_{μ} and d_{μ}^* are certain coefficients that depend on g.

Note that $(2j)/(2M) = c$, we can write (3.3.24) into

$$R_{2j}(g) = \sum_{\mu=3}^{m+1} \tilde{d}_{\mu}(2M)^{\alpha-\mu} + \sum_{\mu=2}^{\mu^*} \tilde{d}_{\mu}^*(2M)^{-2\mu} + o((2M)^{\alpha-m-1}), \quad \text{for } j \to \infty. \tag{3.3.25}$$

Choose

$$c_{\mu} = \frac{1}{-c^{\alpha}\Gamma(-\alpha)\beta - 1/\alpha}\tilde{d}_{\mu}, \quad \mu = 3, 4, \ldots, m+1, \tag{3.3.26}$$
$$c_{\mu}^* = \frac{1}{-c^{\alpha}\Gamma(-\alpha)\beta - 1/\alpha}\tilde{d}_{\mu}^*, \quad \mu = 1, 2, \ldots, \mu^*, \tag{3.3.27}$$

we will prove below that (3.3.22) holds for the coefficents c_{μ}, c_{μ}^* defined in (3.3.26) and (3.3.27).

We shall use mathematical induction to prove (3.3.22). By assumption $e_0 = 0, e_1 = 0$, hence (3.3.22) holds for $l = 0, 1$ with the coefficients given by (3.3.26) and (3.3.27). Let us now consider the case for $l = 2$. We have, noting that $\alpha_{0,l} = \frac{2^{-\alpha}(\alpha+2)(2Mc)^{\alpha}}{(-\alpha)(-\alpha+1)(-\alpha+2)}$ and applying Lemma 3.3.4,

$$e_2 = y(t_2) - y_2 = \frac{1}{c^{\alpha}\Gamma(-\alpha)\beta - \alpha_{0,2}}\Big(\sum_{k=1}^{2} \alpha_{k,2} e_{2-k} + R_2(g)\Big)$$
$$= \frac{1}{c^{\alpha}\Gamma(-\alpha)\beta - \alpha_{0,2}}\Big[\Big(\sum_{\mu=3}^{m+1} c_{\mu}(2M)^{\alpha-\mu} + \sum_{\mu=2}^{\mu^*} c_{\mu}^*(2M)^{-2\mu} + o((2M)^{\alpha-m-1})\Big)$$
$$\cdot \Big(\sum_{k=0}^{2} \alpha_{k,2} - \alpha_{0,2}\Big) + R_2(g)\Big]. \tag{3.3.28}$$

Thus we get, noting that $\sum_{k=0}^{2}\alpha_{k,2} = -1/\alpha$ and $\alpha_{0,2} = \frac{2^{-\alpha}(\alpha+2)(2Mc)^\alpha}{(-\alpha)(-\alpha+1)(-\alpha+2)}$,

$$\begin{aligned}
&\Big[\frac{2^{-\alpha}(\alpha+2)(2Mc)^\alpha}{(-\alpha)(-\alpha+1)(-\alpha+2)} - c^\alpha\Gamma(-\alpha)\beta\Big]e_2 \\
&= \frac{1}{\alpha}\Big[\sum_{\mu=3}^{m+1} c_\mu (2M)^{\alpha-\mu} + \sum_{\mu=2}^{\mu^*} c_\mu^*(2M)^{-2\mu} + o((2M)^{\alpha-m-1})\Big] \\
&- \sum_{\mu=3}^{m+1} \tilde{d}_\mu (2M)^{\alpha-\mu} - \sum_{\mu=2}^{\mu^*} \tilde{d}_\mu^*(2M)^{-2\mu} + o((2M)^{\alpha-m-1}) \\
&+ \frac{2^{-\alpha}(\alpha+2)(2Mc)^\alpha}{(-\alpha)(-\alpha+1)(-\alpha+2)}\Big[\sum_{\mu=3}^{m+1} c_\mu (2M)^{\alpha-\mu} + \sum_{\mu=2}^{\mu^*} c_\mu^*(2M)^{-2\mu} + o((2M)^{\alpha-m-1})\Big].
\end{aligned} \tag{3.3.29}$$

This shows that the sequence e_2 possesses an asymptotic expansion with respect to the powers of $2M$, and it is easy to check that, by comparing with the coefficients of powers of $(2M)$, see [33],

$$e_2 = \sum_{\mu=3}^{m+1} c_\mu (2M)^{\alpha-\mu} + \sum_{\mu=2}^{\mu^*} c_\mu^*(2M)^{-2\mu} + o((2M)^{\alpha-m-1}).$$

Assume that (3.3.22) holds for $l = 0, 1, \ldots, 2j-1$. Then we have, following the same argument for (3.3.29), noting $\sum_{k=0}^{2j}\alpha_{k,2j} = -1/\alpha$ and applying Lemma 3.3.4,

$$\begin{aligned}
&\Big[\frac{2^{-\alpha}(\alpha+2)(2Mc)^\alpha}{(-\alpha)(-\alpha+1)(-\alpha+2)} - c^\alpha\Gamma(-\alpha)\beta\Big]e_{2j} \\
&= \frac{1}{\alpha}\Big[\sum_{\mu=3}^{m+1} c_\mu (2M)^{\alpha-\mu} + \sum_{\mu=2}^{\mu^*} c_\mu^*(2M)^{-2\mu} + o((2M)^{\alpha-m-1})\Big] \\
&- \sum_{\mu=3}^{m+1} \tilde{d}_\mu (2M)^{\alpha-\mu} - \sum_{\mu=2}^{\mu^*} \tilde{d}_\mu^*(2M)^{-2\mu} + o((2M)^{\alpha-m-1}) \\
&+ \frac{2^{-\alpha}(\alpha+2)(2Mc)^\alpha}{(-\alpha)(-\alpha+1)(-\alpha+2)}\Big[\sum_{\mu=3}^{m+1} c_\mu (2M)^{\alpha-\mu} + \sum_{\mu=2}^{\mu^*} c_\mu^*(2M)^{-2\mu} + o((2M)^{\alpha-m-1})\Big].
\end{aligned} \tag{3.3.30}$$

This shows that the sequence e_{2j} possesses an asymptotic expansion with respect to the powers of $2M$, and it is easy to check that, by comparing with the coefficients of powers of $(2M)$, see [33],

$$e_{2j} = \sum_{\mu=3}^{m+1} c_\mu (2M)^{\alpha-\mu} + \sum_{\mu=2}^{\mu^*} c_\mu^*(2M)^{-2\mu} + o((2M)^{\alpha-m-1}).$$

Hence (3.3.22) holds for $l = 2j$.

Finally we assume that (3.3.22) holds for $l = 0, 1, \dots, 2j$. Then we have, following the same argument for (3.3.30), noting $\sum_{k=0}^{2j} \alpha_{k,2j+1} = \sum_{k=0}^{2j} \alpha_{k,2j} = -1/\alpha$, $\alpha_{0,2j+1} = \alpha_{0,2j}$ and applying Lemma 3.3.4,

$$\begin{aligned}
&\Big[\frac{2^{-\alpha}(\alpha+2)(2Mc)^{\alpha}}{(-\alpha)(-\alpha+1)(-\alpha+2)} - c^{\alpha}\Gamma(-\alpha)\beta\Big] e_{2j+1} \\
&= \frac{1}{\alpha}\Big[\sum_{\mu=3}^{m+1} c_{\mu}(2M)^{\alpha-\mu} + \sum_{\mu=2}^{\mu^*} c_{\mu}^{*}(2M)^{-2\mu} + o((2M)^{\alpha-m-1})\Big] \\
&- \sum_{\mu=3}^{m+1} \tilde{d}_{\mu}(2M)^{\alpha-\mu} - \sum_{\mu=2}^{\mu^*} \tilde{d}_{\mu}^{*}(2M)^{-2\mu} + o((2M)^{\alpha-m-1}) \\
&+ \frac{2^{-\alpha}(\alpha+2)(2Mc)^{\alpha}}{(-\alpha)(-\alpha+1)(-\alpha+2)}\Big[\sum_{\mu=3}^{m+1} c_{\mu}(2M)^{\alpha-\mu} + \sum_{\mu=2}^{\mu^*} c_{\mu}^{*}(2M)^{-2\mu} + o((2M)^{\alpha-m-1})\Big].
\end{aligned} \tag{3.3.31}$$

This again shows that the sequence e_{2j+1} possesses an asymptotic expansion with respect to the powers of $2M$, and it is easy to check that, by comparing with the coefficients of powers of $2M$, see [33],

$$e_{2j+1} = \sum_{\mu=3}^{m+1} c_{\mu}(2M)^{\alpha-\mu} + \sum_{\mu=2}^{\mu^*} c_{\mu}^{*}(2M)^{-2\mu} + o((2M)^{\alpha-m-1}).$$

Hence (3.3.22) holds also for $l = 2j + 1$. Together these estimates complete the proof of (3.3.22). Applying $l = 2M$ in (3.3.22), we complete the proof of Theorem 3.3.3.

□

Remark 6. In Theorem 3.3.3, we assume that $y_1 = y(t_1)$ exactly. In practice y_1 can be approximated by using the ideas described in Remark 5.

3.4 Numerical examples

Example 7. *Consider [26]*

$$ {}_0^C D_t^{\alpha} y(t) = \beta y(t) + f(t), \quad t \in [0, 1], \tag{3.4.1}$$

$$ y(0) = y_0, \tag{3.4.2}$$

where $y_0 = 0$, $0 < \alpha < 1$, $\beta = -1$ *and* $f(t) = (t^2 + 2t^{2-\alpha}/\Gamma(3-\alpha)) + (t^3 + 3!t^{3-\alpha}/\Gamma(4-\alpha))$. *The exact solution is* $y(t) = t^2 + t^3$.

The main purpose is to check the order of convergence of the numerical method with respect to the fractional order α. *For various choices of* $\alpha \in (0,1)$, *we computed the errors at* $t = 1$. *We choose the stepsize* $h = 1/(5 \times 2^l), l = 1, 2, \dots, 7$, *i.e, we divided the interval* $[0,1]$ *into* $n = 1/h$ *small intervals with nodes* $0 = t_0 < t_1 < \cdots < t_n = 1$. *Then we compute the error* $e(t_n) = y(t_n) - y_n$. *By Theorem 3.3.3, we have*

$$|e(t_n)| = |y(t_n) - y_n| \leq Ch^{3-\alpha}, \tag{3.4.3}$$

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 stepsize* 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 $3 - \alpha \approx log_2\Big(\frac{|e_{h_l}(t_n)|}{|e_{h_{l+1}}(t_n)|}\Big)$. *In Tables 3.4.1- 3.4.2, we compute the experimentally determined orders of convergence (EOC) for the different values of* α. *The numerical results are consistent with the theoretical results.*

n	EOC($\alpha = .1$)	EOC($\alpha = .2$)	EOC($\alpha = .3$)	EOC ($\alpha = .4$)	EOC ($\alpha = .5$)
10					
20	2.8885	2.7870	2.6836	2.5790	2.4732
40	2.8941	2.7935	2.6919	2.5897	2.4871
80	2.8972	2.7963	2.6961	2.5950	2.4937
160	2.8987	2.7985	2.6981	2.5976	2.4969
320	2.8994	2.7993	2.6991	2.5988	2.4985
640	2.9003	2.7998	2.6995	2.5994	2.4992

Table 3.4.1: Numerical results at $t = 1$ for $\beta = -1$
and $f(t) = (t^2 + 2t(2-\alpha)/\Gamma(3-\alpha)) + (t^3 + 3!t^{3-\alpha}/\Gamma(4-\alpha))$

In Figures 3.4.1 - 3.4.6, we plot the experimentally determined orders of convergence. We have from (3.4.3)

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

n	EOC($\alpha = .6$)	EOC($\alpha = .7$)	EOC($\alpha = .8$)	EOC ($\alpha = .9$)
10				
20	2.3662	2.2579	2.1476	2.0351
40	2.3840	2.2804	2.1760	2.0709
80	2.3923	2.2905	2.1885	2.0861
160	2.3962	2.2954	2.1944	2.0932
320	2.3981	2.2977	2.1972	2.0967
640	2.3991	2.2989	2.1986	2.0983

Table 3.4.2: Numerical results at $t = 1$ for $\beta = -1$
and $f(t) = (t^2 + 2t(2-\alpha)/\Gamma(3-\alpha)) + (t^3 + 3!t^{3-\alpha}/\Gamma(4-\alpha))$

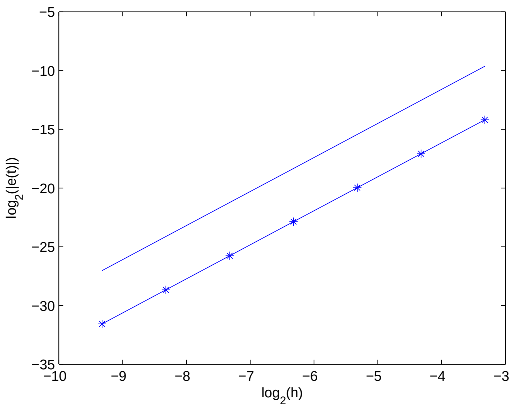

Figure 3.4.1: The experimentally determined orders of convergence ("EOC ") at $t = 1$ in Example 7 with $\alpha = 0.1$

Let $y = log_2(|e(t_n)|)$ *and* $x = log_2(h)$. *In Figure 3.1, we plot the function* $y = y(x)$ *for the different values of* $x = log_2(h)$ *where* $h = 1/(5 \times 2^l), l = 1, 2, \ldots, 7$. *To observe the order of convergence, we also plot the straight line* $y = (3-\alpha)x$, *where* $\alpha = 0.1, 0.2, 0.4, 0.5, 0.7, 0.8$. *We see that these two lines are exactly parallel which means that the order of convergence of the numerical method is* $O(h^{3-\alpha})$.

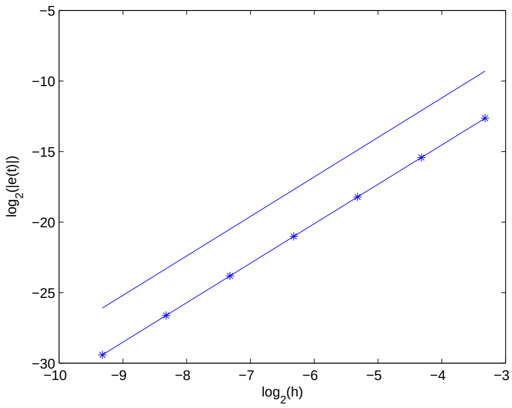

Figure 3.4.2: The experimentally determined orders of convergence (“EOC ”) at $t = 1$ in Example 7 with $\alpha = 0.2$

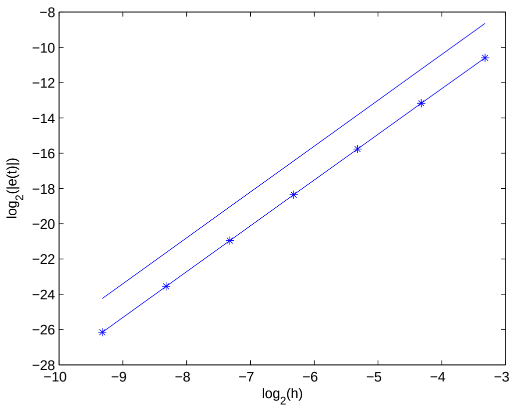

Figure 3.4.3: The experimentally determined orders of convergence (“EOC ”) at $t = 1$ in Example 7 with $\alpha = 0.4$

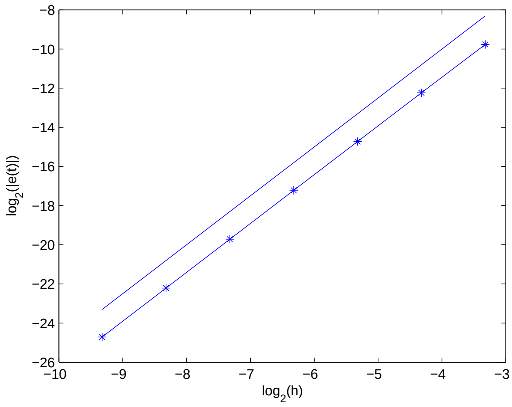

Figure 3.4.4: The experimentally determined orders of convergence (“EOC ”) at $t = 1$ in Example 7 with $\alpha = 0.5$

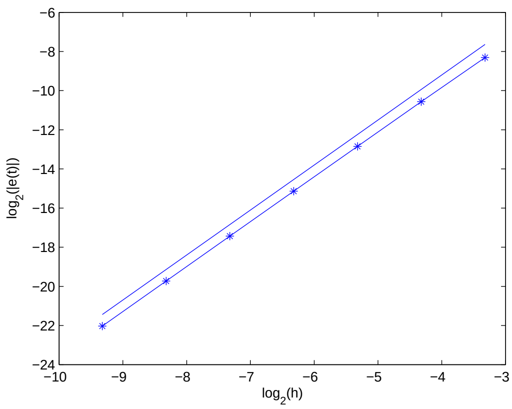

Figure 3.4.5: The experimentally determined orders of convergence (“EOC ”) at $t = 1$ in Example 7 with $\alpha = 0.7$

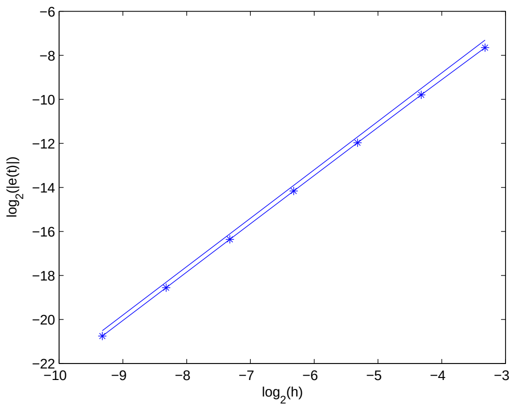

Figure 3.4.6: The experimentally determined orders of convergence (“EOC ”) at $t = 1$ in Example 7 with $\alpha = 0.8$

Chapter 4

Higher order numerical method for fractional ODEs (predictor-corrector method)

4.1 Introduction

A predictor-corrector approximation method [29] for fractional differential equations has been developed by the three well-known mathematicians Kai Diethelm, Neville J. Ford and Alan D. Freed. The popularity of this method is due to its suitability for use both for linear and for nonlinear problems and the easy implementation of a computational algorithm.

We consider numerical methods for solving the fractional differential equations

$$ {}_0^C D_t^\alpha y(t) = f(t, y(t)), \quad 0 < t < T, \tag{4.1.1}$$

$$ y^{(k)}(0) = y_0^k, \quad k = 0, 1, 2, \dots, \lceil \alpha \rceil - 1, \tag{4.1.2}$$

where the y_0^k may be arbitrary real numbers and $\alpha > 0$. Here ${}_0^C D_t^\alpha$ denotes the differential operator in the sense of Caputo denoted by, with $n-1 < \alpha < n$

$$ {}_0^C D_t^\alpha y(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t (t-u)^{n-\alpha-1} y^{(n)}(u)\, du,$$

where $n = \lceil \alpha \rceil$ is the smallest integer $\geq \alpha$.

The approach for solving the fractional differential equation (4.1.1)-(4.1.2) is based on the discretization of the integral in the equivalent form of (4.1.1)-(4.1.2), see [28]. It is well-known that (4.1.1)-(4.1.2) is equivalent to the Volterra integral equation

$$y(t) = \sum_{\nu=0}^{\lceil\alpha\rceil-1} y_0^{(\nu)} \frac{t^\nu}{\nu!} + \frac{1}{\Gamma(\alpha)} \int_0^t (t-u)^{\alpha-1} f(u, y(u))\, du. \tag{4.1.3}$$

In [29], the authors approximated the integral in (4.1.3) by using a piecewise linear interpolation polynomial and introduced a fractional Adams method for solving (4.1.1)-(4.1.2) and proved that the order of convergence of the numerical method is $O(h^2)$ for $1 < \alpha < 2$ and $O(h^{1+\alpha})$ for $0 < \alpha < 1$ if ${}_0^C D_t^\alpha y(t) \in C^2[0,T]$

We will use piecewise quadratic interpolation polynomials to approximate the integral in (4.1.3) and introduce a high order fractional Adams method for solving (4.1.3) and prove that the order of convergence of the numerical method is $\min\{3, 1+2\alpha\}$ for $\alpha \in (0,2]$ if ${}_0^C D_t^\alpha y(t) \in C^3[0,T]$. This method has higher convergence order than the method in [29]. It is easier to implement our numerical algorithm compared with the method in [95] where the Jacobi-Gauss-Lobatto nodes must be calculated at each time level. Our method is simpler than the method in [9] in the sense that we are using a predictor-corrector method and therefore we do not need to solve the nonlinear system at each time level.

4.2 Fractional Adams-type algorithm (quadratic interpolation polynomial)

In this section we will consider a higher order numerical method for solving (4.1.1)-(4.1.2). For simplicity we only consider the case where $0 < \alpha \leq 2$ since the case $\alpha > 2$ does not seem to be of major practical interest [28].

To make sure that (4.1.1)-(4.1.2) has a unique solution, we assume that $f(u, \cdot)$ satisfies a Lipschitz condition, i.e., there exists a constant L such that

$$|f(u,x) - f(u,y)| \leq L|x-y|, \quad \forall\, x, y \in \mathbb{R}. \tag{4.2.1}$$

Let m be a positive integer and let $0 = t_0 < t_1 < t_2 < \cdots < t_{2j} < t_{2j+1} < \cdots < t_{2m} = T$ be a partition of $[0,T]$ and h the stepsize. Note that the system (4.1.1)-(4.1.2) is equivalent to (4.1.3). Let us now consider the discretization of (4.1.3). At node $t = t_{2j}$, $j = 1, 2, \ldots, m$, we have

$$y(t_{2j}) = y_0 + y_0^{(1)} \frac{t_{2j}}{1!} + \frac{1}{\Gamma(\alpha)} \int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} f(u, y(u))\, du. \tag{4.2.2}$$

(The second of the initial conditions only for $1 < \alpha < 2$ of course). At node $t = t_{2j+1}, j = 1, 2, \ldots, m-1$, we have

$$\begin{aligned} y(t_{2j+1}) &= y_0 + y_0^{(1)} \frac{t_{2j+1}}{1!} + \frac{1}{\Gamma(\alpha)} \int_0^{t_{2j+1}} (t_{2j+1} - u)^{\alpha-1} f(u, y(u))\, du \\ &= y_0 + y_0^{(1)} \frac{t_{2j+1}}{1!} + \frac{1}{\Gamma(\alpha)} \int_0^{t_1} (t_{2j+1} - u)^{\alpha-1} f(u, y(u))\, du \\ &\quad + \frac{1}{\Gamma(\alpha)} \int_{t_1}^{t_{2j+1}} (t_{2j+1} - u)^{\alpha-1} f(u, y(u))\, du \\ &= y_0 + y_0^{(1)} \frac{t_{2j+1}}{1!} + \frac{1}{\Gamma(\alpha)} \int_0^{t_1} (t_{2j+1} - u)^{\alpha-1} f(u, y(u))\, du \\ &\quad + \frac{1}{\Gamma(\alpha)} \int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} f(u+h, y(u+h))\, du \end{aligned} \tag{4.2.3}$$

We will replace $f(u, y(u))$ in the integral $\int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} f(u, y(u))\, du$ in (4.2.2) by the following piecewise quadratic polynomial, for $t_{2l} \le u \le t_{2l+2},\ l = 0, 1, 2, \ldots, j-1$ with $j = 1, 2, \ldots, m$,

$$\begin{aligned} f(u, y(u)) \approx P_2(u) =& \frac{(u - t_{2l+1})(u - t_{2l+2})}{(t_{2l} - t_{2l+1})(t_{2l} - t_{2l+2})} f(t_{2l}, y(t_{2l})) \\ &+ \frac{(u - t_{2l})(u - t_{2l+2})}{(t_{2l+1} - t_{2l})(t_{2l+1} - t_{2l+2})} f(t_{2l+1}, y(t_{2l+1})) \\ &+ \frac{(u - t_{2l})(u - t_{2l+1})}{(t_{2l+2} - t_{2l})(t_{2l+2} - t_{2l+1})} f(t_{2l+2}, y(t_{2l+2})). \end{aligned} \tag{4.2.4}$$

Similarly, we will replace $f(u+h, y(u+h))$ in the integral $\int_0^{t_{2j}} (t_{2j}-u)^{\alpha-1} f(u+h, y(u+h))\, du$ in (4.2.3) by the following piecewise quadratic polynomial, for $t_{2l} \le u \le t_{2l+2},\ l = 0, 1, 2, \ldots, j-1,\ j = 1, 2, \ldots, m-1$,

$$\begin{aligned} f(u+h, y(u+h)) \approx Q_2(u) =& \frac{(u - t_{2l+1})(u - t_{2l+2})}{(t_{2l} - t_{2l+1})(t_{2l} - t_{2l+2})} f(t_{2l+1}, y(t_{2l+1})) \\ &+ \frac{(u - t_{2l})(u - t_{2l+2})}{(t_{2l+1} - t_{2l})(t_{2l+1} - t_{2l+2})} f(t_{2l+2}, y(t_{2l+2})) \\ &+ \frac{(u - t_{2l})(u - t_{2l+1})}{(t_{2l+2} - t_{2l})(t_{2l+2} - t_{2l+1})} f(t_{2l+3}, y(t_{2l+3})). \end{aligned} \tag{4.2.5}$$

We then have the following lemma:

Lemma 4.2.1. Let $0 < \alpha \leq 2$. We have

$$\int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} P_2(u)\, du = \sum_{k=0}^{2j} c_{k,2j} f(t_k, y(t_k)), \tag{4.2.6}$$

and

$$\int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} Q_2(u)\, du = \sum_{k=0}^{2j} c_{k,2j} f(t_{k+1}, y(t_{k+1})), \tag{4.2.7}$$

where

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

and

$$\begin{aligned}
F_0(l) &= \alpha(\alpha+1)\Big((2j-2l)^{\alpha+2} - (2j-2l-2)^{\alpha+2}\Big) \\
&\quad + \alpha(\alpha+2)\Big(2(2j) - (2l+1) - (2l+2)\Big)\Big((2j-2l-2)^{\alpha+1} - (2j-2l)^{\alpha+1}\Big) \\
&\quad + (\alpha+1)(\alpha+2)\Big((2j-2l-1)(2j-2l-2)\Big)\Big((2j-2l)^{\alpha} - (2j-2l-2)^{\alpha}\Big), \\
F_1(l) &= \alpha(\alpha+1)\Big((2j-2l)^{\alpha+2} - (2j-2l-2)^{\alpha+2}\Big) \\
&\quad + \alpha(\alpha+2)\Big(2(2j) - (2l) - (2l+2)\Big)\Big((2j-2l-2)^{\alpha+1} - (2j-2l)^{\alpha+1}\Big) \\
&\quad + (\alpha+1)(\alpha+2)\Big((2j-2l)(2j-2l-2)\Big)\Big((2j-2l)^{\alpha} - (2j-2l-2)^{\alpha}\Big), \\
F_2(l) &= \alpha(\alpha+1)\Big((2j-2l)^{\alpha+2} - (2j-2l-2)^{\alpha+2}\Big) \\
&\quad + \alpha(\alpha+2)\Big(2(2j) - (2l) - (2l+1)\Big)\Big((2j-2l-2)^{\alpha+1} - (2j-2l)^{\alpha+1}\Big) \\
&\quad + (\alpha+1)(\alpha+2)\Big((2j-2l)(2j-2l-1)\Big)\Big((2j-2l)^{\alpha} - (2j-2l-2)^{\alpha}\Big),
\end{aligned}$$

Proof. We have

$$\int_0^{t_{2j}}(t_{2j}-u)^{\alpha-1}P_2(u)du=\sum_{l=0}^{j-1}\int_{t_{2l}}^{t_{2l+2}}(t_{2j}-u)^{\alpha-1}\Big(\frac{(u-t_{2l+1})(u-t_{2l+2})}{(t_{2l}-t_{2l+1})(t_{2l}-t_{2l+2})}g(t_{2l})$$
$$+\frac{(u-t_{2l})(u-t_{2l+2})}{(t_{2l+1}-t_{2l})(t_{2l+1}-t_{2l+2})}g(t_{2l+1})+\frac{(u-t_{2l})(u-t_{2l+1})}{(t_{2l+2}-t_{2l})(t_{2l+2}-t_{2l+1})}g(t_{2l+2})\Big)du$$
$$=\sum_{l=0}^{j-1}\Big(\int_{t_{2l}}^{t_{2l+2}}(t_{2j}-u)^{\alpha-1}\frac{(u-t_{2l+1})(u-t_{2l+2})}{(-h)(-2h)}g(t_{2l})du$$
$$+\int_{t_{2l}}^{t_{2l+2}}(t_{2j}-u)^{\alpha-1}\frac{(u-t_{2l})(u-t_{2l+2})}{(h)(-h)}g(t_{2l+1})du$$
$$+\int_{t_{2l}}^{t_{2l+2}}(t_{2j}-u)^{\alpha-1}\frac{(u-t_{2l})(u-t_{2l+1})}{(2h)(h)}g(t_{2l+2})du\Big).$$

Note that,

$$\int_{t_{2l}}^{t_{2l+2}}(t_{2j}-u)^{\alpha-1}(u-t_{2l+1})(u-t_{2l+2})du$$
$$=\int_{t_{2l}}^{t_{2l+2}}(t_{2j}-u)^{\alpha-1}[(u-t_{2j})+(t_{2j}-t_{2l+1})][(u-t_{2j})+(t_{2j}-t_{2l+2})]du$$
$$=\int_{t_{2l}}^{t_{2l+2}}(t_{2j}-u)^{\alpha+1}du-\int_{t_{2l}}^{t_{2l+2}}(t_{2j}-u)^{\alpha}(t_{2j}-t_{2l+1}-t_{2l+2})du$$
$$+\int_{t_{2l}}^{t_{2l+2}}(t_{2j}-u)^{\alpha-1}(t_{2j}-t_{2l+1})(t_{2j}-t_{2l+2})du$$
$$=h^{\alpha+2}\Big(\frac{(2j-2l)^{\alpha+2}-(2j-2l-2)^{\alpha+2}}{\alpha+2}$$
$$+\frac{[2.2j-(2l+1)-(2l+2)][(2j-2l)^{\alpha+1}-(2j-2l-2)^{\alpha+1}]}{\alpha+1}$$
$$+\frac{[2j-(2l+1)][2j-(2l+2)][(2j-2l)^{\alpha}-(2j-2l-2)^{\alpha}]}{\alpha}\Big)$$
$$=\frac{h^{\alpha+2}}{\alpha(\alpha+1)(\alpha+2)}\Big(\alpha(\alpha+1)[(2j-2l)^{\alpha+2}-(2j-2l-2)^{\alpha+2}]$$
$$+\alpha(\alpha+2)[2.2j-(2l+1)-(2l+2)][(2j-2l)^{\alpha+1}-(2j-2l-2)^{\alpha+1}]$$
$$+(\alpha+1)(\alpha+2)(2j-2l-1)(2j-2l-2)[(2j-2l)^{\alpha}-(2j-2l-2)^{\alpha}\Big)$$
$$=\frac{h^{\alpha+2}}{\alpha(\alpha+1)(\alpha+2)}F_0(l),\qquad l=0,1,2,3\ldots,j-1.$$

Similarly, we have,

$$\int_{t_{2l}}^{t_{2l+2}}(t_{2j}-u)^{\alpha-1}(u-t_{2l})(u-t_{2l+2})du$$
$$=\int_{t_{2l}}^{t_{2l+2}}(t_{2j}-u)^{\alpha-1}[(u-t_{2j})+(t_{2j}-t_{2l})][(u-t_{2j})+(t_{2j}-t_{2l+2})]du$$
$$=\int_{t_{2l}}^{t_{2l+2}}(t_{2j}-u)^{\alpha+1}du-\int_{t_{2l}}^{t_{2l+2}}(t_{2j}-u)^{\alpha}(2t_{2j}-t_{2l}-t_{2l+2})du$$
$$+\int_{t_{2l}}^{t_{2l+2}}(t_{2j}-u)^{\alpha-1}(t_{2j}-t_{2l})(t_{2j}-t_{2l+2})du$$
$$=\frac{h^{\alpha+2}}{\alpha(\alpha+1)(\alpha+2)}\Big(\alpha(\alpha+1)[(2j-2l)^{\alpha+2}-(2j-2l-2)^{\alpha+2}]$$
$$+\alpha(\alpha+2)[2.2j-2l-(2l+2)][(2j-2l-2)^{\alpha+1}-(2j-2l)^{\alpha+1}]$$
$$+(\alpha+1)(\alpha+2)(2j-2l)(2j-2l-2)[(2j-2l)^{\alpha}-(2j-2l-2)^{\alpha}\Big)$$
$$=\frac{h^{\alpha+2}}{\alpha(\alpha+1)(\alpha+2)}F_1(l),\qquad l=0,1,2,3\ldots,(j-1).$$

and,

$$\int_{t_{2l}}^{t_{2l+2}}(t_{2j}-u)^{\alpha-1}(u-t_{2l})(u-t_{2l+1})du$$
$$=\int_{t_{2l}}^{t_{2l+2}}(t_{2j}-u)^{\alpha-1}[(u-t_{2j})+(t_{2j}-t_{2l})][(u-t_{2j})+(t_{2j}-t_{2l+1})]du$$
$$=\int_{t_{2l}}^{t_{2l+2}}(t_{2j}-u)^{\alpha+1}du-\int_{t_{2l}}^{t_{2l+2}}(t_{2j}-u)^{\alpha}(2t_{2j}-t_{2l}-t_{2l+1})du$$
$$+\int_{t_{2l}}^{t_{2l+2}}(t_{2j}-u)^{\alpha-1}(t_{2j}-t_{2l})(t_{2j}-t_{2l+1})du$$
$$=h^{\alpha+2}\Big(\frac{(2j-2l)^{\alpha+2}-(2j-2l-1)^{\alpha+2}}{\alpha+2}$$
$$+\frac{[2.2j-2l-(2l+1)][(2j-2l-1)^{\alpha+1}-(2j-2)^{\alpha+1}]}{\alpha+1}$$
$$+\frac{(2j-2l)(2j-2l-1)[(2j-2l)^{\alpha}-(2j-2l-1)^{\alpha}]}{\alpha}\Big)$$
$$=\frac{h^{\alpha+2}}{\alpha(\alpha+1)(\alpha+2)}\Big(\alpha(\alpha+1)[(2j-2l)^{\alpha+2}-(2j-2l-1)^{\alpha+2}]$$
$$+\alpha(\alpha+2)[2.2j-2l-(2l+1)][(2j-2l-1)^{\alpha+1}-(2j-2l)^{\alpha+1}]$$
$$+(\alpha+1)(\alpha+2)(2j-2l)(2j-2l-1)[(2j-2l)^{\alpha}-(2j-2l-1)^{\alpha}\Big)$$
$$=\frac{h^{\alpha+2}}{\alpha(\alpha+1)(\alpha+2)}F_2(l),\qquad l=0,1,2,3\ldots,j-1.$$

Thus we get,

$$
\begin{aligned}
&\int_0^{t_{2j}} (t_{2j}-u)^{\alpha-1} P_2(u)du \\
&= \sum_{l=0}^{j-1} \Big(\frac{h^\alpha}{\alpha(\alpha+1)(\alpha+2)} \frac{F_0(l)}{2} g(t_{2l}) \\
&- \frac{h^\alpha}{\alpha(\alpha+1)(\alpha+2)} \frac{F_1(l)}{2} g(t_{2l+1}) + \frac{h^\alpha}{\alpha(\alpha+1)(\alpha+2)} \frac{F_2(l)}{2} g(t_{2l+2}) \Big) \\
&= \frac{h^\alpha}{\alpha(\alpha+1)(\alpha+2)} \sum_{k=0}^{2j} c_{k,2j} f(t_k, y(t_k)),
\end{aligned}
$$

where, $c_{k,2j}$ is given in (4.2.7) □

We now define a fractional Adams numerical method for solving (4.1.3). Let $y_l \approx y(t_l)$ denote the approximation of $y(t_l)$, $l = 0, 1, 2, \ldots, 2m$. The corrector formula is defined by

$$
y_{2j} = y_0 + y_0^{(1)} \frac{t_{2j}}{1!} + \frac{1}{\Gamma(\alpha)} \Big(\sum_{k=0}^{2j-1} c_{k,2j} f(t_k, y_k) + c_{2j,2j} f(t_{2j}, y_{2j}^P) \Big), \quad j = 1, 2, \ldots, m, \tag{4.2.8}
$$

and

$$
\begin{aligned}
y_{2j+1} &= y_0 + y_0^{(1)} \frac{t_{2j+1}}{1!} + \frac{1}{\Gamma(\alpha)} \int_0^{t_1} (t_{2j+1}-u)^{\alpha-1} f(u, y(u))\, du \\
&+ \frac{1}{\Gamma(\alpha)} \Big(\sum_{k=0}^{2j-1} c_{k,2j} f(t_{k+1}, y_{k+1}) + c_{2j,2j} f(t_{2j+1}, y_{2j+1}^P) \Big), \quad j = 1, 2, \ldots, m-1.
\end{aligned} \tag{4.2.9}
$$

The remaining problem is the determination of the predictor formula required to calculate y_{2j}^P and y_{2j+1}^P. The idea is the same as the one described above: we replace $f(u, y(u))$ and $f(u+h, y(u+h))$ of the integrals on the right-hand sides of equations (4.2.2) and (4.2.3), respectively, by the piecewise linear interpolation polynomials and obtain

$$
y_{2j}^P = y_0 + y_0^{(1)} \frac{t_{2j}}{1!} + \frac{1}{\Gamma(\alpha)} \Big(\sum_{k=0}^{2j-1} a_{k,2j} f(t_k, y_k) + a_{2j,2j} f(t_{2j}, y_{2j}^{PP}) \Big), \quad j = 1, 2, \ldots, m, \tag{4.2.10}
$$

and, with $j = 1, 2, \ldots, m-1$,

$$
y_{2j+1}^P = y_0 + y_0^{(1)} \frac{t_{2j+1}}{1!} + \frac{1}{\Gamma(\alpha)} \Big(\sum_{k=0}^{2j} a_{k,2j+1} f(t_k, y_k) + a_{2j+1,2j+1} f(t_{2j+1}, y_{2j+1}^{PP}) \Big), \tag{4.2.11}
$$

where the weights are [28]

$$a_{k,n+1} = \frac{h^\alpha}{\alpha(\alpha+1)} \begin{cases} n^{\alpha+1} - (n-\alpha)(n+1)^\alpha, \quad \text{if } k = 0, \\ (n-k+2)^{\alpha+1} + (n-k)^{\alpha+1} - 2(n-k+1)^{\alpha+1}, \quad \text{if } 1 \le k \le n, \\ 1, \quad \text{if } k = n+1. \end{cases}$$

Similarly, to calculate y_{2j}^{PP} and y_{2j+1}^{PP}, we replace $f(u, y(u))$ and $f(u+h, y(u+h))$ in the integrals on the right-hand sides of equations (4.2.2) and (4.2.3), respectively, by the piecewise constants and obtain

$$y_{2j}^{PP} = y_0 + y_0^{(1)} \frac{t_{2j}}{1!} + \frac{1}{\Gamma(\alpha)} \sum_{k=0}^{2j-1} b_{k,2j} f(t_k, y_k), \quad j = 1, 2, \ldots, m, \tag{4.2.12}$$

and

$$y_{2j+1}^{PP} = y_0 + y_0^{(1)} \frac{t_{2j+1}}{1!} + \frac{1}{\Gamma(\alpha)} \sum_{k=0}^{2j} b_{k,2j+1} f(t_k, y_k), \quad j = 1, 2, \ldots, m-1. \tag{4.2.13}$$

where the weights are [28]

$$b_{k,n+1} = \frac{h^\alpha}{\alpha} \Big((n+1-k)^\alpha - (n-k)^\alpha \Big). \tag{4.2.14}$$

Our basic fractional Adams method, is completely described now by equations (4.2.8) - (4.2.13).

