Numerical approximation of time-fractional differential equations

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Numerical approximation of time-fractional differential equations

Numerieke benadering van tijds-fractionele differentiaalvergelijkingen

(met een samenvatting in het Nederlands)

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Chapter 1

Preliminary

The motivation of this thesis is to construct a class of continuous piecewise polynomials approximations to the fractional derivatives in Caputo's sense on both a uniform grid and a non-uniform grid, and construct the corresponding numerical schemes for time-fractional differential equations. We investigate the numerical stability and convergence of the proposed numerical methods on the uniform grid. Numerical experiments are made to examine the high-order accuracy of the methods for both a smooth solution and a non-smooth solution.

1.1 Fractional calculus

Fractional calculus, as a generalization of ordinary calculus, has been an intriguing topic for many famous mathematicians since the end of the 17th century. During the last four decades, many scholars have been working on the development of theory for fractional derivatives and integrals, and found their way in the world of fractional calculus and their applications. For plentiful summaries and investigation on the historical background of fractional calculus, we refer the interested reader to the following books: [55, 56], and more detailed information on application to physics, we refer to [60, 52, 28, 32, 5, 48] and [27].

1.1.1 Fractional integrals and derivatives

In this section, we would like to collect some existing main definitions of fractional integrals and fractional derivatives, and their relevant properties. In fractional calculus, the first basic definition needed to be presented is the so-called Riemann-Liouville (R-L) fractional integral. One interpretation of a fractional integral is to see it as a generalization of the n-fold iterated integral to a positive real number α with $\lceil \alpha \rceil = n$.

Definition 1.1.1. *Let $\alpha \in \mathbb{R}^+$, for a function $u(t) \in L^1_{loc}(\mathbb{R})$, $a, b \in \mathbb{R}$, the left hand and right hand Riemann-Liouville fractional integral of α order of $u(t)$ are respectively defined by*

$$ {}_a\mathcal{I}_t^{\alpha} u(t) = \frac{1}{\Gamma(\alpha)} \int_a^t (t-\xi)^{\alpha-1} u(\xi) \mathrm{d}\xi, \qquad -\infty \le a < t < \infty \tag{1.1.1} $$

and

$$ {}_t\mathcal{I}_b^{\alpha} u(t) = \frac{1}{\Gamma(\alpha)} \int_t^b (\xi - t)^{\alpha-1} u(\xi) \mathrm{d}\xi, \qquad -\infty < t < b \le \infty. \tag{1.1.2} $$

In particular, consistent with Riemann's definition, we define

$$ \mathcal{I}^{\alpha} u(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-\xi)^{\alpha-1} u(\xi) \mathrm{d}\xi. \tag{1.1.3} $$

Remark 1.1.1. *It can be noticed that, when taking the case of the left hand fractional integral as an example, the fractional integral of order* $\alpha \in \mathbb{R}^+$ *can be considered as the convolution of the kernel* $t^{\alpha-1}$ *and the function* $u(t)$. *Since it is known that* $t^{\alpha-1} \in L^1_{loc}(\mathbb{R})$ *for* $\alpha \in \mathbb{R}^+$, *the local integrability assumption of* $u(t)$ *in Definition 1.1.1 is sufficient to guarantee* ${}_a\mathcal{I}_t^\alpha u(t) \in L^1_{loc}(\mathbb{R})$ *as well.*

Property 1.1.1. *The fractional integral satisfies the semigroup property , i.e.,*

$$ {}_a\mathcal{I}_t^\beta\, {}_a\mathcal{I}_t^\alpha u = {}_a\mathcal{I}_t^{\beta+\alpha} u, \qquad \alpha,\ \beta \in \mathbb{R}^+. \tag{1.1.4}$$

The semigroup property is an important result of the fractional integral, because in some sense it implies that the fractional integral operator is commutative. On the other hand, this property doesn't apply to the fractional derivatives, which will be defined later.

Taking a particular case into account, if we choose $\beta = n \in \mathbb{N}$ and any positive real number α, and operate the n-th derivative on both sides of (1.1.4), it follows that

$$ {}_a\mathcal{I}_t^\alpha u(t) = \frac{\mathrm{d}^n}{\mathrm{d}t^n} {}_a\mathcal{I}_t^{n+\alpha} u(t), \qquad \alpha \in \mathbb{R}^+. \tag{1.1.5}$$

In addition, if we add some smoothness property on $u(t)$, such that $u(t) \in C^n(a,\infty) \cap L^1_{loc}(a,\infty)$ or $u(t) \in AC^{(n-1)}(a,\infty) \cap L^1_{loc}(a,\infty)$, i.e, there exists a function $v(t) \in C(a,\infty) \cap L^1_{loc}(a,\infty)$ or $v(t) \in L^1_{loc}(a,\infty)$ such that $u^{(n)}(t) = v(t)$ or $u^{(n)}(t) = v(t)$ almost everywhere, we could investigate the condition under which the function $v(t)$ satisfies formula (1.1.5). Actually, in contrast to the ordinary derivative case, the following result states that the differentiation operator $\frac{\mathrm{d}^n}{\mathrm{d}t^n}$ and fractional integral operator ${}_a\mathcal{I}_t^\alpha$ can't commute unless it is satisfied that $u^{(m)}(a) = 0$ for $m = 0, 1, \cdots, n-1$, which can be applicable to the case of the right-handed fractional integral as well.

Property 1.1.2. *If* $u^{(n)}(a) = 0$ *for* $n \in \mathbb{N}$, *then*

$$ {}_a\mathcal{I}_t^\alpha u(t) = {}_a\mathcal{I}_t^{n+\alpha} u^{(n)}(t), \qquad \alpha \in \mathbb{R}^+. \tag{1.1.6}$$

Therefore, operating the n-th derivative on both sides, one obtains

$$ \frac{\mathrm{d}^n}{\mathrm{d}t^n} {}_a\mathcal{I}_t^\alpha u(t) = {}_a\mathcal{I}_t^\alpha u^{(n)}(t), \qquad \alpha \in \mathbb{R}^+. \tag{1.1.7}$$

Proof. The result of formula (1.1.6) can be directly obtained by repeatedly making use of the integration by part technique on the term ${}_a\mathcal{I}_t^\alpha u(t)$. □

Moreover, the validity of formulae (1.1.5) and (1.1.6) for the sufficiently smooth function $u(t)$ provides two approaches to generalize the operator ${}_a\mathcal{I}_t^\alpha u(t)$ to the case $\alpha > -n$, which are defined by the fractional derivative in the sense of Riemann-Liouville and Caputo, respectively.

Definition 1.1.2 (R-L fractional derivative). *Let* $\alpha \in \mathbb{R}^+$, *and* $n = \lceil \alpha \rceil$, *the* α *order left-handed and right-handed Riemann-Liouville fractional derivative of function* $u(t)$, *which is assumed to be absolutely continuous on the subinterval of* $\mathbb{R}$, *is defined by*

$$ {}^R_a\mathcal{D}_t^\alpha u(t) = \frac{1}{\Gamma(n-\alpha)} \frac{\mathrm{d}^n}{\mathrm{d}t^n} \int_a^t (t-\xi)^{n-1-\alpha} u(\xi)\mathrm{d}\xi, \qquad -\infty \le a < t < \infty \tag{1.1.8}$$

and

$$ {}^R_t\mathcal{D}_b^\alpha u(t) = \frac{(-1)^n}{\Gamma(n-\alpha)} \frac{\mathrm{d}^n}{\mathrm{d}t^n} \int_t^b (\xi-t)^{n-\alpha-1} u(\xi)\mathrm{d}\xi, \qquad -\infty < t < b \le \infty \tag{1.1.9}$$

respectively. Especially, in Riemann's sense, we denote by

$$ {}^{R}\mathcal{D}^{\alpha}u(t) = \frac{1}{\Gamma(n-\alpha)}\frac{\mathrm{d}^n}{\mathrm{d}t^n}\int_0^t (t-\xi)^{n-\alpha-1}u(\xi)\mathrm{d}\xi \tag{1.1.10} $$

for convenience of notation.

Definition 1.1.3 (Caputo fractional derivative). *Let $\alpha \in \mathbb{R}^+$ and $n = \lceil \alpha \rceil$, assume that $u^{(n)}(t) \in L^1_{loc}(\mathbb{R})$, the α order left-hand and right-hand Caputo derivatives are defined by*

$$ {}_{a}^{C}\mathcal{D}_{t}^{\alpha}u(t) = \frac{1}{\Gamma(n-\alpha)}\int_a^t (t-\xi)^{n-1-\alpha}\frac{\mathrm{d}^n}{\mathrm{d}\xi^n}u(\xi)\mathrm{d}\xi, $$

and

$$ {}_{t}^{C}\mathcal{D}_{b}^{\alpha}u(t) = \frac{(-1)^n}{\Gamma(n-\alpha)}\int_t^b (\xi-t)^{n-1-\alpha}\frac{\mathrm{d}^n}{\mathrm{d}\xi^n}u(\xi)\mathrm{d}\xi. $$

For the consideration of a series of applications in the subsequent sections, we now particularly pay attention to the definition of the Caputo fractional derivative on $[0,T]$, and make use of some simplified notations.

Definition 1.1.4 ([14]). *Let $\alpha > 0$, and $n = \lceil \alpha \rceil$, the α order Caputo derivative of a function $u(t)$ on $[0,T]$ is defined by*

$$ {}^{C}\mathcal{D}^{\alpha}u(t) = \frac{1}{\Gamma(n-\alpha)}\int_0^t \frac{u^{(n)}(\xi)}{(t-\xi)^{\alpha-n+1}}\mathrm{d}\xi \tag{1.1.11} $$

for $u^{(n)}(t) \in L^1[0,T]$. In particular, the Caputo derivative of order $\alpha \in (0,1)$ is defined by

$$ {}^{C}\mathcal{D}^{\alpha}u(t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t (t-\xi)^{-\alpha}\frac{\mathrm{d}u}{\mathrm{d}\xi}\mathrm{d}\xi, \tag{1.1.12} $$

for $u(t) \in L^1[0,T]$.

Recalling the formulae (1.1.5) and (1.1.6), the definitions of the two fractional derivatives are not equivalent. Moreover, the following conclusion shows a relationship between the α order Riemann-Liouvile derivative and the Caputo derivative.

Proposition 1.1.1 ([28]). *Assume that $\alpha \in \mathbb{R}$ and $n = \lceil \alpha \rceil$, then*

$$ {}_{a}^{R}\mathcal{D}_{t}^{\alpha}u(t) = {}_{a}^{C}\mathcal{D}_{t}^{\alpha}u(t) + \sum_{k=0}^{n-1}\frac{u^{(k)}(a)}{\Gamma(k+1-\alpha)}(t-a)^{k-\alpha} \tag{1.1.13} $$

and

$$ {}_{t}^{R}\mathcal{D}_{b}^{\alpha}u(t) = {}_{t}^{C}\mathcal{D}_{b}^{\alpha}u(t) + \sum_{k=0}^{n-1}\frac{(-1)^k u^{(k)}(b)}{\Gamma(k+1-\alpha)}(b-t)^{k-\alpha}. \tag{1.1.14} $$

If we consider a class of functions $u(t) := t^p$ with $p \in \mathbb{R}$ and $p > -1$, which is a generalization of the power function with $p \in \mathbb{N}$. It can be noted that $u(t) \in L^1_{loc}(\mathbb{R}) \cap C^{\infty}(\mathbb{R}^+)$. The fractional integral and fractional derivatives of the mentioned function in the sense of Riemann-Liouville and Caputo are illustrated as an example.

Example 1.1.1. *Assume the function $u(t) = t^p$ with $p \in \mathbb{R}$ and $p > -1$. For $\alpha \in \mathbb{R}^+$, we have*

$$\mathcal{I}^\alpha u(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-\xi)^{\alpha-1} \xi^p \mathrm{d}\xi = \frac{\Gamma(p+1)}{\Gamma(\alpha+p+1)} t^{p+\alpha}.$$

In addition, we find

$$\frac{\mathrm{d}^n}{\mathrm{d}t^n} t^p = \begin{cases} \frac{\Gamma(p+1)}{\Gamma(p-n+1)} t^{p-n}, & p \neq 0, 1, \cdots, n-1, \\ 0, & p = 0, 1, \cdots, n-1. \end{cases}$$

For $n = \lceil \alpha \rceil$, it follows that

$${}^R\mathcal{D}^\alpha t^p = \frac{\mathrm{d}^n}{\mathrm{d}t^n} {}_a\mathcal{I}_t^{n-\alpha} t^p = \begin{cases} \frac{\Gamma(p+1)}{\Gamma(p-\alpha+1)} t^{p-\alpha}, & p > -1, \ \ p+n-\alpha \neq 0, 1, \cdots, n-1, \\ 0, & p+n-\alpha = 0, 1, \cdots, n-1, \end{cases}$$

and

$${}^C\mathcal{D}^\alpha t^p = {}_a\mathcal{I}_t^{n-\alpha} \frac{\mathrm{d}^n}{\mathrm{d}t^n} t^p = \begin{cases} \frac{\Gamma(p+1)}{\Gamma(p-\alpha+1)} t^{p-\alpha}, & p-n > -1, \\ 0, & p = 0, 1, \cdots, n-1. \end{cases}$$

Remark 1.1.2. *It can be noted that if $u(t)$ is a constant function on $\mathbb{R}$, the α order Riemann-Liouville fractional derivative is nonzero, whereas the Caputo derivative is zero.*

1.1.2 Integral transform of fractional integrals and derivatives

We will collect and derive some basic results on the integral transform of the fractional integral and derivatives, respectively. Especially, the Laplace transform (cf. [66]) and Fourier transform are mainly taken into consideration.