Remark 8. In practice, we need to approximate the integral in (4.2.9). We shall use the same ideas as in Remark 5.

We have thus completed the description of our numerical algorithm. Now we will discuss the error analysis of the scheme.

4.3 Error analysis

We have the following theorem.

Theorem 4.3.1. Let $0 < \alpha \le 2$ and assume that ${}_0^C D_t^\alpha y \in C^3[0, T]$ for some suitable chosen T. Let $y(t_k)$ and $y_k, k = 0, 1, 2, \ldots, 2m$, $t_{2m} = T$ be the solutions of (4.2.2), (4.2.3), (4.2.8), (4.2.9), respectively. Assume that $y_0 = y(0)$ and $y_1 = y(t_1)$ exactly. Then there exists a positive constant $C_0 > 0$ such that

$$\max_{0\le k\le 2m} |y(t_k) - y_k| \le \begin{cases} C_0 h^{1+2\alpha}, & \text{if } 0 < \alpha \le 1, \\ C_0 h^3, & \text{if } 1 < \alpha \le 2. \end{cases}$$

To prove this theorem, we need some lemmas.

Lemma 4.3.2 (Theorem 2.4 [28])**.** Let $0 < \alpha \le 2$. If $z \in C^1[0,T]$, then there is a constant C_1^α depending only on α such that

$$\Big|\int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} z(u)\, du - \sum_{k=0}^{2j-1} b_{k,2j} z(t_k)\Big| \le C_1^\alpha t_{2j}^\alpha h.$$

where $b_{k,2j}$ are the weights defined by,

$$b_{k,2j} = \frac{h^\alpha}{\alpha}\Big((2j-k)^\alpha - (2j-1-k)^\alpha\Big).$$

Lemma 4.3.3 (Theorem 2.5 [28])**.** Let $0 < \alpha \le 2$. If $z \in C^2[0,T]$, then there is a constant C_2^α depending only on α such that

$$\Big|\int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} z(u)\, du - \sum_{k=0}^{2j} a_{k,2j} z(t_k)\Big| \le C_2^\alpha t_{2j}^\alpha h^2.$$

where $a_{k,2j}$ are the weights defined by,

$$a_{k,2j} = \frac{h^\alpha}{\alpha(\alpha+1)} \begin{cases} (2j-1)^{\alpha+1} - (2j-1-\alpha)(2j)^\alpha, & \text{if } k = 0, \\ (2j-k+1)^{\alpha+1} + (2j-1-k)^{\alpha+1} - 2(2j-k)^{\alpha+1}, & \text{if } 1 \le k \le 2j-1, \\ 1, & \text{if } k = 2j. \end{cases}$$

Lemma 4.3.4. Let $0 < \alpha \le 2$. If $z \in C^3[0,T]$, then there is a constant C_3^α depending only on α such that

$$\Big|\int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} z(u)\, du - \sum_{k=0}^{2j} c_{k,2j} z(t_k)\Big| \le C_3^\alpha t_{2j}^\alpha h^3. \tag{4.3.1}$$

and

$$\Big|\int_{t_1}^{t_{2j+1}} (t_{2j+1} - u)^{\alpha-1} z(u)\, du - \sum_{k=0}^{2j} c_{k,2j} z(t_{k+1})\Big| \le C_3^\alpha t_{2j+1}^\alpha h^3, \tag{4.3.2}$$

where $c_{k,2j}$ are the weights defined in 4.2.7

Proof. We have

$$\begin{aligned} I &= \int_0^{t_{2j}} (t_{2j}-u)^{\alpha-1} z(u)\,du - \sum_{k=0}^{2j} c_{k,2j} z(t_k) \\ &= \int_0^{t_{2j}} (t_{2j}-u)^{\alpha-1} z(u)\,du - \int_0^{t_{2j}} (t_{2j}-u)^{\alpha-1} P_2(u)\,du, \end{aligned} \tag{4.3.3}$$

where $P_2(u)$ is the piecewise quadratic interpolation polynomial of $z(u)$, defined by (4.2.4).

Thus we have

$$\begin{aligned} |I| &= \Big| \sum_{k=0}^{j-1} \int_{t_{2k}}^{t_{2k+2}} (t_{2j}-u)^{\alpha-1} \Big(z(u) - P_2(u) \Big)\,du \Big| \\ &= \Big| \sum_{k=0}^{j-1} \int_{t_{2k}}^{t_{2k+2}} (t_{2j}-u)^{\alpha-1} \frac{z'''(\xi)}{3!} (u-t_{2k})(u-t_{2k+1})(u-t_{2k+2})\,du \Big| \\ &\leq \frac{\|f'''\|_\infty}{3!} (2h)^3 \int_0^{t_{2j}} (t_{2j}-u)^{\alpha-1}\,du = C_3^\alpha t_{2j}^\alpha h^3, \end{aligned}$$

which shows (4.3.1). Similarly, we can show (4.3.2).

□

Lemma 4.3.5. [28] Let $0 < \alpha \leq 2$ and m be a positive integer. Let $a_{k,2j}$ and $b_{k,2j}, k = 0, 1, 2, \ldots, 2j,\ j = 1, 2, \ldots, m$ be introduced in (4.2.10) and (4.2.12), respectively. Then we have

$$a_{k,2j} \geq 0, \qquad b_{k,2j} \geq 0, \quad k = 0, 1, 2, \ldots, 2j,$$

and

$$\sum_{k=0}^{2j} a_{k,2j} \leq \frac{1}{\alpha} T^\alpha, \qquad \sum_{k=0}^{2j} b_{k,2j} \leq \frac{1}{\alpha} T^\alpha. \quad j = 1, 2, \ldots, m.$$

Further, there exist constants D_1^α and D_2^α such that

$$a_{2j,2j} = D_2^\alpha h^\alpha, \quad b_{2j,2j} = D_1^\alpha h^\alpha, \quad j = 1, 2, \ldots, m.$$

Lemma 4.3.6. Let $0 < \alpha \leq 2$. Let $c_{k,2j}, k = 0, 1, 2, \ldots, 2j,\ j = 1, 2, \ldots, m$ be introduced in (4.2.8). Then we have

$$c_{k,2j} \geq 0, \quad k = 0, 1, 2, \ldots, 2j, \tag{4.3.4}$$

and

$$\sum_{k=0}^{2j} c_{k,2j} \leq \frac{1}{\alpha} T^{\alpha}. \tag{4.3.5}$$

Further there exists a constant D_3^{α} such that

$$c_{2j,2j} = D_3^{\alpha} h^{\alpha}, \ j = 1, 2, \ldots, m. \tag{4.3.6}$$

Proof. We first show that

$$F_1(l) \leq 0, \quad l = 0, 1, 2, \ldots, j-1. \tag{4.3.7}$$

It is easy to show that

$$F_1(l) = 2\Big((2j-2l)^{\alpha+2} - (\alpha+2)(2j-2l)^{\alpha+1} - (2j-2l-2)^{\alpha+2} \\ - (\alpha+2)(2j-2l-2)^{\alpha+1}\Big), \quad l = 0, 1, 2, \ldots, j-1.$$

Further, after some direct calculations, we can show that

$$(\gamma+1)(n+2)^{\gamma} + (\gamma+1)n^{\gamma} + n^{\gamma+1} - (n+2)^{\gamma+1} \geq 0, \quad \forall\, n \in \mathbb{Z}^+, \ \gamma > 0.$$

By putting $n = 2j - 2l - 2$ and $\gamma = \alpha + 1$, we get (4.3.7).

Next we show

$$F_0(l) + F_2(l-1) \geq 0, \quad l = 1, 2, \ldots, j-1. \tag{4.3.8}$$

It is easy to show that

$$F_0(l) + F_2(l-1) = 2(2j-2l+2)^{\alpha+2} - (\alpha+2)(2j-2l+2)^{\alpha+1} - 6(\alpha+2)(2j-2l)^{\alpha+1} \\ - 2(2j-2l-2)^{\alpha+2} - (\alpha+2)(2j-2l-2)^{\alpha+1}.$$

Further, after some direct calculations, we can show that

$$2(n+4)^{\alpha+2} - (\alpha+2)(n+4)^{\alpha+1} - 6(\alpha+2)(n+2)^{\alpha+1} - 2n^{\alpha+2} - (\alpha+2)n^{\alpha+1} \geq 0, \quad \forall\, n \in \mathbb{Z}^+. \tag{4.3.9}$$

Hence (4.3.8) follows from (4.3.9). Finally we can also show $F_0(0) \geq 0$ and $F_2(j-1) \geq 0$. Hence we prove (4.3.4).

Further (4.3.5) follows from

$$\sum_{k=0}^{2j} c_{k,2j} = \int_0^{t_{2j}} (t_{2j}-u)^{\alpha-1}\, du = \frac{1}{\alpha} t_{2j}^{\alpha} \le \frac{1}{\alpha} T^{\alpha}.$$

For (4.3.6), we have, by Lemma 4.2.1, $c_{2j,2j} = \frac{1}{2}F_2(j-1) = D_3^{\alpha} h^{\alpha}$, with the suitable constant D_3^{α}. Together these estimates complete the proof of Lemma 4.3.6.

□

Proof of Theorem 4.3.1. We first consider the case where $1 < \alpha \le 2$. We will use mathematical induction. Note that, by assumptions, $|y(t_0) - y_0| = 0$, $|y(t_1) - y_1| = 0$. Assume that

$$|y(t_k) - y_k| \le C_0 h^3, \tag{4.3.10}$$

is true for $k = 0, 1, 2, \ldots, 2j-1$, $j = 1, 2, \ldots, m$. We must prove that this also holds for $k = 2j$. In fact, we have, with $j = 1, 2, \ldots, m$,

$$\begin{aligned}
&\Gamma(\alpha)\Big(y(t_{2j}) - y_{2j}\Big) \\
&= \int_0^{t_{2j}} (t_{2j}-u)^{\alpha-1} f(u, y(u))\, du - \Big(\sum_{k=0}^{2j-1} c_{k,2j} f(t_k, y_k) - c_{2j,2j} f(t_{2j}, t_{2j}^P)\Big) \\
&= \int_0^{t_{2j}} (t_{2j}-u)^{\alpha-1} f(u, y(u))\, du - \int_0^{t_{2j}} (t_{2j}-u)^{\alpha-1} P_2(u)\, du \\
&\quad + \int_0^{t_{2j}} (t_{2j}-u)^{\alpha-1} P_2(u)\, du - \Big(\sum_{k=0}^{2j-1} c_{k,2j} f(t_k, y_k) - c_{2j,2j} f(t_{2j}, t_{2j}^P)\Big) \\
&= \Big(\int_0^{t_{2j}} (t_{2j}-u)^{\alpha-1} f(u, y(u))\, du - \int_0^{t_{2j}} (t_{2j}-u)^{\alpha-1} P_2(u)\, du\Big) \\
&\quad + \sum_{k=0}^{2j-1} c_{k,2j}\Big(f(t_k, y(t_k)) - f(t_k, y_k)\Big) + c_{2j,2j}\Big(f(t_{2j}, y(t_{2j})) - f(t_{2j}, t_{2j}^P)\Big) \\
&= I_1 + II_1 + III_1.
\end{aligned}$$

For I_1, we have, by Lemma 4.3.4,

$$|I_1| = \Big|\int_0^{t_{2j}} (t_{2j}-u)^{\alpha-1} f(u, y(u))\, du - \int_0^{t_{2j}} (t_{2j}-u)^{\alpha-1} P_2(u)\, du\Big| \le C_3^{\alpha} T^{\alpha} h^3.$$

For II_1, we have, by Lemma 4.3.6 and the Lipschitz condition (4.2.1),

$$\begin{aligned}
|II_1| &\le \sum_{k=0}^{2j-1} c_{k,2j} |f(t_k, y(t_k)) - f(t_k, y_k)| \le \sum_{k=0}^{2j-1} c_{k,2j} L |y(t_k) - y_k| \\
&\le \frac{1}{\alpha} T^{\alpha} L \max_{0 \le k \le 2j-1} |y(t_k) - y_k|.
\end{aligned}$$

For III_1, we have, by Lemma 4.3.6 and the Lipschitz condition,

$$|III_1| \leq c_{2j,2j}|f(t_{2j}, y(t_{2j})) - f(t_{2j}, y_{2j}^P)| \leq D_3^\alpha h^\alpha L|y(t_{2j}) - y_{2j}^P|.$$

Now let us consider the bound for $|y(t_{2j}) - y_{2j}^P|$. We have

$$\begin{aligned}
&\Gamma(\alpha)\Big(y(t_{2j}) - y_{2j}^P\Big) \\
&= \int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} f(u, y(u))\, du - \Big(\sum_{k=0}^{2j-1} a_{k,2j} f(t_k, y_k) - a_{2j,2j} f(t_{2j}, t_{2j}^{PP})\Big) \\
&= \Big(\int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} f(u, y(u))\, du - \int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} P_1(u)\, du\Big) \\
&\quad + \sum_{k=0}^{2j-1} a_{k,2j}\Big(f(t_k, y(t_k)) - f(t_k, y_k)\Big) + a_{2j,2j}\Big(f(t_{2j}, y(t_{2j})) - f(t_{2j}, t_{2j}^{PP})\Big) \\
&= I_2 + II_2 + III_2.
\end{aligned}$$

For I_2, we have, by Lemma 4.3.3,

$$|I_2| = \Big| \int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} f(u, y(u))\, du - \int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} P_1(u)\, du \Big| \leq C_2^\alpha T^\alpha h^2.$$

For II_2, we have, by Lemma 4.3.5 and the Lipschitz condition (4.2.1),

$$\begin{aligned}
|II_2| &\leq \sum_{k=0}^{2j-1} a_{k,2j}|f(t_k, y(t_k)) - f(t_k, y_k)| \leq \sum_{k=0}^{2j-1} a_{k,2j}|y(t_k) - y_k| \\
&\leq \frac{1}{\alpha} T^\alpha L \max_{0\leq k\leq 2j-1} |y(t_k) - y_k|.
\end{aligned}$$

For III_2, we have, by Lemma 4.3.5 and Lipschitz condition (4.2.1),

$$|III_2| \leq a_{2j,2j}|f(t_{2j}, y(t_{2j})) - f(t_{2j}, y_{2j}^{PP})| \leq D_2^\alpha h^\alpha L|y(t_{2j}) - y_{2j}^{PP}|.$$

We also need to consider the bound for $|y(t_{2j}) - y_{2j}^{PP}|$. We have

$$\begin{aligned}
&\Gamma(\alpha)\Big(y(t_{2j}) - y_{2j}^{PP}\Big) = \int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} f(u, y(u))\, du - \sum_{k=0}^{2j-1} b_{k,2j} f(t_k, y_k) \\
&= \int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} f(u, y(u))\, du - \sum_{k=0}^{2j-1} b_{k,2j} f(t_k, y(t_k)) \\
&\quad + \sum_{k=0}^{2j-1} b_{k,2j}\Big(f(t_k, y(t_k)) - f(t_k, y_k)\Big) = I_3 + II_3.
\end{aligned}$$

For I_3, we have, by Lemma 4.3.2, $|I_3| \leq C_1^\alpha T^\alpha h$.

For II_3, we have, by Lemma 4.3.5 and Lipschitz condition (4.2.1),

$$|II_3| \leq \frac{1}{\alpha} T^\alpha L \max_{0 \leq k \leq 2j-1} |y(t_k) - y_k|.$$

Together these estimates, we have

$$\begin{aligned}
\Gamma(\alpha)|y(t_{2j}) - y_{2j}| &\leq C_3^\alpha T^\alpha h^3 + \frac{1}{\alpha} T^\alpha L \max_{0 \leq k \leq 2j-1} |y(t_k) - y_k| \\
&+ D_3^\alpha h^\alpha L \frac{1}{\Gamma(\alpha)} \Big(C_2^\alpha T^\alpha h^2 + \frac{1}{\alpha} T^\alpha L \max_{0 \leq k \leq 2j-1} |y(t_k) - y_k| \\
&+ D_2^\alpha h^\alpha L \frac{1}{\Gamma(\alpha)} \Big[C_1^\alpha T^\alpha h + \frac{1}{\alpha} T^\alpha L \max_{0 \leq k \leq 2j-1} |y(t_k) - y_k| \Big] \Big) \\
&\leq \Big[C_3^\alpha T^\alpha h^3 + \frac{D_3^\alpha L C_2^\alpha T^\alpha h^{2+\alpha}}{\Gamma(\alpha)} + \frac{D_3^\alpha D_2^\alpha L^2 C_1^\alpha T^\alpha h^{1+2\alpha}}{\Gamma(\alpha)^2} \Big] \\
&\quad + \Big[\frac{1}{\alpha} T^\alpha L + \frac{D_3^\alpha L^2 (\frac{1}{\alpha} T^\alpha) h^\alpha}{\Gamma(\alpha)} + \frac{D_3^\alpha D_2^\alpha (\frac{1}{\alpha} T^\alpha) L^3 h^{2\alpha}}{\Gamma(\alpha)^2} \Big] \max_{0 \leq k \leq 2j-1} |y(t_k) - y_k|.
\end{aligned}$$

By mathematical induction (4.3.10), we have

$$\begin{aligned}
|y(t_{2j}) - y_{2j}| \leq & \Big[\frac{C_3^\alpha T^\alpha h^3}{\Gamma(\alpha)} + \frac{D_3^\alpha L C_2^\alpha T^\alpha h^{2+\alpha}}{\Gamma(\alpha)^2} + \frac{D_3^\alpha D_2^\alpha L^2 C_1^\alpha T^\alpha h^{1+2\alpha}}{\Gamma(\alpha)^3} \Big] \\
& + \Big[\frac{1}{\Gamma(\alpha+1)} T^\alpha L + \frac{D_3^\alpha L^2 (\frac{1}{\alpha} T^\alpha) h^\alpha}{\Gamma(\alpha+1)\Gamma(\alpha)} + \frac{D_3^\alpha D_2^\alpha (\frac{1}{\alpha} T^\alpha) L^3 h^{2\alpha}}{\Gamma(\alpha+1)\Gamma(\alpha)^2} \Big] C_0 h^3.
\end{aligned} \tag{4.3.11}$$

We first choose T sufficiently small, see Lemma 3.1 in [28] such that $\frac{1}{\Gamma(\alpha+1)} T^\alpha L \leq \frac{1}{2}$. Then we fix this value for T and make the sum of the remaining terms in the right hand side of (4.3.11) smaller than $\frac{C_0}{2} h^3$ (for sufficiently small h) by choosing C_0 sufficiently large. Hence we obtain, for $1 < \alpha \leq 2$,

$$|y(t_{2j}) - y_{2j}| \leq \frac{C_0}{2} h^3 + \frac{C_0}{2} h^3 = C_0 h^3. \tag{4.3.12}$$

We also need to show that if (4.3.10) is true for $k = 0, 1, 2, \ldots, 2j$ with $j = 1, 2, \ldots, m-$

1, then it also holds for $k = 2j + 1$. In fact, we have, with $j = 1, 2, \ldots, m-1$,

$$\Gamma(\alpha)\Big(y(t_{2j+1}) - y_{2j+1}\Big) = \int_0^{t_{2j+1}} (t_{2j+1} - u)^{\alpha-1} f(u, y(u))\, du$$
$$- \Big(\int_0^{t_1} (t_{2j+1} - u)^{\alpha-1} f(u, y(u))\, du + \sum_{k=0}^{2j-1} c_{k,2j} f(t_{k+1}, y_{k+1}) + c_{2j,2j} f(t_{2j+1}, y_{2j+1}^P)\Big)$$
$$= \int_{t_1}^{t_{2j+1}} (t_{2j+1} - u)^{\alpha-1} f(u, y(u))\, du - \Big(\sum_{k=0}^{2j-1} c_{k,2j} f(t_{k+1}, y_{k+1}) + c_{2j,2j} f(t_{2j+1}, y_{2j+1}^P)\Big)$$
$$= \Big(\int_{t_1}^{t_{2j+1}} (t_{2j+1} - u)^{\alpha-1} f(u, y(u))\, du - \int_{t_1}^{t_{2j+1}} (t_{2j+1} - u)^{\alpha-1} Q_2(u)\, du \Big)$$
$$+ \sum_{k=0}^{2j-1} c_{k,2j} \Big(f(t_{k+1}, y(t_{k+1})) - f(t_{k+1}, y_{k+1})\Big) + c_{2j,2j}\Big(f(t_{2j+1}, y(t_{2j+1})) - f(t_{2j+1}, y_{2j+1}^P)\Big).$$

Using the same arguments as proving (4.3.12), we can show

$$|y(t_{2j+1}) - y_{2j+1}| \leq C_0 h^3, \quad j = 1, 2, \ldots, m-1.$$

Hence we complete the proof for the case where $1 < \alpha \leq 2$.

For the case $0 < \alpha \leq 1$. Note that, by the assumptions, $|y(t_0) - y_0| = 0$, and $|y(t_1) - y_1| = 0$. Assume that

$$|y(t_k) - y_k| \leq C_0 h^{1+2\alpha}, \tag{4.3.13}$$

for $k = 0, 1, 2, \ldots, 2j-1,\ j = 1, 2, \ldots, m$. We must prove that this also holds for $k = 2j$. In fact, by using the same arguments as showing (4.3.12), we get

$$|y(t_{2j}) - y_{2j}| \leq \Big[\frac{C_3^\alpha T^\alpha h^3}{\Gamma(\alpha)} + \frac{D_3^\alpha L C_2^\alpha T^\alpha h^{2+\alpha}}{\Gamma(\alpha)^2} + \frac{D_3^\alpha D_2^\alpha L^2 C_1^\alpha T^\alpha h^{1+2\alpha}}{\Gamma(\alpha)^3}\Big]$$
$$+ \Big[\frac{1}{\Gamma(\alpha+1)} T^\alpha L + \frac{D_3^\alpha L^2 (\frac{1}{\alpha} T^\alpha) h^\alpha}{\Gamma(\alpha+1)\Gamma(\alpha)} + \frac{D_3^\alpha D_2^\alpha (\frac{1}{\alpha} T^\alpha) L^3 h^{2\alpha}}{\Gamma(\alpha+1)\Gamma(\alpha)^2}\Big] C_0 h^{1+2\alpha}. \tag{4.3.14}$$

As in the case for $1 < \alpha \leq 2$, we first choose T sufficiently small such that $\frac{1}{\Gamma(\alpha+1)} T^\alpha L \leq \frac{1}{2}$. Then we fix this value for T and make the sum of the remaining terms in the right had side of (4.3.14) smaller than $\frac{C_0}{2} h^{1+2\alpha}$ (for sufficiently small h) by choosing C_0 sufficiently large.

Hence we obtain, for $0 < \alpha \leq 1$,

$$|y(t_{2j}) - y_{2j}| \leq \frac{C_0}{2} h^{1+2\alpha} + \frac{C_0}{2} h^{1+2\alpha} = C_0 h^{1+2\alpha}. \tag{4.3.15}$$

Similarly, we can show that if (4.3.13) is true for $k = 0, 1, 2, \ldots, 2j$ with $j = 1, 2, \ldots, m-1$, then it is also true for $k = 2j+1$. Together these estimates complete the proof of Theorem 4.3.1.

□

4.4 Numerical examples

Example 9. *[28] This example deals with the nonlinear fractional differential equation where the unknown solution y has a smooth derivative of order α. Specifically we shall look at the equation*

$$ {}_0^C D_t^{\alpha} y(t) = \frac{40320}{\Gamma(9-\alpha)} t^{8-\alpha} - 3\frac{\Gamma(5+\alpha/2)}{\Gamma(5-\alpha/2)} t^{4-\alpha/2} + \frac{9}{4}\Gamma(\alpha+1) + \left(\frac{3}{2}t^{\alpha/2} - t^4\right)^3 - [y(t)]^{3/2}. $$

The initial conditions were chosen to be homogeneous ($y(0) = 0,\ y'(0) = 0$; the latter only in the case $1 < \alpha < 2$). This equation has been chosen because it exhibits a difficult (nonlinear and nonsmooth) right-hand side, and yet we are able to find its exact solution, thus allowing us to compare the numerical results for this nontrivial case to the exact results. Indeed, the exact solution of this initial value problem is

$$ y(t) = t^8 - 3t^{4+\alpha/2} + \frac{9}{4}t^{\alpha}, $$

and hence

$$ {}_0^C D_t^{\alpha} y(t) = \frac{40320}{\Gamma(9-\alpha)} t^{8-\alpha} - 3\frac{\Gamma(5+\alpha/2)}{\Gamma(5-\alpha/2)} t^{4-\alpha/2} + \frac{9}{4}\Gamma(\alpha+1), $$

which implies ${}_0^C D_t^{\alpha} y \in C^3[0,T]$ for arbitrary $T > 0$ and $0 < \alpha \le 2$, and thus the conditions of Theorem 4.3.1 are fulfilled.

For various choices of $\alpha \in (0, 2]$, we compute the errors at $t_n = 1$. We choose the stepsize $h = 1/(5 \times 2^l), l = 1, 2, \ldots, 7$, i.e, we divided the interval $[0, 1]$ into $n = 1/h$ small subintervals with nodes $0 = t_0 < t_1 < \cdots < t_n = 1$. Then we compute the error $e(t_n) = y(t_n) - y_n$. By Theorem 4.3.1, we have

$$ \max_{0\le k\le 2m} |y(t_k) - y_k| \le \begin{cases} C_0 h^{1+2\alpha}, & \text{if } 0 < \alpha \le 1, \\ C_0 h^3, & \text{if } 1 < \alpha \le 2. \end{cases} $$

In Tables 4.4.1-4.4.2, we compute the orders of convergence for different values of α. *We observe that the order of convergence is* $O(h^{1+2\alpha})$ *for* $0 < \alpha \leq 1$. *But the observed order of convergence is higher than 3 for* $1 < \alpha \leq 2$ *in this example. For example, when* $\alpha = 1.35$, *the experimentally determined order is 3.5. When* $\alpha = 1.65$, *the experimentally determined order of convergence (EOC) is almost 4.*

n	EOC ($\alpha = .35$)	EOC ($\alpha = .40$)	EOC ($\alpha = .45$)	EOC ($\alpha = .50$)
10				
20	1.2475	1.2993	1.2965	1.2037
40	1.5302	1.6834	1.7891	1.8583
80	1.7461	1.8758	1.9787	2.0638
160	1.8293	1.9391	2.0350	2.1232
320	1.8518	1.9482	2.0391	2.1284
640	1.8478	1.9356	2.0233	2.1135

Table 4.4.1: Numerical results at $t = 1$ in Example 9 with the different fractional order $\alpha < 1$

n	EOC ($\alpha = 1.35$)	EOC ($\alpha = 1.40$)	EOC ($\alpha = 1.60$)	EOC ($\alpha = 1.65$)
10				
20	3.4810	3.5611	3.7581	3.7921
40	3.6886	3.7438	3.8753	3.8963
80	3.7695	3.8198	3.9268	3.9414
160	3.7977	3.8517	3.9526	3.99637
320	3.7944	3.8588	3.99667	3.9772
640	3.7662	3.8355	3.9810	3.9380

Table 4.4.2: Numerical results at $t = 1$ in Example 9 with the different fractional order $\alpha > 1$

In Figure 4.4.1, we plot the order of convergence. We have

$$log_2(|e(t_n)|) \leq log_2(C) + (1 + 2\alpha)log_2(h).$$

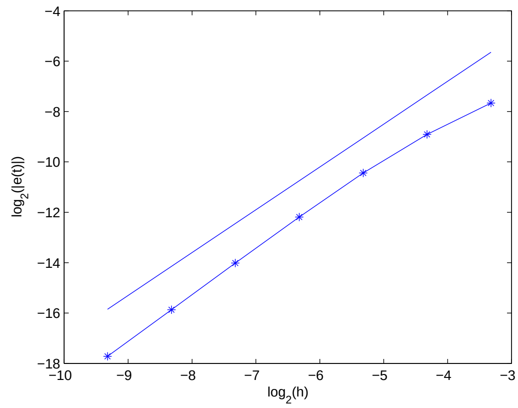

Figure 4.4.1: The experimentally determined orders of convergence ("EOC ") at $t = 1$ in Example 9 with $\alpha = 0.35$

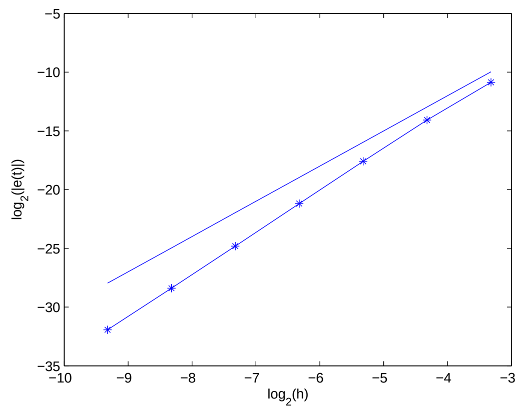

Figure 4.4.2: The experimentally determined orders of convergence ("EOC ") at $t = 1$ in Example 9 with $\alpha = 1.25$

Let $y = log_2(|e(t_n)|)$ and $x = log_2(h)$. 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 $y = (1 + 2\alpha)x$, where $\alpha = 0.35$. We see that these two lines are almost parallel which confirms that the order of convergence of the numerical method is $O(h^{1+2\alpha})$.

In Figure 4.4.2, we will plot the order of convergence for $\alpha = 1.25$. 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 $y = 3x$. We observe that the order of convergence is higher than 3 (almost $1 + 2\alpha$).

Chapter 5

Higher order numerical methods for fractional differential equations by extrapolation

5.1 Introduction

The aim of this chapter is to discuss convergence acceleration methods for fractional differential equation by extrapolation procedure. We will consider Richardson extrapolation algorithms for solving higher order fractional differential equations. Richardson extrapolation is an idea which can often be used to improve the convergence order of the numerical method: from a method of order $O(h^{k_0})$ we can get a method of order $O(h^{k_1}, k_0 < k_1)$.