Definition 1.1.5 (Laplace transform). *The Laplace transform of a function $u(t) \in L^1_{loc}(\mathbb{R}^+)$ is defined by*

$$\mathcal{L}(u)(s) = \int_0^\infty e^{-st} u(t) \mathrm{d}t, \qquad s \in \mathbb{C} \tag{1.1.15}$$

and the inverse Laplace transform of $\mathcal{L}(u)(s)$ is given by

$$\mathcal{L}^{-1}\mathcal{L}(u)(t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{st} \mathcal{L}(u)(s) \mathrm{d}s,$$

where c is a real number such that $\mathcal{L}(u)(s)$ is convergent on the vertical line $\{s : \Re s = c, -\infty < \Im s < \infty\}$.

Property 1.1.3 (convolution property). *The convolution operation of two functions $u(t)$ and $v(t)$ which are locally integrable on $\mathbb{R}^+$ is denoted by*

$$u(t) * v(t) = \int_0^t u(t-\xi) v(\xi) \mathrm{d}\xi.$$

Then

$$\mathcal{L}(u * v)(s) = \mathcal{L}(u)(s)\mathcal{L}(v)(s).$$

A direct consequence of making use of the convolution property is to obtain the Laplace transform of the $\alpha > 0$ order fractional integral, that is

$$\mathcal{L}(\mathcal{I}^\alpha u)(s) = \mathcal{L}\left(\frac{t_+^{\alpha-1}}{\Gamma(\alpha)} * u(t)\right)(s) = s^{-\alpha}\mathcal{L}(u)(s),$$

where the fractional integral is defined in formula (1.1.3) and the last equality can be obtained by means of the definition of Gamma function. Hence the Laplace transform of the fractional derivative can be obtained in combination with the Laplace transform of the n-th order derivative of $u(t)$.

Lemma 1.1.1. *The Laplace transform of the $n-1 < \alpha < n$ order Riemann-Liouville fractional derivative ${}^R\mathcal{D}^\alpha u(t)$ is given by*

$$\mathcal{L}\left({}^R\mathcal{D}^\alpha u(t)\right)(s) = s^\alpha(\mathcal{L}u)(s) - \sum_{m=0}^{n-1} s^m \left({}^R\mathcal{D}^{\alpha-m-1}u(t)\right)\Big|_{t=0}. \tag{1.1.16}$$

Lemma 1.1.2. *The Laplace transform of the $n-1 < \alpha \le n$ order Caputo fractional derivative ${}^C\mathcal{D}^\alpha u(t)$ is given by*

$$\mathcal{L}\left({}^C\mathcal{D}^\alpha u(t)\right)(s) = s^\alpha(\mathcal{L}u)(s) - \sum_{m=0}^{n-1} s^{\alpha-m-1}u^{(m)}(0). \tag{1.1.17}$$

Definition 1.1.6 (Fourier transform). *The Fourier transform of a function $u(x) \in L^1(\mathbb{R})$ is defined by*

$$\mathcal{F}(u)(\omega) = \int_{\mathbb{R}} e^{-i\omega\xi}u(\xi)\mathrm{d}\xi. \tag{1.1.18}$$

In addition, if $\mathcal{F}(u)(\omega) \in L^1(\mathbb{R})$, the inverse Fourier transform of $\mathcal{F}(u)(\omega)$ is defined by

$$\mathcal{F}^{-1}\mathcal{F}(u)(x) = \frac{1}{2\pi}\int_{\mathbb{R}} e^{ix\xi}\mathcal{F}(u)(\xi)\mathrm{d}\xi. \tag{1.1.19}$$

If we look into the requirement on the function $u(x)$ in Definition 1.1.6, it appears to be stricter in comparison with that of the Laplace transform, where the locally integrable restriction can be satisfied by a large class of functions. In the usual sense, most elementary functions, such as power functions $1, x, x^2, \cdots$ are not in $L^1(\mathbb{R})$, and they don't possess Fourier transforms as well. However, for some functions which are not absolutely integrable on $\mathbb{R}$, the Fourier transform of those functions may exist and can be gained in a technical way. In what follows, we would like to testify the existence of Fourier transform of the class of function $f(x) := x_+^\beta$ for $\beta \in (-1, 0)$, in this case, it is noted that $f(x) \notin L^1(\mathbb{R})$.

Lemma 1.1.3. *For $0 < \alpha < 1$, it holds that*

$$\int_0^\infty \xi^{-\alpha}e^{-i\xi\omega}\mathrm{d}\xi = (i\omega)^{\alpha-1}\Gamma(1-\alpha) \tag{1.1.20}$$

and

$$\int_0^\infty \xi^{-\alpha}e^{i\xi\omega}\mathrm{d}\xi = (-i\omega)^{\alpha-1}\Gamma(1-\alpha). \tag{1.1.21}$$

Proof. We first consider the derivation of equality (1.1.21). The change of variable $\eta = \xi\omega$ deduces that

$$\int_0^\infty \xi^{-\alpha} e^{i\xi\omega} \mathrm{d}\xi = \omega^{\alpha-1} \int_0^\infty \eta^{-\alpha} e^{i\eta} \mathrm{d}\eta. \tag{1.1.22}$$

It is noticed that $\lim_{\eta\to 0} \eta^{-\alpha} e^{i\eta} = \infty$ and $\lim_{\eta\to\infty} \eta^{-\alpha} e^{i\eta} = 0$ for $\alpha > 0$. Therefore, we consider a closed curve Γ, such that the integrand is analytic on the domain Ω enclosed by Γ. The Cauchy theorem implies

$$\int_\Gamma \eta^{-\alpha} e^{i\eta} \mathrm{d}\eta = 0,$$

where $\Gamma := \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \cup \Gamma_4 \cup s_\varepsilon$ with a variable $\epsilon > 0, R > 0$ and $\Gamma_1 = \{x : \epsilon \le x \le R\}$, $\Gamma_2 = \{R + ix : 0 \le x \le R\}$, $\Gamma_3 = \{x + iR : 0 \le x \le R\}$, $\Gamma_4 = \{ix : \epsilon \le x \le R\}$ and $s_\epsilon = \{\epsilon e^{-i\theta} : 0 \le \theta \le \pi/2\}$. It follows that

$$\left(\sum_{i=1}^{4} \int_{\Gamma_i} + \int_{s_\epsilon} \right) \eta^{-\alpha} e^{i\eta} \mathrm{d}\eta = 0. \tag{1.1.23}$$

In addition, we have

$$\left| \int_{\Gamma_2} \eta^{-\alpha} e^{i\eta} \mathrm{d}\eta \right| = \left| i \int_0^R (R + iz)^{-\alpha} e^{iR} e^{-z} \mathrm{d}z \right| \le R^{-\alpha} \int_0^R e^{-z} \mathrm{d}z \le R^{-\alpha},$$

$$\left| \int_{\Gamma_3} \eta^{-\alpha} e^{i\eta} \mathrm{d}\eta \right| = \left| \int_0^R (z + iR)^{-\alpha} e^{iz} e^{-R} \mathrm{d}z \right| \le R^{1-\alpha} e^{-R}$$

and

$$\left| \int_{s_\epsilon} \eta^{-\alpha} e^{i\eta} \mathrm{d}\eta \right| = \left| i \int_0^{\frac{\pi}{2}} \epsilon^{1-\alpha} e^{-\epsilon \sin\theta} e^{-i\alpha\theta} e^{i\epsilon\cos\theta} e^{i\theta} \mathrm{d}\theta \right| \le \epsilon^{1-\alpha} \frac{\pi}{2}.$$

Let $\epsilon \to 0$ and $R \to \infty$, for $0 < \alpha < 1$, formula (1.1.23) therefore becomes

$$\int_0^\infty \eta^{-\alpha} e^{i\eta} \mathrm{d}\eta = i^{1-\alpha} \int_0^\infty z^{-\alpha} e^{-z} \mathrm{d}z = i^{1-\alpha} \Gamma(1-\alpha), \tag{1.1.24}$$

together with $i^{1-\alpha} = (e^{\pi/2i})^{1-\alpha} = (e^{-\pi/2i})^{\alpha-1} = (-i)^{\alpha-1}$, the desired result holds. In a similar way, result (1.1.21) can be obtained by choosing $\tilde{\Gamma} = \Gamma_1 \cup \tilde{\Gamma}_2 \cup \tilde{\Gamma}_3 \cup \tilde{\Gamma}_4 \cup \tilde{s}_\epsilon$, where $\tilde{\Gamma}_2 = \{R + ix : -R \le x \le 0\}$, $\tilde{\Gamma}_3 = \{x - iR : 0 \le x \le R\}$, $\tilde{\Gamma}_4 = \{ix : -R \le x \le -\epsilon\}$, and $\tilde{s}_\epsilon = \{\epsilon e^{i\theta} : -\pi/2 \le \theta \le 0\}$. □

Remark 1.1.3. *According to the results in Lemma 1.1.3, we easily get*

$$\int_0^\infty \xi^{-\alpha} \cos(\omega\xi) \mathrm{d}\xi = \omega^{\alpha-1} \Gamma(1-\alpha) \sin(\frac{\alpha\pi}{2}),$$
$$\int_0^\infty \xi^{-\alpha} \sin(\omega\xi) \mathrm{d}\xi = \omega^{\alpha-1} \Gamma(1-\alpha) \cos(\frac{\alpha\pi}{2}).$$

In addition, according to the equivalent relations

$$\int_{-\infty}^\infty e^{-i\omega x} \left(\int_{-\infty}^x (x-\xi)^{\alpha-1} u(\xi) \mathrm{d}\xi \right) \mathrm{d}x = \int_{-\infty}^\infty e^{-i\omega\xi} u(\xi) \mathrm{d}\xi \int_0^\infty x^{\alpha-1} e^{-i\omega x} \mathrm{d}x$$

and

$$\int_{-\infty}^\infty e^{-i\omega x} \left(\int_x^\infty (\xi-x)^{\alpha-1} u(\xi) \mathrm{d}\xi \right) \mathrm{d}x = \int_{-\infty}^\infty e^{-i\omega\xi} u(\xi) \mathrm{d}\xi \int_0^\infty x^{\alpha-1} e^{i\omega x} \mathrm{d}x,$$

together with the results in Lemma 1.1.3, the Fourier transforms of the fractional integrals are obtained as follows:

Lemma 1.1.4 ([28]). *If $u \in L^1(\mathbb{R})$ and $0 < \alpha < 1$, then*

$$\mathcal{F}\left({}_{-\infty}\mathcal{I}_x^{\alpha} u\right)(\omega) = (i\omega)^{-\alpha}\mathcal{F}(u)(\omega), \tag{1.1.25a}$$

$$\mathcal{F}\left({}_{x}\mathcal{I}_{\infty}^{\alpha} u\right)(\omega) = (-i\omega)^{-\alpha}\mathcal{F}(u)(\omega). \tag{1.1.25b}$$

If adding a smoothness condition on the function u and combining with the Fourier transform of the corresponding integer order derivative of u, we obtain the Fourier transform of the Caputo fractional derivatives.

Lemma 1.1.5. *Let $n = \lceil \alpha \rceil > 0$. Assume that $u^{(n)} \in L^1(\mathbb{R})$. Then it holds that*

$$\mathcal{F}\left({}_{-\infty}^{\ \ C}\mathcal{D}_x^{\alpha} u\right)(\omega) = (i\omega)^{\alpha}\mathcal{F}(u)(\omega); \tag{1.1.26a}$$

$$\mathcal{F}\left({}_{x}^{C}\mathcal{D}_{\infty}^{\alpha} u\right)(\omega) = (-i\omega)^{\alpha}\mathcal{F}(u)(\omega). \tag{1.1.26b}$$

The results will be used in the following section to derive the solutions of some specific fractional differential equations.