Suppose that we want to approximate a quantity A, we have available approximation $A(h)$ for stepsize $h > 0$.

For example, we want to approximate

$$A = f'(x_0).$$

By Taylor formula,

$$A = f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{f''(x_0)}{2!}h - \frac{f'''(x_0)}{3!}h^2 - \dots$$

Denote

$$A_0(h) = \frac{f(x_0+h) - f(x_0)}{h},$$

we have

$$A = A_0(h) + a_0 h + a_1 h^2 + \dots \tag{5.1.1}$$

we note that $A_0(h)$ is a numerical method of order $O(h)$.

We use the stepsize $\frac{h}{t}, t > 0$, for example $t = 2$, we get the approximate $A_0(\frac{h}{t})$ i.e.,

$$A = A_0(\frac{h}{t}) + a_0(\frac{h}{t}) + a_1(\frac{h}{t})^2 + \dots \tag{5.1.2}$$

Multiplying t in both sides of (5.1.2) we get

$$tA = tA_0(\frac{h}{t}) + a_0 h + a_1 t(\frac{h}{t})^2 + \dots. \tag{5.1.3}$$

Subtracting (5.1.1) from (5.1.3), we get

$$(t-1)A = [tA_0(\frac{h}{t}) - A_0(h)] + O(h^2).$$

i.e.

$$A = \frac{tA_0(\frac{h}{t}) - A_0(h)}{t-1} + O(h^2),$$

Denote

$$A_1(h) = \frac{tA_0(\frac{h}{t}) - A_0(h)}{t-1},$$

we get

$$A = A_1(h) + O(h^2).$$

Thus we see that $A_1(h)$ is a numerical method of $O(h^2)$. Let $t = 2$, we get the extrapolation formula

$$A_1(h) = 2A_0(\frac{h}{2}) - A_0(h).$$

5.2 Richardson extrapolation

Let us now consider the general idea of the Richardson extrapolation. Assume that $A(h)$ is the approximation of a quantity A, where h is the stepsize . We also assume that

$$A = A_0(h) + a_0 h^{k_0} + a_1 h^{k_1} + a_2 h^{k_2} + \dots \tag{5.2.1}$$

with $0 < k_0 < k_1 < k_2 < \dots$, we use the stepsize $\frac{h}{t}, t > 0$. (for example $t = 2$) to get the approximation $A_0(\frac{h}{t})$, i.e.

$$A = A_0(\frac{h}{t}) + a_0(\frac{h}{t})^{k_0} + a_1(\frac{h}{t})^{k_1} + a_2(\frac{h}{t})^{k_2} + \dots . \tag{5.2.2}$$

Multiplying t^{k_0} in both sides, we get

$$t^{k_0} A = t^{k_0} A_0(\frac{h}{t}) + a_0(h)^{k_0} + a_1 t^{k_0}(\frac{h}{t})^{k_1} + a_2 t^{k_0}(\frac{h}{t})^{k_2} + \dots . \tag{5.2.3}$$

Subtracting (5.2.1) from (5.2.3), we have

$$A = \frac{t^{k_0} A_0(\frac{h}{t}) - A_0(h)}{t^{k_0} - 1} + b_1 h^{k_1} + b_2 h^{k_2} + \dots$$

Denote

$$A_1(h) = \frac{t^{k_0} A_0(\frac{h}{t}) - A_0(h)}{t^{k_0} - 1},$$

we have

$$A = A_1(h) + b_1 h^{k_1} + b_2 h^{k_2} + \dots$$

Thus $A_1(h)$ is a numerical method of convergence order $O(h^{k_1})$, we can continue this process to construct the numerical methods of order $O(h^{k_2}), O(h^{k_3}), \dots$. Choose $t = 2$ we first calculate $A_0(h), \quad A_0(\frac{h}{2}), \quad A_0(\frac{h}{2^2}), \quad A_0(\frac{h}{2^3})$ which has convergence order $O(h^{k_0})$. We next calculate $A_1(h), \quad A_1(\frac{h}{2}), \quad A_1(\frac{h}{2^2}), \dots$ which has convergence order $O(h^{k_1})$. Similarly, we can calculate $A_2(h), \quad A_2(\frac{h}{2}), \quad A_2(\frac{h}{2^2}), \dots$ which has convergence order $O(h^{k_2})$.

We proceed by setting up a triangular array (so-called Romberg tableau) of approximation value for A of the form

$A_0(h)$

$A_0(\frac{h}{2}) \quad A_1(h)$

$A_0(\frac{h}{2^2}) \quad A_1(\frac{h}{2}) \quad A_2(h)$

$A_0(\frac{h}{2^3}) \quad A_1(\frac{h}{2^2}) \quad A_2(\frac{h}{2})$

$A_0(\frac{h}{2^4}) \quad A_1(\frac{h}{2^3}) \quad A_2(\frac{h}{2^2})$

. . .

. . .

. . .

Here

$$A_1(h) = \frac{2^{k_0}A_0(\frac{h}{2}) - A_0(h)}{2^{k_0}-1}, \quad A_1(\frac{h}{2}) = \frac{2^{k_0}A_0(\frac{h}{2^2}) - A_0(\frac{h}{2})}{2^{k_0}-1},$$

$$A_2(h) = \frac{2^{k_1}A_1(\frac{h}{2}) - A_1(h)}{2^{k_1}-1}, \quad A_2(\frac{h}{2}) = \frac{2^{k_1}A_1(\frac{h}{2^2}) - A_1(\frac{h}{2})}{2^{k_1}-1}$$

To observe the order $O(h^{k_0})$ from $A_0(h), A_0(\frac{h}{2}), A_0(\frac{h}{2^2}), \dots$ we can use the following idea.

Note that,

$$|e_0(h)| = |A - A_0(h)| \leq Ch^{k_0}.$$

$$|e_0(\frac{h}{2})| = |A - A_0(\frac{h}{2})| \leq C(\frac{h}{2})^{k_0}.$$

Thus

$$\frac{|e_0(h)|}{|e_0(\frac{h}{2})|} \approx \frac{h^{k_0}}{(\frac{h}{2})^{k_0}} = 2^{k_0}, \quad k_0 = \log_2 \frac{|e_0(h)|}{|e_0(\frac{h}{2})|}.$$

Hence one can calculat all the values

$$\log_2 \frac{|e_0(h)|}{|e_0(\frac{h}{2})|}, \quad \log_2 \frac{|e_0(\frac{h}{2})|}{|e_0(\frac{h}{2^2})|}, \quad \log_2 \frac{|e_0(\frac{h}{2^2})|}{|e_0(\frac{h}{2^3})|}, \dots$$

and observe that the values should be k_0 approximately.

Similarly, we can calculate

$$\log_2 \frac{|e_1(h)|}{|e_1(\frac{h}{2})|}, \quad \log_2 \frac{|e_1(\frac{h}{2})|}{|e_1(\frac{h}{2^2})|}, \quad \log_2 \frac{|e_1(\frac{h}{2^2})|}{|e_1(\frac{h}{2^3})|}, \dots$$

and observe that the values should be k_1 approximately.

In this chapter we will consider two extrapolation algorithms for solving fractional differential equations. One algorithm is for solving a linear fractional differential equation which is based on the direct discretization of the fractional differential operator. Another algorithm is for solving the nonlinear fractional differential equation which is based on the discretization of the equivalent integral form of the fractional differential equation. We also discuss in detail how to determine the starting values and the starting integrals in the numerical methods for quadratic interpolation polynomials. Numerical results show that the approximate solutions of these two numerical methods have the expected asymptotic expansions.

We consider the Richardson extrapolation algorithms for solving the following fractional order differential equation

$$ {}_0^C D_t^{\alpha} y(t) = f(t, y(t)), \quad 0 < t \le T, \tag{5.2.4} $$
$$ y^{(k)}(0) = y_0^{(k)}, \quad k = 0, 1, 2, \ldots, \lceil \alpha \rceil - 1, \tag{5.2.5} $$

where the $y_0^{(k)}$ may be arbitrary real numbers and $\alpha > 0$. Here ${}_0^C D_t^{\alpha}$ denotes the differential operator in the sense of Caputo defined by,

$$ {}_0^C D_t^{\alpha} y(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t (t-u)^{n-\alpha-1} y^{(n)}(u)\, du, $$

where $n = \lceil \alpha \rceil$ is the smallest integer $\ge \alpha$.

Extrapolation can be used to accelerate the convergence of a given sequence, [6, 7, 92]. Its applicability depends on the fact that a given sequence of the approximate solutions of the problem possesses an asymptotic expansion. Let us review some extrapolation algorithms for solving fractional differential equations. For the linear fractional differential equation, Diethelm [26] introduced an algorithm for solving the following linear differential equation of fractional order, with $0 < \alpha < 1$,

$$ {}_0^C D_t^{\alpha} y(t) = \beta y(t) + f(t), \quad 0 \le t \le 1, \tag{5.2.6} $$
$$ y(0) = y_0, \tag{5.2.7} $$

where $\beta < 0$ and f is a given function on $[0, 1]$. Diethelm and Walz [33] proved that the approximate solution of the numerical algorithm in [26] has an asymptotic expansion. For the general nonlinear fractional differential equation (5.2.4) -(5.2.5),Diethelm, Ford and Freed [28] introduced a fractional Adams-type predictor-corrector method for solving (5.2.4)-(5.2.5) and numerical evidence suggests that the approximate solution of the numerical method in [28] has also an asymptotic expansion.

Recently, Yan, Pal and Ford [93] extended the numerical method in [26] and obtained a high order numerical method for solving (5.2.6) - (5.2.7) and proved that the approximate solution has an asymptotic expansion.

5.3 The linear fractional differential equation

5.3.1 The numerical method

In this section we will consider a higher order numerical method for solving (5.2.6)-(5.2.7). It is well-known that (5.2.6)-(5.2.7) is equivalent to, with $0 < \alpha < 1$,

$$ {}_0^R D_t^{\alpha}[y(t) - y_0] = \beta y(t) + f(t), \quad 0 \le t \le 1, \tag{5.3.1} $$

where ${}_0^R D_t^{\alpha} y(t)$ denotes the Riemann-Liouville fractional derivative defined by, with $0 < \alpha < 1$,

$$ {}_0^R D_t^{\alpha} y(t) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_0^t (t-u)^{-\alpha} y(u)\, du. \tag{5.3.2} $$

By using the Hadamard finite-part integral, ${}_0^R D_t^{\alpha} y(t)$ can be written as

$$ {}_0^R D_t^{\alpha} y(t) = \frac{1}{\Gamma(-\alpha)} \oint_0^t (t-u)^{-1-\alpha} y(u)\, du. \tag{5.3.3} $$

Here the integral $\oint$ denotes a Hadamard finite-part integral [25].

Let M be a positive integer and let $0 = t_0 < t_1 < \cdots < t_j < \cdots < t_M = 1$ be a partition of $[0, 1]$. At $t = t_j$, we have

$$ {}_0^R D_t^{\alpha}[y(t_j) - y_0] = \beta y(t_j) + f(t_j), \quad j = 1, 2, \dots, M. $$

Note that

$$ {}_0^R D_t^{\alpha} y(t_j) = \frac{1}{\Gamma(-\alpha)} \oint_0^{t_j} (t_j - u)^{-1-\alpha} y(u)\, du = \frac{t_j^{-\alpha}}{\Gamma(-\alpha)} \oint_0^1 w^{-1-\alpha} y(t_j - t_j w)\, dw. \tag{5.3.4} $$

For every j, we denote $g(w) = y(t_j - t_j w)$ and approximate $\oint_0^1 w^{-1-\alpha} g(w)\, dw$ by $\oint_0^1 w^{-1-\alpha} g_1(w)\, dw$, where $g_1(w)$ is the piecewise linear interpolation polynomial on the nodes $0, \frac{1}{j}, \frac{2}{j}, \dots, \frac{j}{j} = 1$. We then obtain

$$\begin{aligned}
{}_0^R D_t^\alpha y(t_j) &= \frac{t_j^{-\alpha}}{\Gamma(-\alpha)} \oint_0^1 w^{-1-\alpha} y(t_j - t_j w)\, dw \\
&= \frac{t_j^{-\alpha}}{\Gamma(-\alpha)} \Big(\sum_{k=1}^{j} \oint_{t_{k-1}}^{t_k} w^{-1-\alpha} g_1(w)\, dw + R_j(g) \Big) \\
&= \frac{t_j^{-\alpha}}{\Gamma(-\alpha)} \Big(\sum_{k=0}^{j} \alpha_{k,j} y(t_{j-k}) + R_j(g) \Big),
\end{aligned}$$

where $\alpha_{k,j}, k = 0, 1, 2, \dots, j$ are weights and $R_j(g)$ is the remainder term. Thus (5.3.1) satisfies, with $j = 1, 2, \dots, M$,

$$\begin{aligned}
y(t_j) = &\frac{1}{\alpha_{0,j} - t_j^\alpha \Gamma(-\alpha)\beta} \Big[t_j^\alpha \Gamma(-\alpha) f(t_j) \\
&- \sum_{k=1}^{j} \alpha_{k,j} y(t_{j-k}) + y_0 \sum_{k=0}^{j} \alpha_{k,j} - R_j(g) \Big].
\end{aligned} \tag{5.3.5}$$

Let $y_j \approx y(t_j)$ be the approximate solutions of $y(t_j)$. We define the following finite difference method for solving (5.2.6) - (5.2.7), with $j = 1, 2, \dots, M$,

$$y_j = \frac{1}{\alpha_{0,j} - t_j^\alpha \Gamma(-\alpha)\beta} \Big[t_j^\alpha \Gamma(-\alpha) f(t_j) - \sum_{k=1}^{j} \alpha_{k,j} y_{j-k} + y_0 \sum_{k=0}^{j} \alpha_{k,j} \Big]. \tag{5.3.6}$$

Diethelm and Walz [33] proved the following asymptotic expansion theorem.

Theorem 5.3.1 (Theorem 2.1 in [33])**.** Let $0 < \alpha < 1$ and M be a positive integer. Let $0 = t_0 < t_1 < t_2 < \cdots < t_j < \cdots < t_M = 1$ be a partition of $[0, 1]$ and h the stepsize. Let $y(t_j)$ and y_j be the exact and the approximate solutions of (5.3.5) and (5.3.6), respectively. Assume that the function $y \in C^{m+2}[0, 1],\ m \geq 2$. Then there exist coefficients $c_\mu = c_\mu(\alpha)$ and $c_\mu^* = c_\mu^*(\alpha)$ such that the sequence $\{y_l\}, l = 0, 1, 2, \dots, M$ possesses an asymptotic expansion of the form

$$y(t_M) - y_M = \sum_{\mu=2}^{m+1} c_\mu (M)^{\alpha-\mu} + \sum_{\mu=1}^{\mu^*} c_\mu^* (M)^{-2\mu} + o((M)^{\alpha-m-1}), \quad \text{for } M \to \infty,$$

that is,

$$y(t_M) - y_M = \sum_{\mu=2}^{m+1} c_\mu h^{\mu-\alpha} + \sum_{\mu=1}^{\mu^*} c_\mu^* h^{2\mu} + o(h^{m+1-\alpha}), \quad \text{for } h \to 0,$$

where μ^* is the integer satisfying $2\mu^* < m + 1 - \alpha < 2(\mu^* + 1)$, and c_μ and c_μ^* are certain coefficients that depend on y.

Yan, Pal and Ford [93] extended the numerical method in Diethelm and Walz [33] and obtained a high order numerical method for solving (5.2.6)- (5.2.7). Let M be a fixed positive integer and let $0 = t_0 < t_1 < t_2 < \cdots < t_{2j} < t_{2j+1} < \cdots < t_{2M} = 1$ be a partition of $[0, 1]$ and h the stepsize. At the nodes $t_{2j} = \frac{2j}{2M}$, the equations (5.2.6)- (5.2.7) satisfy

$$ {}_0^R D_t^\alpha [y(t_{2j}) - y_0] = \beta y(t_{2j}) + f(t_{2j}), \quad j = 1, 2, \ldots, M, $$

and at the nodes $t_{2j+1} = \frac{2j+1}{2M}$, the equations (5.2.6)- (5.2.7) satisfy

$$ {}_0^R D_t^\alpha [y(t_{2j+1}) - y_0] = \beta y(t_{2j+1}) + f(t_{2j+1}), \quad j = 0, 1, 2, \ldots, M-1. \tag{5.3.7} $$

Note that

$$ {}_0^R D_t^\alpha y(t_{2j}) = \frac{1}{\Gamma(-\alpha)} \oint_0^{t_{2j}} (t_{2j}-u)^{-1-\alpha} y(u)\, du = \frac{t_{2j}^{-\alpha}}{\Gamma(-\alpha)} \oint_0^1 w^{-1-\alpha} y(t_{2j}-t_{2j}w)\, dw. \tag{5.3.8} $$

For every j, we denote $g(w) = y(t_{2j} - t_{2j}w)$ and approximate $\oint_0^1 w^{-1-\alpha} g(w)\, dw$ by $\oint_0^1 w^{-1-\alpha} g_2(w)\, dw$, where $g_2(w)$ is the piecewise quadratic interpolation polynomials on the nodes $w_l = l/2j,\ l = 0, 1, 2, \ldots, 2j$. More precisely, we have, for $k = 1, 2, \ldots, j$,

$$ \begin{aligned} g_2(w) = & \frac{(w - w_{2k-1})(w - w_{2k})}{(w_{2k-2} - w_{2k-1})(w_{2k-2} - w_{2k})} g(w_{2k-2}) \\ & + \frac{(w - w_{2k-2})(w - w_{2k})}{(w_{2k-1} - w_{2k-2})(w_{2k-1} - w_{2k})} g(w_{2k-1}) \\ & + \frac{(w - w_{2k-2})(w - w_{2k-1})}{(w_{2k} - w_{2k-2})(w_{2k} - w_{2k-1})} g(w_{2k}), \quad \text{for } w \in [w_{2k-2}, w_{2k}]. \end{aligned} $$

Thus

$$ \begin{aligned} {}_0^R D_t^\alpha y(t_{2j}) &= \frac{t_{2j}^{-\alpha}}{\Gamma(-\alpha)} \oint_0^1 w^{-1-\alpha} y(t_{2j} - t_{2j}w)\, dw \\ &= \frac{t_{2j}^{-\alpha}}{\Gamma(-\alpha)} \Big(\sum_{k=1}^{j} \oint_{w_{2k-2}}^{w_{2k}} w^{-1-\alpha} g_2(w)\, dw + R_{2j}(g) \Big) \\ &= \frac{t_{2j}^{-\alpha}}{\Gamma(-\alpha)} \Big(\sum_{k=0}^{2j} \alpha_{k,2j} y(t_{2j-k}) + R_{2j}(g) \Big) \end{aligned} $$

where $R_{2j}(g)$ is the remainder term and $\alpha_{k,2j}, k = 0, 1, 2, \ldots, 2j$ are weights given by

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

Here

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

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

and

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

Hence (5.3.1) satisfies, with $j = 1, 2, \ldots, M$,

$$
y(t_{2j}) = \frac{1}{\alpha_{0,2j} - t_{2j}^{\alpha}\Gamma(-\alpha)\beta}\Big[t_{2j}^{\alpha}\Gamma(-\alpha)f(t_{2j}) - \sum_{k=1}^{2j}\alpha_{k,2j}y(t_{2j-k}) + y_0\sum_{k=0}^{2j}\alpha_{k,2j} - R_{2j}(g)\Big]. \tag{5.3.9}
$$

At the nodes $t_{2j+1} = \frac{2j+1}{2M},\ j = 0, 1, 2, \dots, M-1$, we have

$$
\begin{aligned}
{}_0^R D_t^\alpha y(t_{2j+1}) &= \frac{1}{\Gamma(-\alpha)} \oint_0^{t_{2j+1}} (t_{2j+1} - u)^{-1-\alpha} y(u)\, du \\
&= \frac{1}{\Gamma(-\alpha)} \oint_0^{t_1} (t_{2j+1} - u)^{-1-\alpha} y(u)\, du \\
&\quad + \frac{t_{2j+1}^{-\alpha}}{\Gamma(-\alpha)} \oint_0^{\frac{2j}{2j+1}} w^{-1-\alpha} y(t_{2j+1} - t_{2j+1} w)\, dw.
\end{aligned}
$$

For every j, we denote $g(w) = y(t_{2j+1} - t_{2j+1} w)$ and approximate $\oint_0^{\frac{2j}{2j+1}} w^{-1-\alpha} g(w)\, dw$ by $\oint_0^{\frac{2j}{2j+1}} w^{-1-\alpha} g_2(w)\, dw$, where $g_2(w)$ is the piecewise quadratic interpolation polynomials on the nodes $w_l = \frac{l}{2j+1},\ l = 0, 1, 2, \dots, 2j$. We then get

$$
\begin{aligned}
{}_0^R D_t^\alpha y(t_{2j+1}) &= \frac{1}{\Gamma(-\alpha)} \int_0^{t_1} (t_{2j+1} - u)^{-1-\alpha} y(u)\, du \\
&\quad + \frac{t_{2j+1}^{-\alpha}}{\Gamma(-\alpha)} \Big(\sum_{k=1}^{j} \oint_{w_{2k-2}}^{w_{2k}} w^{-1-\alpha} g_2(w)\, dw + R_{2j+1}(g) \Big) \\
&= \frac{1}{\Gamma(-\alpha)} \int_0^{t_1} (t_{2j+1} - u)^{-1-\alpha} y(u)\, du \\
&\quad + \frac{t_{2j+1}^{-\alpha}}{\Gamma(-\alpha)} \Big(\sum_{k=0}^{2j} \alpha_{k,2j+1} y(t_{2j+1-k}) + R_{2j+1}(g) \Big)
\end{aligned}
$$

where $R_{2j+1}(g)$ is the remainder term and $\alpha_{k,2j+1} = \alpha_{k,2j},\ k = 0, 1, 2, \dots, 2j$. Hence

$$
\begin{aligned}
y(t_{2j+1}) &= \frac{1}{\alpha_{0,2j+1} - t_{2j+1}^\alpha \Gamma(-\alpha)\beta} \Big[t_{2j+1}^\alpha \Gamma(-\alpha) f(t_{2j+1}) - \sum_{k=1}^{2j} \alpha_{k,2j+1} y(t_{2j+1-k}) \\
&\qquad + y_0 \sum_{k=0}^{2j} \alpha_{k,2j+1} - R_{2j+1}(g) - t_{2j+1}^\alpha \int_0^{t_1} (t_{2j+1} - u)^{-1-\alpha} y(u)\, du \Big]. \qquad (5.3.10)
\end{aligned}
$$

Here $\alpha_{0,l} - t_l^\alpha \Gamma(-\alpha)\beta < 0,\ l = 2j, 2j+1$, which follow from $\Gamma(-\alpha) < 0$, $\beta < 0$ and $\alpha_{0,2j+1} = \alpha_{0,2j}$.

Let $y_{2j} \approx y(t_{2j})$ and $y_{2j+1} \approx y(t_{2j+1})$ denote the approximate solutions of $y(t_{2j})$ and $y(t_{2j+1})$, respectively. We define the following numerical methods for solving (5.2.6)-(5.2.7), with $j = 1, 2, \dots, M$,

$$
y_{2j} = \frac{1}{\alpha_{0,2j} - t_{2j}^\alpha \Gamma(-\alpha)\beta} \Big[t_{2j}^\alpha \Gamma(-\alpha) f(t_{2j}) - \sum_{k=1}^{2j} \alpha_{k,2j} y_{2j-k} + y_0 \sum_{k=0}^{2j} \alpha_{k,2j} \Big], \qquad (5.3.11)
$$

and, with $j = 1, 2, \ldots, M-1$,

$$y_{2j+1} = \frac{1}{\alpha_{0,2j+1} - t_{2j+1}^{\alpha}\Gamma(-\alpha)\beta}\Big[t_{2j+1}^{\alpha}\Gamma(-\alpha)f(t_{2j+1}) - \sum_{k=1}^{2j}\alpha_{k,2j+1}y_{2j+1-k}$$
$$+ y_0\sum_{k=0}^{2j}\alpha_{k,2j+1} - t_{2j+1}^{\alpha}\int_0^{t_1}(t_{2j+1}-u)^{-1-\alpha}y(u)\,du\Big]. \tag{5.3.12}$$

Yan, Pal and Ford [93] proved the following Theorem.

Theorem 5.3.2 (for proof see the Theorem 3.3.3)**.** Let $0 < \alpha < 1$ and M be a positive integer. Let $0 = t_0 < t_1 < t_2 < \cdots < t_{2j} < t_{2j+1} < \cdots < t_{2M} = 1$ be a partition of $[0,1]$ and h the stepsize. Let $y(t_{2j}), y(t_{2j+1}), y_{2j}$ and y_{2j+1} be the exact and the approximate solutions of (5.3.9) - (5.3.12), respectively. Assume that $y \in C^{m+2}[0,1]$, $m \geq 3$. Further assume that we can approximate the starting value y_1 and the starting integral $\int_0^{t_1}(t_{2j+1}-\tau)^{-1-\alpha}y(\tau)\,d\tau$ in (5.3.12) by using some numerical methods and obtain the required accuracy. Then there exist coefficients $c_\mu = c_\mu(\alpha)$ and $c_\mu^* = c_\mu^*(\alpha)$ such that the sequence $\{y_l\}, l = 0, 1, 2, \ldots, 2M$ possesses an asymptotic expansion of the form

$$y(t_{2M}) - y_{2M} = \sum_{\mu=3}^{m+1} c_\mu (2M)^{\alpha-\mu} + \sum_{\mu=2}^{\mu^*} c_\mu^*(2M)^{-2\mu} + o((2M)^{\alpha-m-1}), \quad \text{for } M \to \infty,$$

that is,

$$y(t_{2M}) - y_{2M} = \sum_{\mu=3}^{m+1} c_\mu h^{\mu-\alpha} + \sum_{\mu=2}^{\mu^*} c_\mu^* h^{2\mu} + o(h^{m+1-\alpha}), \quad \text{for } h \to 0,$$

where μ^* is the integer satisfying $2\mu^* < m+1-\alpha < 2(\mu^*+1)$, and c_μ and c_μ^* are certain coefficients that depend on y.

5.3.2 Approximating the starting values and the starting integrals

To obtain the approximate solutions $y_l, l = 0, 1, 2, \ldots, 2M$ numerically, we need to approximate the starting value y_1 and the initial integral $\int_0^{t_1}(t_{2j+1}-u)^{-1-\alpha}y(u)\,du$ in (5.3.12). We shall consider these issues in this subsection and follow the idea in Cao and Xu [9].

At $t = t_1$, we have

$${}_0^R D_t^{\alpha} y(t_1) = \frac{1}{\Gamma(-\alpha)}\oint_0^{t_1}(t_1-u)^{-1-\alpha}y(u)\,du = \frac{t_1^{-\alpha}}{\Gamma(-\alpha)}\oint_0^1 w^{-1-\alpha}y(t_1 - t_1 w)\,dw.$$

We denote $g(w) = y(t_1 - t_1 w)$ and approximate $\oint_0^1 w^{-1-\alpha} g(w)\, dw$ by $\oint_0^1 w^{-1-\alpha} g_2(w)\, dw$, where $g_2(w)$ is the quadratic interpolation polynomial on the nodes $0, \frac{1}{2}, 1$ defined by

$$\begin{aligned} g_2(w) = & \frac{(w-\frac{1}{2})(w-1)}{(0-\frac{1}{2})(0-1)} g(0) + \frac{(w-0)(w-1)}{(\frac{1}{2}-0)(\frac{1}{2}-1)} g(\frac{1}{2}) \\ & + \frac{(w-0)(w-\frac{1}{2})}{(1-0)(1-\frac{1}{2})} g(1), \quad \text{for } w \in [0,1]. \end{aligned} \tag{5.3.13}$$

We then get

$$\begin{aligned} {}_0^R D_t^\alpha y(t_1) &= \frac{t_1^{-\alpha}}{\Gamma(-\alpha)} \oint_0^1 w^{-1-\alpha} g(w)\, dw = \frac{t_1^{-\alpha}}{\Gamma(-\alpha)} \Big(\oint_0^1 w^{-1-\alpha} g_2(w)\, dw + R_2^{(1)} \Big) \\ &= \frac{t_1^{-\alpha}}{\Gamma(-\alpha)} \Big(w_1^0 y(t_1) + w_1^1 y(t_{\frac{1}{2}}) + w_1^2 y(t_0) + R_2^{(1)} \Big), \end{aligned} \tag{5.3.14}$$

where

$$\begin{aligned} w_1^0 &= \oint_0^1 w^{-1-\alpha} \frac{(w-\frac{1}{2})(w-1)}{(0-\frac{1}{2})(0-1)}\, dw, \qquad w_1^1 = \oint_0^1 w^{-1-\alpha} \frac{(w-0)(w-1)}{(\frac{1}{2}-0)(\frac{1}{2}-1)}\, dw, \\ w_1^2 &= \oint_0^1 w^{-1-\alpha} \frac{(w-0)(w-\frac{1}{2})}{(1-0)(1-\frac{1}{2})}\, dw, \end{aligned} \tag{5.3.15}$$

and the remainder term $R_2^{(1)}$ satisfies, [26]

$$|R_2^{(1)}| \le C t_1^3 |y'''|_\infty.$$

Further we approximate the value $y(t_{\frac{1}{2}})$ by, [9]

$$y(t_{\frac{1}{2}}) = \frac{3}{8} y(t_0) + \frac{3}{4} y(t_1) - \frac{1}{8} y(t_2) + R_2^{(2)},$$

where $R_2^{(2)} = \frac{1}{12} h^3 y'''(c)$. Hence we have

$${}_0^R D_t^\alpha y(t_1) = \frac{t_1^{-\alpha}}{\Gamma(-\alpha)} \Big(\hat{B}_0 y(t_2) + \hat{B}_1 y(t_1) + \hat{B}_2 y(t_0) + R_2^{(1)} + R_2^{(2)} \Big), \tag{5.3.16}$$

where

$$\hat{B}_2 = w_1^2 + \frac{3}{8} w_1^1, \quad \hat{B}_1 = w_1^0 + \frac{3}{4} w_1^1, \quad \hat{B}_0 = -\frac{1}{8} w_1^1.$$

Therefore we have, at $t = t_1$,

$$\begin{aligned} y(t_1) = \frac{1}{\hat{B}_1 - t_1^\alpha \Gamma(-\alpha)\beta} \Big(& t_1^\alpha \Gamma(-\alpha) f(t_1) - \hat{B}_0 y(t_2) - \hat{B}_2 y(t_0) \\ & + y_0 \sum_{k=0}^{2} \hat{B}_k - R_2^{(1)} - R_2^{(2)} \Big). \end{aligned} \tag{5.3.17}$$

At $t = t_2$, we have

$$ {}_0^R D_t^\alpha y(t_2) = \frac{1}{\Gamma(-\alpha)} \oint_0^{t_2} (t_2 - u)^{-1-\alpha} y(u)\, du = \frac{t_2^{-\alpha}}{\Gamma(-\alpha)} \oint_0^1 w^{-1-\alpha} y(t_2 - t_2 w)\, dw. $$

We denote $g(w) = y(t_2 - t_2 w)$ and approximate the integral $\oint_0^1 w^{-1-\alpha} g(w)\, dw$ by $\oint_0^1 w^{-1-\alpha} g_2(w)\, dw$, where $g_2(w)$ is defined as in (5.3.13). We have

$$ \begin{aligned} {}_0^R D_t^\alpha y(t_2) &= \frac{t_2^{-\alpha}}{\Gamma(-\alpha)} \oint_0^1 w^{-1-\alpha} g(w)\, dw = \frac{t_2^{-\alpha}}{\Gamma(-\alpha)} \Big(\oint_0^1 w^{-1-\alpha} g_2(w)\, dw + R_2^{(3)} \Big) \\ &= \frac{t_2^{-\alpha}}{\Gamma(-\alpha)} \Big(w_1^0 y(t_2) + w_1^1 y(t_1) + w_1^2 y(t_0) + R_2^{(3)} \Big), \end{aligned} \tag{5.3.18} $$

where $w_1^j, j = 0, 1, 2$ are defined as in (5.3.15) and the remainder term $R_2^{(3)}$ satisfies, [26]

$$ |R_2^{(3)}| \le C t_2^3 |y'''|_\infty. $$

Therefore we have, at $t = t_2$,

$$ y(t_2) = \frac{1}{w_1^0 - t_2^\alpha \Gamma(-\alpha)\beta} \Big(t_2^\alpha \Gamma(-\alpha) f(t_2) - \sum_{k=1}^{2} w_1^k y(t_{2-k}) + y_0 \sum_{k=0}^{2} w_1^k - R_2^{(3)} \Big). \tag{5.3.19} $$

Let $y_l \approx y(t_l), l = 1, 2$, be the approximate solutions of $y(t_l)$. We define the following numerical methods for solving $y_l, l = 1, 2$.

$$ y_1 = \frac{1}{\hat{B}_1 - t_1^\alpha \Gamma(-\alpha)\beta} \Big(t_1^\alpha \Gamma(-\alpha) f(t_1) - \hat{B}_0 y_2 - \hat{B}_2 y_0 + y_0 \sum_{k=0}^{2} \hat{B}_k \Big), \tag{5.3.20} $$

$$ y_2 = \frac{1}{w_1^0 - t_2^\alpha \Gamma(-\alpha)\beta} \Big(t_2^\alpha \Gamma(-\alpha) f(t_2) - \sum_{k=1}^{2} w_1^k y_{2-k} + y_0 \sum_{k=0}^{2} w_1^k \Big). \tag{5.3.21} $$

Let $e_l = y(t_l) - y_l, l = 1, 2$, denote the errors, we then have

$$ e_1 = \frac{1}{\hat{B}_1 - t_1^\alpha \Gamma(-\alpha)\beta} \Big(\hat{B}_0 e_2 + \hat{B}_2 e_0 - R_2^{(1)} - R_2^{(2)} \Big), \tag{5.3.22} $$

$$ e_2 = \frac{1}{w_1^0 - t_2^\alpha \Gamma(-\alpha)\beta} \Big(\sum_{k=1}^{2} w_1^k e_{2-k} - R_2^{(3)} \Big). \tag{5.3.23} $$

By using Gronwall's Lemma, we get, [9]

$$ |e_2| \le C |R_2^{(3)}| \le C h^3, $$

and

$$|e_1| \le C(|R_2^{(1)}| + |R_2^{(2)}|) \le Ch^3.$$

We next consider how to approximate the starting integral $\int_0^{t_1} (t_{2j+1} - u)^{-1-\alpha} y(u)\, du$ in (5.3.12) with $j \ge 1$. Note that this integral is the usual integral since $j \ge 1$ and

$$\int_0^{t_1} (t_{2j+1} - u)^{-1-\alpha} y(u)\, du = t_1 \int_0^1 (t_{2j} + t_1 w)^{-1-\alpha} y(t_1 - t_1 w)\, dw.$$

Denoting $g(w) = y(t_1 - t_1 w)$ and approximating the integral $\int_0^1 (t_{2j} + t_1 w)^{-1-\alpha} g(w)\, dw$ by $\int_0^1 (t_{2j} + t_1 w)^{-1-\alpha} g_2(w)\, dw$, where $g_2(w)$ is defined by (5.3.13), we have

$$\int_0^{t_1} (t_{2j+1} - u)^{-1-\alpha} y(u)\, du = t_1 \Big(w_j^0 y(t_1) + w_j^1 y(t_{\frac{1}{2}}) + w_j^2 y(t_0) + R_j^{(1)} \Big), \tag{5.3.24}$$

where

$$\begin{aligned} w_j^0 &= \int_0^1 (t_{2j} + t_1 w)^{-1-\alpha} \frac{(w - \frac{1}{2})(w - 1)}{(0 - \frac{1}{2})(0 - 1)}\, dw, \\ w_j^1 &= \int_0^1 (t_{2j} + t_1 w)^{-1-\alpha} \frac{(w - 0)(w - 1)}{(\frac{1}{2} - 0)(\frac{1}{2} - 1)}\, dw, \\ w_j^2 &= \int_0^1 (t_{2j} + t_1 w)^{-1-\alpha} \frac{(w - 0)(w - \frac{1}{2})}{(1 - 0)(1 - \frac{1}{2})}\, dw, \end{aligned}$$

and the remainder term $R_j^{(1)}$ satisfies, [26]

$$|R_j^{(1)}| \le \int_0^1 (t_{2j} + t_1 w)^{-1-\alpha} (C t_1^3)\, dw \le Ch^3 t_{2j}^{-\alpha} \le Ch^{3-\alpha}.$$

Further we approximate the value $y(t_{\frac{1}{2}})$ by

$$y(t_{\frac{1}{2}}) = \frac{3}{8} y(t_0) + \frac{3}{4} y(t_1) - \frac{1}{8} y(t_2) + R_2^{(2)},$$

where $R_2^{(2)} = \frac{1}{12} h^3 y'''(c)$. Hence we have

$$\int_0^{t_1} (t_{2j+1} - u)^{-1-\alpha} y(u)\, du = t_1 \Big(\hat{B}_{0,j} y(t_2) + \hat{B}_{1,j} y(t_1) + \hat{B}_{2,j} y(t_0) + R_j^{(1)} + R_j^{(2)} \Big),$$

where

$$\hat{B}_{2,j} = w_j^2 + \frac{3}{8} w_j^1, \quad \hat{B}_{1,j} = w_j^0 + \frac{3}{4} w_j^1, \quad \hat{B}_{0,j} = -\frac{1}{8} w_j^1.$$

We shall approximate the integral $\int_0^{t_1} (t_{2j+1} - u)^{-1-\alpha} y(u)\, du$ by

$$\int_0^{t_1} (t_{2j+1} - u)^{-1-\alpha} y(u)\, du \approx t_1 \Big(\hat{B}_{0,j} y_2 + \hat{B}_{1,j} y_1 + \hat{B}_{2,j} y_0 \Big), \tag{5.3.25}$$

and it is easy to show that

$$\Big| \int_0^{t_1} (t_{2j+1} - u)^{-1-\alpha} y(u)\, du - t_1 \Big(\hat{B}_{0,j} y_2 + \hat{B}_{1,j} y_1 + \hat{B}_{2,j} y_0 \Big) \Big|$$
$$= \Big| t_1 \Big(\sum_{k=0}^{2} \hat{B}_{k,j} e_{2-k} + R_j^{(1)} + R_2^{(2)} \Big) \Big| \leq C t_1 (C h^3 + C h^{3-\alpha}) \leq C h^{4-\alpha}.$$

After obtaining y_1 and y_2 by (5.3.20) and (5.3.21), we then use (5.3.11), (5.3.12) and (5.3.25) to calculate $y_3, y_4, \ldots, y_{2M}$.