1.2 Time-fractional differential equations

The applications of fractional calculus on modeling equations possessing terms with fractional derivatives in the time- or space- or time-space direction have become very important in the areas of physical, chemistry, engineering. Particularly, in recent years a huge amount of interesting and surprising fractional models have been proposed. Here, we just mention a few typical applications: in the theory of Hankel transforms [19], in financial models [62, 67], in elasticity theory [4], in medical applications [61, 34], in geology [7, 38], in physics [12, 6, 51] and many more. In practical applications, the solution of an ordinary differential equation generally depicts the trajectory of a state variable (a point in mathematics) along with the time direction. From an ordinary differential equation to a partial differential equation, all the points in a domain of space which can be considered as a flow are taken into consideration. The corresponding solution of a partial differential equation represents the evolution of the flow with the time. As a generalization of classical differential equations, the time-fractional ordinary differential equation (TFODE) and partial differential equation (TFPDE) are proposed to explain some particular physical phenomena, and are characterized in a general form by replacing the integer order derivative with respect to time by the fractional derivative of α order with $\alpha \in \mathbb{R}^+$, such as those defined in the previous section. In terms of the TFODE, we mainly focus on its relation with Volterra integral equations and some qualitative properties, such as the existence and uniqueness, stability behaviour and the smoothness of the solution. In the case of a TFPDE, we review a general class of fractional diffusion equations and fractional wave equations including some physical interpretations and representations of the solutions, and their related properties.

1.2.1 Time-fractional ordinary differential equations

We are mainly concerned with some analytical properties of the time-fractional ordinary differential equation, which is expressed in a general form of

$$\begin{cases} {}^{C}\mathcal{D}^{\alpha} u(t) = f(t, u(t)), & t \in [0, T], \ \ \alpha \in \mathbb{R}^+, \\ u^{(m)}(0) = u_0^{(m)}, & m = 0, 1, \cdots, \lfloor \alpha \rfloor, \end{cases} \tag{1.2.1}$$

where the integer order operator with respect to time is replaced by the α order Caputo fractional derivative${}^{C}\mathcal{D}^{\alpha}$ defined in Definition 1.1.4. In this situation, the initial values can be prescribed in a usual way.

It is known that a time-fractional ordinary differential equation has a close relationship with a Volterra integral equation. On the one hand, if operating $\mathcal{I}^{\alpha}$ on both sides of (1.2.1) and making use of the property (1.1.4), equation (1.2.1) becomes

$$u(t)=\sum_{m=0}^{\lfloor\alpha\rfloor}\frac{u_0^{(m)}}{\Gamma(m+1)}t^m+\frac{1}{\Gamma(\alpha)}\int_0^t(t-\xi)^{\alpha-1}f(\xi,u(\xi))\mathrm{d}\xi,\qquad t\in[0,T],\ \alpha\in\mathbb{R}^+,\tag{1.2.2}$$

on the other hand, according to [15], we have

Lemma 1.2.1. *If the function f is continuous, then the initial value problem (1.2.1) is equivalent to the nonlinear Volterra integral equation (1.2.2). In other words, each solution of the Volterra equation (1.2.2) is also a solution of problem (1.2.1), and vice versa.*

The equivalent result stated in Lemma 1.2.1 indicates an approach to regard fractional differential equation (1.2.1) as the Volterra integral equation with a special kind of convolution kernel. Therefore, in what follows, we incorporate some qualitative properties of the problem (1.2.1) in terms of the theory on Volterra integral equation in a general form. In terms of the analytic properties of the Volterra integral equation, the existence and uniqueness properties and smoothness of the solution are investigated detailed in [37, 10, 53].

Theorem 1.2.1. *For the nonlinear Volterra integral equation in a general form of*

$$u(t)=g(t)+\int_0^t K(t,s,u(s))\mathrm{d}s,\tag{1.2.3}$$

let $K(t,s,u)\in C([0,T]\times[0,t]\times\mathbb{R})$, and suppose that K satisfies the Lipschitz condition

$$|K(t,s,u)-K(t,s,v)|\le L\,|u-v|\,,\tag{1.2.4}$$

where the Lipschitz constant $L>0$ is independent of u and v. Then for each $g\in C([0,T])$ the equation (1.2.3) possesses a unique solution $u\in C([0,T])$.

Theorem 1.2.2. *If the nonlinear Volterra integral of the convolution form*

$$u(t)=g(t)+\int_0^t a(t-s)K(s,u(s))\mathrm{d}s,\tag{1.2.5}$$

satisfies the following assumptions:

i) *equation (1.2.5) has a unique solution $u\in C([0,T])$,*

ii) *g and K are of class C^{n+1} for some integer $n\ge 1$,*

iii) *$a(t)\in C^{n-1}([0,T])\cap C^n((0,T])$ and $|a^{(n)}(t)|\le\rho(t)$, where ρ is nonincreasing and $\rho\in L^1((0,T))\cap C((0,T])$.*

Then the solution of (1.2.5) satisfies $u\in C^n([0,T])\cap C^{n+1}((0,T])$ and $u^{(n+1)}\in L^1((0,T))$.

Furthermore, it is observed that if $0<\alpha<1$ in (1.2.1), the corresponding convolution kernel $a(t):=t^{\alpha-1}/\Gamma(\alpha)$ in (1.2.2) is not continuous on $[0,T]$. In the case $a(t)\in C((0,T])\cap L^1([0,T])$, it is shown that the smoothness of given functions g and K only makes $u\in C([0,T])\cap C^{\infty}((0,T])$, there is no effect on the smoothness of the solution at $t=0$. Therefore, in the following, we particularly focus on the case of weakly singular kernel $a(t)=t^{-\beta}/\Gamma(1-\beta)$ when $0<\beta<1$. We first consider the linear equation of the form

$$u(t)=g(t)+\int_0^t(t-s)^{-\alpha}K(t,s)u(s)\mathrm{d}s,\qquad t\in[0,T],\quad 0<\alpha<1,\tag{1.2.6}$$

according to [37, 10], the following result is reviewed.

Theorem 1.2.3. *Suppose the functions $g(t)$ and $K(t,s)$ are continuous on $[0,T]$ and $S := [0,T] \times [0,t]$, respectively. Then equation* (1.2.6) *has a unique solution $u \in C([0,T])$ given by*

$$u(t) = g(t) + \int_0^t (t-s)^{-\alpha} \rho(t,s,\alpha) g(s) \mathrm{d}s, \tag{1.2.7}$$

with $\rho \in C(S)$ for each $0 < \alpha < 1$. Furthermore, ρ satisfies

$$\rho(t,s,\alpha) = K(t,s) + (t-s)^{\alpha} \int_s^t (t-\tau)^{-\alpha} (\tau - s)^{-\alpha} K(t,s) \rho(\tau, s, \alpha) \mathrm{d}\tau. \tag{1.2.8}$$

Next consider the nonlinear Volterra integral equation

$$u(t) = g(t) + \int_0^t (t-s)^{-\alpha} K(t,s,u(s)) \mathrm{d}s, \qquad t \in [0,T], \quad 0 < \alpha < 1, \tag{1.2.9}$$

and it is proved that

Theorem 1.2.4. *Let $K(t,s,u(s))$ be continuous for all (t,s) with $0 \le s \le t \le T$ and all u, and suppose that K satisfies the Lipschitz condition, i.e.,*

$$|K(t,s,u) - K(t,s,v)| \le L |u - v| . \tag{1.2.10}$$

Then for each $g \in C([0,T])$, equation (1.2.9) *possesses a unique solution $u \in C([0,T])$.*

Remark 1.2.1. *As shown in [37], the existence and uniqueness property of the solution of the linear and nonlinear Volterra integral equation with weakly singular kernel in continuous function space can be generalized to systems of equations without essential difficulties.*

As a natural generalization, the well-posedness and smoothness of the solution of equation (1.2.1) are obtained as well (for example, see [14]).

Theorem 1.2.5. *Let the function $f : [0,T] \times \mathbb{R} \to \mathbb{R}$ be continuous and fulfill a Lipschitz condition with respect to the second variable. Then there exists a unique solution $u(t) \in C([0,T])$ solving problem* (1.2.1).

Theorem 1.2.6. *Let $\alpha \in \mathbb{R}^+$ and f be continuous and satisfy the Lipschitz condition with respect to the second variable. Let u be the exact solution of problem* (1.2.1). *Then it holds that $u \in C^{\lceil \alpha \rceil - 1}([0,T])$.*

Theorem 1.2.7. *Assume the hypotheses of Theorem 1.2.6. Moreover, assume $f \in C^k([0,T] \times \mathbb{R})$ for some $k \in \mathbb{N}$ and $k < \alpha$, then $u \in C^{\lceil \alpha \rceil + k - 1}((0,T])$. Furthermore, $u \in C^{\lceil \alpha \rceil + k - 1}([0,T])$ if and only if f has a k-fold zero at the origin.*

Remark 1.2.2. *It is known from Theorem 1.2.2 and 1.2.7 that the smoothness conditions for the given source term and the nonlinear term don't lead to the smoothness of the solution on the closed interval $[0,T]$ for the problems* (1.2.5) *and* (1.2.1), *which is different from the classical counterpart. This is because the derivatives of the solution are unbounded at the origin $t = 0$. On the other hand, it is noticed that the integer order derivative of any smooth function on a compact interval I still preserves to be smooth on I, however, the α order fractional derivative of the smooth function isn't a smooth function. This implies that for some source term and nonlinear term that are continuous, the solution may be smooth on I. Analogous analysis on this issue is provided partially in [13, 9, 42]. The main results are reviewed.*

Theorem 1.2.8. *Assume that the source term in* (1.2.9) *has the form of* $g(t) = g_1(t) + t^\beta g_2(t)$, $\beta > 0$, $\beta \notin \mathbb{N}$. *Let* $g_1, g_2 \in C^n(I)$ *with* $n \geq 1$, *and the kernel* $K(t, s, u(s)) \in C^m([0,T] \times [0,t] \times \mathbb{R})$. *Then the solution of* (1.2.9) *has the representation of*

$$u(t) = g(t) + \sum_{n=1}^{\infty} \left(\varphi_n(t) + t^\beta \psi_n(t)\right) t^{n(1-\alpha)}, \tag{1.2.11}$$

where $\varphi_n(t), \psi_n(t) \in C^n(I)$.

In the sequel, we present the results on the linear stability behavior of the solution. In the case $K(t,s) = \lambda$, there follows the stability property of the solution.

Theorem 1.2.9 ([45]). *Consider the linear scalar Volterra integral equation*

$$u(t) = g(t) + \frac{\lambda}{\Gamma(\alpha)} \int_0^t (t-\xi)^{\alpha-1} u(\xi) d\xi, \qquad 0 < \alpha \leq 1$$

with $g \in C(\mathbb{R})$, *and* $|\arg(\lambda) - \pi| < \left(1 - \frac{1}{2}\alpha\right)\pi$. *Then there exists a unique solution* $u \in C[0,\infty)$ *which satisfies*

i) $u(t) \to 0$ *as* $t \to \infty$ *when* $g(t)$ *has a finite limit as* $t \to \infty$;

ii) $u(t)$ *is bounded on* $[0,\infty)$ *when* $g(t)$ *is bounded.*

In a similar way, the generalization of the above result to a system of fractional differential equations is provided in [49], i.e.,

Theorem 1.2.10. *Consider the system of time-fractional differential equations in the form of*

$${}^C D^\alpha \mathbf{u}(t) = A\mathbf{u}(t), \qquad t \in \mathbb{R}^+, \ 0 < \alpha < 1, \tag{1.2.12}$$

in combination with the initial value $\mathbf{u}(0) = \mathbf{u}_0$, *where* A *is a square matrix. Then*

i) $\|\mathbf{u}(t)\| \to 0$ *as* $t \to \infty$ *if and only if* $|\arg(\rho(A))| > \frac{\alpha\pi}{2}$,

ii) $\|\mathbf{u}(t)\|$ *is bounded on* $[0,\infty)$ *as* $\|\mathbf{u}_0\|$ *is bounded if and only if those critical eigenvalues which satisfy* $|\arg(\rho(A))| = \frac{\alpha\pi}{2}$ *have geometric multiplicity one.*

where $\rho(A)$ *is denoted by the spectral radius of matrix* A *and* $\|\cdot\|$ *is the discrete* L^2 *norm.*