5.4 The nonlinear fractional differential equation

5.4.1 The numerical method

In this subsection we will introduce the fractional Adams-type predictor-corrector method for solving (5.2.4)-(5.2.5). Note that (5.2.4)-(5.2.5) is equivalent to the integral form, with $0 < \alpha \leq 2$,

$$y(t) = y_0 + y_0^{(1)} \frac{t}{1!} + \frac{1}{\Gamma(\alpha)} \int_0^t (t-u)^{\alpha-1} f(u, y(u))\, du. \tag{5.4.1}$$

(The second of the initial conditions is only for $1 < \alpha \leq 2$ of course).

Let M be a positive integer and let $0 = t_0 < t_1 < t_2 < \cdots < t_j < \cdots < t_M = T$ be a partition of $[0, T]$ and h the stepsize. At $t = t_j$, we have

$$y(t_j) = y_0 + y_0^{(1)} \frac{t_j}{1!} + \frac{1}{\Gamma(\alpha)} \int_0^{t_j} (t_j - u)^{\alpha-1} f(u, y(u))\, du. \tag{5.4.2}$$

Approximating $f(u, y(u))$ in (5.4.2) by the piecewise linear interpolation polynomial $P_1(u)$ on the nodes $0 = t_0 < t_1 < \cdots < t_j$, we obtain

$$\int_0^{t_j} (t_j - u)^{\alpha-1} f(u, y(u))\, du \approx \int_0^{t_j} (t_j - u)^{\alpha-1} P_1(u)\, du = \sum_{k=0}^{j} a_{k,j} f(t_k, y(t_k)),$$

where $a_{k,j}, k = 0, 1, 2, \ldots, j$ are some weights, see [29].

Let $y_j \approx y(t_j)$ denote the approximate solution of $y(t_j), j = 0, 1, 2, \ldots, M$. We define the corrector formula of (5.4.2) by

$$y_j = y_0 + y_0^{(1)} \frac{t_j}{1!} + \frac{1}{\Gamma(\alpha)} \Big(\sum_{k=0}^{j-1} a_{k,j} f(t_k, y_k) + a_{j,j} f(t_j, y_j^P) \Big), \; j = 1, 2, \ldots, M. \tag{5.4.3}$$

To determine the predictor formula for y_j^P, we approximate $f(u, y(u))$ in (5.4.2) by the piecewise constant function $P_0(u)$ on the nodes $0 = t_0 < t_1 < t_2, \cdots < t_j$ and obtain

$$\int_0^{t_j} (t_j - u)^{\alpha-1} f(u, y(u))\, du \approx \int_0^{t_j} (t_j - u)^{\alpha-1} P_0(u)\, du = \sum_{k=0}^{j} b_{k,j} f(t_k, y(t_k)),$$

where $b_{k,j}, k = 0, 1, 2, \ldots, j-1$ are some weights, see [29]. The predictor formula is defined by

$$y_j^P = y_0 + y_0^{(1)} \frac{t_j}{1!} + \frac{1}{\Gamma(\alpha)} \sum_{k=0}^{j-1} b_{k,j} f(t_k, y_k),\ j = 1, 2, \ldots, M. \tag{5.4.4}$$

The fractional Adams-type predictor-corrector method for solving (5.2.4)-(5.2.5) is completely described now by (5.4.3) and (5.4.4) with the weights $a_{k,j}, k = 0, 1, 2, \ldots, j$ and $b_{k,j}, k = 0, 1, 2, \ldots, j$. Diethelm, Ford and Freed [29] obtained the error estimates for the methods (5.4.3) and (5.4.4).

In [93], Yan, Pal and Ford introduced a high order fractional Adams-type predictor-corrector method for solving (5.2.4)-(5.2.5). Let M be a positive integer and let $0 = t_0 < t_1 < t_2 < \cdots < t_{2j} < t_{2j+1} < \cdots < t_{2M} = T$ be a partition of $[0, T]$ and h the stepsize. Note that the system (5.2.4)-(5.2.5) is equivalent to (5.4.1). Let us now consider the discretization of (5.4.1). At the nodes $t = t_{2j},\ j = 1, 2, \ldots, M$, we have

$$y(t_{2j}) = y_0 + y_0^{(1)} \frac{t_{2j}}{1!} + \frac{1}{\Gamma(\alpha)} \int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} f(u, y(u))\, du. \tag{5.4.5}$$

At the nodes $t = t_{2j+1}, j = 0, 1, 2, \ldots, M-1$, we have

$$\begin{aligned} y(t_{2j+1}) &= y_0 + y_0^{(1)} \frac{t_{2j+1}}{1!} + \frac{1}{\Gamma(\alpha)} \int_0^{t_1} (t_{2j+1} - u)^{\alpha-1} f(u, y(u))\, du \\ &\quad + \frac{1}{\Gamma(\alpha)} \int_{t_1}^{t_{2j+1}} (t_{2j+1} - u)^{\alpha-1} f(u, y(u))\, du \\ &= y_0 + y_0^{(1)} \frac{t_{2j+1}}{1!} + \frac{1}{\Gamma(\alpha)} \int_0^{t_1} (t_{2j+1} - u)^{\alpha-1} f(u, y(u))\, du \\ &\quad + \frac{1}{\Gamma(\alpha)} \int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} f(u + h, y(u + h))\, du. \end{aligned} \tag{5.4.6}$$

We will replace $f(u, f(u))$ of the integral $\int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} f(u, y(u))\, du$ in (5.4.5) by the following piecewise quadratic polynomial $P_2(u)$, $t_{2l} \le u \le t_{2l+2},\ l = 0, 1, 2, \ldots, j-1$ with

$j = 1, 2, \ldots, M$, where

$$
\begin{aligned}
P_2(u) =& \frac{(u - t_{2l+1})(u - t_{2l+2})}{(t_{2l} - t_{2l+1})(t_{2l} - t_{2l+2})} f(t_{2l}, y(t_{2l})) \\
&+ \frac{(u - t_{2l})(u - t_{2l+2})}{(t_{2l+1} - t_{2l})(t_{2l+1} - t_{2l+2})} f(t_{2l+1}, y(t_{2l+1})) \\
&+ \frac{(u - t_{2l})(u - t_{2l+1})}{(t_{2l+2} - t_{2l})(t_{2l+2} - t_{2l+1})} f(t_{2l+2}, y(t_{2l+2})),
\end{aligned} \tag{5.4.7}
$$

and

$$f(u, y(u)) - P_2(u) = R_l^{(1)},$$

where

$$R_l^{(1)} = \frac{f'''(c_l, y(c_l))}{3!}(u - t_{2l})(u - t_{2l+1})(u - t_{2l+2}), \ t_{2l} \leq c_l \leq t_{2l+2}.$$

Similarly, we will replace $f(u + h, f(u + h))$ in the integral $\int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} f(u + h, y(u + h))\, du$ in (5.4.6) by the following piecewise quadratic polynomial $Q_2(u)$, for $t_{2l} \leq u \leq t_{2l+2}, \ l = 0, 1, 2, \ldots, j - 1, \ j = 1, 2, \ldots, M - 1$, where

$$
\begin{aligned}
Q_2(u) =& \frac{(u - t_{2l+1})(u - t_{2l+2})}{(t_{2l} - t_{2l+1})(t_{2l} - t_{2l+2})} f(t_{2l+1}, y(t_{2l+1})) \\
&+ \frac{(u - t_{2l})(u - t_{2l+2})}{(t_{2l+1} - t_{2l})(t_{2l+1} - t_{2l+2})} f(t_{2l+2}, y(t_{2l+2})) \\
&+ \frac{(u - t_{2l})(u - t_{2l+1})}{(t_{2l+2} - t_{2l})(t_{2l+2} - t_{2l+1})} f(t_{2l+3}, y(t_{2l+3})),
\end{aligned} \tag{5.4.8}
$$

and

$$f(u + h, y(u + h)) - Q_2(u) = R_l^{(2)},$$

where

$$R_l^{(2)} = \frac{f'''(d_l, y(d_l))}{3!}(u - t_{2l})(u - t_{2l+1})(u - t_{2l+2}), \ t_{2l} \leq d_l \leq t_{2l+2}.$$

We then have, with $0 < \alpha \leq 2$, see [93],

$$\int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} P_2(u)\, du = \sum_{k=0}^{2j} c_{k,2j} f(t_k, y(t_k)),$$

and

$$\int_0^{t_{2j}} (t_{2j} - u)^{\alpha-1} Q_2(u)\, du = \sum_{k=0}^{2j} c_{k,2j} f(t_{k+1}, y(t_{k+1})),$$

where

$$c_{k,2j} = \frac{h^\alpha}{\alpha(\alpha+1)(\alpha+2)} \begin{cases} \frac{1}{2}F_0(0), & \text{if } k = 0, \\ \frac{1}{2}F_0(l) + \frac{1}{2}F_2(l-1), & \text{if } k = 2l,\ l = 1, 2, \ldots, j-1, \\ -F_1(l), & \text{if } k = 2l+1,\ l = 0, 1, 2, \ldots, j-1, \\ \frac{1}{2}F_2(j-1), & \text{if } k = 2j, \end{cases}$$

and

$$\begin{aligned} F_0(l) &= \alpha(\alpha+1)\Big((2j-2l)^{\alpha+2} - (2j-2l-2)^{\alpha+2}\Big) \\ &\quad + \alpha(\alpha+2)\Big(2(2j) - (2l+1) - (2l+2)\Big)\Big((2j-2l-2)^{\alpha+1} - (2j-2l)^{\alpha+1}\Big) \\ &\quad + (\alpha+1)(\alpha+2)\Big((2j-2l-1)(2j-2l-2)\Big)\Big((2j-2l)^{\alpha} - (2j-2l-2)^{\alpha}\Big), \\ F_1(l) &= \alpha(\alpha+1)\Big((2j-2l)^{\alpha+2} - (2j-2l-2)^{\alpha+2}\Big) \\ &\quad + \alpha(\alpha+2)\Big(2(2j) - (2l) - (2l+2)\Big)\Big((2j-2l-2)^{\alpha+1} - (2j-2l)^{\alpha+1}\Big) \\ &\quad + (\alpha+1)(\alpha+2)\Big((2j-2l)(2j-2l-2)\Big)\Big((2j-2l)^{\alpha} - (2j-2l-2)^{\alpha}\Big), \\ F_2(l) &= \alpha(\alpha+1)\Big((2j-2l)^{\alpha+2} - (2j-2l-2)^{\alpha+2}\Big) \\ &\quad + \alpha(\alpha+2)\Big(2(2j) - (2l) - (2l+1)\Big)\Big((2j-2l-2)^{\alpha+1} - (2j-2l)^{\alpha+1}\Big) \\ &\quad + (\alpha+1)(\alpha+2)\Big((2j-2l)(2j-2l-1)\Big)\Big((2j-2l)^{\alpha} - (2j-2l-2)^{\alpha}\Big). \end{aligned}$$

Let $y_l \approx y(t_l)$ denote the approximate solutions of $y(t_l),\ l = 0, 1, 2, \ldots, 2M$. We now define a fractional Adams numerical method for solving (5.2.4)-(5.2.5). The corrector formula is defined by, with $j = 1, 2, \ldots, M$,

$$y_{2j} = y_0 + y_0^{(1)} \frac{t_{2j}}{1!} + \frac{1}{\Gamma(\alpha)} \Big(\sum_{k=0}^{2j-1} c_{k,2j} f(t_k, y_k) + c_{2j,2j} f(t_{2j}, y_{2j}^P) \Big), \tag{5.4.9}$$

and, with $j = 0, 1, 2, \ldots, M-1$,

$$\begin{aligned} y_{2j+1} &= y_0 + y_0^{(1)} \frac{t_{2j+1}}{1!} + \frac{1}{\Gamma(\alpha)} \int_0^{t_1} (t_{2j+1} - u)^{\alpha-1} f(u, y(u))\, du \\ &\quad + \frac{1}{\Gamma(\alpha)} \Big(\sum_{k=0}^{2j-1} c_{k,2j} f(t_{k+1}, y_{k+1}) + c_{2j+1,2j+1} f(t_{2j+1}, y_{2j+1}^P) \Big), \end{aligned} \tag{5.4.10}$$

The remaining problem is the determination of the predictor formula required to calculate y_{2j}^P and y_{2j+1}^P. The idea is the same as the one described above: we replace $f(u, y(u))$

and $f(u+h, y(u+h))$ of the integrals on the right-hand sides of equations (5.4.5) and (5.4.6), respectively, by the piecewise linear interpolation polynomials and obtain, with $j = 1, 2, \ldots, M$,

$$y_{2j}^{P} = y_0 + y_0^{(1)} \frac{t_{2j}}{1!} + \frac{1}{\Gamma(\alpha)} \Big(\sum_{k=0}^{2j-1} a_{k,2j} f(t_k, y_k) + a_{2j,2j} f(t_{2j}, y_{2j}^{PP}) \Big), \tag{5.4.11}$$

and, with $j = 0, 1, 2, \ldots, M-1$,

$$y_{2j+1}^{P} = y_0 + y_0^{(1)} \frac{t_{2j+1}}{1!} + \frac{1}{\Gamma(\alpha)} \Big(\sum_{k=0}^{2j} a_{k,2j+1} f(t_k, y_k) + a_{2j+1,2j+1} f(t_{2j+1}, y_{2j+1}^{PP}) \Big), \tag{5.4.12}$$

where the weights [28]

$$a_{k,n+1} = \frac{h^\alpha}{\alpha(\alpha+1)} \begin{cases} n^{\alpha+1} - (n-\alpha)(n+1)^\alpha, & \text{if } k = 0, \\ (n-k+2)^{\alpha+1} + (n-k)^{\alpha+1} - 2(n-k+1)^{\alpha+1} & \text{if } 1 \le k \le n, \\ 1, & \text{if } k = n+1. \end{cases}$$

Similarly, to calculate y_k^{PP}, we replace $f(u, y(u))$ and $f(u+h, y(u+h))$ in the integrals in (5.4.5) and (5.4.6), respectively by the piecewise constants and obtain

$$y_{2j}^{PP} = y_0 + y_0^{(1)} \frac{t_{2j}}{1!} + \frac{1}{\Gamma(\alpha)} \sum_{k=0}^{2j-1} b_{k,2j} f(t_k, y_k), \quad j = 1, 2, \ldots, M, \tag{5.4.13}$$

and

$$y_{2j+1}^{PP} = y_0 + y_0^{(1)} \frac{t_{2j+1}}{1!} + \frac{1}{\Gamma(\alpha)} \sum_{k=0}^{2j} b_{k,2j+1} f(t_k, y_k), \quad j = 1, 2, \ldots, M-1, \tag{5.4.14}$$

where the weights [28]

$$b_{k,n+1} = \frac{h^\alpha}{\alpha} \Big((n+1-k)^\alpha - (n-k)^\alpha \Big). \tag{5.4.15}$$

Our basic fractional Adams method, is completely described now by equations (5.4.9) - (5.4.14). Assume that the starting value y_1 and the starting integral $\int_0^{t_1} (t_{2j+1} - u)^{-1-\alpha} f(u, y(u))\, du$ in (5.4.10) can be approximate by using some numerical methods and satisfy the required accuracy, Yan, Pal and Ford [93] proved the error estimates for $y_l - y(t_l), l = 1, 2, \ldots, 2M$.

5.4.2 Approximating the starting values and the starting integrals

In this subsection we shall consider how to approximate the starting value y_1 and the initial integral $\int_0^{t_1}(t_{2j+1}-u)^{-1-\alpha}y(u)\,du$ in (5.4.10). We will follow the idea in Cao and Xu [9].

At $t=t_1$, we have

$$y(t_1) = y_0 + y_0^{(1)}\frac{t_1}{1!} + \frac{1}{\Gamma(\alpha)}\int_0^{t_1}(t_1-u)^{\alpha-1}f(u,y(u))\,du.$$

Approximating $g(u)=f(u,y(u))$ on $[0,t_1]$ by the following quadratic interpolation polynomial

$$\begin{aligned}P_2(u) &= \frac{(u-t_{\frac12})(u-t_1)}{(t_0-t_{\frac12})(t_0-t_1)}f(0,y(0)) + \frac{(u-t_0)(u-t_1)}{(t_{\frac12}-t_0)(t_{\frac12}-t_1)}f(t_{\frac12},y(t_{\frac12}))\\ &\quad + \frac{(u-t_0)(u-t_{\frac12})}{(t_1-t_0)(t_1-t_{\frac12})}f(t_1,y(t_1)) \quad \text{for } u\in[t_0,t_1],\end{aligned}$$

where

$$f(u,y(u)) - P_2(u) = R_1^{(1)}(u) = \frac{f'''(c_1)}{3!}(u-0)(u-t_{\frac12})(u-t_1),\ c_1\in(0,t_1).$$

Further we approximate the value $f(t_{\frac12},y(t_{\frac12}))$ by

$$f(t_{\frac12},y(t_{\frac12})) \approx \frac38 f(t_0,y(t_0)) + \frac34 f(t_1,y(t_1)) - \frac18 f(t_2,y(t_2)),$$

where

$$f(t_{\frac12},y(t_{\frac12})) - \Big(\frac38 f(t_0,y(t_0)) + \frac34 f(t_1,y(t_1)) - \frac18 f(t_2,y(t_2))\Big) = R_1^{(2)}(u),$$

and $R_1^{(2)}(u) = \frac{1}{16}f'''(c_2)h^3,\ c_2\in(0,t_2)$.

We then obtain

$$\begin{aligned}y(t_1) &= y_0 + y_0^{(1)}\frac{t_1}{1!} + \frac{1}{\Gamma(\alpha)}\int_0^{t_1}(t_1-u)^{\alpha-1}f(u,y(u))\,du\\ &= y_0 + y_0^{(1)}\frac{t_1}{1!} + \frac{1}{\Gamma(\alpha)}\Big(\sum_{i=0}^{2}\hat{B}_i f(t_i,y(t_i))\\ &\quad + \int_0^{t_1}(t_1-u)^{\alpha-1}R_1^{(1)}(u)\,du + \int_0^{t_1}(t_1-u)^{\alpha-1}R_1^{(2)}(u)\,du,\end{aligned} \tag{5.4.16}$$

where

$$\hat{B}_0 = \int_0^{t_1} (t_1-u)^{\alpha-1} \frac{(u-t_{\frac{1}{2}})(u-t_1)}{(t_0-t_{\frac{1}{2}})(t_0-t_1)}\, du + \frac{3}{8}\int_0^{t_1} (t_1-u)^{\alpha-1} \frac{(u-t_0)(u-t_1)}{(t_{\frac{1}{2}}-t_0)(t_{\frac{1}{2}}-t_1)}\, du,$$
$$\hat{B}_1 = \frac{3}{4}\int_0^{t_1} (t_1-u)^{\alpha-1} \frac{(u-t_0)(u-t_1)}{(t_{\frac{1}{2}}-t_0)(t_{\frac{1}{2}}-t_1)}\, du + \int_0^{t_1} (t_1-u)^{\alpha-1} \frac{(u-t_0)(u-t_1)}{(t_1-t_0)(t_1-t_{\frac{1}{2}})}\, du,$$
$$\hat{B}_2 = -\frac{1}{8}\int_0^{t_1} (t_1-u)^{\alpha-1} \frac{(u-t_0)(u-t_1)}{(t_{\frac{1}{2}}-t_0)(t_{\frac{1}{2}}-t_1)}\, du.$$

Let $y_l \approx y(t_l), l = 0, 1, 2$, denote the approximations of $y(t_l)$ and we define the following numerical method for y_1.

$$y_1 = y_0 + y_0^{(1)}\frac{t_1}{1!} + \frac{1}{\Gamma(\alpha)}\sum_{i=0}^{2} \hat{B}_i f(t_i, y_i). \tag{5.4.17}$$

At $t = t_2$, we have

$$y(t_2) = y_0 + y_0^{(1)}\frac{t_2}{1!} + \frac{1}{\Gamma(\alpha)}\int_0^{t_2} (t_2-u)^{\alpha-1} f(u, y(u))\, du.$$

Approximating $g(u) = f(u, y(u))$ on $[0, t_2]$ by the following quadratic interpolation polynomial

$$P_2(u) = \frac{(u-t_1)(u-t_2)}{(t_0-t_1)(t_0-t_2)} f(0, y(0)) + \frac{(u-t_0)(u-t_2)}{(t_1-t_0)(t_1-t_2)} f(t_1, y(t_1))$$
$$+ \frac{(u-t_0)(u-t_1)}{(t_2-t_0)(t_2-t_1)} f(t_2, y(t_2)), \quad \text{for } u \in [t_0, t_2],$$

where

$$f(u, y(u)) - P_2(u) = R_2^{(1)}(u) = \frac{f'''(c_3)}{3!}(u-t_0)(u-t_1)(u-t_2),\ c_3 \in (t_0, t_2).$$

We obtain

$$y(t_2) = y_0 + y_0^{(1)}\frac{t_2}{1!} + \frac{1}{\Gamma(\alpha)}\int_0^{t_2} (t_2-u)^{\alpha-1} f(u, y(u))\, du$$
$$= y_0 + y_0^{(1)}\frac{t_2}{1!} + \frac{1}{\Gamma(\alpha)}\Big(\sum_{i=0}^{2} \tilde{B}_i f(t_i, y(t_i)) + \int_0^{t_2} (t_2-u)^{\alpha-1} R_2^{(1)}(u)\, du\Big), \tag{5.4.18}$$

where

$$\tilde{B}_0 = \int_0^{t_2} (t_2-u)^{\alpha-1} \frac{(u-t_1)(u-t_2)}{(t_0-t_1)(t_0-t_2)}\, du,$$
$$\tilde{B}_1 = \int_0^{t_2} (t_2-u)^{\alpha-1} \frac{(u-t_0)(u-t_2)}{(t_1-t_0)(t_1-t_2)}\, du,$$
$$\tilde{B}_2 = \int_0^{t_2} (t_2-u)^{\alpha-1} \frac{(u-t_0)(u-t_1)}{(t_2-t_0)(t_2-t_1)}\, du.$$

We then define the following numerical method for y_2.

$$y_2 = y_0 + y_0^{(1)} \frac{t_2}{1!} + \frac{1}{\Gamma(\alpha)} \Big(\tilde{B}_0 f(t_0, y_0) + \tilde{B}_1 f(t_1, y_1) + \tilde{B}_2 f(t_2, y_2) \Big), \tag{5.4.19}$$

Similarly, we can approximate the starting integral $\int_0^{t_1} (t_{2j+1} - u)^{\alpha-1} f(u, y(u))\, du$ in (5.4.10) by using the same idea as in (5.4.16) and obtain

$$\begin{aligned}
&\int_0^{t_1} (t_{2j+1} - u)^{\alpha-1} f(u, y(u))\, du \\
&= \Big(\hat{B}_{0,j} f(t_0, y_0) + \hat{B}_{1,j} f(t_1, y_1) + \hat{B}_{2,j} f(t_2, y_2) \Big) \\
&+ \int_0^{t_1} (t_{2j+1} - u)^{\alpha-1} R_1^{(1)}(u)\, du + \int_0^{t_1} (t_{2j+1} - u)^{\alpha-1} R_1^{(2)}(u)\, du,
\end{aligned} \tag{5.4.20}$$

where

$$\begin{aligned}
\hat{B}_{0,j} &= \int_0^{t_1} (t_{2j+1} - u)^{\alpha-1} \frac{(u - t_{\frac{1}{2}})(u - t_1)}{(t_0 - t_{\frac{1}{2}})(t_0 - t_1)}\, du + \frac{3}{8} \int_0^{t_1} (t_{2j+1} - u)^{\alpha-1} \frac{(u - t_0)(u - t_1)}{(t_{\frac{1}{2}} - t_0)(t_{\frac{1}{2}} - t_1)}\, du, \\
\hat{B}_{1,j} &= \frac{3}{4} \int_0^{t_1} (t_{2j+1} - u)^{\alpha-1} \frac{(u - t_0)(u - t_1)}{(t_{\frac{1}{2}} - t_0)(t_{\frac{1}{2}} - t_1)}\, du + \int_0^{t_1} (t_{2j+1} - u)^{\alpha-1} \frac{(u - t_0)(u - t_1)}{(t_1 - t_0)(t_1 - t_{\frac{1}{2}})}\, du, \\
\hat{B}_{2,j} &= -\frac{1}{8} \int_0^{t_1} (t_{2j+1} - u)^{\alpha-1} \frac{(u - t_0)(u - t_1)}{(t_{\frac{1}{2}} - t_0)(t_{\frac{1}{2}} - t_1)}\, du.
\end{aligned}$$

We now introduce the following corrector fractional Adams method.

$$y_1 = y_0 + y_0^{(1)} \frac{t_1}{1!} + \frac{1}{\Gamma(\alpha)} \Big(\hat{B}_0 f(t_0, y_0) + \hat{B}_1 f(t_1, y_1) + \hat{B}_2 f(t_2, y_2) \Big), \tag{5.4.21}$$

$$y_2 = y_0 + y_0^{(1)} \frac{t_2}{1!} + \frac{1}{\Gamma(\alpha)} \Big(\tilde{B}_0 f(t_0, y_0) + \tilde{B}_1 f(t_1, y_1) + \tilde{B}_2 f(t_2, y_2) \Big), \tag{5.4.22}$$

and, with $j = 1, 2, \ldots, M$,

$$y_{2j} = y_0 + y_0^{(1)} \frac{t_{2j}}{1!} + \frac{1}{\Gamma(\alpha)} \Big(\sum_{k=0}^{2j-1} c_{k,2j} f(t_k, y_k) + c_{2j,2j} f(t_{2j}, y_{2j}^P) \Big), \tag{5.4.23}$$

and, with $j = 0, 1, 2, \ldots, M-1$,

$$\begin{aligned}
y_{2j+1} = y_0 + y_0^{(1)} \frac{t_{2j+1}}{1!} &+ \frac{1}{\Gamma(\alpha)} \Big(\hat{B}_{0,j} f(t_0, y_0) + \hat{B}_{1,j} f(t_1, y_1) + \hat{B}_{2,j} f(t_2, y_2) \Big) \\
&+ \frac{1}{\Gamma(\alpha)} \Big(\sum_{k=0}^{2j-1} c_{k,2j} f(t_{k+1}, y_{k+1}) + c_{2j,2j} f(t_{2j+1}, y_{2j+1}^P) \Big),
\end{aligned} \tag{5.4.24}$$

where the predictor terms y_{2j}^P and y_{2j+1}^P can be obtained by (5.4.11) and (5.4.12). We then have the following error estimates.

Theorem 5.4.1. Let $0 < \alpha \leq 2$ and assume that ${}_0^C D_t^\alpha y \in C^3[0, T]$ for some suitable T. Let $y(t_k)$ and $y_k, k = 0, 1, 2, \dots, 2M$, $t_{2M} = T$ be the solutions of (5.4.1) and (5.4.21) - (5.4.24). Then, for sufficiently small h, there exists a positive constant $C_0 > 0$ such that

$$\max_{0 \leq k \leq 2M} |y(t_k) - y_k| \leq \begin{cases} C_0 h^{1+2\alpha}, & \text{if } 0 < \alpha \leq 1, \\ C_0 h^3, & \text{if } 1 < \alpha \leq 2. \end{cases}$$

5.5 Numerical simulations

5.5.1 The linear fractional differential equation

In this section we will consider two examples for solving the linear differential equation (5.2.6)-(5.2.7) by using the algorithm (5.3.11)-(5.3.12). Theorem 5.3.2 shows that the approximate solution y_{2M} has the asymptotic expansion

$$y(t_{2M}) - y_{2M} = \sum_{\mu=3}^{m+1} c_\mu h^{\mu-\alpha} + \sum_{\mu=2}^{\mu^*} c_\mu^* h^{2\mu} + o(h^{m+1-\alpha}), \quad \text{as } h \to 0,$$

where μ^* is the integer satisfying $2\mu^* < m + 1 - \alpha < 2(\mu^* + 1)$, and c_μ and c_μ^* are certain coefficients that depend on y.

Let $A = y(t_{2M}), t_{2M} = 1$ and assume that $A_0(h) = y_{2M}$ is the approximate solution of A with stepsize h. We then have by Theorem 5.3.2, with $0 < \alpha < 1$,

$$A = A_0(h) + a_1 h^{\lambda_1} + a_2 h^{\lambda_2} + a_3 h^{\lambda_3} + \dots, \tag{5.5.1}$$

where $\lambda_1 = 3 - \alpha, \lambda_2 = 4 - \alpha, \lambda_3 = 4, \lambda_4 = 5 - \alpha, \dots$. It is obvious that the convergence order of $A_0(h)$ is λ_1, that is

$$|A - A_0(h)| = O(h^{\lambda_1}).$$

Let $A_0(h/2)$ denote the approximate solution of A with stepsize $h/2$. Then we have

$$A = A_0(h/2) + a_1 (h/2)^{\lambda_1} + a_2 (h/2)^{\lambda_2} + a_3 (h/2)^{\lambda_3} + \dots. \tag{5.5.2}$$

Multiplying 2^{λ_1} in both sides of (5.5.2), we have

$$2^{\lambda_1} A = 2^{\lambda_1} A_0(h/2) + 2^{\lambda_1} a_1 (h/2)^{\lambda_1} + 2^{\lambda_1} a_2 (h/2)^{\lambda_2} + 2^{\lambda_1} a_3 (h/2)^{\lambda_3} + \dots. \tag{5.5.3}$$

Subtracting (5.5.3) from (5.5.2), we get

$$A = A_1(h) + b_1 h^{\lambda_2} + b_2 h^{\lambda_3} + b_3 h^{\lambda_4} + \dots,$$

where

$$A_1(h) = \frac{2^{\lambda_1} A_0(h/2) - A_0(h/2)}{2^{\lambda_1} - 1},$$

which implies that $A_1(h)$ is an approximation of A with the convergence order $O(h^{\lambda_2})$, that is

$$|A - A_1(h)| = O(h^{\lambda_2}).$$

Continuing these processes, we obtain the high order approximations $A_2(h), A_3(h), \dots$ of A. In Table 5.5.1, we proceed by setting up a triangle array (a so-called Romberg tableau) of approximate values for A.

$A_0(h)$				
$A_0(h/2)$	$A_1(h)$			
$A_0(h/2^2)$	$A_1(h/2)$	$A_2(h)$		
$A_0(h/2^3)$	$A_1(h/2^2)$	$A_2(h/2)$	$A_3(h)$	
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\dots$

Table 5.5.1: Romberg tableau of approximate solutions

The convergence order of the approximate solution $A_k(h)$ is λ_{k+1}, $k = 1, 2, \dots$. To obtain the experimentally determined order of convergence ("EOC") we will calculate the following ratios

$$\frac{|A - A_k(h/2^l)|}{|A - A_k(h/2^{l+1})|} = \frac{O((h/2^l)^{\lambda_{k+1}})}{O((h/2^{l+1})^{\lambda_{k+1}})} \approx 2^{\lambda_{k+1}}, \quad k = 0, 1, 2, \dots, \quad l = 0, 1, 2, \dots,$$

which implies that

$$\lambda_{k+1} \approx \log_2 \Big(\frac{|A - A_k(h/2^l)|}{|A - A_k(h/2^{l+1})|} \Big), \quad k = 0, 1, 2, \dots. \tag{5.5.4}$$

Example 10. *Consider, [26]*

$${}_0^C D_t^{\alpha} y(t) + y(t) = t^3 + \frac{3!}{\Gamma(4-\alpha)} t^{3-\alpha}, \quad t \in [0, 1], \tag{5.5.5}$$

$$y(0) = 0, \tag{5.5.6}$$

whose exact solution is given by $y(t) = t^3$.