1.2.2 Time-fractional partial differential equations

Fractional integrals and derivatives in mathematical models that consist of both time and space continuous variables generalize the normal diffusion and wave equations of form

$$\begin{aligned} \frac{\partial^m u(x,t)}{\partial t^m} &= \Delta u(x,t), \qquad (x,t) \in \mathbb{R}^n \times \mathbb{R}^+, \quad m = 1,2, \\ \left.\frac{\partial^k u(x,t)}{\partial t^k}\right|_{t=0} &= u^k(x), \qquad 0 \leq k \leq m-1 \end{aligned} \tag{1.2.13}$$

into fractional order cases [63] by reformulating (1.2.13) into an integral form and replacing the integer number $m = 1, 2$ by $\alpha \in \mathbb{R}$ with $m = \lceil \alpha \rceil$. Therefore, the so-called fractional diffusion and fractional wave equations are represented by

$$u(x,t) = \sum_{k=0}^{m-1} \frac{t^k u^k(x)}{\Gamma(k+1)} + \frac{1}{\Gamma(\alpha)} \int_0^t (t-\xi)^{\alpha-1} \Delta u(x,t), \qquad (x,t) \in \mathbb{R}^n \times \mathbb{R}^+ \tag{1.2.14}$$

in the cases $0 < \alpha < 1, m = 1$ and $1 < \alpha < 2, m = 2$, respectively, where we denote that $\Delta := \sum_{i=1}^{n} \partial^2/\partial x_i^2$. In addition, if operating the fractional integral $\mathcal{I}^{1-\alpha}$ defined in (1.1.3) on both sides of equation (1.2.14) and making use of the result from Proposition 1.1.1, one obtains a reformulation of (1.2.14) in the form of

$$\begin{aligned} &{}^{C}\mathcal{D}^{\alpha}u(x,t) = \Delta u(x,t), \qquad (x,t) \in \mathbb{R}^n \times \mathbb{R}^+, \quad \lceil \alpha \rceil = 1, 2, \\ &\frac{\partial^k u(x,t)}{\partial t^k}\Big|_{t=0} = u^k(x), \qquad 0 \le k \le \lceil \alpha \rceil - 1, \end{aligned} \tag{1.2.15}$$

where ${}^{C}\mathcal{D}^{\alpha}u$ is denoted by the fractional derivative of Caputo's approach defined by (1.1.11).

Denote $\hat{u}(x,s)$ by the Laplace transform of $u(x,t)$ with respect to temporal variable. It follows from (1.2.14) that

$$\Delta \hat{u}(x,s) - s^{\alpha}\hat{u}(x,s) = -\sum_{k=0}^{m-1} u^k(x) s^{\alpha-k-1}. \tag{1.2.16}$$

With the help of the Mellin transform of some special functions, a technical way is employed in [63] to solve (1.2.16) by

$$\hat{u}(x,s) = \sum_{k=0}^{m-1} \int_{\mathbb{R}^n} \hat{G}_k^{\alpha}(|x-y|,s) u^k(y) \mathrm{d}y, \tag{1.2.17}$$

where the convolution kernel $\hat{G}_k^{\alpha}(x,s)$ is denoted by the Laplace transform of a function $G_k^{\alpha}(x,t)$. Therefore, operating the inverse Laplace transform on (1.2.17) yields the explicit solution of (1.2.14) in the form of

$$u(x,t) = \sum_{k=0}^{m-1} \int_{\mathbb{R}^n} G_k^{\alpha}(|x-y|,t) u^k(y) \mathrm{d}y, \tag{1.2.18}$$

where the representation of G_k^{α} is given by

$$G_k^{\alpha}(x,t) = \pi^{-n/2} 2^{-1-2k/\alpha} x^{-n+2k/\alpha} H_{1,2}^{2,0}\left(\frac{1}{2} x t^{-\alpha/2} \Big|_{(n/2-k/\alpha,1/2),(1-k/\alpha,1/2)}^{(1,\alpha/2)}\right) \tag{1.2.19}$$

in terms of the Fox's H function $H_{p,q}^{m,n}$ (see Appendix A.1). Based on (1.2.19), the moments of the function $G_k^{\alpha}(x,t)$ of the form

$$M(l_1, l_2, \cdots, l_n) = \int_{\mathbb{R}^n} G_k^{\alpha}(|x|,t) x_1^{l_1} x_2^{l_2} \cdots x_n^{l_n} \mathrm{d}x$$

are confirmed to be finite for all $n \ge 1$, and in the case of the time-fractional diffusion equation, the mean square displacement is shown to be

$$\int_{\mathbb{R}^n} G_0^{\alpha}(|x|,t)|x|^2 \mathrm{d}x = \frac{2n}{\Gamma(1+\alpha)} t^{\alpha}, \qquad 0 < \alpha \le 1. \tag{1.2.20}$$

The time-fractional diffusion and wave equations can be used to characterize the anomalous diffusion process of some physical quantities in disordered systems. In particular, the time-fractional diffusion equation describes a subdiffusive process in contrast to its normal diffusion counterpart, since the mean square displacement of the solution $u(x,t)$ of the problem (1.2.14) follows the power-law pattern

$$\int_{\mathbb{R}^n} u(|x|,t)|x|^2 \mathrm{d}x \sim t^{\alpha}, \qquad \text{for } 0 < \alpha < 1.$$

Another derivation of time-fractional diffusion equation arises from a stochastic process such as the continuous time random walk (CTRW) [51]. If assuming $u(x,t)$ as a probability distribution function denoting the probability density of certain diffusive entity at the position $x \in \mathbb{R}^n$ and at time t, together with an initial state at the origin $x = 0$ and at $t = 0$, one considers a decoupled form of $u(x,t) = \lambda(x)w(t)$, where the function $\lambda(x)$ represents the probability density at the displacement x for all waiting times, defined by

$$\lambda(x) = \int_0^\infty u(x,t)\mathrm{d}t,$$

and the function $w(t)$ represents the probability density of waiting time t for all positions

$$w(t) = \int_{\mathbb{R}^n} u(x,t)\mathrm{d}x.$$

Note that $\lambda(x)$ is independent of $w(t)$. The CTRW process described by [54] produces

$$u(\xi,s) = \frac{1-\mathcal{L}(w)(s)}{s}\frac{\mathcal{F}(u^0)(\xi)}{1-\mathcal{F}(\lambda)(\xi)\mathcal{L}(w)(s)}, \tag{1.2.21}$$

where $u(\xi,s)$ is denoted by the Laplace transform and Fourier transform of $u(x,t)$ with respect to temporal variable and spatial variable, respectively. In the case that CTRW is characterized by $w(t) \sim t^{-1-\alpha}, 0 < \alpha < 1$ as $t \to \infty$ such that the first moment of probability distribution function of waiting time is infinite, i.e., $\tau_1 = \int_0^\infty w(t)t\mathrm{d}t = \infty$, the Laplace transform of $w(t)$ obeys

$$\mathcal{L}(w)(s) \sim 1 - c_\alpha s^\alpha, \qquad s \to 0, \tag{1.2.22}$$

and all the moments of $\lambda(x)$, denoted by $\sigma_k = \int_{\mathbb{R}^n} \lambda(x)|x|^k \mathrm{d}x,\ k = 0,1,\cdots$ are finite. In addition, we obtain

$$\mathcal{F}(\lambda)(\xi) = \int_{\mathbb{R}^n} e^{-i\xi x}\lambda(x)\mathrm{d}x = 1 - \frac{1}{2}\sigma_2|\xi|^2 + O(|\xi|^4). \tag{1.2.23}$$

Substituting (1.2.22) and (1.2.23) into (1.2.21) yields

$$u(\xi,s) = \frac{\mathcal{F}(u^0)(\xi)}{s}\frac{1}{1+K_\alpha s^{-\alpha}\xi^2} \tag{1.2.24}$$

for $\xi \to 0, s \to 0$, where $K_\alpha = \sigma_2/(2c_\alpha)$ is a finite constant. Therefore, applying the inverse Laplace and inverse Fourier transforms to (1.2.24), one derives the time-fractional diffusion equation

$$u(x,t) = u^0(x) + K_\alpha \mathcal{I}^\alpha \Delta u(x,t) \tag{1.2.25}$$

for $0 < \alpha < 1$, which can be reformulated to the form (1.2.15) similarly.

1.3 Numerical discretization of fractional differential equations

The investigation of the numerical approximation of fractional differential equations started its development recently. Before that, there existed lots of work on the numerical methods for Volterra type integral equations. In terms of designing numerical methods for the two types of equations, one of the essential difficulties arises from the numerical approximation to the integral term with an irregular kernel. For example, if we consider the problem (1.2.1) in the case $0 < \alpha < 1$, the Caputo derivative ${}^C\mathcal{D}^\alpha u(t)$ defined in (1.1.12) can be regarded as a convolution of the weakly singular kernel $t_+^{-\alpha}/\Gamma(1-\alpha)$ and $u^{(1)}(t)$, in which case the integrand is unbounded and integrable on $[0,T]$ with finite $T > 0$, if the function $u^{(1)}(t)$ is well-behaved. In practical implementation, it is known that standard numerical integration techniques are not applicable to this case. Therefore, two available approaches, that are called the product integration and the fractional linear multistep methods, are proposed, respectively, to numerically approximate some irregular integrals. In the following, we mainly recall these methods with the basic ideas and applications on numerically solving time-fractional differential equations.

1.3.1 Product integration method

As mentioned in [36], the product integration method was employed to evaluate an integral in the form of

$$\mathcal{I} = \int_a^b g(s)f(s)\mathrm{d}s,$$

where g is unbounded and integrable on the interval $[a, b]$ and f is a well-behaved function. The general idea of the product integration is to replace f by its approximation δf, and let

$$\delta\mathcal{I} = \int_a^b g(s)\delta f(s)\mathrm{d}s$$

be the numerical approximation to $\mathcal{I}$. By making use of the analytical property of kernel g, it is readily obtained

$$|\mathcal{I} - \delta\mathcal{I}| \leq \|f - \delta f\|_\infty \int_a^b |g(s)|\,\mathrm{d}s = O(\|f - \delta f\|_\infty). \tag{1.3.1}$$

Therefore, provided that $\|f - \delta f\|_\infty = O\left(\Delta t^p\right)$ through the numerical approximations, it is easy to know that the error between $\mathcal{I}$ and $\delta\mathcal{I}$ will be at least of p-th order accuracy with respect to Δt. As an application, this technique is first applied to numerically solve the nonlinear Volterra integral equation including a specific irregular kernel

$$u(t) = g(t) + \int_0^t (t-s)^{-\alpha} K(t, s, u(s))\mathrm{d}s. \tag{1.3.2}$$

A general discretized formula to (1.3.2) is proposed in the form of

$$u_n = g(t_n) + \sum_{j=0}^{n} W_{n,j} K(t_n, t_j, u_j) \qquad n \geq 1$$

by choosing some quadrature rules on the term $K(t, s, u(s))$, for instance, the combination of quadratic and cubic piecewise polynomial interpolation approximation is taken into consideration in [36] for $\alpha = 1/2$. In a similar way, higher order methods are constructed in [13] to approximate the problem (1.3.2) for $\alpha = 1/2$, and furthermore generalized by [11] for the case $0 \leq \alpha < 1$. In addition, the so-called backward difference product integration methods are proposed in [11]. These construct the piecewise polynomial approximation to the term $K(t_n, s, u(s))$ under the condition of interpolating at $(k+1)$ points $t_{j+1}, t_j, \cdots, t_{j+1-k}$ on each subinterval $[t_j, t_{j+1}]$ for $j \geq k-1$. On the subinterval $[t_0, t_{k-1}]$, polynomials of degree k interpolating at $t_0, \cdots, t_{k-1}$ are employed to generate the starting weights. Accordingly, the k starting values can be computed with other numerical methods. In this case, the discretized formula to problem (1.3.2) is written in the form of

$$u_n = g(t_n) + (\Delta t)^{1-\alpha} \sum_{j=0}^{k} w_{n,j} K(t_n, t_j, u_j) + (\Delta t)^{1-\alpha} \sum_{j=0}^{n} \omega_{n-j} K(t_n, t_j, u_j), \qquad n \geq k. \tag{1.3.3}$$

In terms of consistency, in [17] the local truncation error of the linear case of (1.3.2) is concerned, when the solution has an unbounded derivative at the origin (cf. Theorem 1.2.8). It is presented that $\tau_n = O\left(t_n^{-\alpha}\Delta t^{2-\alpha} + \Delta t^{p+1}\right)$ when piecewise polynomials of degree p are employed to approximate the kernel $K(t, s, u(s))$, where τ_n denotes the local truncation error at the n-th time step, and Δt is the stepsize of a uniform discretization. The relation between the consistency and convergence analysis of numerical method is also given in [11]:

Theorem 1.3.1. *If the discretized scheme is consistent of order p, and the starting values are convergent of order p, then the global error* $|u(t_n) - u_n|$ *is of p-th order accuracy.*

Alternative starting weights of (1.3.3) are introduced in [45], named the implicit Adams method, since for the case $\alpha = 1$, all of the methods reduce to the classical implicit Adams method. In addition, the numerical linear stability analysis of the methods, especially in terms of $A(\theta)$-stability , are fully developed:

i). The implicit Euler method and the trapezoidal rule are $A(\frac{\pi}{2})$-stable for all $0 < \alpha \leq 1$.

ii). For each k, there exists $\alpha_k > 0$ such that the k step implicit Adams method is $A(\frac{\pi}{2})$-stable for all α with $0 < \alpha \leq \alpha_k$.

iii). For $\alpha = \frac{1}{2}$, the k step implicit Adams methods are $A(\frac{\pi}{2})$-stable for $k = 0, 1, 2$.