Choose the stepsize $h = 1/10$. *In Table 5.5.2, we display the errors of the algorithms* (5.3.11)-(5.3.12) *at* $t = 1$ *and of the first two extrapolation steps in the Romberg tableau with* $\alpha = 0.3$. *In Table 5.5.3, we display the experimentally determined orders of convergence ("EOC ") at* $t = 1$. *We observe that the first column (the errors of the basic algorithm without extrapolation) converges as* $h^{3-\alpha}$. *The second column (errors using one extrapolation step) converges as* $h^{4-\alpha}$, *and the last column (two extrapolation steps) converges as* h^4. *In Tables 5.5.4-5.5.5, we display the errors and the experimentally determined order of convergence ("EOC ") with* $\alpha = 0.5$. *In Tables 5.5.6-5.5.7, we display the errors and the experimentally determined order of convergence ("EOC ") with* $\alpha = 0.9$. *In all cases of* α *under consideration, we observe that the first column converges as* $h^{3-\alpha}$. *The second column converges as* $h^{4-\alpha}$ *and the last column converges as* h^4.

Step size	Error of the method	1st extra. error	2nd extra. error
1/10	3.3237e-004		
1/20	5.1939e-005	9.3242e-007	
1/40	8.0506e-006	6.8029e-008	4.0268e-009
1/80	1.2432e-006	5.0402e-009	2.1066e-010
1/160	1.9164e-007	3.7765e-010	1.1023e-011
1/320	2.9516e-008	2.8511e-011	5.9381e-013

Table 5.5.2: Errors for equations (5.5.5)-(5.5.6) with $\alpha = 0.3$, taken at $t = 1$.

Step size	The method	1st extrapolation	2nd extrapolation
1/10			
1/20	2.68		
1/40	2.69	3.78	
1/80	2.70	3.75	4.26
1/160	2.70	3.74	4.26
1/320	2.70	3.73	4.21

Table 5.5.3: Orders ("EOC ") for equations (5.5.5)-(5.5.6) with $\alpha = 0.3$, taken at $t = 1$.

Step size	Error of the method	1st extra. error	2nd extra. error
1/10	1.1296e-003		
1/20	2.0412e-004	5.3779e-006	
1/40	3.6454e-005	4.5025e-007	2.7527e-008
1/80	6.4759e-006	3.8539e-008	1.3800e-009
1/160	1.1475e-006	3.3431e-009	6.9354e-011
1/320	2.0310e-007	2.9225e-010	3.5604e-012

Table 5.5.4: Errors for equations (5.5.5)-(5.5.6) with $\alpha = 0.5$, taken at $t = 1$.

Step size	The method	1st extrapolation	2nd extrapolation
1/10			
1/20	2.46		
1/40	2.49	3.58	
1/80	2.49	3.55	4.32
1/160	2.5	3.53	4.31
1/320	2.5	3.52	4.28

Table 5.5.5: Orders ("EOC ") for equations (5.5.5)-(5.5.6) with $\alpha = 0.5$, taken at $t = 1$.

Step size	Error of the method	1st extra. error	2nd extra. error
1/10	7.6048e-003		
1/20	1.8568e-003	1.0809e-004	
1/40	4.4205e-004	1.1665e-005	1.0659e-006
1/80	1.0412e-004	1.3139e-006	5.2739e-008
1/160	2.4402e-005	1.5070e-007	2.8748e-009
1/320	5.7054e-006	1.7432e-008	1.6257e-010

Table 5.5.6: Errors for equations (5.5.5)-(5.5.6) with $\alpha = 0.9$, taken at $t = 1$.

Example 11. *Consider, [33]*

$$ {}_0^C D_t^{\alpha} y(t) + y(t) = t^4 - \frac{1}{2}t^3 - \frac{3!}{\Gamma(4-\alpha)}t^{3-\alpha} + \frac{24}{\Gamma(5-\alpha)}t^{4-\alpha}, \quad t \in [0,1], \tag{5.5.7} $$

$$ y(0) = 0, \tag{5.5.8} $$

Step size	The method	1st extrapolation	2nd extrapolation
1/10			
1/20	2.03		
1/40	2.07	3.21	
1/80	2.09	3.15	4.34
1/160	2.09	3.12	4.20
1/320	2.10	3.11	4.14

Table 5.5.7: Orders ("EOC ") for equations (5.5.5)-(5.5.6) with $\alpha = 0.9$, taken at $t = 1$.

whose exact solution is given by $y(t) = t^4 - \frac{1}{2}t^3$.

Choose the stepsize $h = 1/10$. *In Tables 5.5.8 - 5.5.13, we display the errors of the algorithms* (5.3.11)-(5.3.12) *at* $t = 1$ *and of the first two extrapolation steps in the Romberg tableau with* $\alpha = 0.3, 0.5, 0.9$. *In all cases of* α *under consideration, we observe that the first column converges as* $h^{3-\alpha}$. *The second column converges as* $h^{4-\alpha}$ *and the last column converges as* h^4. *We observe that when* α *is close to* 1, *the convergence seems to be even a bit faster. But when* α *is close to* 0, *the convergence is a bit slower than expected.*

Step size	Error of the method	1st extra. error	2nd extra. error
1/10	1.4571e-004		
1/20	2.3118e-005	8.2097e-007	
1/40	3.6127e-006	6.5021e-008	2.0039e-009
1/80	5.6030e-007	5.1186e-009	1.2514e-010
1/160	8.6565e-008	4.0106e-010	7.8051e-012
1/320	1.3348e-008	3.1315e-011	4.9268e-013

Table 5.5.8: Errors for equations (5.5.7)-(5.5.8) with $\alpha = 0.3$, taken at $t = 1$.

Step size	The method	1st extrapolation	2nd extrapolation
1/10			
1/20	2.66		
1/40	2.68	3.66	
1/80	2.69	3.67	4.00
1/160	2.70	3.67	4.00
1/320	2.70	3.68	3.98

Table 5.5.9: Orders ("EOC ") for equations (5.5.7)-(5.5.8) with $\alpha = 0.3$, taken at $t = 1$.

Step size	Error of the method	1st extra. error	2nd extra. error
1/10	5.0921e-004		
1/20	9.2881e-005	3.4801e-006	
1/40	1.6676e-005	3.1186e-007	4.6709e-009
1/80	2.9708e-006	2.7831e-008	2.9143e-010
1/160	5.2721e-007	2.4764e-009	1.8053e-011
1/320	9.3380e-008	2.1991e-010	1.1328e-012

Table 5.5.10: Errors for equations (5.5.7)-(5.5.8) with $\alpha = 0.5$, taken at $t = 1$.

Step size	The method	1st extrapolation	2nd extrapolation
1/10			
1/20	2.45		
1/40	2.48	3.48	
1/80	2.49	3.49	4.00
1/160	2.50	3.49	4.01
1/320	2.50	3.50	3.99

Table 5.5.11: Orders ("EOC ") for equations (5.5.7)-(5.5.8) with $\alpha = 0.5$, taken at $t = 1$.

5.5.2 The nonlinear fractional differential equation

In this subsection we will consider one example for solving (5.2.4)-(5.2.5) by using the algorithm (5.4.9)-(5.4.14). We will numerically check that, with $1 < \alpha \leq 2$,

$$y(t_{2M}) - y_{2M} = a_1 h^{\lambda_1} + a_2 h^{\lambda_2} + a_3 h^{\lambda_3} + \dots,$$

Step size	Error of the method	1st extra. error	2nd extra. error
1/10	3.5534e-003		
1/20	8.5873e-004	3.8951e-005	
1/40	2.0381e-004	4.5703e-006	3.1078e-008
1/80	4.7950e-005	5.3459e-007	1.7728e-009
1/160	1.1233e-005	6.2442e-008	1.0563e-010
1/320	2.6257e-006	7.2882e-009	6.3909e-012

Table 5.5.12: Errors for equations (5.5.7)-(5.5.8) with $\alpha = 0.9$, taken at $t = 1$.

Step size	The method	1st extrapolation	2nd extrapolation
1/10			
1/20	2.05		
1/40	2.08	3.09	
1/80	2.09	3.10	4.13
1/160	2.10	3.10	4.07
1/320	2.10	3.10	4.05

Table 5.5.13: Orders (“EOC ”) for equations (5.5.7)-(5.5.8) with $\alpha = 0.9$, taken at $t = 1$.

where $\lambda_1 = 2 + \alpha$, $\lambda_2 = 4$, $\lambda_3 = 3 + \alpha, \dots$.

Example 12. *Consider, with $1 < \alpha \leq 2$, [28]*

$$ {}_0^C D_t^\alpha y(t) = \frac{40320}{\Gamma(9-\alpha)} t^{8-\alpha} - 3\frac{\Gamma(5+\alpha/2)}{\Gamma(5-\alpha/2)} t^{4-\alpha/2} + \frac{9}{4}\Gamma(\alpha+1) + \left(\frac{3}{2}t^{\alpha/2} - t^4\right)^3 - [y(t)]^{3/2}. \quad (5.5.9) $$

The initial conditions were chosen to be homogeneous, i.e., $y(0) = 0$, $y'(0) = 0$. This equation has been chosen because it exhibits a difficult (nonlinear and nonsmooth) right-hand side, and yet we are able to find its exact solution, thus allowing us to compare the numerical results for this nontrivial case to the exact results. Indeed, the exact solution of this initial value problem is

$$ y(t) = t^8 - 3t^{4+\alpha/2} + \frac{9}{4}t^\alpha, $$

Choose the stepsize $h = 1/10$. In Tables 5.5.14-5.5.19, we display the errors of the algorithms (5.4.9) -(5.4.14) *at $t = 1$ and of the first two extrapolation steps in the Romberg* *tableau with* $\alpha = 1.3, 1.5, 1.9$. *In all cases of* α *under consideration, we observe that the first column converges as* $h^{2+\alpha}$. *The second column converges as* h^4 *and the last column converges as* $h^{3+\alpha}$. *We also observe that when* α *is close to* 2, *the convergence seems to be even a bit faster. But when* α *is close to* 1, *the convergence is a bit slower than expected.*

Step size	Error of the method	1st extra. error	2nd extra. error	3rd extra error
1/10	7.1066e-004			
1/20	6.8623e-005	3.9303e-006		
1/40	5.6000e-006	1.5219e-006	1.3613e-006	
1/80	4.3070e-007	1.5346e-007	6.2236e-008	7.2391e-009
1/160	3.2640e-008	1.2343e-008	2.9345e-009	2.3700e-010
1/320	2.5021e-009	9.0367e-010	1.4107e-010	8.3232e-012

Table 5.5.14: Errors for equation (5.5.9) with $\alpha = 1.3$, taken at $t = 1$.

Step size	The method	1st extrapolation	2nd extrapolation	3rd extrapolation
1/10				
1/20	3.37			
1/40	3.62	1.39		
1/80	3.70	3.31	4.45	
1/160	3.72	3.64	4.41	4.93
1/320	3.71	3.77	4.38	4.83

Table 5.5.15: Orders ("EOC ") for equation (5.5.9) with $\alpha = 1.3$, taken at $t = 1$.

Step size	Error of the method	1st extra. error	2nd extra. error	3rd extra error
1/10	1.3107e-003			
1/20	1.0256e-004	1.4581e-005		
1/40	7.2525e-006	1.9886e-006	1.1491e-006	
1/80	4.9046e-007	1.6518e-007	4.3614e-008	7.5021e-009
1/160	3.2450e-008	1.1957e-008	1.7426e-009	1.9344e-010
1/320	2.1236e-009	8.1682e-010	7.4128e-011	3.0170e-012

Table 5.5.16: Errors for equation (5.5.9) with $\alpha = 1.5$, taken at $t = 1$.

Step size	The method	1st extrapolation	2nd extrapolation	3rd extrapolation
1/10				
1/20	3.68			
1/40	3.82	2.87		
1/80	3.89	3.59	4.72	
1/160	3.92	3.79	4.65	5.28
1/320	3.93	3.87	4.56	6.00

Table 5.5.17: Orders ("EOC ") for equation (5.5.9) with $\alpha = 1.5$, taken at $t = 1$.

Step size	Error of the method	1st extra. error	2nd extra. error	3rd extra error
1/10	1.9057e-003			
1/20	1.2585e-004	1.9355e-006		
1/40	8.0391e-006	4.1927e-007	3.1819e-007	
1/80	5.0764e-007	3.3082e-008	7.3362e-009	3.4360e-009
1/160	3.1910e-008	2.2452e-009	1.8944e-010	5.8225e-011
1/320	2.0046e-009	1.4248e-010	2.2910e-012	4.1943e-012

Table 5.5.18: Errors for equation (5.5.9) with $\alpha = 1.9$, taken at $t = 1$.

Step size	The method	1st extrapolation	2nd extrapolation	3rd extrapolation
1/10				
1/20	3.92			
1/40	3.97	2.21		
1/80	3.99	3.66	5.44	
1/160	3.99	3.88	5.28	5.88
1/320	3.99	3.98	6.36	3.80

Table 5.5.19: Orders ("EOC ") for equation (5.5.9) with $\alpha = 1.9$, taken at $t = 1$.

Chapter 6

Finite difference method (FDM) for space-fractional PDEs

6.1 Introduction

Space fractional derivatives are used to model anomalous diffusion or dispersion, a phenomenon observed in many problems, where particles spread faster than the classical models predict. When a fractional derivative replaces the second derivative in a diffusion or dispersion model, it leads to enhanced diffusion (also called superdiffusion), see Meerschaert and Tadjeran [66]. Space-fractional diffusion equations have been investigated by West and Seshadri [91] and Gorenflo and Mainardi [48] and Gorenflo [47] . A linear interpolation polynomial was used to approximate the Hadamard integral generated by fractional derivative and the rate of the convergence of the proposed numerical method is $O(h^{2-\alpha})$ [26].

In this chapter we will discuss a finite difference method for solving space-fractional partial differential equation. The space-fractional derivatives are the left-handed and right-handed Riemann-Liouville fractional derivatives which can be expressed by using the Hadamard finite-part integrals.

We will examine the stability, consistency and convergence of the proposed finite difference method. The Hadamard finite-part integrals are approximated by using piecewise quadratic interpolation polynomials and a numerical approximation scheme of the space-fractional derivative with convergence order $O(\Delta x^{3-\alpha})$ $(1 < \alpha < 2)$ is obtained. A shifted implicit finite difference method is introduced for solving two-sided space-fractional partial differential equations and we prove that the order of convergence of the finite difference method is $O(\Delta t + \Delta x^{\min(3-\alpha,\beta)}), 1 < \alpha < 2, \beta > 0$, where $\Delta t, \Delta x$ denote the time and space stepsizes, respectively, and β is related to the smoothness of the exact solution u.

6.2 Brief reviews of FDM for solving space-fractional PDEs

Consider the following two-sided space-fractional partial differential equation, with $1 < \alpha < 2$, $t > 0$,

$$u_t(t,x) = C_+(t,x)\,{}_0^R D_x^\alpha u(t,x), + C_-(t,x)\,{}_x^R D_1^\alpha u(t,x) + f(t,x), \quad 0 < x < 1, \quad (6.2.1)$$

$$u(t,0) = \varphi_1(t), \quad u(t,1) = \varphi_2(t), \quad (6.2.2)$$

$$u(0,x) = u_0(x), \quad 0 < x < 1. \quad (6.2.3)$$

Here the function $f(t,x)$ is a source/sink term. The functions $C_+(t,x) \geq 0$ and $C_-(t,x) \geq 0$ may be interpreted as transport related coefficients. The addition of a classical advective term $-\nu(t,x)\frac{\partial u(t,x)}{\partial x}$ in (6.2.1) does not impact the analysis performed in this chapter, and has been omitted to simplify the notation. The left-handed fractional derivative ${}_0^R D_x^\alpha f(x)$ and right-handed fractional derivative ${}_x^R D_1^\alpha f(x)$ in (6.2.1) are Riemann-Liouville fractional derivatives of order α defined by, with $1 < \alpha < 2$,

$${}_0^R D_x^\alpha f(x) = \frac{1}{\Gamma(2-\alpha)} \frac{d^2}{dx^2} \int_0^x (x-\xi)^{1-\alpha} f(\xi)\, d\xi, \quad (6.2.4)$$

and

$${}_x^R D_1^\alpha f(x) = \frac{1}{\Gamma(2-\alpha)} \frac{d^2}{dx^2} \int_x^1 (\xi - x)^{1-\alpha} f(\xi)\, d\xi. \quad (6.2.5)$$

There are several ways to approximate the Riemann- Liouville fractional derivative. Let $0 = x_0 < x_1 < \cdots < x_j < \cdots < x_M = 1$ be a partition of $[0,1]$ and Δx the stepsize. Based on the definition of the Grünwald-Letnikov derivative, one can approximate the left-handed and right-handed Riemann-Liouville fractional derivatives by see [66])

$${}_0^R D_x^\alpha f(x_j) = \Delta x^{-\alpha} \sum_{k=0}^{j} w_k^{(\alpha)} f(x_{j-k}) + O(\Delta x), \quad (6.2.6)$$

and

$$ {}_{x}^{R}D_{1}^{\alpha} f(x_j) = \Delta x^{-\alpha} \sum_{k=0}^{M-j} w_k^{(\alpha)} f(x_{j+k}) + O(\Delta x), \tag{6.2.7} $$

where $w_k^{(\alpha)}$ are some weights and the order of convergence in (6.2.6) or (6.2.7) is $O(\Delta x)$ for any $\alpha > 0$. Meerschaert and Tadjeran [64] proposed finite difference approximations for fractional advection-dispersion flow equations. They used the Grünwald method to approximate the space-fractional derivative and proved that the standard finite difference method is unconditionally unstable, but the shifted finite difference method is unconditionally stable.

Lubich [53] obtained approximations of order 2 - 6 in the form of (6.2.6), where the coefficients $w_k^{(\alpha)}$ are just the coefficients of the Taylor series expansions of some generating functions $w_l^{(\alpha)}(z)$, $l = 2, 3, 4, 5, 6$. The $L2$ scheme and its modification $L2C$ scheme are introduced in Oldham and Spanier [72], Lynch, et al. [62] as follows. Note that, with $1 < \alpha < 2$,

$$ \begin{aligned} {}_{0}^{R}D_{x}^{\alpha} f(x_j) = {} & \frac{f(x_0)(x_j - x_0)^{-\alpha}}{\Gamma(1-\alpha)} + \frac{f'(x_0)(x_j - x_0)^{1-\alpha}}{\Gamma(2-\alpha)} \\ & + \frac{1}{2-\alpha} \sum_{l=0}^{j-1} \int_{x_l}^{x_{l+1}} s^{1-\alpha} f''(x_j - s)\, ds. \end{aligned} $$

On each interval $[x_l, x_{l+1}]$, $f''(x_j - s)$ is approximated by $\frac{f(x_j - x_l) - 2f(x_j - x_{l+1}) + f(x_j - x_{l+2})}{\Delta x^2}$, then the so-called $L2$ scheme is obtained and the convergence order is $O(\Delta x)$. Similarly, one can obtain $L2C$ scheme. Diethelm [25, 26] expressed the Riemann-Liouville fractional derivative into the equivalent Hadamard finite-part integral and then approximated the Hadamard finite-part integral by piecewise linear interpolation polynomials to obtain an approximation scheme to the fractional derivative for $0 < \alpha < 1$. More precisely, Diethelm [26] obtained, with $0 < \alpha < 1$,

$$ \begin{aligned} {}_{0}^{R}D_{x}^{\alpha} f(x_j) &= \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_0^{x_j} (x_j - \xi)^{-\alpha}\, d\xi = \frac{1}{\Gamma(-\alpha)} \oint_0^{x_j} (x_j - \xi)^{-\alpha-1} f(\xi)\, d\xi \\ &= \Delta x^{-\alpha} \sum_{k=0}^{j} w_{k,j} f(x_{j-k}) + O(\Delta x^{2-\alpha}), \end{aligned} $$

where $\oint_0^{x_j}$ denotes the Hadamard finite-part integral and $w_{k,j}$ are some weights.

Odibat [70, 71] introduced a computational algorithm for approximating the Caputo fractional derivative and the convergence order is $O(\Delta x^2)$, see also Sousa [84]. The idea is as follows. Note that, with $1 < \alpha < 2$,

$$
\begin{aligned}
{}_{0}^{C}D_{x}^{\alpha} f(x_j) &= \frac{1}{\Gamma(2-\alpha)} \int_{0}^{x_j} (x_j - \xi)^{1-\alpha} f''(\xi)\, d\xi \\
&= \frac{1}{\Gamma(2-\alpha)} \sum_{l=0}^{j-1} \int_{x_l}^{x_{l+1}} (x_j - \xi)^{1-\alpha} f''(\xi)\, d\xi.
\end{aligned}
$$

On each subinterval $[x_l, x_{l+1}]$, one approximates the integral by using the linear interpolation polynomial $P_1(\xi) = \frac{\xi - x_{l+1}}{x_l - x_{l+1}} f''(x_l) + \frac{\xi - x_l}{x_{l+1} - x_l} f''(x_{l+1})$ and obtains, with some weights $\bar{w}_{k,j}, k = 0, 1, 2, \ldots, j$,

$$
{}_{0}^{C}D_{x}^{\alpha} f(x_j) \approx \frac{1}{\Gamma(2-\alpha)} \sum_{l=0}^{j-1} \int_{x_l}^{x_{l+1}} (x_j - \xi)^{1-\alpha} P_1(\xi)\, d\xi = \Delta x^{2-\alpha} \sum_{k=0}^{j} \bar{w}_{k,j} f''(x_k).
$$

Further, Odibat [70] approximated $f''(x_k)$ by $\frac{f(x_{k+1}) - 2f(x_k) + f(x_{k-1})}{\Delta x^2}$ and obtained a second order approximation scheme to ${}_{0}^{C}D_{x}^{\alpha} f(x_j)$. More recently, Dimitrov [34] obtained a second and third order approximations for the Grünwald and shifted Grünwald formulae with weighted averages of Caputo derivatives.

Let us review some numerical methods for solving space-fractional partial differential equations. There are many different numerical methods for solving space-fractional partial differential equations in literature: Choi at al. [12] applied the backward Euler finite difference method with the right-shifted Grünward formula for the Riemann-Liouville space fractional derivative term and proved the existence using Leray-Schauder fixed point theorem and finally the convergence order $O(\Delta x + \Delta t)$ are considered. By using shifted Grünwald-Letnikov formulae (6.2.6) and (6.2.7), Meerschaert and Tadjeran [66] introduced a finite difference method for solving two-sided space-fractional partial differential equations (6.2.1)- (6.2.3) and proved that the convergence order of spatial discretization is $O(\Delta x)$. Meerschaert and Tadjeran (2004) [64] also considered the finite difference method for solving the 1D fractional advection-dispersion equation, with $1 < \alpha < 2$,

$$
\frac{\partial u(t,x)}{\partial t} = -\nu(x) \frac{\partial u(t,x)}{\partial x} + d(x) \frac{\partial^{\alpha} u(t,x)}{\partial x^{\alpha}} + f(t,x),
$$

by using the shifted Grünwald-Letnikov formula on a finite domain and they proved that the convergence order of spatial discretization is $O(\Delta x)$. Tadjeran, Meerschaert and Scheffler [88] and Tadjeran and Meerschaert [89] applied the shifted Grünwald-Letnikov formula and extrapolation techniques to fractional diffusion equations in 1D and 2D and obtained a second-order accurate finite difference method. Liu et al. [61] transformed the fractional advection-dispersion equation into a system of ordinary differential equations, which was then solved using backward difference formulae. Chen and Liu [11] used a technique combining the alternating direction implicit-Euler method with Richardson extrapolation to establish an unconditionally stable second-order accuracy difference method to approximate a 2D fractional advection-dispersion equation with variable coefficients on a finite domain. Podlubny et al. [77] developed a matrix approach to discretize fractional diffusion equations with various combinations of time-space-fractional derivatives. Shen et al. [79, 80] presented explicit and implicit difference approximations for the Riesz fractional advection-dispersion equations and the space-time Riesz-Caputo fractional advection-dispersion equations. Shen et al. [81] considered a novel numerical approximation for the space fractional advection-dispersion equation. See also [2, 13, 60, 65, 82, 83, 85, 94, 86].

There are other numerical methods for solving space-fractional partial differential equations: the finite element methods, see [20, 21, 38, 39, 37, 40] and the spectral methods [57, 58].

In this chapter, we will use the idea in Diethelm [26] to define a finite difference method for solving (6.2.1)- (6.2.3), see recent works for this method [93, 43, 45, 46]. We first express the fractional derivative by using the Hadamard finite-part integral, i.e., with $1 < \alpha < 2$,

$$ {}_0^R D_x^\alpha f(x) = \frac{1}{\Gamma(2-\alpha)} \frac{d^2}{dx^2} \int_0^x (x-\xi)^{1-\alpha} f(\xi)\, d\xi = \frac{1}{\Gamma(-\alpha)} \oint_0^x (x-\xi)^{-\alpha-1} f(\xi)\, d\xi. $$

Then we approximate $f(\xi)$ by using piecewise quadratic interpolation polynomials and obtain an approximation scheme of Riemann-Liouville fractional derivative. Similarly, we can approximate the right-handed Riemann-Liouville fractional derivative ${}_x^R D_1^\alpha f(x)$. Based on these approximation schemes, we define a shifted finite difference method for solving (6.2.1)-(6.2.3). We proved that the convergence order of the numerical method is $O(\Delta t + \Delta x^{\min(3-\alpha,\beta)}), 1 < \alpha < 2, \beta > 0$.

6.3 FDM based on linear interpolation

In this section, we will introduce a finite difference method for solving (6.2.1)-(6.2.3) by using the idea in Diethelm [25]. For simplicity, we assume $C_+(t,x) = C_-(t,x) = 1$ and $\varphi_1(t) = \varphi_2(t) = 0$. Recall that the Riemann-Liouville fractional derivative has the form, with $1 < \alpha < 2$,

$$ {}_0^R D_x^\alpha f(x) = \frac{1}{\Gamma(-\alpha)} \oint_0^x (x-\xi)^{-1-\alpha} f(\xi)\, d\xi, \tag{6.3.1}$$

where $\oint_0^x (x-\xi)^{-1-\alpha} f(\xi)\, d\xi$ denotes the Hadamard finite-part integral [25].

Let $0 = x_0 < x_1 < x_2 < \cdots < x_j < \cdots < x_M = 1$ be a partition of $[0,1]$ and Δx the stepsize. We then have, at $x = x_j$, $j = 1, 2, \ldots, M$,

$$\begin{aligned} {}_0^R D_x^\alpha f(x_j) &= \frac{1}{\Gamma(-\alpha)} \oint_0^{x_j} (x_j-\xi)^{-1-\alpha} f(\xi)\, d\xi = \frac{x_j^{-\alpha}}{\Gamma(-\alpha)} \oint_0^1 w^{-1-\alpha} f(x_j - x_j w)\, dw \\ &= \frac{x_j^{-\alpha}}{\Gamma(-\alpha)} \sum_{l=1}^{j} \oint_{\frac{l-1}{j}}^{\frac{l}{j}} w^{-1-\alpha} f(x_j - x_j w)\, dw. \end{aligned} \tag{6.3.2}$$

Denoting $g(w) = f(x_j - x_j w)$ and substituting $g(w)$ in (6.3.2) by the following linear interpolation polynomial $P_1(w)$ on $[\frac{l-1}{j}, \frac{l}{j}], l = 1, 2, \ldots, j$,

$$P_1(w) = \frac{w - \frac{l}{j}}{\frac{l-1}{j} - \frac{l}{j}} g\Big(\frac{l-1}{j}\Big) + \frac{w - \frac{l-1}{j}}{\frac{l}{j} - \frac{l-1}{j}} g\Big(\frac{l}{j}\Big),$$

we obtain an approximation to ${}_0^R D_x^\alpha f(x_j)$, $1 < \alpha < 2$,

$$ {}_0^R D_x^\alpha f(x_j) = \Delta x^{-\alpha} \sum_{k=0}^{j} w_{k,j} f(x_{j-k}) + O(\Delta x^{2-\alpha}), \tag{6.3.3}$$

where

$$\Gamma(2-\alpha) w_{k,j} = \begin{cases} 1, & \text{for } k = 0, \\ 2^{1-\alpha} - 2, & \text{for } k = 1, \\ (k+1)^{1-\alpha} - 2k^{1-\alpha} + (k-1)^{1-\alpha}, & \text{for } k = 2, 3, \ldots, j-1, \\ -j^{1-\alpha} + (j-1)^{1-\alpha} - (\alpha-1) j^{-\alpha}, & \text{for } k = j. \end{cases}$$

Remark 13. The coefficients $w_{k,j}$ in (6.3.3) can also be written

$$\Gamma(2-\alpha)w_{k,j} = \begin{cases} b_0, & \text{for } k=0, \\ b_1 - b_0, & \text{for } k=1, \\ b_k - b_{k-1}, & \text{for } k=2,3,\dots,j-1, \\ \bar{b}_j - b_{j-1}, & \text{for } k=j, \end{cases}$$

where $b_k = (k+1)^{1-\alpha} - k^{1-\alpha}$, $0 \leq k \leq j-1$, $\bar{b}_j = (1-\alpha)j^{-\alpha}$. These are the same coefficients as in the L2 scheme defined in [72, 61].

Lemma 6.3.1. Let $1 < \alpha < 2$. The coefficients $w_{k,j}$ in (6.3.3) satisfy

$$w_{1,j} < 0, \quad \text{and} \quad w_{k,j} > 0,\ k \neq 1,\ k = 0,2,3,\dots,j,$$
$$\Gamma(2-\alpha)\sum_{k=0}^{j} w_{k,j} = \bar{b}_j = (1-\alpha)j^{1-\alpha} < 0.$$

Proof. From the properties of w_{kj} it is obvious that $w_{1,j} < 0$ and $w_{k,j} > 0$ We can show that the sum of coefficients w_{kj} are always negative. For example, Let, j=3 we have,

$$\Gamma(2-\alpha)w_{k3} = \begin{cases} b_0, & k=0, \\ b_0 - b_1, & k=1, \\ b_2 - b_1, & k=2, \\ \overline{b_3} - b_2, & k=3, \end{cases}$$

Therefore,

$$\begin{aligned} \sum_{k=0}^{3} w_{k3} &= b_0 + \ (b_1 - b_0) + (b_2 - b_1) + (\overline{b_3} - b_2) \\ &= \bar{b}_3 = (1-\alpha)3^{-\alpha} < 0. \end{aligned} \tag{6.3.4}$$

In general, we have

$$\begin{aligned} \sum_{k=0}^{j} w_{kj} &= b_0 + (b_1 - b_0) + (b_2 - b_1) + \cdots + (b_j - b_{j-1}) + (\overline{b_{j+1}} - b_j) \\ &= \bar{b}_{j+1} = (1-\alpha)(j+1)^{-\alpha} < 0. \end{aligned} \tag{6.3.5}$$

Further, we have, when $j \to \infty$

$$\sum_{k=0}^{j} w_{kj} = 0.$$

□

Similarly, we can obtain an approximation scheme for the right-handed Riemann-Liouville fractional derivative ${}_x^R D_1^\alpha f(x)$. We have

$$ {}_x^R D_1^\alpha f(x_j) = \Delta x^{-\alpha} \sum_{k=0}^{M-j} w_{k,M-j} f(x_{j+k}) + O(\Delta x^{2-\alpha}), \quad j = 0, 1, 2, \ldots, M-1, \tag{6.3.6} $$

where $w_{k,M-j},\ k = 0, 1, 2, \ldots, M-j,\ j = 0, 1, 2, \ldots, M-1$ are defined as in (6.3.3).

Discretizing $u_t(t_n, x_j)$ by using forward Euler method at t_n and discretizing ${}_0^R D_x^\alpha u(t_n, x_j)$ and ${}_x^R D_1^\alpha u(t_n, x_j)$ by using (6.3.3) and (6.3.6) at x_j respectively, we get, with $u_j^n = u(t_n, x_j)$, $f_j^n = f(t_n, x_j)$,

$$ \begin{aligned} &\Delta t^{-1}(u_j^{n+1} - u_j^n) - (\Delta x)^{-\alpha} \Big(\sum_{k=0}^{j} w_{k,j} u_{j-k}^n + \sum_{k=0}^{M-j} w_{k,M-j} u_{j+k}^n \Big) \\ &= f_j^n + \tau_j^n, \end{aligned} \tag{6.3.7} $$

where the truncation error $\tau_j^n = O(\Delta t + \Delta x^{2-\alpha})$ [25], [26].

Let $U_j^n \approx u(t_n, x_j)$ be the approximate solution of $u(t_n, x_j)$ at the node (t_n, x_j). We define an explicit finite difference method for solving (6.2.1) - (6.2.3), with $j = 1, 2, \ldots, M-1$,

$$ \Delta t^{-1}\big(U_j^{n+1} - U_j^n\big) = \Delta x^{-\alpha} \Big(\sum_{k=0}^{j} w_{k,j} U_{j-k}^n + \sum_{k=0}^{M-j} w_{k,M-j} U_{j+k}^n \Big) + f_j^n, \tag{6.3.8} $$

with $U_0^n = U_M^n = 0$, and $U_j^0 = u_0(x_j), j = 0, 1, 2, \ldots, M-1$. Here the weights $w_{k,j}$ and $w_{k,M-j}$, are given in (6.3.3).

Lemma 6.3.2. The explicit finite difference method (6.3.8) is unconditionally unstable

Proof. Let $n = 0$. With $\lambda = \Delta t / \Delta x^\alpha$, (6.3.8) can be written as, $j = 1, 2, \ldots, M-1$,

$$ U_j^1 = \big(1 + w_{0j}\lambda + w_{0,(M-j)}\lambda\big) U_j^0 + \lambda \sum_{k=1}^{j} w_{kj} U_{j-k}^0 + \lambda \sum_{k=1}^{M-j} w_{k,(M-j)} U_{j+k}^0 + \Delta t f_j^0. \tag{6.3.9} $$

Assume that we have some errors in the starting values U_j^0, i.e.,

$$ \bar{U}_j^0 = U_j^0 + \epsilon_j^0, \quad j = 0, 1, 2, \ldots, M. $$

To consider the stability, we assume that only the term U_i^0, for some fixed i, has the error, and other terms have no errors, i.e.,

$$\epsilon_j^0 = 0, \quad j \neq i.$$

Then we have

$$\bar{U}_i^1 = \big(1 + w_{0i}\lambda + w_{0,(M-j)}\lambda\big)\bar{U}_i^0 + \lambda \sum_{k=1}^{i} w_{ki}\bar{U}_{i-k}^0 + \lambda \sum_{k=1}^{M-i} w_{k,M-i}\bar{U}_{i+k}^0 + \Delta t f_i^0. \quad (6.3.10)$$

Subtracting (6.3.9) from (6.3.10) , we obtain

$$\epsilon_i^1 = \big(1 + w_{0i}\lambda + w_{0,(M-i)}\big)\epsilon_i^0.$$

That is, the error is amplified by the factor $\mu_i = 1 + w_{0i}\lambda + w_{0,(M-i)}$ when the finite difference equation is advanced by one time step. After n time steps, one may write

$$\epsilon_i^n = \big(1 + w_{0i}\lambda + w_{0,(M-i)}\big)^n \epsilon_i^0.$$

Note that, by Lemma 6.3.1, $w_{0i} = 1/\Gamma(2-\alpha) > 0$, and $w_{0,(M-i)} = 1/\Gamma(2-\alpha) > 0$ we have $1 + w_{0i}\lambda + w_{0,(M-i)} > 1$. Thus $|\epsilon_i^n| \to \infty$ as $n \to \infty$, which implies that the method is unstable.

□

Next we consider an implicit Euler method for solving (6.2.1)-(6.2.3), we define an implicit finite difference method for solving (6.2.1) - (6.2.3), with $j = 1, 2, \ldots, M-1$,

$$\Delta t^{-1}\big(U_j^{n+1} - U_j^n\big) = \Delta x^{-\alpha}\Big(\sum_{k=0}^{j} w_{k,j}U_{j-k}^{n+1} + \sum_{k=0}^{M-j} w_{k,M-j}U_{j+k}^{n+1}\Big) + f_j^{n+1}, \qquad (6.3.11)$$

with $U_0^n = U_M^n = 0$, and $U_j^0 = u_0(x_j), j = 0, 1, 2, \ldots, M-1$. Here the weights $w_{k,j}$ and $w_{k,M-j}$, are given in (6.3.3).

Lemma 6.3.3. The implicit finite difference method (6.3.11) is unconditionally unstable

Proof. We have, with $\lambda = \Delta t/\Delta x^\alpha$,

$$(1 - w_{0j}\lambda - w_{0,M-j}\lambda)U_j^{n+1} = U_j^n + \lambda \sum_{k=1}^{j} w_{kj}U_{j-k}^{n+1} + \lambda \sum_{k=1}^{M-j} w_{k,M-j}U_{j+k}^{n+1} + \Delta t f_j^{n+1}. \quad (6.3.12)$$

Although this is an implicit Euler method, the problem can be solved explicitly by a left-to -right sweep across the x domain due to the Dirichlet boundary condition at the left boundary. For example, the value U_3^1 can be explicitly determined by U_0^1, U_1^1, U_2^1 and U_3^0. Now let us consider the stability. Let $\epsilon_j^0 = \bar{U}_j^0 - U_j^0,\ j = 0, 1, 2, \dots, M$ be the error generated by U_j^0. Assume that $\epsilon_j^0 = 0,\ j \neq i$, that is U_i^0 is the only term that has an error for fixed i. Let $n = 0$, we have

$$U_i^1 = \frac{1}{1 - w_{0i}\lambda - w_{0,M-i}\lambda} U_i^0 + \frac{1}{1 - w_{0i}\lambda - w_{0,M-i}\lambda} \Big(\lambda \sum_{k=1}^{i} w_{ki} U_{i-k}^1 + \lambda \sum_{k=1}^{M-i} w_{k,M-i} U_{i+k}^1 + \Delta t f_i^1 \Big), \tag{6.3.13}$$

and

$$\bar{U}_i^1 = \frac{1}{1 - w_{0i}\lambda - w_{0,M-i}\lambda} \bar{U}_i^0 + \frac{1}{1 - w_{0i}\lambda - w_{0,M-i}\lambda} \Big(\lambda \sum_{k=1}^{i} w_{ki} \bar{U}_{i-k}^1 + \lambda \sum_{k=1}^{M-i} w_{k,M+i} \bar{U}_{i+k}^1 + \Delta f_i^1 \Big). \tag{6.3.14}$$

Denote $\epsilon_i^1 = \bar{U}_i^1 - U_i^1$, we get, subtracting (6.3.13) from (6.3.14),

$$\epsilon_i^1 = \frac{1}{1 - w_{0i}\lambda - w_{0,M-i}\lambda} \epsilon_i^0.$$

After n time steps, we may write

$$\epsilon_i^n = \Big(\frac{1}{1 - w_{0i}\lambda - w_{0,M-i}\lambda} \Big)^n \epsilon_i^0.$$

Note that, by Lemma 6.3.1, $w_{0i} > 0$, and $w_{0,M-i} > 0$ which implies that $1 - w_{0i}\lambda - w_{0,M-i} < 1$ and therefore

$$\Big| \frac{1}{1 - w_{0i}\lambda - w_{0,M-i}} \Big| > 1.$$

Thus $|\epsilon_i^n| \to \infty$ as $n \to \infty$, which means that the method is unconditionally unstable.

$\square$

We now introduce the shifted Diethelm's FDM for space-fractional PDEs. At the node (t_{n+1}, x_j), we may write the equation (6.2.1) into the shifted form, with $j = 1, 2, \dots, M-1$,

$$u_t(t_{n+1}, x_j) - \Big({}_0^R D_x^\alpha u(t_{n+1}, x_{j+1}) + {}_x^R D_1^\alpha u(t_{n+1}, x_{j-1}) \Big) = f_j^{n+1} + \sigma_j^{n+1}, \tag{6.3.15}$$

where $f_j^{n+1} = f(t_{n+1}, x_j)$ and

$$\sigma_j^{n+1} = -\Big({}_0^R D_x^\alpha u(t_{n+1}, x_{j+1}) - {}_0^R D_x^\alpha u(t_{n+1}, x_j) \Big) - \Big({}_x^R D_1^\alpha u(t_{n+1}, x_{j-1}) - {}_x^R D_1^\alpha u(t_{n+1}, x_j) \Big).$$

Discretizing $u_t(t_{n+1}, x_j)$ at t_{n+1} by using the backward Euler method and discretizing ${}_0^R D_x^\alpha u(t_{n+1}, x_{j+1})$ and ${}_x^R D_1^\alpha u(t_{n+1}, x_{j-1})$ by using (6.3.3) and (6.3.6) at x_{j+1} and x_{j-1} respectively, we get, with $u_j^n = u(t_n, x_j)$, $f_j^n = f(t_n, x_j)$,

$$\begin{aligned} &\Delta t^{-1}(u_j^{n+1} - u_j^n) - (\Delta x)^{-\alpha} \Big(\sum_{k=0}^{j+1} w_{k,j+1} u_{j+1-k}^{n+1} + \sum_{k=0}^{M-(j-1)} w_{k,M-(j-1)} u_{j-1+k}^{n+1} \Big) \\ &= f_j^{n+1} + \sigma_j^{n+1} + \tau_j^{n+1}, \end{aligned} \tag{6.3.16}$$

where the truncation error $\tau_j^{n+1} = O(\Delta t + \Delta x^{2-\alpha})$ [25, 26].

Let $U_j^n \approx u(t_n, x_j)$ be the approximate solution of $u(t_n, x_j)$ at the node (t_n, x_j). We define an implicit shifted finite difference method for solving (6.2.1) - (6.2.3), with $j = 1, 2, \dots, M-1$,

$$\Delta t^{-1}\big(U_j^{n+1} - U_j^n\big) = \Delta x^{-\alpha} \Big(\sum_{k=0}^{j+1} w_{k,j+1} U_{j+1-k}^{n+1} + \sum_{k=0}^{M-(j-1)} w_{k,M-(j-1)} U_{j-1+k}^{n+1} \Big) + f_j^{n+1}, \tag{6.3.17}$$

with $U_0^{n+1} = U_M^{n+1} = 0$, and $U_j^0 = u_0(x_j), j = 0, 1, 2, \dots, M-1$. Here the weights $w_{k,j+1}$ and $w_{k,M-(j-1)}$, are given in (6.3.3).

Theorem 6.3.4. The shifted implicit method (6.3.17) is unconditionally stable.

Proof. With $\lambda = \Delta t / \Delta x^\alpha$, (6.3.17) can be written as, $j = 1, 2, \dots, M-1$,

$$\begin{aligned} &\Big(-\lambda w_{0,j+1} - \lambda w_{2,M-(j-1)} \Big) U_{j+1}^{n+1} + \Big(1 - \lambda w_{1,j+1} - \lambda w_{1,M-(j-1)} \Big) U_j^{n+1} \\ &- \lambda \Big(\sum_{k=2}^{j+1} w_{k,j+1} U_{j+1-k}^{n+1} + \sum_{k=2}^{M-(j-1)} w_{k,M-(j-1)} U_{j-1+k}^{n+1} \Big) = U_j^n + \Delta t f_j^{n+1}, \end{aligned} \tag{6.3.18}$$

$$U_0^{n+1} = U_M^{n+1} = 0, \tag{6.3.19}$$

or in the matrix form,

$$AU^{n+1} = U^n + \Delta t F^{n+1},$$

where

$$A = \begin{pmatrix} 1-\lambda w_{12}-\lambda w_{1M} & -\lambda w_{02}-\lambda w_{2M} & \cdots & -\lambda w_{M-1,M} \\ \\ -\lambda w_{23}-\lambda w_{0,M-1} & 1-\lambda w_{13}-\lambda w_{1,M-1} & \cdots & -\lambda w_{M-2,M-1} \\ -\lambda w_{34} & -\lambda w_{24}-\lambda w_{0,M-2} & \cdots & -\lambda w_{M-3,M-2} \\ \vdots & \vdots & \vdots & \vdots \\ -\lambda w_{M-1,M} & -\lambda w_{M-2,M} & -\lambda w_{2,M}-\lambda w_{0,2} & 1-\lambda w_{1,M}-\lambda w_{12} \end{pmatrix},$$

and

$$U^{n+1} = \begin{pmatrix} U_1^{n+1} \\ U_2^{n+1} \\ \vdots \\ U_{M-1}^{n+1} \end{pmatrix}, \quad U^n = \begin{pmatrix} U_1^n \\ U_2^n \\ \vdots \\ U_{M-1}^n \end{pmatrix}, \quad F^{n+1} = \begin{pmatrix} f_1^{n+1} \\ f_2^{n+1} \\ \vdots \\ f_{M-1}^{n+1} \end{pmatrix}.$$

Let μ denote an eigenvalue of A and $\xi = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_{M-1} \end{pmatrix} \neq 0$ the corresponding eigenvector, that is,

$$A\xi = \mu\xi.$$

Denote

$$|x_i| = \max_j \{|x_j|,\ j = 1, 2, \ldots, M-1\},$$

we have, for fixed i,

$$\sum_{j=1}^{M-1} a_{ij} x_j = \mu x_i,$$

or

$$\mu = a_{ii} + \sum_{j=1, j\neq i}^{M-1} a_{ij} \frac{x_j}{x_i}.$$

Note that

$$\begin{aligned}
&a_{i,1} = -\lambda w_{i,i+1},\ \ldots, a_{i,i-2} = -\lambda w_{3,i+1},\\
&a_{i,i-1} = -\lambda w_{2,i+1} - \lambda w_{0,M-(i-1)},\ a_{ii} = 1 - \lambda w_{1,i+1} - \lambda w_{1,M-(i-1)},\\
&a_{i,i+1} = -\lambda w_{0,i+1} - \lambda w_{2,M-(i-1)},\\
&a_{i,i+2} = -\lambda w_{3,M-(i-1)},\ \ldots, a_{i,M-1} = -\lambda w_{M-(i-1)-1,M-(i-1)},
\end{aligned}$$

we have

$$\begin{aligned}
\mu = 1 &- \lambda\Big(w_{0,i+1}\frac{x_{i+1}}{x_i} + w_{1,i+1} + w_{2,i+1}\frac{x_{i-1}}{x_i} + \cdots + w_{i,i+1}\frac{x_1}{x_i}\Big)\\
&- \lambda\Big(w_{0,M-(i-1)}\frac{x_{i-1}}{x_i} + w_{1,M-(i-1)} + w_{2,M-(i-1)}\frac{x_{i+1}}{x_i} + \cdots + w_{i,M-(i-1)}\frac{x_{M-1}}{x_i}\Big).
\end{aligned}$$

Since $\frac{x_j}{x_i} < 1$, $j \neq i$ and, by Lemma 6.3.1, $w_{k,i+1} > 0$, $k \neq 1$ and $\sum_{k=0}^{i} w_{k,i+1} < \sum_{k=0}^{i+1} w_{k,i+1} = (1-\alpha)(i+1)^{-\alpha} < 0$, and $\sum_{k=0}^{M-(i-1)-1} w_{k,M-(i-1)} < \sum_{k=0}^{M-(i-1)} w_{k,M-(i-1)} = (1-\alpha)(M-(i-1))^{-\alpha} < 0$, we have

$$\begin{aligned}
&w_{0,i+1}\frac{x_{i+1}}{x_i} + w_{1,i+1} + w_{2,i+1}\frac{x_{i-1}}{x_i} + \cdots + w_{i,i+1}\frac{x_1}{x_i}\\
&\quad + w_{0,M-(i-1)}\frac{x_{i-1}}{x_i} + w_{1,M-(i-1)} + w_{2,M-(i-1)}\frac{x_{i+1}}{x_i} + \cdots + w_{i,M-(i-1)}\frac{x_{M-1}}{x_i}\\
&< \Big(w_{0,i+1} + w_{1,i+1} + w_{2,i+1} + \cdots + w_{i,i+1}\Big)\\
&\quad + \Big(w_{0,M-(i-1)} + w_{1,M-(i-1)} + w_{2,M-(i-1)} + \cdots + w_{i,M-(i-1)}\Big) < 0,
\end{aligned}$$

which implies that $\mu > 1$.

Since all the eigenvalues μ of matrix A satisfy $|\mu| \geq 1$, the matrix A is invertible and all eigenvalues of A^{-1} are less than 1. Hence there exists a matrix norm $\|\cdot\|$ such that $\|A^{-1}\| \leq 1$ and

$$\begin{aligned}
\|U^{n+1}\| = \|A^{-1}(U^n + kF^{n+1})\| &\leq \|U^n\| + k\|F^{n+1}\|\\
&\leq \cdots \leq \|U^0\| + k\sum_{j=1}^{n+1}\|F^j\|\\
&\leq \|U^0\| + t_{n+1}\max_{t\geq 0}\|f(t)\| \leq C,
\end{aligned}$$

which implies that the numerical method is stable.

We may use the Gershgorin lemma to simplify the proof above. In fact, we have, noting that $w_{1,j} < 0,\ w_{k,j} > 0,\ k \neq 1,\ k = 0, 2, 3, \dots, j$,

$$
\begin{aligned}
r_i = \sum_{k=1,k\neq i}^{M-1} |a_{ik}| &= \lambda(w_{0,i+1} + w_{2,i+1} + w_{3,i+1} + \cdots + w_{i,i+1}) \\
&+ \lambda\big(w_{0,M-(i-1)} + w_{2,M-(i-1)} + w_{3,M-(i-1)} + \cdots + w_{M-i,M-(i-1)}\big),
\end{aligned}
$$

for $i = 1, 2, \dots, M-1$.

Since $a_{ii} = 1 - \lambda w_{1,i+1} - \lambda w_{1,M-i+1},\ i = 1, 2, \dots, M-1$, we have

$$
\begin{aligned}
a_{ii} - r_i =& 1 - \lambda(w_{0,i+1} + w_{1,i+1} + w_{2,i+1} + \cdots + w_{i,i+1}) \\
&- \lambda\big(w_{0,M-(i-1)} + w_{1,M-(i-1)} + w_{2,M-(i-1)} + \cdots + w_{M-i,M-(i-1)}\big),
\end{aligned}
$$

which implies that, by Lemma 6.3.1,

$$a_{ii} - r_i > 1, \quad i = 1, 2, \dots, M-1.$$

By Gershgorin lemma, all the eigenvalues μ of A satisfy

$$1 < a_{ii} - r_i < \mu < a_{ii} + r_i.$$

Thus all the eigenvalues of A are larger than or equal to 1, which implies that the matrix A is invertible and there exists a matrix norm $\| \cdot \|$ such that $\|A^{-1}\| \leq 1$. Hence the numerical method (6.3.17) is unconditionally stable.

The proof of the Theorem 6.3.4 is complete.

□

We now consider the error estimates of the shifted finite difference method (6.3.17).

Theorem 6.3.5. Let $u(t_{n+1}, x_j)$ and U_j^{n+1} be the solutions of (6.3.15) and (6.3.17), respectively. Assume that $u(t,x)$ satisfies the Lipschitz conditions, with some $\beta > 0$,

$$\left| {}_0^R D_x^\alpha u(t,x) - {}_0^R D_x^\alpha u(t,y) \right| \leq C_\alpha |x-y|^\beta, \tag{6.3.20}$$

$$\left| {}_x^R D_1^\alpha u(t,x) - {}_x^R D_1^\alpha u(t,y) \right| \leq C_\alpha |x-y|^\beta. \tag{6.3.21}$$

Then we have

$$\max_j |u(t_{n+1}, x_j) - U_j^{n+1}| \leq C(\Delta t + \Delta x^{\min(\beta, 2-\alpha)}).$$

Proof. Let $e_j^{n+1} = u(t_{n+1}, x_j) - U_j^{n+1}$. Subtracting (6.3.17) from (6.3.16), we obtain the following error equation,

$$\Delta t^{-1}\big(e_j^{n+1} - e_j^n\big) - \Delta x^{-\alpha}\Big(\sum_{k=0}^{j+1} w_{k,j+1} e_{j+1-k}^{n+1} + \sum_{k=0}^{M-(j-1)} w_{k,M-(j-1)} e_{j-1+k}^{n+1}\Big)$$
$$= \sigma_j^{n+1} + \tau_j^{n+1}.$$

With $\lambda = \Delta t/\Delta x^\alpha$, we have

$$\begin{aligned}
&(1 - \lambda w_{1,j+1} - \lambda w_{1,M-(j-1)})e_j^{n+1} \\
&- \lambda\big(w_{0,j+1}e_{j+1}^{n+1} + w_{2,j+1}e_{j-1}^{n+1} + \cdots + w_{j,j+1}e_1^{n+1} + w_{j+1,j+1}e_0^{n+1}\big) \\
&- \lambda\big(w_{0,M-(j-1)}e_{j-1}^{n+1} + w_{2,M-(j-1)}e_{j+1}^{n+1} + \cdots + w_{M-(j-1),M-(j-1)}e_M^{n+1}\big) \\
=\ & e_j^n + \Delta t\sigma_j^{n+1} + \Delta t\tau_j^{n+1}.
\end{aligned}$$

Using Lemma 6.3.1 and assumptions (6.3.20)- (6.3.21), we have, with $R = (\Delta t + \Delta x^{\min(2-\alpha,\beta)}$,

$$\begin{aligned}
|e^1|_\infty = \sup_j |e_j^1| = |e_l^1| \le |e_l^1|\Big(&1 - \lambda(w_{0,l+1} + w_{1,l+1} + \cdots + w_{l+1,l+1}) \\
&- \lambda(w_{0,M-(l-1)} + w_{1,M-(l-1)} + \cdots + w_{M-(l-1),M-(l-1)})\Big) \\
=\ & |e_l^1| - \lambda w_{0,l+1}|e_l^1| - \lambda w_{1,l+1}|e_l^1| - \cdots - \lambda w_{l+1,l+1}|e_l^1| \\
& - \lambda w_{0,M-(l-1)}|e_l^1| - \lambda w_{1,M-(l-1)}|e_l^1| - \cdots - \lambda w_{M-(l-1),M-(l-1)}|e_l^1| \\
\le\ & |e_l^1| - \lambda w_{0,l+1}|e_{l+1}^1| - \lambda w_{1,l+1}|e_l^1| - \cdots - \lambda w_{l+1,l+1}|e_0^1| \\
& - \lambda w_{0,M-(l-1)}|e_{l-1}^1| - \lambda w_{1,M-(l-1)}|e_l^1| - \cdots - \lambda w_{M-(l-1),M-(l-1)}|e_M^1| \\
\le\ & |e_l^1 - \lambda w_{0,l+1}e_{l+1}^1 - \lambda w_{1,l+1}e_l^1 - \cdots - \lambda w_{l+1,l+1}e_0^1 \\
& - \lambda w_{0,M-(l-1)}e_{l-1}^1 - \lambda w_{1,M-(l-1)}e_l^1 - \cdots - \lambda w_{M-(l-1),M-(l-1)}e_M^1| \\
=\ & |e_l^0 + \Delta t\sigma_l^1 + \Delta t\tau_l^1| \\
\le\ & |e_l^0| + \Delta t R.
\end{aligned}$$

Further, for simplicity, we assume that $e_l^0 = 0$. Then we have

$$|e^1|_\infty \le \Delta t R.$$

Similarly, we can show that

$$|e^2|_\infty \le |e_l^1| + \Delta t R \le t_2 R,$$

and in general, with $0 \leq t_n \leq T$,

$$|e^n|_\infty \leq t_n R \leq C(\Delta t + \Delta x^{\min(2-\alpha,\beta)}).$$

The proof of Theorem 6.3.5 is now complete.

□

6.4 FDM based on quadratic interpolation

In this section, we will introduce a new finite difference method for solving (6.2.1)- (6.2.3). For simplicity, we assume $C_+(t,x) = C_-(t,x) = 1$ and $\varphi_1(t) = \varphi_2(t) = 0$.

The Riemann-Liouville fractional derivative ${}_0^R D_x^\alpha f(x)$ can be written as [26]

$${}_0^R D_x^\alpha f(x) = \frac{1}{\Gamma(-\alpha)} \oint_0^x (x-\xi)^{-1-\alpha} f(\xi)\, d\xi. \tag{6.4.1}$$

Here the integral $\oint$ denotes the Hadamard finite-part integral.

Let m be a fixed positive integer and $M = 2m$. Let $0 = x_0 < x_1 < x_2 < \cdots < x_{2j} < x_{2j+1} < \cdots < x_{2m} = 1$ be a partition of $[0,1]$ and Δx the stepsize.

At the nodes $x_{2j} = \frac{2j}{2m}, j = 1, 2, \ldots, m$, we have

$${}_0^R D_x^\alpha f(x_{2j}) = \frac{1}{\Gamma(-\alpha)} \oint_0^{x_{2j}} (x_{2j}-\xi)^{-1-\alpha} f(\xi)\, d\xi = \frac{x_{2j}^{-\alpha}}{\Gamma(-\alpha)} \oint_0^1 w^{-1-\alpha} f(x_{2j} - x_{2j} w)\, dw. \tag{6.4.2}$$

For every j, we replace $g(w) = f(x_{2j} - x_{2j}w)$ in the integral in (6.4.2) by piecewise quadratic interpolation polynomials with the equispaced nodes $0, \frac{1}{2j}, \frac{2}{2j}, \ldots, \frac{2j}{2j}$. We then have

$$\oint_0^1 w^{-1-\alpha} g(w)\, dw = \oint_0^1 w^{-1-\alpha} P_2(w)\, dw + R_{2j}(g), \tag{6.4.3}$$

where $P_2(w)$ is the piecewise quadratic interpolation polynomial of $g(w)$ defined on the equispaced nodes $0, \frac{1}{2j}, \frac{2}{2j}, \ldots, \frac{2j}{2j}$ and $R_{2j}(g)$ is the remainder term.

At the node $x_{2j+1} = \frac{2j+1}{2m}$, $j = 1, 2, \ldots, m-1$ we have

$$\begin{aligned}
{}_0^R D_x^\alpha f(x_{2j+1}) &= \frac{1}{\Gamma(-\alpha)} \oint_0^{x_{2j+1}} (x_{2j+1}-\xi)^{-1-\alpha} f(\xi)\, d\xi \\
&= \frac{1}{\Gamma(-\alpha)} \int_0^{x_1} (x_{2j+1}-\xi)^{-1-\alpha} f(\xi)\, d\xi \\
&\quad + \frac{x_{2j+1}^{-\alpha}}{\Gamma(-\alpha)} \oint_0^{\frac{2j}{2j+1}} w^{-1-\alpha} f(x_{2j+1} - x_{2j+1} w)\, dw.
\end{aligned} \tag{6.4.4}$$

For every j, $j = 1, 2, \dots, m-1$, we replace $g(w) = f(x_{2j+1} - x_{2j+1}w)$ by a piecewise quadratic interpolation polynomial with the equispaced nodes $0, \frac{1}{2j+1}, \frac{2}{2j+1}, \dots, \frac{2j}{2j+1}$ and obtain

$$\oint_0^{\frac{2j}{2j+1}} w^{-1-\alpha} g(w)\, dw = \oint_0^{\frac{2j}{2j+1}} w^{-1-\alpha} Q_2(w)\, dw + R_{2j+1}(g), \tag{6.4.5}$$

where $Q_2(w)$ is the piecewise quadratic interpolation polynomial of $g(w)$ defined on the nodes $0, \frac{1}{2j+1}, \frac{2}{2j+1}, \dots, \frac{2j}{2j+1}$ and $R_{2j+1}(g)$ is the remainder term.

We have,

Lemma 6.4.1. [93]. Let $1 < \alpha < 2$ and let $M = 2m$ where m is a fixed positive integer. Let $0 = x_0 < x_1 < x_2 < \cdots < x_{2j} < x_{2j+1} < \cdots < x_M = 1$ be a partition of $[0,1]$. Assume that $f(x)$ is a sufficiently smooth function. Then we have, with $j = 1, 2, \dots, m$,

$$\begin{aligned} {}_0^R D_x^\alpha f(x)\Big|_{x=x_{2j}} &= \frac{x_{2j}^{-\alpha}}{\Gamma(-\alpha)} \Big(\sum_{l=0}^{2j} \alpha_{l,2j} f(x_{2j-l}) + R_{2j}(f) \Big) \\ &= \Delta x^{-\alpha} \sum_{l=0}^{2j} w_{l,2j} f(x_{2j-l}) + \frac{x_{2j}^{-\alpha}}{\Gamma(-\alpha)} R_{2j}(f), \end{aligned} \tag{6.4.6}$$

and, with $j = 1, 2, \dots, m-1$,

$$\begin{aligned} {}_0^R D_x^\alpha f(x)\Big|_{x=x_{2j+1}} &= \frac{1}{\Gamma(-\alpha)} \int_0^{x_1} (x_{2j+1} - \xi)^{-1-\alpha} f(\xi)\, d\xi \\ &+ \frac{x_{2j+1}^{-\alpha}}{\Gamma(-\alpha)} \Big(\sum_{l=0}^{2j} \alpha_{l,2j+1} f(x_{2j+1-l}) + R_{2j+1}(f) \Big) \\ = \frac{1}{\Gamma(-\alpha)} \int_0^{x_1} (x_{2j+1} - \xi)^{-1-\alpha} f(\xi)\, d\xi &+ \Delta x^{-\alpha} \sum_{l=0}^{2j} w_{l,2j+1} f(x_{2j+1-l}) + \frac{x_{2j+1}^{-\alpha}}{\Gamma(-\alpha)} R_{2j+1}(f), \end{aligned} \tag{6.4.7}$$

where

$$
(-\alpha)(-\alpha+1)(-\alpha+2)(2j)^{-\alpha}\alpha_{l,2j}
$$

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

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

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

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

Further we have, with $l=0,1,2,\dots,2j$,

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

and

$$
\alpha_{l,2j+1}=\alpha_{l,2j}, \quad w_{l,2j+1}=w_{l,2j}.
$$

The remainder term $R_l(f)$ satisfies, for every $f\in C^3(0,1)$,

$$
|R_l(f)|\le C\Delta x^{3-\alpha}\|f'''\|_\infty,\ l=2,3,4,\dots,M,\ \text{with}\, M=2m.
$$

Proof. By the relationship between Riemann-Liouville and Hadamard finite-part integral, for fixed $2j$, let $0 < \frac{1}{2j} < \frac{2}{2j} < \cdots < \frac{2j}{2j} = 1$ be a partition of [0,1]. We then have

$$\oint_0^1 \omega^{-1-\alpha} g(\omega) d\omega = [\oint_0^{\frac{2}{2j}} + \int_{\frac{2}{2j}}^{\frac{4}{2j}} + \cdots + \int_{\frac{2j-2}{2j}}^{\frac{2j}{2j}}]\omega^{-1-\alpha} g(\omega) d\omega.$$

Here the integral denotes the Hadamard finite-part integral [3]. We approximate $g(\omega)$ on [0,1] by the quadratic interpolation polynomials $g_2(\omega)$, where

$$\begin{aligned} g_2(\omega) \quad = \quad & \frac{(\omega - \frac{2k-1}{2j})(\omega - \frac{2k}{2j})}{(\frac{2k-2}{2j} - \frac{2k-1}{2j})(\frac{2k-2}{2j} - \frac{2k}{2j})} g(\frac{2k-2}{2j}) \\ & + \frac{(\omega - \frac{2k-2}{2j})(\omega - \frac{2k}{2j})}{(\frac{2k-1}{2j} - \frac{2k-2}{2j})(\frac{2k-1}{2j} - \frac{2k}{2j})} g(\frac{2k-1}{2j}) \\ & + \frac{(\omega - \frac{2k-2}{2j})(\omega - \frac{2k-1}{2j})}{(\frac{2k}{2j} - \frac{2k-2}{2j})(\frac{2k}{2j} - \frac{2k-1}{2j})} g(\frac{2k}{2j}), \quad for \quad \omega \in [\frac{2k-2}{2j}, \frac{2k}{2j}], \quad k = 1, 2, \ldots, j. \end{aligned} \tag{6.4.8}$$

Let us now find the values of

$$\oint_0^1 \omega^{-1-\alpha} g_2(\omega) d\omega = [\oint_0^{\frac{2}{2j}} + \int_{\frac{2}{2j}}^{\frac{4}{2j}} + \cdots + \int_{\frac{2j-2}{2j}}^{\frac{2j}{2j}}]\omega^{-1-\alpha} g_2(\omega) d\omega,$$

where the integral $\oint_0^{\frac{2}{2j}} g_2(\omega)\omega^{-1-\alpha} d\omega$ is a Hadamard finite-part integral. By the definition of the Hadamard finite-part integral, we get

$$\begin{aligned} \oint_0^{\frac{2}{2j}} g_2(\omega)\omega^{-1-\alpha} d\omega \quad = \quad & \frac{g_2(0)(\frac{2}{2j})^{-\alpha}}{-\alpha} + \int_0^{\frac{2}{2j}} \omega^{-1-\alpha}[\int_0^{\omega} g_2'(y) dy] d\omega \\ = \quad & \frac{2^{-\alpha}}{(-\alpha)(2j)^{-\alpha}} g_2(0) + \int_0^{\frac{2}{2j}} \omega^{-1-\alpha}(g_2(\omega) - g_2(0)) d\omega \\ = \quad & \frac{2^{-\alpha}}{(-\alpha)(2j)^{-\alpha}} g(0) + \int_0^{\frac{2}{2j}} \omega^{-1-\alpha}\Big[\frac{(2j)^2}{2}(\omega^2 - (\frac{1}{2j} + \frac{2}{2j})\omega) g(0) \\ & + \frac{(2j)^2}{-1}(\omega^2 - (0 + \frac{2}{2j})\omega) g(\frac{1}{2j}) + \frac{(2j)^2}{2}(\omega^2 - (0 + \frac{1}{2j})\omega) g(\frac{2}{2j})\Big] d\omega \\ = \quad & \frac{2^{-\alpha}(\alpha+2)}{(-\alpha)(-\alpha+1)(-\alpha+2)(2j)^{-\alpha}} g(0) \\ & + \frac{2^{2-\alpha}}{(-\alpha+1)(-\alpha+2)(2j)^{-\alpha}} g(\frac{1}{2j}) \\ & + \frac{-2^{-\alpha}\alpha}{(-\alpha+1)(-\alpha+2)(2j)^{-\alpha}} g(\frac{2}{2j}) \end{aligned} \tag{6.4.9}$$

Similarly, we have

$$(-\alpha)(-\alpha+1)(-\alpha+2)(2j)^{-\alpha}\int_{\frac{2k}{2j}}^{\frac{2k-2}{2j}} g_2(\omega)\omega^{-1-\alpha}d\omega$$
$$=\frac{1}{2}F_0(k)g(\frac{2k-2}{2j})+(-1)F_1(k)g(\frac{2k-1}{2j})+\frac{1}{2}F_2(k)g(\frac{2k}{2j}),$$

where $F_i(k), i=0,1,2$ and $k=1,2,3,\dots,j$ are defined as above.

Together these estimates complete the proof of Lemma 6.4.1. $\square$

The weights $w_{l,2j}$ have some special properties which are summarized in the following Lemma 6.4.2 .