Recently, there are more discussions and developments on fractional ordinary differential equations. In [16], fractional Adams methods are discussed with respect to the error estimation.

From the time-fractional ordinary differential equations to partial differential equations, in the framework of product integration rules, the so-called $L1$ scheme is proposed in [35] to numerically solve the time-fractional diffusion equation (1.2.15) in one-dimension in space. The method approximates the solution $u(t, x)$ by a piecewise linear polynomial $P^1(t)$ interpolating at points t_i and t_{i+1} on each subinterval $[t_i, t_{i+1}]$ in the time direction. The local truncation error in terms of time is proved to be of $(2-\alpha)$-order accuracy. In terms of the spatial discretization, the central difference method and the so-called Legendre spectral collocation method are applied seperately. The global error is theoretically and experimentally confirmed to be $O(\Delta t^{2-\alpha} + \Delta x^l)$ $(l \geq 2)$ under the assumption that the solution $u(t, x)$ possesses certain smoothness property on $[0, T]$. One idea to improve the order of accuracy is by employing the piecewise interpolation with a higher degree to approximate the solution. As discussed in [22], a discretization to the Caputo derivative of order $0 < \alpha < 1$ is constructed, which is named $L1$-2-formula. The approximation polynomial to u, denoted by $P_1^2(t)$, is the piecewise quadratic interpolating polynomial on the subintervals $[t_i, t_{i+1}]$ for $i \geq 1$ using interpolation points (t_{i-2}, f_{i-2}), (t_{i-1}, f_{i-1}) and (t_i, f_i), and on $[t_0, t_1]$, is a linear function. Consequently, the Caputo fractional derivative of $P_1^2(t)$ is considered as the approximation to ${}^C\mathcal{D}^\alpha u(t)$ for $t_1 < t \leq T$. Here, the starting value at $t = t_1$ is computed by the $L1$-method. Because of the construction, it seems to be very hard to carry on the convergence analysis for this scheme. The consistency analysis tells:

Theorem 1.3.2 ([22]). *Suppose* $u(t) \in C^3[0, t_n]$ *for* $n \geq 1$. *Then*

$$\begin{aligned}
\left|{}^C\mathcal{D}^\alpha\left(u(t_1) - P^1(t_1)\right)\right| &\leq c_\alpha \max_{t_0 \leq t \leq t_1} |u^{(2)}(t)| \Delta t^{2-\alpha}, \\
\left|{}^C\mathcal{D}^\alpha\left(u(t_n) - P_1^2(t_n)\right)\right| &\leq \tilde{c}_\alpha\Big(\max_{t_0 \leq t \leq t_1} |u^{(2)}(t)|(t_n - t_1)^{-\alpha-1}\Delta t^3 \\
&\quad + \max_{t_0 \leq t \leq t_n} |u^{(3)}(t)|\Delta t^{3-\alpha}\Big), \qquad n \geq 2,
\end{aligned}$$

where constants c_α *and* $\tilde{c}_\alpha$ *are independent of* Δt.

Another modified scheme of the $L1$-2 formula is investigated in [47] to numerically solve the problem (1.2.15). This scheme is based on a modified quadratic piecewise polynomial $P_2^2(t_n)$ as an approximation to the solution $u(t_n)$ by means of the interpolating conditions at the points t_{j-1}, t_j and t_{j+1} on each $[t_{j-1}, t_j]$ for $1 \le j \le n-1$, and at points t_{n-2}, t_{n-1} and t_n on $[t_{n-1}, t_n]$. A similar result as Theorem 1.3.2 is presented by means of providing a uniform $(3-\alpha)$-order accuracy of local truncation error τ_n with $n \ge 2$. In combination with the spectral method for the spatial discretization, the semidiscretized formula of the problem is proved to be unconditionally stable under a certain norm. The corresponding convergence order is confirmed to be preserved of $(3-\alpha)$-order with respect to time. For other analogous results applied to the variable fractional diffusion equation, we refer to [3].

On the other hand, it is noticed the regularity condition to the solution isn't always proper, as mentioned before in Theorem 1.2.2, and also in [31]: the solution has an unbounded derivative with respect to time at $t = 0$ for the homogeneous case of problem (1.2.15) with a smooth initial value. In that case, the $(2-\alpha)$-order convergence of the global error can't be preserved, instead, an $O(\Delta t)$ convergence rate in terms of time is proved on a uniform grid in [31] together with a spatial discretization in the continuous piecewise linear finite element space:

$$X = \{u \in H_0^1(\Omega) : \ u \text{ is a linear polynomial on each element of } \Omega\}.$$

In addition, a global error estimation with nonsmooth initial value $u^0(x) \in L^2(\Omega)$ is provided:

Theorem 1.3.3. *Let $u(t,x)$ be the solution of (1.2.15) with $f = 0$, $U(t,x)$ be the solution of the corresponding numerical scheme based on the $L1$ discretization in time and continuous piecewise linear finite element approximation in space with $U^0(x) = \tilde{u}^0(x)$, where $\tilde{u}^0(x)$ is denoted by the $L^2(\Omega)$-orthogonal projection of $u^0(x)$ into space X. Then*

$$\|u(t_n,x) - U(t_n,x)\|_2 \le C\left(t_n^{-1}\Delta t + t_n^{-\alpha}\Delta x^2\right)\|u^0(x)\|_2, \qquad n \ge 1, \tag{1.3.4}$$

where $\|\cdot\|_2$ is the L^2-norm.

1.3.2 Fractional linear multistep method

Another approach called the fractional linear multistep method, was originally proposed in [39] and later extended in [40] to approximate the convolution integral

$$\mathcal{I}(t) = \int_0^t f(t-s)g(s)\mathrm{d}s = \int_0^t f(s)g(t-s)\mathrm{d}s \tag{1.3.5}$$

in the case that f is locally integrable on $\mathbb{R}^+$. The discretized form is constructed with the help of the Laplace transform of f. If $F(s)$ denotes the Laplace transform of f, then (1.3.5) is rewritten to

$$\mathcal{I}(t) = \frac{1}{2\pi i}\int_\Gamma F(s)\left(\int_0^t e^{st}g(t-s)\mathrm{d}t\right)\mathrm{d}s = \frac{1}{2\pi i}\int_\Gamma F(s)y(t;s)\mathrm{d}s, \tag{1.3.6}$$

where $y(t;s)$ satisfies the differential equation

$$y'(t) = sy(t) + g(t), \qquad y(0) = 0. \tag{1.3.7}$$

Remark 1.3.1. *It is known that the linear first order differential equation*

$$y'(t) + P(t)y(t) = Q(t), \qquad y(0) = 0$$

has the explicit solution expressed by

$$y(t) = e^{-\int_0^t P(\tau)\mathrm{d}\tau} \int_0^t e^{\int_0^\xi P(\tau)\mathrm{d}\tau} Q(\xi)\mathrm{d}\xi. \tag{1.3.8}$$

This yields that $y(t) = \int_0^t e^{s(t-\xi)} g(\xi)\mathrm{d}\xi = \int_0^t e^{s\xi} g(t-\xi)\mathrm{d}\xi$ *when replacing* $P(t)$ *by* $-s$ *and* $Q(t)$ *by* $g(t)$ *separately into the expression* (1.3.8).

If approximating y by δy, and accordingly, one defines that

$$\delta\mathcal{I}(t) = \frac{1}{2\pi i}\int_\Gamma F(s)\delta y(t;s)\mathrm{d}s \tag{1.3.9}$$

as an approximation to $\mathcal{I}(t)$. In [39], the k-step linear multistep methods (ρ,σ) [25, 24, 29] are employed to obtain δy. The general form of linear multistep method for (1.3.7) is denoted by

$$\sum_{j=0}^{k} \alpha_j \delta y_{n+j-k} = \Delta t \sum_{j=0}^{k} \beta_j \left(s\delta y_{n+j-k} + g_{n+j-k}\right), \qquad n \geq 0, \tag{1.3.10}$$

and the starting values and $g_{-k},\cdots,g_{-1}$ are chosen zero. In addition, rewriting (1.3.10) into a power series form yields

$$\rho(1/\xi)\delta y(\xi) = \Delta t\sigma(1/\xi)\left(s\delta y(\xi) + g(\xi)\right) \tag{1.3.11}$$

with the series denoted by

$$\rho(\xi) = \sum_{j=0}^{k}\alpha_j\xi^j, \quad \sigma(\xi) = \sum_{j=0}^{k}\beta_j\xi^j, \quad \delta y(\xi) = \sum_{n=0}^{\infty}\delta y_n\xi^n, \quad g(\xi) = \sum_{n=0}^{\infty} g_n\xi^n.$$

Substituting (1.3.11) into (1.3.9), one has

$$\delta\mathcal{I}(\xi) = \frac{1}{2\pi i}\int_\Gamma F(s)\left(\frac{\omega(\xi)}{\Delta t} - s\right)^{-1} g(\xi)\mathrm{d}s = F\left(\frac{\omega(\xi)}{\Delta t}\right) g(\xi), \tag{1.3.12}$$

where $\omega(\xi) = \rho(1/\xi)/\sigma(1/\xi)$. It is noted that the last equality of (1.3.12) holds based on the Cauchy integral formula and the assumptions that

i) $F(s)$ is analytic in the sector $S_{\varphi,c} = \{s \in \mathbb{C} : |\arg(s-c)| < \pi - \varphi\}$ with $\varphi < \pi/2$ and $c \in \mathbb{R}$, and is bounded by

$$|F(s)| \leq M|s|^{-\mu}, \qquad \mu \in \mathbb{R}^+.$$

ii) the linear multistep method (ρ,σ) is strongly zero-stable, $A(\theta)$-stable for some $\theta > \varphi$ such that point $\omega(\xi)/\Delta t$ for $|\xi| \leq 1$ falls in the sector $S_{\varphi,c}$, and is consistent of order $p \geq 1$.

Hence, the corresponding coefficients satisfy

$$\delta\mathcal{I}_n = \sum_{j=0}^{n}\omega_{n-j}^{\mu} g_j \qquad \text{for } n \geq 0,$$

where the convolution quadrature weights $\{\omega_n^\mu\}_{n=0}^\infty$ are the generating coefficients of the series $F\left(\frac{\omega(\xi)}{\Delta t}\right)$, i.e., $F\left(\frac{\omega(\xi)}{\Delta t}\right) = \sum_{n=0}^\infty \omega_n^\mu \xi^n$. Based on (1.3.6) and (1.3.9), the convolution error is obtained by

$$\mathcal{I}(t_n) - \delta\mathcal{I}_n = \frac{1}{2\pi i}\int_\Gamma F(s)\left(y(t_n;s) - \delta y(t_n;s)\right)\mathrm{d}s. \tag{1.3.13}$$

An estimate in [39] states that

$$\begin{aligned}|\mathcal{I}(t_n) - \delta\mathcal{I}_n| \le & C t_n^{\mu-1} \max_{s\in\Gamma} |y(t_n;s) - \delta y(t_n;s)| \\ \le & C t_n^{\mu-1} \left(\sum_{k=0}^{p-1} (\Delta t)^{k+1} |g^{(k)}(0)| + (\Delta t)^p t_n \max_{0\le t\le t_n} |g^{(p)}(t)| \right), \qquad n \ge 1,\end{aligned} \tag{1.3.14}$$

where the time step Δt is sufficiently small and $g \in C^p[0,T]$.

The original application of fractional linear multistep methods is to numerically solve the problem (1.2.2) for the case $\alpha \in (0,1)$, where the initial condition u^0 is substituted by a general source term $g(t)$. The discretization form

$$I^\alpha f(t_n, u_n) = (\Delta t)^\alpha \sum_{j=0}^{s} w_{n,j}^\alpha f(t_j, u_j) + (\Delta t)^\alpha \sum_{j=0}^{n} \omega_{n-j}^\alpha f(t_j, u_j) \tag{1.3.15}$$

is proposed to approximate the fractional integral $\mathcal{I}^\alpha f(t, u(t))$ included in (1.2.2), which can be regarded as a particular convolution integral form of the formula (1.3.5). For example, it is well known that the classical zero-stable BDF methods have the following generating polynomials

$$(\rho, \sigma) = \left(\sum_{i=1}^{k} \frac{\nabla_k^i \xi^k}{i}, \xi^k \right), \qquad k = 1, \cdots, 6, \tag{1.3.16}$$

where $\nabla_k \xi^k = \xi^k - \xi^{k-1}$ and $\nabla_k^{i+1}\xi^k = \nabla_k^i \xi^k - \nabla_k^i \xi^{k-1}$. Therefore, according to $\mathcal{L}\left(t_+^{\alpha-1}/\Gamma(\alpha)\right) = s^{-\alpha}$ with $\Re s > 0$ and equality (1.3.12), the convolution quadrature weights $\{\omega_n^\alpha\}$ in (1.3.15) are constructed by

$$\sum_{n=0}^{\infty} \omega_n^\alpha \xi^n = \left(\sum_{i=1}^{k} \frac{(1-\xi)^i}{i} \right)^{-\alpha}, \qquad k = 1, \cdots, 6. \tag{1.3.17}$$

In the case $u(t) \in C^p([0,T])$, the starting quadrature weights $\{w_{n,j}\}$ are uniquely determined by

$$(\Delta t)^\alpha \sum_{j=0}^{n} \omega_{n-j}^\alpha t_j^k + (\Delta t)^\alpha \sum_{j=0}^{p-2} w_{n,j} t_j^k = \mathcal{I}^\alpha t_n^k, \qquad k = 0, 1, \cdots, p-2.$$

And in the other case $u(t) = U(t, t^\alpha)$ for $U \in C^1$, the starting quadrature weights $\{w_{n,j}\}$ satisfy

$$(\Delta t)^\alpha \sum_{j=0}^{n} \omega_{n-j}^\alpha t_j^\gamma + (\Delta t)^\alpha \sum_{j=0}^{p-2} w_{n,j} t_j^\gamma = \mathcal{I}^\alpha t_n^\gamma, \qquad \gamma = k + l\alpha.$$

Therefore, the consistency result can be a direct consequence of (1.3.14), or discussed in another way in [44]. An estimate of the global error is given in [43] to show that if $w_{n,j} = O(n^{\alpha-1})$, then there exists a constant $C > 0$ which is independent of n and Δt, such that the difference between the numerical solution u_n and the exact solution $u(t_n)$ satisfies

$$|u_n - u(t_n)| \le C t_n^{\beta-1} (\Delta t)^p, \qquad \beta > \alpha. \tag{1.3.18}$$

Furthermore, the stability of the numerical methods is investigated in [45]. The stability regions S of the methods are proved to be

$$S = \mathbb{C} \backslash \{\lambda(\Delta t)^\alpha : 1/\left(\sum_{n=0}^{\infty} \omega_n^\alpha \xi^n \right) \text{ for } |\xi| \le 1\}, \tag{1.3.19}$$

which is equivalent to saying that for any $\lambda(\Delta t)^\alpha \in S$, the numerical solution $u_n \to 0$ as $n \to \infty$ with arbitrary bounded $f(t_n)$. Accordingly, the stability result of convolution quadrature $\{\omega_n^\alpha\}$ connecting to the corresponding linear multistep method (ρ, σ) can be readily presented:

Theorem 1.3.4 ([43]). *Assume that the linear multistep method (ρ,σ) satisfies the strong root condition and $A(\theta)$-stability for some $0<\theta\le\pi/2$, and define*

$$\omega^{\alpha}(\xi) := (\delta(\xi))^{\alpha} = (\sigma(1/\xi)/\rho(1/\xi))^{\alpha}.$$

Let S_{ω^α} and S_δ denote the stability regions of ω^α and δ, respectively. Then, one has

i). $(\mathbb{C}\backslash S_{\omega^\alpha}) = (\mathbb{C}\backslash S_\delta)^{\alpha}$.

ii). *ω^α is absolutely stable iff δ is absolutely stable.*

iii). *ω^α is $A(\pi-\alpha(\pi-\theta))$-stable iff δ is $A(\theta)$-stable.*

Furthermore, [46] treats the integro-differential equation of the form

$$\begin{aligned}&\frac{\partial u(x,t)}{\partial t}+\frac{1}{\Gamma(\alpha)}\int_0^t (t-\xi)^{\alpha-1}Au(x,\xi)\mathrm{d}\xi = f(x,t), \qquad (x,t)\in\Omega\times[0,T],\\ &u(0,x)=u^0(x), \qquad u(t,x)|_{x\in\partial\Omega}=c,\end{aligned} \tag{1.3.20}$$

where $0<\alpha<1$ and A is assumed to be a self-adjoint positive definite second-order elliptic operator or a positive definite linear operator in a real Hilbert space H. In terms of the time discretization, the first-order and second-order fractional BDF methods of (1.3.17) are employed to approximate the integral term in (1.3.20), respectively. And the implicit Euler method and second-order BDF method are accordingly used to replace the first-order time derivative. The semidiscrete formulae with respect to time are written in the forms

$$U_h^n(x)-U_h^{n-1}(x)+(\Delta t)^{1+\alpha}\sum_{j=0}^{n}\omega_{n-j}^{\alpha,1}AU_h^j(x)=\Delta t f^n(x), \qquad n\ge 1 \tag{1.3.21a}$$

and

$$\frac{3}{2}U_h^n(x)-2U_h^{n-1}(x)+\frac{1}{2}U_h^{n-2}(x)+(\Delta t)^{1+\alpha}\left(\frac{1}{2}\omega_{n-1}^{\alpha,2}AU_h^0(x)+\sum_{j=1}^{n}\omega_{n-j}^{\alpha,2}AU_h^j(x)\right)=\Delta t f^n(x), \ \ n\ge 2, \tag{1.3.21b}$$

where $\{\omega_j^{\alpha,k}\}$ are the generating coefficients of the series (1.3.17) for $k=1,2$. In the case of (1.3.21b), the starting value $U_h^1(x)$ is computed in advance by a suitable scheme. In the homogenous case of (1.3.20), global error estimates can be found:

$$\|U_h^n-u(t_n)\|\le\|U_h^n-u_h(t_n)\|+\|u_h(t_n)-u(t_n)\|\le C\left(\Delta t^k t_n^{-k}+h^2 t_n^{-\alpha-1}\right)\|u^0\|,$$

where $k=1,2$ and $n\ge 1$.

In this part, we mainly recall some basic definitions and properties of fractional calculus and time-fractional differential equations. Two types of well-known methods are briefly introduced to numerically solve fractional differential equations. In the following chapters, we construct the numerical approximations to time-fractional differential equations, and investigate the consistency, stability and convergence of the numerical schemes.

Chapter 2

Continuous piecewise polynomial approximation

In order to numerically solve a system of time-fractional differential equations of the form

$$^{C}\mathcal{D}^{\alpha}\mathbf{u}(t) = \mathbf{f}(t, \mathbf{u}(t)), \qquad 0 < \alpha < 1, \tag{2.0.1}$$

with prescribed initial conditions $\mathbf{u}(0)$ and given vector function $\mathbf{f}$, we are mainly concerned with constructing a series of numerical approximations to the Caputo fractional derivative of a function $u(t)$ in the case $0 < \alpha < 1$. As remarked before, recently, the so-called $L1$ method [35], $L1$-2 method [22] and $L2$-1_σ method [3] are designed to approximate the Caputo fractional derivative for solving time-fractional diffusion equations. These methods are based on piecewise linear or quadratic interpolating polynomials approximation in the framework of the product integration method. It is natural to generalize the approach by improving the degree of the piecewise polynomial to approximate a function that possesses suitable smoothness, in which situation a higher order of accuracy can be obtained. In the following sections, we shall derive a series of discretized schemes on uniform and non-uniform temporal grids by making use of continuous piecewise polynomials as approximations to solution $u(t)$, and consequently, the α order Caputo derivative of the polynomials as the approximations to $^{C}\mathcal{D}^{\alpha}u(t)$. Some properties of the quadrature weights are analyzed. The local truncation errors of the numerical schemes are discussed correspondingly.

2.1 Uniform grid approximation of Caputo fractional derivative

Let $I = [0, T]$ be an interval and the $M + 1$ nodes $\{t_i\}_{i=0}^{M}$ define a partition

$$0 = t_0 < t_1 \cdots < t_{M-1} < t_M = T. \tag{2.1.1}$$

If the solution $u(t)$ is assumed to be continuous on the interval I, and we think about a piecewise polynomial approximation to $u(t)$, it is reasonable to find the approximate solution at least in the continuous piecewise polynomial space, which is defined by

$$C_p(I) = \{v(t) \in C(I) : \ \ v(t) \text{ is a polynomial on each subinterval } I_j = [t_{j-1}, t_j]\}.$$

Specifically, denoting the space of continuous piecewise polynomial of degree at most k by

$$C_p^k(I) = \{v(t) \in C(I) : \ \ v(t) = \sum_{l=0}^{k} a_{j,l} t^l \text{ on } I_j\},$$

we construct a class of approximate solutions of $u(t)$ in the space $C_p^k(I)$. Here the Lagrangian interpolation technique by prescribing interpolation conditions on distinct $k+1$ nodes is used, such that the coefficients $\{a_{j,l}\}$ for $0 \le l \le k$ on each I_j are uniquely determined. In addition, assume that $u(t)$ is not a constant function, then we only need to focus on the case $k \ge 1$ in view of the continuity restriction. The choice of the interpolating points is provided in the following way.

We define a class of polynomials $p_{j,q}^k(t)$ that are of degree $k \ge 1$ and have a compact support I_j. The coefficients of the polynomials are uniquely determined by the following $k+1$ interpolation conditions

$$p_{j,q}^k(t_n) = u(t_n), \qquad n = j+q-1, j+q-2, \cdots, j+q-k-1. \tag{2.1.2}$$

Here the index q records the number of shifts of the $k+1$ interpolating nodes $\{t_n\}_{n=j-1-k}^{j-1}$, and the sign of q indicates the direction of the shift. Based on (2.1.2), the polynomials can be represented by a Lagrange form

$$p_{j,q}^k(t) = \sum_{n=j+q-k-1}^{j+q-1} \prod_{\substack{m=j+q-k-1 \\ m \neq n}}^{j+q-1} \frac{t - t_m}{t_n - t_m} u(t_n). \tag{2.1.3}$$

In particular, if the partition (2.1.1) is equidistant, i.e., $t_n = n\Delta t$ and $\Delta t = \frac{T}{M}$ as $M \in \mathbb{N}^+$, the alternative Newton expression is given by

$$p_{j,q}^k(t) = \sum_{n=0}^{k} \frac{\nabla^n u(t_{j+q-1})}{n!(\Delta t)^n} \prod_{l=0}^{n-1} (t - t_{j+q-1-l}). \tag{2.1.4}$$

For convenience of notation, we rewrite (2.1.4) by changing the variable $t = t_{j-1} + s\Delta t$ to obtain

$$p_{j,q}^k(t) = p_{j,q}^k(t_{j-1} + s\Delta t) = \sum_{r=0}^{k} \binom{s-q+r-1}{r} \nabla^r u(t_{j+q-1}), \tag{2.1.5}$$

where the r-th order backward difference operator ∇^r is commonly defined by

$$\nabla^0 u(t_i) = u(t_i), \quad \nabla^r u(t_i) = \nabla^{r-1} u(t_i) - \nabla^{r-1} u(t_{i-1})$$

and $\binom{s-q+r-1}{r}$ is the binomial coefficient. In addition, it follows that

$$\frac{\mathrm{d}^m p_{j,q}^k}{\mathrm{d}s^m} = \sum_{r=0}^{k} \frac{\mathrm{d}^m}{\mathrm{d}s^m} \binom{s-q+r-1}{r} \nabla^r u_{j+q-1}, \qquad m \in \mathbb{N}. \tag{2.1.6}$$

In the following, we construct a class of approximate solutions $P_i^k(t) \in C_p^k(I)$ to $u(t)$ on the uniform grid for $1 \le i \le k \le 6$. The general representations are proposed by

$$P_i^k(t) = \sum_{j=1}^{k-i} p_{j,k-j}^{k-1}(t) + \sum_{j=k}^{n} p_{j-i+1,i}^k(t) + \sum_{j=n-i+2}^{n} p_{j,n+1-j}^k(t) \tag{2.1.7}$$

for $t \in (t_{n-1}, t_n]$ and $1 \le n \le M$, where $\sum_{j=1}^{k-i} p_{j,k-j}^{k-1}(t) = 0$ and $\sum_{j=n-i+2}^{n} p_{j,n+1-j}^k(t) = 0$ if $k - i < 1$ and $n - i + 2 > n$, respectively.