Lemma 6.4.2. Let $1<\alpha<2$. The coefficients $w_{l,2j}$ in (6.4.6) satisfy

$$w_{1,2j}<0, \tag{6.4.10}$$

$$w_{l,2j}>0, \quad l\neq 1,\ l=0,2,3,\dots,2j, \tag{6.4.11}$$

$$\Gamma(3-\alpha)\sum_{l=0}^{2j} w_{l,2j}<0. \tag{6.4.12}$$

Proof. It is easy to show that $w_{0,2j}>0$ and $w_{1,2j}<0$. We now prove that $w_{k,2j}>0$, $k=2,3,\dots,2j$. We first show that

$$w_{2l-1,2j}>0, \quad l=2,3,\dots,j.$$

Note that

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

Let $m=2l$. It is sufficient to show that, with $m=4,6,\dots$,

$$I(m)=(m-2)^{-\alpha+2}-m^{-\alpha+2}+(-\alpha+2)(m-2)^{-\alpha+1}+(-\alpha+2)m^{-\alpha+1}>0.$$

In fact, we have, by using binomial expansion,

$$\begin{aligned} I(m)=&m^{-\alpha+2}\Big(-1+(-\alpha+2)\frac{1}{m}+(1-\frac{2}{m})^{-\alpha+2}+(-\alpha+2)(1-\frac{2}{m})^{-\alpha+1}\frac{1}{m}\Big)\\ &=m^{-\alpha+2}\Big(\frac{(-\alpha+2)(-\alpha+1)(-\alpha)}{m^3}\Big(-\frac{2^3}{3!}+\frac{2^2}{2!}\Big)\\ &+\frac{(-\alpha+2)(-\alpha+1)(-\alpha)(-\alpha-1)}{m^4}\Big(\frac{2^4}{4!}-\frac{2^3}{3!}\Big)\\ &+\frac{(-\alpha+2)(-\alpha+1)(-\alpha)(-\alpha-1)}{m^5}\Big(\frac{-2^5}{5!}+\frac{2^4}{4!}\Big)+\dots\Big). \end{aligned}$$

Note that the sequence $a_n = \frac{2^n}{n!}$ is decreasing. Hence we see that, with $1 < \alpha < 2$,

$$I(m) > 0.$$

We next prove that

$$w_{2l,2j} > 0,\ l = 1, 2, \ldots, j-1.$$

Note that, with $l = 2, 3, \ldots, j-1$,

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

Let $m = 2l$. It is sufficient to show that, with $m = 4, 6, \ldots,$

$$\begin{aligned}I(m) &= -6(-\alpha+2)m^{-\alpha+1} + (-2)(m-2)^{-\alpha+2}\\ &\quad + (-1)(-\alpha+2)(m-2)^{-\alpha+1} + 2(m+2)^{-\alpha+2} + (-1)(-\alpha+2)(m+2)^{-\alpha+1} > 0.\end{aligned}$$

In fact, we have, by using binomial expansion,

$$\begin{aligned}I(m) =& m^{-\alpha+2}\Big(+ (-2)(1-\frac{2}{m})^{-\alpha+2} + (-1)(-\alpha+2)(1-\frac{2}{m})^{-\alpha+1}\frac{1}{m}\\ &+ 2(1+\frac{2}{m})^{-\alpha+2} + (-1)(-\alpha+2)(1+\frac{2}{m})^{-\alpha+1}\frac{1}{m}\Big)\\ =& m^{-\alpha+2}\Big(\frac{2(-\alpha+2)(-\alpha+1)(-\alpha)(-\alpha-1)(-\alpha-2)}{m^3}\Big(-\frac{2^3\cdot 2}{3!} + \frac{2^2}{2!}\Big)\\ &+ \frac{2(-\alpha+2)(-\alpha+1)(-\alpha)(-\alpha-1)(-\alpha-2)}{m^5}\Big(\frac{2^5\cdot 2}{5!} - \frac{2^4}{4!}\Big)\\ &+ \frac{2(-\alpha+2)(-\alpha+1)(-\alpha)(-\alpha-1)(-\alpha-2)}{m^7}\Big(\frac{2^7\cdot 2}{7!} - \frac{2^6}{6!}\Big) + \ldots\Big)\\ =& \frac{1}{m^{1+\alpha}}\Big(\frac{2(-\alpha+2)(-\alpha+1)(-\alpha)}{m^0}\Big(\frac{2^3\cdot 2}{3!} - \frac{2^2}{2!}\Big)\\ &+ \quad \frac{2(-\alpha+2)(-\alpha+1)(-\alpha)(-\alpha-1)(-\alpha-2)}{m^2}\Big(\frac{2^5\cdot 2}{5!} - \frac{2^4}{4!}\Big)\\ &+ \quad \frac{2(-\alpha+2)(-\alpha+1)(-\alpha)(-\alpha-1)(-\alpha-2)(-\alpha-3)(-\alpha-4)}{m^4}\\ &\Big(\frac{2^7\cdot 2}{7!} - \frac{2^6}{6!}\Big) + \ldots\Big).\end{aligned}$$

Note that

$$\frac{2^n\cdot 2}{n!} - \frac{2^{n-1}}{(n-1)!} = \frac{2^{n-1}}{(n-1)!}\Big(\frac{2\cdot 2}{n} - 1\Big) \le 0,\ n \ge 4.$$

Hence we get

$$
\begin{aligned}
I(m) \geq & \frac{2^{1+\alpha}}{m^{1+\alpha}} \frac{1}{2^{1+\alpha}} \Big[\frac{2(-\alpha+2)(-\alpha+1)(-\alpha)}{m^0} \Big(\frac{2^3 \cdot 2}{3!} - \frac{2^2}{2!} \Big) \\
& + \frac{2(-\alpha+2)(-\alpha+1)(-\alpha)(-\alpha-1)(-\alpha-2)}{2^2} \Big(\frac{2^5 \cdot 2}{5!} - \frac{2^4}{4!} \Big) \\
& + \frac{2(-\alpha+2)(-\alpha+1)(-\alpha)(-\alpha-1)(-\alpha-2)(-\alpha-3)(-\alpha-4)}{2^4} \Big(\frac{2^7 \cdot 2}{7!} - \frac{2^6}{6!} \Big) + \dots \Big] \\
= & \frac{2^{1+\alpha}}{m^{1+\alpha}} I(2), \quad m = 2, 3, 4, \dots .
\end{aligned}
$$

It is easy to show that, with $1 < \alpha < 2$,

$$
I(2) = 2^{-\alpha+2} \Big(3\alpha - 6 + 2^{-\alpha}(6+\alpha) \Big) > 0.
$$

Thus we get

$$
I(m) > 0, \quad m = 2, 3, 4, \dots .
$$

Similarly, we can show that $w_{2j,2j} > 0$.

Finally we shall prove $\Gamma(3-\alpha) \sum_{l=0}^{2j} w_{l,2j} < 0$. We have

$$
\Gamma(3-\alpha) \sum_{l=0}^{2j} w_{l,2j} = \frac{-3(-\alpha+2)}{2} (2j)^{-\alpha+1} - (2j)^{-\alpha+2} + \frac{\alpha-2}{2} (2j+2)^{-\alpha+1} + (2j+2)^{-\alpha+2}.
$$

Let $m = 2j+2$, it is sufficient to show that, with $m = 4, 6, 8, \dots$,

$$
I(m) = -3(-\alpha+2)(m-2)^{-\alpha+1} - 2(m-2)^{-\alpha+2} + (\alpha-2)m^{-\alpha+1} + 2 \cdot m^{-\alpha+2} < 0.
$$

In fact, by using binomial expansion, we have

$$
\begin{aligned}
I(m) = & m^{-\alpha+2} \Big((3\alpha-6)(1-\frac{2}{m})^{-\alpha+1} \frac{1}{m} - 2(1-\frac{2}{m})^{-\alpha+2} + (\alpha-2)\frac{1}{m} + 2 \Big) \\
= & \frac{(-\alpha+2)(-\alpha+1)}{m^2} \Big((-3)\frac{(-2)}{1!} + (-2)\frac{(-2)^2}{2!} \Big) \\
& + \frac{(-\alpha+2)(-\alpha+1)(-\alpha)}{m^3} \Big((-3)\frac{(-2)^2}{2!} + (-2)\frac{(-2)^3}{3!} \Big) \\
& + \frac{(-\alpha+2)(-\alpha+1)(-\alpha)(-\alpha-1)}{m^4} \Big((-3)\frac{(-2)^3}{3!} + (-2)\frac{(-2)^4}{4!} \Big) + \dots .
\end{aligned}
$$

Note that

$$
\begin{aligned}
& (-3)\frac{(-2)^n}{n!} + (-2)\frac{(-2)^(n+1)}{(n+1)!} = \frac{(-2)^n}{n!} \Big((-3) + (-2)\frac{-2}{n+1} \Big) \\
= & \frac{(-2)^n}{n!} \Big((-3) + \frac{4}{n+1} \Big) = \frac{-3n+1}{(n+1)!} (-2)^n,
\end{aligned}
$$

which implies that

$$I(m) < 0, m = 4, 6, 8, \ldots.$$

Together these estimates complete the proof of Lemma 6.4.2.

□

Similarly, we can consider the approximation of right-handed fractional derivative ${}_x^R D_1^\alpha f(x)$ at $x = x_l, l = 0, 1, 2, \ldots, 2m-2$. Using the same argument as for the approximation of ${}_0^R D_x^\alpha f(x)$ at $x = x_l$, we can show that, with $j = 0, 1, 2, \ldots, m-1$,

$$ {}_x^R D_1^\alpha f(x)\Big|_{x=x_{2j}} = \Delta x^{-\alpha} \sum_{l=0}^{M-2j} w_{l,M-2j} f(x_{2j+l}) + \frac{x_{2j}^{-\alpha}}{\Gamma(-\alpha)} R_{2j}(f), \tag{6.4.13}$$

and, with $j = 0, 1, 2, \ldots, m-2$,

$$\begin{aligned} {}_x^R D_1^\alpha f(x)\Big|_{x=x_{2j+1}} &= \frac{1}{\Gamma(-\alpha)} \int_{x_{M-1}}^{x_M} (\xi - x_{2j+1})^{-1-\alpha} f(\xi)\, d\xi \\ &+ \Delta x^{-\alpha} \sum_{l=0}^{M-(2j+1)-1} w_{l,M-(2j+1)} f(x_{2j+1+l}) + \frac{x_{2j+1}^{-\alpha}}{\Gamma(-\alpha)} R_{2j+1}(f). \end{aligned} \tag{6.4.14}$$

Let $U_{2j}^n \approx u(t_n, x_{2j})$ and $U_{2j+1}^n \approx u(t_n, x_{2j+1})$ denote the approximate solutions of $u(t_n, x_{2j})$ and $u(t_n, x_{2j+1})$, respectively. We define the following explicit numerical method for solving (6.2.1) - (6.2.3).

$$\begin{aligned} \Delta t^{-1}\big(U_{2j}^{n+1} - U_{2j}^n\big) &= \Delta x^{-\alpha}\Big(\sum_{k=0}^{2j} w_{k,2j} U_{2j-k}^n + \sum_{k=0}^{M-2j} w_{k,M-2j} u_{2j+k}^n\Big) \\ &+ f_{2j}^n, \ j = 1, 2, \ldots, m-1, \end{aligned} \tag{6.4.15}$$

$$\begin{aligned} \Delta t^{-1}\big(U_{2j+1}^{n+1} - U_{2j+1}^n\big) &= \Delta x^{-\alpha}\Big(\sum_{k=0}^{2j+1} w_{k,2j+1} U_{2j+1-k}^n + \sum_{k=0}^{M-2j-1} w_{k,M-2j-1} U_{2j+1+k}^n\Big) \\ &+ \bar{f}_{2j+1}^n + Q_{2j}^n, \ j = 0, 1, 2, \ldots, m-1, \end{aligned} \tag{6.4.16}$$

where Q_{2j}^n is defined as in (6.4.24) below.

Lemma 6.4.3. The standard explicit numerical method (6.4.15) - (6.4.16) is unconditionally unstable.

Proof. Let $n = 0$. We have, with $\lambda = \Delta t/\Delta x^{\alpha}$,

$$U_{2j}^{1} = \big(1 + w_{0,2j}\lambda + +w_{0,M-2j}\lambda\big)U_{2j}^{0} + \lambda\sum_{k=1}^{2j} w_{k,2j}U_{2j-k}^{0}$$
$$+ \lambda\sum_{k=1}^{M-2j} w_{k,M-2j}U_{2j+k}^{0} + \Delta t f_{2j}^{0} + \Delta t Q_{2j}^{0}, \tag{6.4.17}$$

$$U_{2j+1}^{1} = \big(1 + w_{0,2j+1}\lambda + w_{0,M-2j-1}\lambda\big)U_{2j+1}^{0} + \lambda\sum_{k=1}^{2j} w_{k,2j+1}U_{2j+1-k}^{0}$$
$$+ \lambda\sum_{k=1}^{M-2j-1} w_{k,M-2j-1}U_{2j+1+k}^{0} + \Delta t\bar{f}_{2j+1}^{0}, \tag{6.4.18}$$

where

$$\bar{f}_{2j+1}^{0} = f_{2j+1}^{0} + \frac{1}{\Gamma(-\alpha)}\int_{0}^{x_1}(x_{2j+1}-\xi)^{-1-\alpha}u(\xi, t_{n+1})\,d\xi.$$

Assume that we have some errors in the starting values U_l^0, i.e.,

$$\bar{U}_l^0 = U_l^0 + \epsilon_l^0, \quad l = 0, 1, 2, \dots, 2j, 2j+1, \dots, 2m.$$

To consider the stability, we assume that only the term $U_{2j_0}^0$, for some fixed j_0, has the error, and other terms have no errors. That is

$$\epsilon_l^0 = 0, \quad l \neq 2j_0.$$

Then we have

$$\bar{U}_{2j_0}^{1} = \big(1+w_{0,2j_0}\lambda+w_{0,M-2j_0}\lambda\big)\bar{U}_{2j_0}^{0}+\lambda\sum_{k=1}^{2j_0} w_{k,2j_0}\bar{U}_{2j_0-k}^{0}+\lambda\sum_{k=1}^{M-2j_0} w_{k,M-2j_0}\bar{U}_{2j_0-k}^{0}+\Delta t f_{2j_0}^{0}. \tag{6.4.19}$$

Subtracting (6.4.17) from (6.4.19), we obtain

$$\epsilon_{2j_0}^{1} = \big(1 + w_{0,2j_0}\lambda + w_{0,M-2j_0}\lambda\big)\epsilon_{2j_0}^{0}.$$

That is, the error is amplified by the factor $\mu_{2j_0} = 1 + w_{0,2j_0}\lambda + w_{0,M-2j_0}\lambda$ when the finite difference equation is advanced by one time step. After n time steps, one may write

$$\epsilon_{2j_0}^{n} = \big(1 + w_{0,2j_0}\lambda + w_{0,M-2j_0}\lambda\big)^{n}\epsilon_{2j_0}^{0}.$$

Note that $w_{0,2j_0} = 1/\Gamma(3-\alpha) > 0$, and $+w_{0,M-2j_0} = 1/\Gamma(3-\alpha) > 0$ we have $1 + w_{0,2j_0}\lambda + w_{0,M-2j_0}\lambda > 1$. Thus $|\epsilon_{2j_0}^{n}| \to \infty$ as $n \to \infty$, which implies that the method is unstable. □

Similarly, we can introduce the standard implicit numerical method and show that the standard implicit numerical method is also unconditionally unstable.

We now introduce the shifted Diethelm FDM for space-fractional PDEs. Let $0 = t_0 < t_1 < t_2 < \cdots < t_n < \ldots$ be the time partition and Δt the time stepsize. At the nodes $x_{2j} = \frac{2j}{2m}, j = 1, 2, \ldots, m-1$, we have, by (6.2.1),

$$u_t(t_{n+1}, x_{2j}) - \Big({}_0^R D_x^\alpha u(t_{n+1}, x_{2j+1}) + {}_x^R D_1^\alpha u(t_{n+1}, x_{2j-1}) \Big) = f_{2j}^{n+1} + \sigma_{2j}^{n+1}, \quad (6.4.20)$$

and at the nodes $x_{2j+1} = \frac{2j+1}{2m}, j = 1, 2, \ldots, m-1$,

$$u_t(t_{n+1}, x_{2j+1}) - \Big({}_0^R D_x^\alpha u(t_{n+1}, x_{2j+2}) + {}_x^R D_1^\alpha u(t_{n+1}, x_{2j}) \Big) = f_{2j+1}^{n+1} + \sigma_{2j+1}^{n+1}, \quad (6.4.21)$$

where

$$\begin{aligned}
\sigma_{2j}^{n+1} &= -\Big({}_0^R D_x^\alpha u(t_{n+1}, x_{2j+1}) - {}_0^R D_x^\alpha u(t_{n+1}, x_{2j}) \Big) \\
&\quad - \Big({}_x^R D_1^\alpha u(t_{n+1}, x_{2j-1}) - {}_x^R D_1^\alpha u(t_{n+1}, x_{2j}) \Big), \\
\sigma_{2j+1}^{n+1} &= -\Big({}_0^R D_x^\alpha u(t_{n+1}, x_{2j+2}) - {}_0^R D_x^\alpha u(t_{n+1}, x_{2j+1}) \Big) \\
&\quad - \Big({}_x^R D_1^\alpha u(t_{n+1}, x_{2j}) - {}_x^R D_1^\alpha u(t_{n+1}, x_{2j+1}) \Big).
\end{aligned}$$

Discretizing $u_t(t_{n+1}, x_l)$ by using the backward Euler method and discretizing ${}_0^R D_x^\alpha u(t_{n+1}, x_l)$ and ${}_x^R D_1^\alpha u(t_{n+1}, x_l)$ by using (6.4.6) - (6.4.7) and (6.4.13) - (6.4.14), respectively, we get, with $u_j^n = u(t_n, x_j)$, $f_j^n = f(t_n, x_j)$

$$\begin{aligned}
\Delta t^{-1}\big(u_{2j}^{n+1} - u_{2j}^n\big) &= \Delta x^{-\alpha} \Big(\sum_{k=0}^{2j} w_{k,2j+1} u_{2j+1-k}^{n+1} + \sum_{k=0}^{M-(2j-1)-1} w_{k,M-(2j-1)} u_{2j-1+k}^{n+1} \Big) \\
&\quad + f_{2j}^{n+1} + Q_{2j}^{n+1} + \sigma_{2j}^{n+1} + \tau_{2j}^{n+1}, \ j = 1, 2, \ldots, m-1, \qquad (6.4.22) \\
\Delta t^{-1}\big(u_{2j+1}^{n+1} - u_{2j+1}^n\big) &= \Delta x^{-\alpha} \Big(\sum_{k=0}^{2j+2} w_{k,2j+2} u_{2j+2-k}^{n+1} + \sum_{k=0}^{M-2j} w_{k,M-2j} u_{2j+k}^{n+1} \Big) \\
&\quad + f_{2j+1}^{n+1} + \sigma_{2j+1}^{n+1} + \tau_{2j+1}^{n+1}, \ j = 0, 1, 2, \ldots, m-1, \qquad (6.4.23)
\end{aligned}$$

where the truncation errors $\tau_l^{n+1} = O(\Delta t + \Delta x^{3-\alpha}), l = 1, 2, \ldots, \dot{M} - 1$ [25], [26] and

$$Q_{2j}^{n+1} = \frac{1}{\Gamma(-\alpha)} \int_0^{x_1} (x_{2j+1} - \xi)^{-1-\alpha} u(\xi, t_{n+1})\, d\xi + \frac{1}{\Gamma(-\alpha)} \int_{x_{M-1}}^{x_M} (\xi - x_{2j+1})^{-1-\alpha} u(\xi, t_{n+1})\, d\xi. \quad (6.4.24)$$

Let $U_{2j}^n \approx u(t_n, x_{2j})$ and $U_{2j+1}^n \approx u(t_n, x_{2j+1})$ denote the approximate solutions of $u(t_n, x_{2j})$ and $u(t_n, x_{2j+1})$, respectively. We define the following implicit shifted numerical method for solving (6.2.1) - (6.2.3).

$$\Delta t^{-1}\big(U_{2j}^{n+1} - U_{2j}^n\big) = \Delta x^{-\alpha}\Big(\sum_{k=0}^{2j} w_{k,2j+1} U_{2j+1-k}^{n+1} + \sum_{k=0}^{M-(2j-1)-1} w_{k,M-(2j-1)} u_{2j-1+k}^{n+1}\Big)$$
$$+ f_{2j}^{n+1} + Q_{2j}^{n+1},\ j = 1, 2, \ldots, m-1, \tag{6.4.25}$$
$$\Delta t^{-1}\big(U_{2j+1}^{n+1} - U_{2j+1}^n\big) = \Delta x^{-\alpha}\Big(\sum_{k=0}^{2j+2} w_{k,2j+2} U_{2j+2-k}^{n+1} + \sum_{k=0}^{M-2j} w_{k,M-2j} U_{2j+k}^{n+1}\Big)$$
$$+ f_{2j+1}^{n+1},\ j = 0, 1, 2, \ldots, m-1, \tag{6.4.26}$$

where Q_{2j}^{n+1} is defined below in (6.4.24).

Lemma 6.4.4. The shifted implicit method (6.4.25)- (6.4.26) is unconditionally stable.

Proof. For simplicity, we only consider the left-hand Riemman-Liouville fractional derivative for stability analysis. With $\lambda = \Delta t/\Delta x^\alpha$ we write (6.4.25)-(6.4.26) into one equation, with $l = 1, 2, \ldots, 2j, 2j+1, \ldots, 2m-1$,

$$-\lambda w_{0,l+1} U_{l+1}^{n+1} + (1 - \lambda w_{1,l+1}) U_l^{n+1} - \lambda \sum_{k=2}^{l+1} w_{k,l+1} U_{l+1-k}^{n+1} = U_l^n + k F_l^{n+1}, \tag{6.4.27}$$

with the boundary conditions $U_0^{n+1} = U_{2m}^{n+1} = 0$, where

$$F_l^{n+1} = \begin{cases} \bar{f}_l^{n+1}, & l = 2j,\ j = 1, 2, \ldots, m, \\ f_l^{n+1}, & l = 2j+1,\ j = 1, 2, \ldots, m-1, \end{cases}$$

and $\bar{f}_l^{n+1}$ is defined as follows:

$$\bar{f}_{2j}^{n+1} = \frac{1}{\Gamma(-\alpha)} \int_0^{x_1} (x_{2j+1} - \xi)^{-1-\alpha} u(\xi, t_{n+1})\, d\xi + f_{2j}^{n+1}.$$

Further we write (6.4.27) into the following linear system with $2m-1$ equations and $2m-1$ unknowns.

$$AU^{n+1} = U^n + kF^{n+1},$$

where

$$A = \begin{pmatrix} 1-\lambda w_{12} & -\lambda w_{02} & & \\ & & & \\ -\lambda w_{23} & 1-\lambda w_{13} & -\lambda w_{03} & \\ \vdots & \vdots & \ddots & \\ -\lambda w_{2m-1,2m} & -\lambda w_{2m-2,2m} & \dots & 1-\lambda w_{1,2m} \end{pmatrix},$$

and

$$U^{n+1} = \begin{pmatrix} U_1^{n+1} \\ U_2^{n+1} \\ \vdots \\ U_{2m-1}^{n+1} \end{pmatrix}, \quad U^n = \begin{pmatrix} U_1^n \\ U_2^n \\ \vdots \\ U_{2m-1}^n \end{pmatrix}, \quad F^{n+1} = \begin{pmatrix} F_1^{n+1} \\ F_2^{n+1} \\ \vdots \\ F_{2m-1}^{n+1} \end{pmatrix}.$$

Let μ be an eigenvalue of A. Let $\xi = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_{2m-1} \end{pmatrix} \neq 0$ be the corresponding eigenvector.

Then we have

$$A\xi = \mu\xi.$$

Denote

$$|x_i| = \max_j \{|x_j|,\ j = 1, 2, \dots, 2m-1\}.$$

We have, for fixed i,

$$\sum_{j=1}^{2m-1} a_{ij} x_j = \mu x_i,$$

i.e.,

$$\mu = a_{ii} + \sum_{j=1, j\neq i}^{2m-1} \frac{x_j}{x_i}.$$

Note that $a_{ii} = 1 - \lambda w_{1,i+1}$, $a_{i,i+1} = -\lambda w_{0,i+1}$, $a_{i,i-1} = -\lambda w_{2,i+1}, \dots, a_{i,1} = -\lambda w_{i,i+1}$. We have

$$\begin{aligned} \mu &= (1 - \lambda w_{1,i+1}) - \lambda w_{0,i+1} \frac{x_{i+1}}{x_i} - \lambda \sum_{j=1}^{i-1} w_{i-j+1,i+1} \frac{x_j}{x_i} \\ &= 1 - \lambda\Big(w_{0,i+1} \frac{x_{i+1}}{x_i} + w_{1,i+1} + w_{2,i+1} \frac{x_{i-1}}{x_i} + \dots + w_{i,i+1} \frac{x_1}{x_i} \Big). \end{aligned}$$

Note that $\frac{x_j}{x_i} < 1$, $j \neq i$ and $w_{k,i+1} > 0$, $k \neq 1$ and, by Lemma 6.3.1, $\sum_{k=0}^{i+1} w_{k,i+1} < 0$, we have

$$\begin{aligned} & w_{0,i+1}\frac{x_{i+1}}{x_i} + w_{1,i+1} + w_{2,i+1}\frac{x_{i-1}}{x_i} + \cdots + w_{i,i+1}\frac{x_1}{x_i} \\ & < w_{0,i+1} + w_{1,i+1} + w_{2,i+1} + \ldots w_{i,i+1} < 0. \end{aligned}$$

Hence

$$\mu = 1 - \lambda\Big(w_{0,i+1}\frac{x_{i+1}}{x_i} + w_{1,i+1} + w_{2,i+1}\frac{x_{i-1}}{x_i} + \cdots + w_{i,i+1}\frac{x_1}{x_i}\Big) > 1.$$

Since all the eigenvalues μ of matrix A satisfy $|\mu| \geq 1$, the matrix A is invertible and all eigenvalues of A^{-1} are less than 1, which implies that there exists a matrix norm $\| \cdot \|$ such that $\|A^{-1}\| \leq 1$ and

$$\begin{aligned} \|U^{n+1}\| &= \|A^{-1}(U^n + kF^{n+1})\| \leq \|U^n\| + k\|F^{n+1}\| \\ &\leq \cdots \leq \|U^0\| + k\sum_{j=1}^{n+1} \|F^j\| \leq \|U^0\| + t_{n+1} \max_{0 \leq t \leq T} \|f(t)\| \leq C, \end{aligned}$$

which means that the numerical method is stable.

We may also use the following lemma to prove the stability.

Lemma 6.4.5. The eigenvalues of the matrix A lie in the disks centered at a_{ii} with radius $r_i = \sum_{k \neq i} |a_{ik}|$.

By using Lemma 6.4.5, we shall prove all the eigenvalues of A are larger than or equal to 1. In fact, we have

$$r_i = \sum_{k=1, k \neq i}^{2m-1} |a_{ik}| = \lambda(w_{0,i+1} + w_{2,i+1} + w_{3,i+1} + \cdots + w_{i,i+1}).$$

We have, with $a_{ii} = 1 - \lambda w_{1,i+1}$,

$$a_{ii} - r_i = 1 - \lambda(w_{0,i+1} + w_{1,i+1} + w_{2,i+1} + \cdots + w_{i,i+1}).$$

By Lemma 3.4.2 we have $w_{0,i+1} + w_{1,i+1} + w_{2,i+1} + \cdots + w_{i,i+1} < 0$, which implies that $a_{ii} - r_i > 1$ and therefore all the eigenvalues μ of A satisfy

$$1 < a_{ii} - r_i < \mu < a_{ii} + r_i.$$

□

6.4.1 Initial integral approximation

To approximate the integral $\frac{1}{\Gamma(-\alpha)}\int_0^{x_1}(x_{2j+1}-\xi)^{-1-\alpha}u(t_{n+1},\xi)\,d\xi$ in (6.4.24), we denote $g(\xi)=u(t_{n+1},\xi)$ and approximate $g(\xi)$ on $[0,x_1]$ by the following quadratic interpolation polynomials, [9],

$$\begin{aligned}P_2(\xi) &= \frac{(\xi-x_{\frac{1}{2}})(\xi-x_1)}{(x_0-x_{\frac{1}{2}})(x_0-x_1)}u(t_{n+1},x_0)+\frac{(\xi-x_0)(\xi-x_1)}{(x_{\frac{1}{2}}-x_0)(x_{\frac{1}{2}}-x_1)}u(t_{n+1},x_{\frac{1}{2}})\\ &\quad+\frac{(\xi-x_0)(\xi-x_{\frac{1}{2}})}{(x_1-x_0)(x_1-x_{\frac{1}{2}})}u(t_{n+1},x_1),\quad \text{for } \xi\in[x_0,x_1],\end{aligned}$$

where

$$u(t_{n+1},\xi)-P_2(\xi)=R_1^{(1)}(\xi)=\frac{u'''(t_{n+1},c_1)}{3!}(\xi-x_0)(\xi-x_{\frac{1}{2}})(\xi-x_1),\ c_1\in(0,x_1).$$

Further we approximate the value $u(t_{n+1},x_{\frac{1}{2}})$ by

$$u(t_{n+1},x_{\frac{1}{2}})\approx\frac{3}{8}u(t_{n+1},x_0)+\frac{3}{4}u(t_{n+1},x_1)-\frac{1}{8}u(t_{n+1},x_2),$$

where

$$u(t_{n+1},x_{\frac{1}{2}})-\Big(\frac{3}{8}u(t_{n+1},x_0)+\frac{3}{4}u(t_{n+1},x_1)-\frac{1}{8}u(t_{n+1},x_2)\Big)=R_1^{(2)}(\xi),$$

and $R_1^{(2)}(\xi)=\frac{1}{16}u'''(t_{n+1},c_2)h^3,\ c_2\in(0,x_2)$.

We then have

$$\frac{1}{\Gamma(-\alpha)}\int_0^{x_1}(x_{2j+1}-\xi)^{-1-\alpha}u(t_{n+1},\xi)\,d\xi=\sum_{i=0}^{2}\hat{B}_i u(t_{n+1},x_i)+R_1,$$

where

$$\begin{aligned}\hat{B}_0 &= \int_0^{x_1}(x_1-\xi)^{\alpha-1}\frac{(\xi-x_{\frac{1}{2}})(\xi-x_1)}{(x_0-x_{\frac{1}{2}})(x_0-x_1)}\,d\xi+\frac{3}{8}\int_0^{x_1}(x_1-\xi)^{\alpha-1}\frac{(\xi-x_0)(\xi-x_1)}{(x_{\frac{1}{2}}-x_0)(x_{\frac{1}{2}}-x_1)}\,d\xi,\\ \hat{B}_1 &= \frac{3}{4}\int_0^{x_1}(x_1-\xi)^{\alpha-1}\frac{(\xi-x_0)(\xi-x_1)}{(x_{\frac{1}{2}}-x_0)(x_{\frac{1}{2}}-x_1)}\,d\xi+\int_0^{x_1}(x_1-\xi)^{\alpha-1}\frac{(\xi-x_0)(\xi-x_1)}{(x_1-x_0)(x_1-x_{\frac{1}{2}})}\,d\xi,\\ \hat{B}_2 &= -\frac{1}{8}\int_0^{x_1}(x_1-\xi)^{\alpha-1}\frac{(\xi-x_0)(\xi-x_1)}{(x_{\frac{1}{2}}-x_0)(x_{\frac{1}{2}}-x_1)}\,d\xi,\end{aligned}$$

and

$$R_1=\int_0^{x_1}(x_{2j+1}-\xi)^{-1-\alpha}R_1^{(1)}(\xi)\,d\xi+\int_0^{x_1}(x_{2j+1}-\xi)^{-1-\alpha}R_1^{(2)}(\xi)\,d\xi.$$

It is easy to show that

$$
\begin{aligned}
|R_1| &\leq \int_0^{x_1} (x_{2j+1}-\xi)^{-1-\alpha} |R_1^{(1)}(\xi)|\, d\xi + \int_0^{x_1} (x_{2j+1}-\xi)^{-1-\alpha} |R_1^{(2)}(\xi)|\, d\xi \\
&\leq \int_0^{x_1} (x_{2j+1}-\xi)^{-1-\alpha} C\Delta x^3 \, d\xi \leq C\Delta x^3 \Delta x^{-\alpha} = C\Delta x^{3-\alpha}.
\end{aligned}
$$

Hence, we have

$$
\int_0^{x_1} (x_{2j+1}-\xi)^{-1-\alpha} u(t_{n+1},\xi)\, d\xi - \sum_{i=0}^{2} \hat{B}_i u_i^{n+1} = O(\Delta x^{3-\alpha}).
$$

Similarly, we have, for some suitable weights $\tilde{B}_i, i = 0, 1, 2,$

$$
\int_{x_{M-1}}^{x_M} (\xi - x_{2j+1})^{-1-\alpha} u(t_{n+1},\xi)\, d\xi - \sum_{i=M-2}^{M} \tilde{B}_i U_i^{n+1} = O(\Delta x^{3-\alpha}).
$$

Based on the analysis above, we approximate Q_{2j}^{n+1} in (6.4.25) by

$$
S_{2j}^{n+1} = \frac{1}{\Gamma(-\alpha)} \sum_{i=0}^{2} \hat{B}_i U_i^{n+1} + \frac{1}{\Gamma(-\alpha)} \sum_{i=M-2}^{M} \tilde{B}_i U_i^{n+1}. \tag{6.4.28}
$$

It is easy to say that

$$
Q_{2j}^{n+1} - \frac{1}{\Gamma(-\alpha)} \Big(\sum_{i=0}^{2} \hat{B}_i u_i^{n+1} + \sum_{i=M-2}^{M} \tilde{B}_i u_i^{n+1} \Big) = O(\Delta x^{3-\alpha}).
$$

6.4.2 Error estimates of the shifted Diethelm FDMs

Theorem 6.4.6. Let $1 < \alpha < 2$ and let $u(t_{n+1}, x_l)$ and $U_l^{n+1}, l = 1, 2, \dots, M-1$ be the solutions of (6.4.22)- (6.4.23) and (6.4.25)-(6.4.26), respectively. Assume that $u(t,x)$ satisfies the Lipschitz conditions, with some $\beta > 0$,

$$
\Big| {}_0^R D_x^\alpha u(t,x) - {}_0^R D_x^\alpha u(t,y) \Big| \leq C_\alpha |x-y|^\beta, \tag{6.4.29}
$$

$$
\Big| {}_x^R D_1^\alpha u(t,x) - {}_x^R D_1^\alpha u(t,y) \Big| \leq C_\alpha |x-y|^\beta. \tag{6.4.30}
$$

We have

$$
\max_{1 \leq l \leq M-1} |u(t_{n+1}, x_l) - U_l^{n+1}| \leq C(\Delta t + \Delta x^{\min(\beta, 3-\alpha)}).
$$

Proof of Theorem 6.4.6. Let $e_l^{n+1} = u(t_{n+1}, x_l) - U_l^{n+1}, l = 1, 2, \dots, M-1$. Subtracting (6.4.22) - (6.4.23) from (6.4.25)-(6.4.26), We obtain the following error equation, for $l = 2j, j = 1, 2 \dots, m-1$, with $R = (\Delta t + \Delta x^{\min(3-\alpha,\beta)})$,

$$\Delta t^{-1}\Big(e_{2j}^{n+1} - e_{2j}^{n}\Big) - \Delta x^{-\alpha}\Big(\sum_{k=0}^{2j} w_{k,2j+1} e_{2j+1-k}^{n+1} + \sum_{k=0}^{M-(2j-1)-1} w_{k,M-(2j-1)} e_{2j-1+k}^{n+1}\Big) + R,$$

and, for $l = 2j+1, j = 0, 1, 2 \dots, m-1$,

$$\Delta t^{-1}\Big(e_{2j+1}^{n+1} - e_{2j+1}^{n}\Big) - \Delta x^{-\alpha}\Big(\sum_{k=0}^{2j+2} w_{k,M-(2j+2)} e_{2j+2+k}^{n+1} + \sum_{k=0}^{M-2j} w_{k,M-2j} e_{2j+k}^{n+1}\Big) + R.$$

With $\lambda = \Delta t / \Delta x^{\alpha}$, we have, for $l = 2j, j = 1, 2 \dots, m-1$,

$$\begin{aligned}
&(1 - \lambda w_{1,2j+1} - \lambda w_{1,M-(2j-1)}) e_{2j}^{n+1} \\
&- \lambda\Big(w_{0,2j+1} e_{2j+1}^{n+1} + w_{2,2j+1} e_{2j-1}^{n+1} + \cdots + w_{2j,2j+1} e_{1}^{n+1}\Big) \\
&- \lambda\Big(w_{0,M-(2j-1)} e_{2j-1}^{n+1} + w_{2,M-(2j-1)} e_{2j+1}^{n+1} + \cdots + w_{M-(2j-1)-1,M-(2j-1)} e_{M-1}^{n+1}\Big) \\
= {}& e_{2j}^{n} + \Delta t R,
\end{aligned}$$

and, for $l = 2j+1, j = 0, 1, 2 \dots, m-1$,

$$\begin{aligned}
&(1 - \lambda w_{1,2j+2} - \lambda w_{1,M-2j}) e_{2j+1}^{n+1} \\
&- \lambda\Big(w_{0,2j+2} e_{2j+2}^{n+1} + w_{2,2j+2} e_{2j}^{n+1} + \cdots + w_{2j+2,2j+2} e_{0}^{n+1}\Big) \\
&- \lambda\Big(w_{0,M-2j} e_{2j}^{n+1} + w_{2,M-2j} e_{2j+2}^{n+1} + \cdots + w_{M-2j,M-2j} e_{M}^{n+1}\Big) \\
= {}& e_{2j+1}^{n} + \Delta t R.
\end{aligned}$$

Assume that $|e^1|_\infty = \sup_l |e_l^1| = |e_{2k}|$ for some k, we get, by Lemma 6.4.2, with $R = (\Delta t + \Delta x^{\min(3-\alpha,\beta)})$,

$$\begin{aligned}
|e^1|_\infty = \sup_l |e_l^1| = |e_{2k}^1| \le |e_{2k}^1|\Big(&1 - \lambda(w_{0,2k+1} + w_{1,2k+1} + \dots w_{2k,2k+1}) \\
&- \lambda(w_{0,M-(2k-1)} + w_{1,M-(2k-1)} + \cdots + w_{M-(2k-1)-1,M-(2k-1)})\Big) \\
\le {}& |e_{2k}^1| - \lambda w_{0,2k+1}|e_{2k+1}^1| - \lambda w_{1,2k+1}|e_{2k}^1| - \cdots - \lambda w_{2k,2k+1}|e_1^1| \\
- {}& \lambda w_{0,M-(2k-1)}|e_{2k-1}^1| - \lambda w_{1,M-(2k-1)}|e_{2k}^1| - \cdots - \lambda w_{M-(2k-1)-1,M-(2k-1)})|e_{M-1}^1| \\
\le {}& |e_{2k}^1| - \lambda w_{0,2k+1}|e_{2k+1}^1| - \lambda w_{1,2k+1}|e_{2k}^1| - \cdots - \lambda w_{2k,2k+1}|e_1^1| \\
&- \lambda w_{0,M-(2k-1)}|e_{2k-1}^1| - \lambda w_{1,M-(2k-1)}|e_{2k}^1| - \cdots - \lambda w_{M-(2k-1)-1,M-(2k-1)}|e_{M-1}^1| \\
\le {}& |e_{2k}^0| + \Delta t R.
\end{aligned}$$

Assume that $|e^1|_\infty = \sup_l |e_l^1| = |e_{2k+1}|$ for some k, we get, by Lemma 6.4.2, with $R = (\Delta t + \Delta x^{\min(3-\alpha,\beta)})$,

$$
\begin{aligned}
|e^1|_\infty = \sup_l |e_l^1| = |e_{2k+1}^1| \leq |e_{2k+1}^1| \Big(& 1 - \lambda(w_{0,2k+2} + w_{1,2k+2} + \dots w_{2k+2,2k+2}) \\
& - \lambda(w_{0,M-2k} + w_{1,M-2k} + \cdots + w_{M-2k,M-2k}) \Big) \\
= & |e_{2k+1}^1| - \lambda w_{0,2k+2}|e_{2k+2}^1| - \lambda w_{1,2k+2}|e_{2k+1}^1| - \cdots - \lambda w_{2k+2,2k+2}|e_0^1| \\
& - \lambda w_{0,M-2k}|e_{2k}^1| - \lambda w_{1,M-2k}|e_{2k+1}^1| + \cdots - \lambda w_{M-2k,M-2k})|e_M^1| \\
\leq & |e_{2k+1}^1| - \lambda w_{0,2k+2}|e_{2k+1}^1| - \lambda w_{1,2k+2}|e_{2k+1}^1| - \cdots - \lambda w_{2k+2,2k+2}|e_0^1| \\
& - \lambda w_{0,M-2k}|e_{2k}^1| - \lambda w_{1,M-2k}|e_{2k+1}^1| - \cdots - \lambda w_{M-2k,M-2k}|e_M^1| \\
\leq & |e_{2k+1}^0| + \Delta t R.
\end{aligned}
$$

Hence we obtain

$$\sup_l |e_l^1| \leq \sup_l |e_l^0| + \Delta t R.$$

Further, for simplicity, we assume that $e_l^0 = 0$. Then we have

$$|e^1|_\infty \leq \Delta t R.$$

Similarly, we can show that

$$|e^2|_\infty \leq |e^1|_\infty + \Delta t R \leq t_2 R,$$

and in general, with $0 \leq t_n \leq T$,

$$|e^n|_\infty \leq t_n R \leq C(\Delta t + \Delta x^{\min(3-\alpha,\beta)}).$$

The proof of Theorem 6.4.6 is now complete.