Remark 2.1.1. *The construction of polynomials $P_i^k(t)$ is mainly based on the continuity requirement on interval I, i.e., the interpolation conditions*

$$p_{j,q}^k(t_n) = u(t_n), \qquad n = j-1,\ j \tag{2.1.8}$$

should be satisfied. It yields that on each subinterval I_j, according to (2.1.2), both conditions $j+q-1 \geq j$ and $j+q-k-1 \leq j-1$ should be satisfied, which indicates $1 \leq q \leq k$. Therefore, in the case $k=1$, there is a unique continuous piecewise linear polynomial, denoted by $P_1^1(t)$, in the space $C_p^1(I)$. According to (2.1.7), it is expressed by

$$P_1^1(t) = \sum_{j=1}^{n} p_{j,1}^1(t),$$

which presents that on each I_j with $1 \leq j \leq n$, $P_1^1(t) = p_{j,1}^1(t)$ holds and the condition (2.1.2) is satisfied. In the other case $k=2$, there are three options on each I_j, that is, $p_{j,1}^1(t)$, $p_{j,1}^2(t)$ and $p_{j,2}^2(t)$ to constitute the interpolating polynomial that belongs to space $C_p^2(I)$. It is known that the construction of $P^2(t)$ is therefore not unique. In order to preserve the convolution property as much as possible, we propose three available continuous piecewise polynomials in forms of

$$P_1^2(t) = p_{1,1}^1(t) + \sum_{j=2}^{n} p_{j,1}^2(t), \qquad P_2^2(t) = \sum_{j=1}^{n-1} p_{j,2}^2(t) + p_{n,1}^2(t) \tag{2.1.9}$$

and

$$P_3^2(t) = p_{1,2}^2(t) + \sum_{j=2}^{n} p_{j,1}^2(t)$$

when $t \in (t_{n-1}, t_n]$. In addition, as shown in (2.1.7), we restrict our further discussion to the case $i \leq k$. This is because in that situation, the least starting values are prescribed.

As a consequence, the operator

$$D_{k,i}^\alpha u(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-\xi)^{-\alpha} \frac{\mathrm{d}P_i^k}{\mathrm{d}\xi} \mathrm{d}\xi \tag{2.1.10}$$

is proposed on $t \in I$ as the approximations to ${}^C\mathcal{D}^\alpha u(t)$. In the case $t = t_n$, formula (2.1.10) can also be rewritten as

$$\begin{aligned} D_{k,i}^\alpha u_n &= \frac{(\Delta t)^{-\alpha}}{\Gamma(1-\alpha)} \sum_{j=1}^{n} \int_0^1 (n-j+1-s)^{-\alpha} \frac{\mathrm{d}P_i^k(t_{j-1}+s\Delta t)}{\mathrm{d}s} \mathrm{d}s \\ &= (\Delta t)^{-\alpha} \sum_{j=0}^{k-1} w_{n,j}^{(k,i)} u_j + (\Delta t)^{-\alpha} \sum_{j=0}^{n} \omega_{n-j}^{(k,i)} u_j, \end{aligned} \tag{2.1.11}$$

where $u_n := u(t_n)$. In the following part, we will present the weight coefficients $\{w_{n,j}^{(k,i)}\}$ and $\{\omega_j^{(k,i)}\}$ in the cases $1 \leq i \leq k \leq 3$ as examples. We first define a class of integral of forms

$$I_{n,q}^r = \begin{cases} \frac{1}{\Gamma(1-\alpha)} \int_0^1 (n+1-s)^{-\alpha} \mathrm{d}\left(s-q+r-1 \atop r\right), & n \geq 0, \\ 0, & n < 0, \end{cases} \tag{2.1.12}$$

where $q, r \in \mathbb{N}^+$ and $n \in \mathbb{Z}$. In addition, note that

$$I_n := I^1_{n,q}, \quad \forall\, q = 1, 2, \cdots,$$
$$\nabla^k I^r_{n,q} = \nabla^{k-1} I^r_{n,q} - \nabla^{k-1} I^r_{n-1,q}, \quad \forall\, k \in \mathbb{N}^+.$$

Then the weight coefficients can be expressed in terms of integrals $I^r_{n,q}$ by

$$\begin{cases} (k,i) = (1,1): \; w_{m,0} = -I_m, \quad m \geq 1, \quad \omega_n = \nabla I_n, \quad n \geq 0, \\ (k,i) = (2,1): \; w_{m,0} = 2I^2_{m-1,1} - I^2_{m,1} - I_m, \quad w_{m,1} = -I^2_{m-1,1}, \; m \geq 2, \\ \qquad \omega_n = \nabla I_n + \nabla^2 I^2_{n,1}, \quad n \geq 0, \\ (k,i) = (2,2): \; w_{m,0} = -\nabla I^2_{m+1,1} + I^2_{m,2}, \quad w_{m,1} = -I^2_{m,1}, \quad m \geq 2, \\ \qquad \omega_0 = I_0 + I_1 + I^2_{0,1} + I^2_{1,2}, \quad \omega_1 = \nabla I_2 - I_0 + I^2_{2,2} - 2I^2_{0,1} - 2I^2_{1,2}, \\ \qquad \omega_2 = \nabla I_3 + \nabla^2 I^2_{3,2} + I^2_{0,1}, \quad \omega_n = \nabla I_{n+1} + \nabla^2 I^2_{n+1,2}, \; n \geq 3, \end{cases}$$

and by more complicated formulae of forms

i). $(k,i) = (3,1)$,

$$\begin{cases} w_{m,0} = -\nabla I_m - I^2_{m,1} + 2I^2_{m-1,1} + I^2_{m-1,2} - I^3_{m,1} + 3I^3_{m-1,1} - 3I^3_{m-2,1}, \\ w_{m,1} = -2I_{m-1} - 2I^2_{m-1,2} - I^2_{m-1,1} - I^3_{m-1,1} + 3I^3_{m-2,1}, \\ w_{m,2} = I_{m-1} + I^2_{m-1,2} - I^3_{m-2,1}, \qquad m \geq 3, \\ \omega_n = \nabla I_n + \nabla^2 I^2_{n,1} + \nabla^3 I^3_{n,1}, \qquad n \geq 0, \end{cases} \tag{2.1.13}$$

ii). $(k,i) = (3,2)$,

$$\begin{cases} w_{m,0} = -\nabla I_{m+1} - I^2_{m+1,2} + 2I^2_{m,2} - I^3_{m+1,2} + 3I^3_{m,2} - 3I^3_{m-1,2}, \\ w_{m,1} = -I_m - I^2_{m,2} - I^3_{m,2} + 3I^3_{m-1,2}, \\ w_{m,2} = -I^3_{m-1,2}, \quad m \geq 3, \\ \omega_0 = I_0 + I_1 + I^2_{1,2} + I^2_{0,1} + I^3_{1,2} + I^3_{0,1}, \\ \omega_1 = \nabla I_2 - I_0 + I^2_{2,2} - 2I^2_{1,2} - 2I^2_{0,1} + I^3_{2,2} - 3I^3_{1,2} - 3I^3_{0,1}, \\ \omega_2 = \nabla I_3 + \nabla^2 I^2_{3,2} + I^2_{0,1} + I^3_{3,2} - 3I^3_{2,2} + 3I^3_{1,2} + 3I^3_{0,1}, \\ \omega_3 = \nabla I_4 + \nabla^2 I^2_{4,2} + \nabla^3 I^3_{4,2} - I^3_{0,1}, \\ \omega_n = \nabla I_{n+1} + \nabla^2 I^2_{n+1,2} + \nabla^3 I^3_{n+1,2}, \quad n \geq 4, \end{cases} \tag{2.1.14}$$

iii). $(k,i) = (3,3)$,

$$\begin{cases} w_{m,0} = -\nabla I_{m+2} - \nabla^2 I^2_{m+2,3} - I^3_{m+2,3} + 3I^3_{m+1,3} - 3I^3_{m,3}, \\ w_{m,1} = -\nabla I_{m+1} - I^2_{m+1,3} + 2I^2_{m,3} - I^3_{m+1,3} + 3I^3_{m,3}, \\ w_{m,2} = -I_m - I^2_{m,3} - I^3_{m,3}, \quad m \geq 3, \\ \omega_0 = I_0 + I_1 + I_2 + I^2_{0,1} + I^2_{1,2} + I^2_{2,3} + I^3_{0,1} + I^3_{1,2} + I^3_{2,3}, \\ \omega_1 = \nabla I_3 - I_0 - I_1 + I^2_{3,3} - 2I^2_{2,3} - 2I^2_{1,2} - 2I^2_{0,1} + I^3_{3,3} - 3I^3_{2,3} - 3I^3_{1,2} - 3I^3_{0,1}, \\ \omega_2 = \nabla I_4 + \nabla^2 I^2_{4,3} + I^2_{1,2} + I^2_{0,1} + I^3_{4,3} - 3I^3_{3,3} + 3I^3_{2,3} + 3I^3_{0,1} + 3I^3_{1,2}, \\ \omega_3 = \nabla I_5 + \nabla^2 I^2_{5,3} + \nabla^3 I^3_{5,3} - I^3_{1,2} - I^3_{0,1}, \\ \omega_n = \nabla I_{n+2} + \nabla^2 I^2_{n+2,3} + \nabla^3 I^3_{n+2,3}, \quad n \geq 4. \end{cases} \tag{2.1.15}$$

In addition, it is observed that when $\alpha \to 1$, the difference operator $D^{\alpha}_{k,i}u_n$ in (2.1.11) recovers to a k-step BDF method.

Remark 2.1.2. *The construction process of operator* (2.1.10) *can be extended to the case* $\alpha > 1$ *as well. In a general case* $\lceil\alpha\rceil - 1 < \alpha < \lceil\alpha\rceil$*, the interpolating polynomials* $P^k_i(t) \in C^k_p(I)$ *could be constructed as the approximations to* $u(t)$ *under the condition that* $k \geq \lceil\alpha\rceil$*, and the* α *order Caputo derivative of* $P^k_i(t)$ *are proposed in a similar way by*

$$D^{\alpha}_{k,i}u(t) = \frac{1}{\Gamma(\lceil\alpha\rceil - \alpha)}\int_0^t (t-\xi)^{-\alpha+\lceil\alpha\rceil-1}\frac{\mathrm{d}^{\lceil\alpha\rceil}P^k_i}{\mathrm{d}\xi^{\lceil\alpha\rceil}}\mathrm{d}\xi$$

as the approximation to ${}^{C}D^{\alpha}u(t)$*. Here the condition of* $k \geq \lceil\alpha\rceil$ *is required such that the* $\lceil\alpha\rceil$ *order derivative of* $P^k_i(t)$ *is nonzero a.e.. We take the case* $\lceil\alpha\rceil = 2$ *as an example. Assume that* $\beta = \alpha - 1 \in (0,1)$*, the polynomials* $P^2_i(t)$ *denoted by* (2.1.9) *are in the space* $C^2_p(I)$*, and it follows that*

$$\begin{aligned} D^{\alpha}_{2,i}u(t_n) =& \frac{1}{\Gamma(1-\beta)}\sum_{j=1}^{n}\int_{t_{j-1}}^{t_j}(t_n-\xi)^{-\beta}\frac{\mathrm{d}^2P^2_i}{\mathrm{d}\xi^2}\mathrm{d}\xi \\ =& \frac{(\Delta t)^{-\alpha}}{\Gamma(1-\beta)}\sum_{j=1}^{n}\int_0^1 (n-j+1-s)^{-\beta}\frac{\mathrm{d}^2P^2_i(t_{j-1}+s\Delta t)}{\mathrm{d}s^2}\mathrm{d}s, \end{aligned}$$

where the last equality holds based on the relation $\frac{\mathrm{d}^2P^k_i(\xi(s))}{\mathrm{d}s^2} = \frac{\mathrm{d}^2P^k_i(\xi)}{\mathrm{d}\xi^2}\left(\frac{\mathrm{d}\xi}{\mathrm{d}s}\right)^2 + \frac{\mathrm{d}P^k_i(\xi)}{\mathrm{d}\xi}\frac{\mathrm{d}^2\xi}{\mathrm{d}s^2}$*. Moreover, it can be rewritten as a form analogous to* (2.1.11)*, and the corresponding weights coefficients* $\{w_{n,i}\}$ *and* $\{\omega_n\}$ *are therefore derived by*

$$\begin{cases} \omega^{(2,1)}_j = \nabla^2 I_j, \quad j \geq 0, \quad w^{(2,1)}_{n,0} = -\left(I_n - 2I_{n-1}\right), \quad w^{(2,1)}_{n,1} = -I_{n-1}, \quad n \geq 2, \\ \omega^{(2,2)}_0 = I_0 + I_1, \quad \omega^{(2,2)}_1 = I_2 - 2I_1 - 2I_0, \quad \omega^{(2,2)}_2 = \nabla^2 I_3 + I_0, \\ \omega^{(2,2)}_j = \nabla^2 I_{j+1}, \quad j \geq 3, \quad w^{(2,2)}_{n,0} = -I_{n+1} + 2I_n, \quad w^{(2,2)}_{n,1} = -I_n, \quad n \geq 2. \end{cases} \tag{2.1.16}$$

Here the integrals $I^r_{n,q} = I^r_{n,q}(\beta)$ *are defined by* (2.1.12) *where the index* α *is replaced by* β*.*

First, we explore the completely monotonic property of the sequence $\{I^r_{n,q}\}^{\infty}_{n=0}$.