□

6.5 Numerical simulations

In this section, we will give some numerical examples. Let us consider the following space-fractional partial differential equation with nonhomogeneous Dirichlet boundary conditions, with $1 < \alpha < 2$,

$$\frac{\partial u(t,x)}{\partial t} - {}_0^R D_x^\alpha u(t,x) = f(t,x), \quad 0 < x < 1, \ t > 0, \tag{6.5.1}$$

$$u(t,0) = \varphi_1(t), \quad u(t,1) = \varphi_2(t), \tag{6.5.2}$$

$$u(0,x) = u_0(x), \tag{6.5.3}$$

where $\varphi_1(t), \varphi_2(t)$ are some suitable functions of t and $u_0(x)$ is the initial condition.

Let us recall the numerical method introduced in the previous section. Let m be a positive integer and let $0 = x_0 < x_1 < x_2 < \cdots < x_{2m} = 1$ be a space partition of $[0,1]$ and Δx the space stepsize. Let $0 = t_0 < t_1 < t_2 < \cdots < x_N = 1$ be a time partition of $[0,1]$ and Δt the time stepsize.

At $x = x_l, t = t_n$, we have, with $l = 1, 2, \ldots, 2m-1$, and $n = 1, 2, \ldots, N$,

$$\frac{\partial u(t,x)}{\partial t}\Big|_{x=x_l,t=t_n} - {}_0^R D_x^\alpha u(t,x)\Big|_{x=x_l,t=t_n} = f(t,x)\Big|_{x=x_l,t=t_n}, \tag{6.5.4}$$

$$u(t_n,0) = \varphi_1(t_n), \quad u(t_n,1) = \varphi_2(t_n), \tag{6.5.5}$$

$$u(0,x_l) = u_0(x_l), \tag{6.5.6}$$

To get a stable finite difference scheme for this time-dependent problem, we need to consider the following shifted equation, that is,

$$\frac{\partial u(t,x)}{\partial t}\Big|_{x=x_l,t=t_n} - {}_0^R D_x^\alpha u(t,x)\Big|_{x=x_{l+1},t=t_n} = f(t,x)\Big|_{x=x_l,t=t_n} + \rho_l(t_n), \tag{6.5.7}$$

$$u(t_n,0) = \varphi_1(t_n), \quad u(t_n,1) = \varphi_2(t_n), \tag{6.5.8}$$

$$u(0,x_l) = u_0(x_l), \tag{6.5.9}$$

where

$$\rho_l(t_n) = -\Big({}_0^R D_x^\alpha u(t,x)\Big|_{x=x_{l+1},t=t_n} - {}_0^R D_x^\alpha u(t,x)\Big|_{x=x_l,t=t_n} \Big).$$

Note that,

$$\frac{\partial u(t,x)}{\partial t}\Big|_{x=x_l,t=t_n} = \frac{u(t_n,x_l) - u(t_{n-1},x_l)}{\Delta t} + O(\Delta t),$$

and, with $l = 2j, j = 1, 2, \dots, m-1$,

$$
\begin{aligned}
{}_0^R D_x^{\alpha} u(t,x)\Big|_{x=x_{l+1}, t=t_n} &= \frac{1}{\Gamma(-\alpha)} \oint_{x_0}^{x_{2j+1}} (x_{2j+1}-\xi)^{-1-\alpha} u(t_n,\xi)\, d\xi \\
&= \frac{1}{\Gamma(-\alpha)} \int_0^{x_1} (x_{2j+1}-\xi)^{-1-\alpha} u(t_n,\xi)\, d\xi \\
&+ \Delta x^{-\alpha} \sum_{k=0}^{2j} w_{k,2j+1} u(t_n, x_{2j+1-k}) + O(\Delta x^{3-\alpha}),
\end{aligned}
$$

and, with $l = 2j+1, j = 0, 1, 2, \dots, m-1$,

$$
\begin{aligned}
{}_0^R D_x^{\alpha} u(t,x)\Big|_{x=x_{l+1}, t=t_n} &= \frac{1}{\Gamma(-\alpha)} \int_0^{x_{2j+2}} (x_{2j+2}-\xi)^{-1-\alpha} u(t_n,\xi)\, d\xi \\
&= \Delta x^{-\alpha} \sum_{k=0}^{2j+2} w_{k,2j+2} u(t_n, x_{2j+2-k}) + O(\Delta x^{3-\alpha}),
\end{aligned}
$$

where $w_{k,2j+1}, w_{k,2j+2}$ are defined as in (6.4.6) and (6.4.7).

Denote $U_j^n \approx u(t_n, x_j)$. We define the following backward Euler method for solving (6.5.1)-(6.5.3),

$$
\begin{aligned}
&\frac{U_{2j}^n - U_{2j}^{n-1}}{\Delta t} - \Delta x^{-\alpha} \sum_{k=0}^{2j} w_{k,2j+1} U_{2j+1-k}^n = f(x_{2j}, t_n) + \rho_{2j}^n \\
&\qquad + \frac{1}{\Gamma(-\alpha)} \int_0^{x_1} (x_{2j+1}-\xi)^{-1-\alpha} u(\xi, t_n)\, d\xi, \ j = 1, 2, \dots, m-1, \\
&\frac{U_{2j+1}^n - U_{2j+1}^{n-1}}{\Delta t} - \Delta x^{-\alpha} \sum_{k=0}^{2j+2} w_{k,2j+2} U_{2j+2-k}^n = f(x_{2j+1}, t_n) + \rho_{2j+1}^n \\
&\qquad + \frac{1}{\Gamma(-\alpha)} \int_0^{x_1} (x_{2j+1}-\xi)^{-1-\alpha} u(\xi, t_n)\, d\xi, \ j = 0, 1, 2, \dots, m-1,
\end{aligned}
$$

or, with $\lambda = \frac{\Delta t}{\Delta x^{\alpha}}$,

$$
\begin{aligned}
U_{2j}^n - \lambda \sum_{k=0}^{2j} w_{k,2j+1} U_{2j+1-k}^n &= U_{2j}^{n-1} + \Delta t f(x_{2j}, t_n) + \Delta t \rho_{2j}^n \\
&+ \Delta t \frac{1}{\Gamma(-\alpha)} \int_0^{x_1} (x_{2j+1}-\xi)^{-1-\alpha} u(\xi, t_n)\, d\xi, \quad j = 1, 2, \dots, m-1,
\end{aligned} \tag{6.5.10}
$$

$$
U_{2j+1}^n - \lambda \sum_{k=0}^{2j+2} w_{k,2j+2} U_{2j+2-k}^n = U_{2j+1}^{n-1} + \Delta t f(x_{2j+1}, t_n) + \Delta t \rho_{2j+1}^n, \quad j = 0, 1, 2, \dots, M-1. \tag{6.5.11}
$$

The numerical methods (6.5.10) - (6.5.11) can be written into the following matrix form

$$AU^n = U^{n-1} + \Delta t F^n + \Delta t \rho^n + \Delta t I^n + B_l^n + B_r^n,$$

where

$$U^n = \begin{bmatrix} U_1^n \\ U_2^n \\ U_3^n \\ \vdots \\ U_{2m-1}^n \end{bmatrix}, \quad F^n = \begin{bmatrix} f(x_1, t_n) \\ f(x_2, t_n) \\ f(x_3, t_n) \\ \vdots \\ f(x_{2m-1}, t_n) \end{bmatrix}, \quad \rho^n = \begin{bmatrix} -\Big({}_0^R D_x^\alpha u(x_2, t_n) - {}_0^R D_x^\alpha u(x_1, t_n) \Big) \\ -\Big({}_0^R D_x^\alpha u(x_3, t_n) - {}_0^R D_x^\alpha u(x_2, t_n) \Big) \\ -\Big({}_0^R D_x^\alpha u(x_4, t_n) - {}_0^R D_x^\alpha u(x_3, t_n) \Big) \\ \vdots \\ -\Big({}_0^R D_x^\alpha u(x_{2m}, t_n) - {}_0^R D_x^\alpha u(x_{2m-1}, t_n) \Big) \end{bmatrix},$$

and

$$I^n = \begin{bmatrix} 0 \\ \frac{1}{\Gamma(-\alpha)} \int_0^{x_1} (x_3 - \xi)^{-1-\alpha} u(t_n, \xi) \, d\xi \\ 0 \\ \vdots \\ \frac{1}{\Gamma(-\alpha)} \int_0^{x_1} (x_{2m-1} - \xi)^{-1-\alpha} u(t_n, \xi) \, d\xi \\ 0 \end{bmatrix},$$

$$B_l^n = \begin{bmatrix} \lambda w_{2,2} u(t_n, x_0) \\ 0 \\ \lambda w_{4,4} u(t_n, x_0) \\ 0 \\ \vdots \\ 0 \\ \lambda w_{2m,2m} u(t_n, x_0) \end{bmatrix}, \ B_r^n = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ \lambda w_{0,2m} u(t_n, x_{2m}) \end{bmatrix},$$

and

$$A = \begin{bmatrix} 1 - \lambda w_{1,2} & -\lambda w_{0,2} & 0 & 0 & \dots & 0 \\ -\lambda w_{2,3} & 1 - \lambda w_{1,3} & -\lambda w_{0,3} & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ -\lambda w_{2m-2,2m-1} & -\lambda w_{2m-3,2m-1} & \dots & \dots & 1 - \lambda w_{1,2m-1} & -\lambda w_{0,2m-1} \\ -\lambda w_{2m-1,2m} & -\lambda w_{2m-2,2m} & \dots & \dots & -\lambda w_{2,2m} & 1 - \lambda w_{1,2m} \end{bmatrix}.$$

Here B_l^n and B_r^n are determined by the Dirichlet boundary conditions $u(t_n, x_0)$ and $u(t_n, x_{2m})$. We then use MATLAB to obtain all the approximate solutions $U^n, n = 1, 2, \ldots, N$.

Example 14. *Consider [12]*

$$u_t(t,x) = {}_0^R D_x^\alpha u(t,x) + f(t,x), \quad 0 < x < 2,\ t > 0 \tag{6.5.12}$$

$$u(t,0) = 0, \quad u(t,2) = 0, \tag{6.5.13}$$

$$u(0,x) = 4x^2(2-x)^2, \quad 0 < x < 1, \tag{6.5.14}$$

where

$$\begin{aligned} f(t,x) = -4e^{-t}x^2(2-x)^2 - 4e^{-t}\Big(4\frac{\Gamma(2+1)}{\Gamma(2-\alpha+1)}x^{2-\alpha} \\ - 4\frac{\Gamma(3+1)}{\Gamma(3-\alpha+1)}x^{3-\alpha} + \frac{\Gamma(4+1)}{\Gamma(4-\alpha+1)}x^{4-\alpha}\Big), \end{aligned}$$

The exact solution is $u(t,x) = 4e^{-t}x^2(2-x)^2$.

By Theorem 6.4.6, we have

$$|e^N|_\infty = |U^N - u(t_N)|_\infty \leq C(\Delta t + \Delta x^\gamma), \text{ with } \gamma = \min(3-\alpha, \beta),$$

where $|e^N|_\infty$ denotes the L^∞-norm of the error at time $t_N = 1$. In our numerical example, we know the exact solution u, so we can exactly calculate ρ^n. In general, we may need to approximate ρ^n by using the computed solutions U^n with some higher order numerical methods.

To observe the convergence order with respect to Δx, we choose $\Delta t = 2^{-10}$ sufficiently small and the different space stepsizes $h_l = \Delta x = 2^{-l}$, $l = 3, 4, 5, 6, 7$. Hence the error will be dominated by Δx^γ. Now let $|e_l^N|_\infty = |U^N - u(t_N)|_\infty$ denote the L^∞-norm at $t_N = 1$ obtained by using the space stepsize h_l. For the fixed space stepsize $h_l = 2^{-l}$, $l = 3, 4, 5, 6, 7$, we have

$$|e_l^N|_\infty \approx C h_l^\gamma, \tag{6.5.15}$$

which implies that

$$\frac{|e_l^N|_\infty}{|e_{l+1}^N|_\infty} \approx \frac{h_l^\gamma}{h_{l+1}^\gamma} = 2^\gamma.$$

Hence the convergence order satisfies

$$\gamma \approx \log_2\Big(\frac{|e_l^N|_\infty}{|e_{l+1}^N|_\infty}\Big). \tag{6.5.16}$$

In Table 6.5.1, we obtain the experimentally determined orders of convergence (EOC) for the different $\alpha = 1.2, 1.4, 1.6, 1.8$. We see that the convergence order is almost $3-\alpha$ which is consistent with our theoretical convergence order $\gamma = \min(3-\alpha, \beta)$. The order $3-\alpha$ term dominates the convergence order in this example. Here and below we will call our numerical method “the Shifted Diethelm method ”.

In Figures 6.5.1- 6.5.2, we plot the convergence orders with $\alpha = 1.20$ and $\alpha = 1.80$, respectively. The convergence order is $O(\Delta x^{3-\alpha})$ as produced in the Table 6.5.1.

Δt	Δx	$\alpha = 1.2$	$\alpha = 1.4$	$\alpha = 1.6$	$\alpha = 1.8$
2^{-10}	2^{-3}				
2^{-10}	2^{-4}	1.5009	1.5203	1.4714	1.5419
2^{-10}	2^{-5}	1.5813	1.4978	1.3432	1.3221
2^{-10}	2^{-6}	1.7058	1.5597	1.3262	1.2168
2^{-10}	2^{-7}	1.8136	1.6285	1.3504	1.1905

Table 6.5.1: The experimentally determined orders of convergence (EOC) at $t = 1$ in Example 14 by using the shifted Diethelm method

In [66], the shifted Grünwald difference operator

$$A_{h,p}^{\alpha} u(x) = \Delta x^{-\alpha} \sum_{k=0}^{\infty} g_k^{(\alpha)} u(x-(k-p)\Delta x)$$

approximates the Riemann-Liouville fractional derivative uniformly with first order accuracy, i.e.,

$$A_{h,p}^{\alpha} u(x) = {}_{-\infty}^{\ R}D_x^{\alpha} u(x) + O(\Delta x),$$

where p is a positive integer and $g_k^{(\alpha)} = (-1)^k \binom{\alpha}{k}$. Considering a well defined function $u(x)$ on a bounded interval $[a,b]$ if $u(a) = 0$ or $u(b) = 0$, the function $u(x)$ can be zero extended for $x < a$ or $x > b$. And then the α order left and right Riemann-Liouville fractional derivatives of $u(x)$ at each point x can be approximated by the shifted

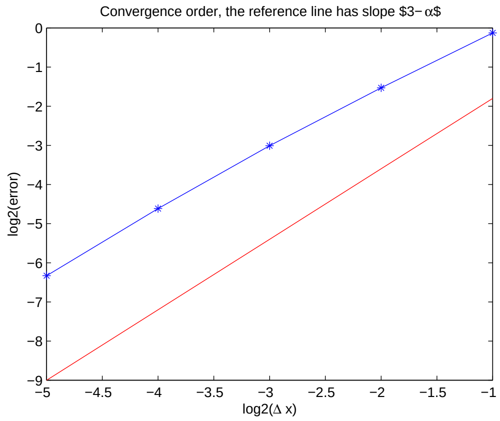

Figure 6.5.1: The experimentally determined orders of convergence ("EOC ") at $t = 1$ in Example 14 with $\alpha = 1.20$

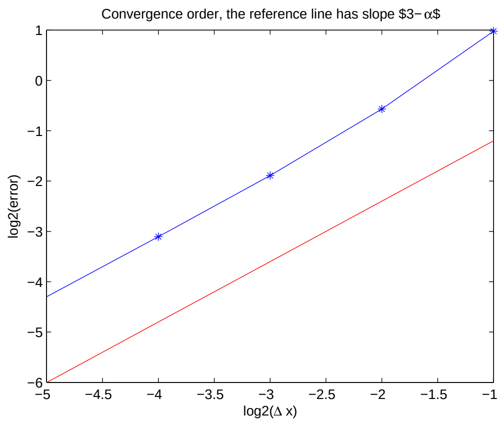

Figure 6.5.2: The experimentally determined orders of convergence ("EOC ") at $t = 1$ in Example 14 with $\alpha = 1.80$

Grünwald difference operator $A^{\alpha}_{h,p}u(x)$. In [90], the authors introduced a weighted and shifted Grünwald difference operator which has second order accuracy to approximate the Riemann-Liouville fractional derivative. However the approximation of the left or right Riemann-Liouville fractional derivatives in [66, 90] by using the shifted Grünwald difference operator on finite interval $[a, b]$ requires that $u(a) = 0$ or $u(b) = 0$ respectively. In Table 6.5.2, we obtain the experimentally determined orders of convergence (EOC) for the different $\alpha = 1.2, 1.4, 1.6, 1.8$ by using the Grünwand difference method in [66]. We only observe the first order convergence.

Δt	Δx	$\alpha = 1.2$	$\alpha = 1.4$	$\alpha = 1.6$	$\alpha = 1.8$
2^{-10}	2^{-3}				
2^{-10}	2^{-4}	0.8970	0.9660	1.1971	1.7665
2^{-10}	2^{-5}	0.9304	0.9997	1.0878	1.4690
2^{-10}	2^{-6}	0.9571	1.0004	1.0340	1.1946
2^{-10}	2^{-7}	0.9792	1.0033	1.0166	1.0674

Table 6.5.2: The experimentally determined orders of convergence (EOC) at $t = 1$ in Example 14 by using the shifted Grünwald method

Example 15. *We consider the same equation as in Example 14, but with the nonhomogeneous Dirichlet boundary condition,*

$$u_t(t,x) = {}_0^R D_x^{\alpha} u(t,x) + f(t,x), \quad 0 < x < 2, \ t > 0 \tag{6.5.17}$$

$$u(t,0) = 5, \quad u(t,2) = 5, \tag{6.5.18}$$

$$u(0,x) = 4x^2(2-x)^2 + 5, \quad 0 < x < 1, \tag{6.5.19}$$

where

$$f(t,x) = -4e^{-t}x^2(2-x)^2 - 4e^{-t}\Big(4\frac{\Gamma(2+1)}{\Gamma(2-\alpha+1)}x^{2-\alpha} - 4\frac{\Gamma(3+1)}{\Gamma(3-\alpha+1)}x^{3-\alpha} + \frac{\Gamma(4+1)}{\Gamma(4-\alpha+1)}x^{4-\alpha} + 5\frac{\Gamma(1)}{\Gamma(1-\alpha)}x^{-\alpha}\Big).$$

The exact solution is $u(t,x) = 4e^{-t}x^2(2-x)^2 + 5$.

We use the same notations as in Example 14. In Table 6.5.3, we obtain the experimentally determined orders of convergence (EOC) for the different $\alpha = 1.2, 1.4, 1.6, 1.8$. We see that the convergence order is less than $3-\alpha$. This is because of the nonhomogeneous boundary conditions.

The approximation of the Riemann-Liouville fractional derivative by using the Grünwald difference operator on $[a, b]$ in Meerschaert and Tadjeran [66] requires that the function has the zero extension for $x < a$ and $x > b$. Hence we require that the function should have zero boundary conditions on the finite interval in order to get good approximation of the fractional derivative of such function by using the Grünwald difference operator. In this example, since the Dirichlet boundary conditions are not homogeneous, we observe that in Table 6.5.4 the convergence order of the algorithm by using the Grünwald difference method is rather low. However the shifted Diethelm method works well for the nonhomogeneous Dirichlet boundary conditions and the convergence order is approximately equal to 1 in this example. This is another advantage of using the shifted Diethelm's method compared with the Grünwald difference method in Meerschaert and Tadjeran [66].

Δt	Δx	$\alpha = 1.2$	$\alpha = 1.4$	$\alpha = 1.6$	$\alpha = 1.8$
2^{-10}	2^{-3}				
2^{-10}	2^{-4}	1.4510	1.4687	1.5479	1.6511
2^{-10}	2^{-5}	1.4388	1.2905	1.2426	1.2030
2^{-10}	2^{-6}	1.3686	1.1039	0.9791	1.0037
2^{-10}	2^{-7}	1.0667	0.8199	0.7011	0.7089

Table 6.5.3: The experimentally determined orders of convergence (EOC) at $t = 1$ in Example 15 by using the shifted Diethelm method

Example 16. *Consider [12]*

$$u_t(t, x) = {}_0^R D_x^\alpha u(t, x) + f(t, x), \quad 0 < x < 1, \ t > 0 \tag{6.5.20}$$

$$u(t, 0) = 0, \quad u(t, 1) = e^{-t}, \tag{6.5.21}$$

$$u(0, x) = x^{\alpha_1}, \quad 0 < x < 1, \tag{6.5.22}$$

Δt	Δx	$\alpha = 1.2$	$\alpha = 1.4$	$\alpha = 1.6$	$\alpha = 1.8$
2^{-10}	2^{-3}				
2^{-10}	2^{-4}	0.7821	0.3548	0.6070	1.1859
2^{-10}	2^{-5}	0.5424	0.2148	0.2738	0.5377
2^{-10}	2^{-6}	0.4045	0.2604	0.2348	0.2664
2^{-10}	2^{-7}	0.3801	0.3191	0.2580	0.1939

Table 6.5.4: The experimentally determined orders of convergence (EOC) at $t = 1$ in Example 15 by using the shifted Grünwald method

where

$$f(t,x) = -e^{-t}x^{\alpha_1} - e^{-t}\frac{\Gamma(\alpha_1+1)}{\Gamma(\alpha_1+1-\alpha)}x^{\alpha_1-\alpha}.$$

The exact solution is $u(t,x) = e^{-t}x^{\alpha_1}$. In our numerical simulations, we first consider the nonsmooth solutions with $\alpha_1 = \alpha$. we then consider the smooth solutions with $\alpha_1 = 3$.

For the case $\alpha_1 = \alpha$, we have

$${}_0^R D_x^\alpha(x^{\alpha_1}) = D^2\left({}_0^R D_x^{\alpha-2}\right)(x^{\alpha_1}) = D^2\frac{1}{\Gamma(2-\alpha)}\int_0^x (x-\tau)^{1-\alpha}\tau^{\alpha_1}\,d\tau = CD^2(x^2) = C,$$

for some constant C, which implies that the following Lipschitz condition holds for any $\beta > 0$,

$$\left|{}_0^R D_x^\alpha u(t,x) - {}_0^R D_y^\alpha u(t,y)\right| = 0 \leq C|x-y|^\beta.$$

In Table 6.5.5, we obtain the experimentally determined orders of convergence (EOC) for the different $\alpha = 1.2, 1.4, 1.6, 1.8$. We see that the convergence order is less than $3-\alpha$. This is because the exact solution u is not sufficiently smooth in this case.

For the case $\alpha_1 = 3$, we obtain, in Table 6.5.6, the experimentally determined orders of convergence (EOC) for the different $\alpha = 1.2, 1.4, 1.6, 1.8$. We see that the convergence order is almost $3 - \alpha$.

Δt	Δx	$\alpha = 1.2,\ \alpha_1 = 1.2$	$\alpha = 1.4,\ \alpha_1 = 1.4$	$\alpha = 1.6,\ \alpha_1 = 1.6$	$\alpha = 1.8,\ \alpha_1 = 1.8$
2^{-10}	2^{-3}				
2^{-10}	2^{-4}	1.2981	1.1479	1.0375	0.9583
2^{-10}	2^{-5}	1.4639	1.3352	1.1884	1.0637
2^{-10}	2^{-6}	1.4405	1.4178	1.2836	1.1379
2^{-10}	2^{-7}	1.2192	1.4118	1.3292	1.1831

Table 6.5.5: The experimentally determined orders of convergence (EOC) at $t = 1$ in Example 16 for $\alpha_1 = \alpha$

Δt	Δx	$\alpha = 1.2,\ \alpha_1 = 3$	$\alpha = 1.4,\ \alpha_1 = 3$	$\alpha = 1.6,\ \alpha_1 = 3$	$\alpha = 1.8,\ \alpha_1 = 3$
2^{-10}	2^{-3}				
2^{-10}	2^{-4}	1.3625	1.2416	1.1532	1.0745
2^{-10}	2^{-5}	1.5740	1.3951	1.2398	1.1111
2^{-10}	2^{-6}	1.7143	1.5008	1.3099	1.1440
2^{-10}	2^{-7}	1.8557	1.5754	1.3585	1.1690

Table 6.5.6: The experimentally determined orders of convergence (EOC) at $t = 1$ in Example 16 for $\alpha_1 = 3$

Example 17. *Consider the same equation as in Example 16, but with nonhomogeneous boundary conditions.*

$$u_t(t,x) = {}_0^R D_x^{\alpha} u(t,x) + f(t,x), \quad 0 < x < 1,\ t > 0 \tag{6.5.23}$$

$$u(t,0) = 1, \quad u(t,1) = e^{-t} + 1, \tag{6.5.24}$$

$$u(0,x) = x^{\alpha_1} + 1, \quad 0 < x < 1, \tag{6.5.25}$$

where

$$f(t,x) = -e^{-t} x^{\alpha_1} - e^{-t} \frac{\Gamma(\alpha_1 + 1)}{\Gamma(\alpha_1 + 1 - \alpha)} x^{\alpha_1 - \alpha}.$$

The exact solution is $u(t,x) = e^{-t}x^{\alpha_1} + 1$. *In our numerical simulations, we consider the smooth solution with* $\alpha_1 = 3$.

In Table 6.5.7, we obtain the experimentally determined orders of convergence (EOC) for the different $\alpha = 1.2, 1.4, 1.6, 1.8$. We see that the convergence order is almost $3-\alpha$ even under the nonhomogeneous boundary conditions.

Δt	Δx	$\alpha = 1.2,\ \alpha_1 = 3$	$\alpha = 1.4,\ \alpha_1 = 3$	$\alpha = 1.6,\ \alpha_1 = 3$	$\alpha = 1.8,\ \alpha_1 = 3$
2^{-10}	2^{-3}				
2^{-10}	2^{-4}	1.3961	1.2732	1.1686	1.0791
2^{-10}	2^{-5}	1.5847	1.4090	1.2514	1.1165
2^{-10}	2^{-6}	1.7003	1.5015	1.3149	1.1474
2^{-10}	2^{-7}	1.7823	1.5581	1.3562	1.1698

Table 6.5.7: The experimentally determined orders of convergence (EOC) at $t = 1$ in Example 17 for $\alpha_1 = 3$

Example 18. *Consider the following two-sided space-fractional partial differential equation, [66]*

$$u_t(t,x) = c_+(t,x)\,{}_0^R D_x^{\alpha} u(t,x) + c_-(t,x)\,{}_x^R D_1^{\alpha} u(t,x) + f(t,x), \quad 0 < x < 2,\ t > 0 \tag{6.5.26}$$

$$u(t,0) = u(t,2) = 0, \tag{6.5.27}$$

$$u(0,x) = 4x^2(2-x)^2, \quad 0 < x < 2, \tag{6.5.28}$$

where

$$c_+(t,x) = \Gamma(1.2)x^{1.8} \quad \textit{and} \quad c_-(t,x) = \Gamma(1.2)(2-x)^{1.8}$$

$$f(t,x) = -32e^{-t}\Big(x^2 + (2-x)^2 - 2.5(x^3 + (2-x)^3) + \frac{25}{22}(x^4 + (2-x)^4)\Big).$$

The exact solution is $u(t,x) = 4e^{-t}x^2(2-x)^2$.

We use the same notations as in Example 14. In Table 6.5.8, we obtain the experimentally determined orders of convergence (EOC) for the different $\alpha = 1.2, 1.4, 1.6, 1.8$. We see that the convergence order is almost $3-\alpha$. The order $3-\alpha$ term dominates the convergence order in this example.

Δt	Δx	$\alpha = 1.2$	$\alpha = 1.4$	$\alpha = 1.6$	$\alpha = 1.8$
2^{-10}	2^{-3}				
2^{-10}	2^{-4}	1.3872	1.2531	1.1841	1.1424
2^{-10}	2^{-5}	1.5540	1.2676	1.1884	1.1425
2^{-10}	2^{-6}	1.6878	1.4151	1.2607	1.1280
2^{-10}	2^{-7}	1.7892	1.4580	1.1861	1.1961

Table 6.5.8: The experimentally determined orders of convergence (EOC) at $t = 1$ in Example 18 by using the shifted Diethelm method

Chapter 7

Conclusions and possibilities for further work

This thesis has extended the existing numerical methods (Diethelm's numerical method and Fractional Adams-type method) to obtain higher orders convergence in the solution to fractional order differential equations.

Applying quadratic interpolation polynomial to discretize Hadamard finite-part integral in Diethelm's method the convergence order is $O(h^{3-\alpha})$ when, $0 < \alpha < 1$, whereas, the existing order of convergence is $O(h^{2-\alpha})$ when, $0 < \alpha < 1$. And in the Adams-type approximation method we have found the convergence order is $O(h^{1+2\alpha})$ for $0 < \alpha < 1$ and $O(h^3)$ for $1 < \alpha < 2$ which are higher than the existing results. The advantage of the method is we can solve non-linear fractional differential equations as well as linear fractional differential equations and we can avoid non-linear calculations in the Newton iteration process.

In Chapter 5 the Richardson extrapolation algorithm was discussed as a tool to accelerate the order of convergence for our considered numerical methods. The extrapolation algorithm is applicable if the sequence of the approximate solutions of the problem possesses an asymptotic expansion and it was proved that the two approximate methods that we considered possess an asymptotic expansion. We also discussed how to approximate the initial value and the initial integrals of the proposed numerical methods.

Finally, we consider the finite difference method for solving space-fractional partial differential equations. We proved that both the standard explicit finite difference method and implicit finite difference methods are unconditionally unstable. To find a stable finite difference method we introduce implicit shifted Diethelm finite difference method for solving two-sided space-fractional partial differential equations. We proved that, the method is unconditionally stable and the order of convergence of the finite difference method is $O(\Delta t + \Delta x^{\min(3-\alpha,\beta)}), 1 < \alpha < 2$, $\beta > 0$, where $\Delta t, \Delta x$ denote the time and space stepsizes, respectively.

The importance of research into fractional order differential equations and their significance to future applications warrant continued study. We propose some possible research topics in this active research area:

- Higher order numerical methods for solving fractional differential equation with variable steps.
- Higher order numerical methods for solving time-fractional PDEs.
- Higher order numerical methods for solving time-space-fractional PDEs.

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