Lemma 2.1.1. *Assume that* $I^r_{n,q}$ *is defined by* (2.1.12)*, then for* $n \geq k$ *with* $k \in \mathbb{N}$*, it holds that*

$$(-1)^{k+r+1}\nabla^k I^r_{n,q} \geq 0 \tag{2.1.17}$$

in the case $r \leq q$*, and*

$$(-1)^{k+q+1}\nabla^k I^r_{n,q} \geq 0 \tag{2.1.18}$$

in the case $r > q$*.*

Proof. We begin with the case $r \leq q$, according to the definition of $I^r_{n,q}$ in (2.1.12), it holds that

$$\begin{aligned} I^r_{n,q} =& \frac{1}{\Gamma(1-\alpha)}\int_0^1 (n+1-s)^{-\alpha}\mathrm{d}\binom{s-q+r-1}{r} \\ =& \frac{1}{\Gamma(1-\alpha)}\int_0^1 (n+1-s)^{-\alpha}\sum_{n=0}^{r-1}\frac{1}{(s-q+n)}\binom{s-q+r-1}{r}\mathrm{d}s, \end{aligned} \tag{2.1.19}$$

since $(s-q+n)\le 0$ for $0\le s\le 1$ and $n=0,\cdots,r-1$, it yields that $(-1)^r\binom{s-q+r-1}{r}\ge 0$, and consequently $(-1)^{r+1}\frac{\mathrm{d}}{\mathrm{d}s}\binom{s-q+r-1}{r}\ge 0$, combined with $(n+1-s)^{-\alpha}>0$ for any $n\ge 0$ and $\alpha>0$, it leads to $(-1)^{r+1}I_{n,q}^r\ge 0$. In addition, by definition, we may see that

$$\begin{aligned}\nabla I_{n,q}^r=&\frac{1}{\Gamma(1-\alpha)}\int_0^1\Big((n+1-s)^{-\alpha}-(n-s)^{-\alpha}\Big)\mathrm{d}\binom{s-q+r-1}{r}\\=&\frac{-\alpha}{\Gamma(1-\alpha)}\int_0^1\int_n^{n+1}(\xi-s)^{-\alpha-1}\mathrm{d}\xi\mathrm{d}\binom{s-q+r-1}{r}\\=&\frac{-\alpha}{\Gamma(1-\alpha)}\int_0^1\int_0^1(\xi+n-s)^{-\alpha-1}\mathrm{d}\xi\mathrm{d}\binom{s-q+r-1}{r},\end{aligned}\tag{2.1.20}$$

with $(\xi+n-s)^{-\alpha-1}\ge 0$ for $n\ge 1$ and $0\le\xi,s\le 1$, then $(-1)^{r+2}\nabla I_{n,q}^r\ge 0$.

Assume that for $k\ge 2$, it holds that

$$\nabla^{k-1}I_{n,q}^r=\frac{(-\alpha)_{k-1}}{\Gamma(1-\alpha)}\int_{[0,1]^k}\Big(\sum_{i=1}^{k-1}\xi_i+n-k+2-s\Big)^{-\alpha-k+1}\mathrm{d}^{k-1}\xi\mathrm{d}\binom{s-q+r-1}{r},$$

where we define $(\alpha)_{k-1}=\alpha(\alpha-1)\cdots(\alpha-k+2)$ and $\mathrm{d}^{k-1}\xi=\mathrm{d}\xi_1\cdots\mathrm{d}\xi_{k-1}$. Then

$$\begin{aligned}\nabla^k I_{n,q}^r=&\nabla^{k-1}I_{n,q}^r-\nabla^{k-1}I_{n-1,q}^r\\=&\frac{(-\alpha)_{k-1}}{\Gamma(1-\alpha)}\int_{[0,1]^k}\nabla\Big(\sum_{i=1}^{k-1}\xi_i+n-k+2-s\Big)^{-\alpha-k+1}\mathrm{d}^{k-1}\xi\mathrm{d}\binom{s-q+r-1}{r}\\=&\frac{(-\alpha)_k}{\Gamma(1-\alpha)}\int_{[0,1]^k}\int_{n+1}^{n+2}\Big(\sum_{i=1}^{k}\xi_i-k-s\Big)^{-\alpha-k}\mathrm{d}\xi_k\mathrm{d}^{k-1}\xi\mathrm{d}\binom{s-q+r-1}{r}\\=&\frac{(-\alpha)_k}{\Gamma(1-\alpha)}\int_{[0,1]^{k+1}}\Big(\sum_{i=1}^{k}\xi_i+n-k+1-s\Big)^{-\alpha-k}\mathrm{d}^k\xi\mathrm{d}\binom{s-q+r-1}{r}.\end{aligned}$$

Since $(\sum_{i=1}^{k}\xi_i+n-k+1-s)\ge 0$ for $n\ge k\ge 1$ and $0\le\xi_i,s\le 1$, then (2.1.17) holds.

In the other case $r\ge q+1$, integrating by part yields that

$$\begin{aligned}I_{n,q}^r=&\frac{1}{\Gamma(1-\alpha)}\int_0^1(n+1-s)^{-\alpha}\mathrm{d}\binom{s-q+r-1}{r}\\=&\frac{-\alpha}{\Gamma(1-\alpha)}\int_0^1(n+1-s)^{-\alpha-1}\binom{s-q+r-1}{r}\mathrm{d}s,\end{aligned}\tag{2.1.21}$$

since $\binom{s-q+r-1}{r}$ includes a factor $s(s-1)$ for $r\ge q+1, q\in\mathbb{N}^+$. The sign of $\binom{s-q+r-1}{r}$ equals the sign of $\prod_{i=1}^{q}(s-i)$, thus $(-1)^q\binom{s-q+r-1}{r}\ge 0$, and it holds that $(-1)^{q+1}I_{n,q}^r\ge 0$ for $n\ge 0$. Furthermore, an induction process demonstrates that

$$\nabla^k I_{n,q}^r=\frac{(-\alpha)_{k+1}}{\Gamma(1-\alpha)}\int_{[0,1]^{k+1}}\Big(\sum_{i=1}^{k}\xi_i+n-k+1-s\Big)^{-\alpha-k-1}\binom{s-q+r-1}{r}\mathrm{d}^k\xi\mathrm{d}s\tag{2.1.22}$$

for $n\ge k\ge 1$, which arrives at (2.1.18). □

Moreover, we discuss the complete monotonicity of a general class of sequences. That is if a function $\sigma(s)$ is non-decreasing and satisfies $\sigma(0)=\sigma(1)=0$, or in the other case when the derivative $\psi(s)$ of the function exists and keeps positive, we can obtain the complete monotonicity of sequence as well.

Lemma 2.1.2. *The sequence* $\{s_n\}_{n=0}^{\infty}$ *is defined by*

$$s_n = \frac{1}{\Gamma(1-\alpha)} \int_0^1 (n+1-s)^{-\alpha} \varphi(s) \mathrm{d}s, \qquad n \geq 0,$$

where $\varphi(s) \geq 0$ *for* $0 \leq s \leq 1$. *Then for* $n \geq k$, *it holds that* $(-1)^k \nabla^k s_n \geq 0$.

Proof. It is easy to check that $s_n \geq 0$ for all $n \geq 0$, since for $n \geq 0$, $0 \leq s \leq 1$, it holds that $(n+1-s)^{-\alpha} > 0$ and $\varphi(s) \geq 0$ by assumption. The definition of s_n implies that

$$\begin{aligned}\nabla s_n &= \frac{1}{\Gamma(1-\alpha)} \int_0^1 \left((n+1-s)^{-\alpha} - (n-s)^{-\alpha}\right) \varphi(s) \mathrm{d}s \\ &= \frac{-\alpha}{\Gamma(1-\alpha)} \int_0^1 \int_0^1 (n+\xi-s)^{-\alpha-1} \varphi(s) \mathrm{d}\xi \mathrm{d}s,\end{aligned}$$

where

$$\begin{aligned}(n+1-s)^{-\alpha} - (n-s)^{-\alpha} &= (-\alpha) \int_n^{n+1} (\xi - s)^{-\alpha-1} \mathrm{d}\xi \\ &= (-\alpha) \int_0^1 (n+\xi-s)^{-\alpha-1} \mathrm{d}\xi.\end{aligned}$$

Since $(n+\xi-s)^{-\alpha-1} > 0$ and $\varphi(s) \geq 0$ for $n \geq 1$ and $0 \leq s, \xi \leq 1$, thus $\nabla s_n \leq 0$ holds. An induction process yields that

$$\nabla^k s_n = \frac{(-\alpha)_n}{\Gamma(1-\alpha)} \int_{[0,1]^{k+1}} (\sum_{i=1}^{k} \xi_i + n - k + 1 - s)^{-\alpha-k} \varphi(s) \mathrm{d}^k \xi \mathrm{d}s,$$

Since for $n \geq k$ and $0 \leq s, \xi_i \leq 1$, it holds that $\sum_{i=1}^{k} \xi_i + n - k + 1 - s)^{-\alpha-k} \varphi(s) \geq 0$, thus we can obtain that $(-1)^k \nabla^k s_n \geq 0$ for $n \geq k$. □

Corollary 2.1.1. *The sequence* $\{q_n\}_{n=0}^{\infty}$ *is defined by*

$$q_n = \frac{-\alpha}{\Gamma(1-\alpha)} \int_0^1 (n+1-s)^{-\alpha-1} \varphi(s) \mathrm{d}s, \tag{2.1.23}$$

where the function satisfying $\varphi(s) \leq 0$ *for* $0 \leq s \leq 1$. *Then for* $n \geq k$, *it holds that* $(-1)^k \nabla^k q_n \geq 0$.

Proof. Since for $0 \leq s \leq 1, 0 < \alpha < 1$ and $n \geq 0$, it holds that $(n+1-s)^{-\alpha} > 0$ and $(n+1-s)^{-\alpha-1} > 0$, therefore according to (2.1.23), there are $p_n \geq 0$ and $q_n \geq 0$ for any $n \geq 0$. For $n \geq k \geq 1$, it can be verified by induction that

$$\nabla^k q_n = \frac{(-\alpha)_{k+1}}{\Gamma(1-\alpha)} \int_{[0,1]^{k+1}} (\sum_{i=1}^{k} \xi_i + n - k + 1 - s)^{-\alpha-k-1} \varphi(s) \mathrm{d}^k \xi \mathrm{d}s,$$

from which we obtain the result. □

2.1.1 Local truncation error analysis

Next, we construct the numerical scheme

$$D^{\alpha}_{k,i}u_n = f(t_n, u_n), \qquad n \ge k, \tag{2.1.24}$$

as the approximation to the problem (2.0.1) of the scalar case. Then the local truncation error of the n-th step is defined by

$$\tau_n^{(k,i)} = D^{\alpha}_{k,i}u(t_n) - {}^{C}\mathcal{D}^{\alpha}u(t_n), \qquad n \ge k, \;\; n \in \mathbb{N}^+,$$

where $u(t)$ is the exact solution of (2.0.1).

Theorem 2.1.2. *Assume that $u(t) \in C^{k+1}[0,T]$ and $0 < \alpha < 1$, then in the cases $1 \le i < k \le 6$ and $n \ge k$, it holds that*

$$D^{\alpha}_{k,i}u(t_n) - {}^{C}\mathcal{D}^{\alpha}u(t_n) = O\left((t_{n-k+i})^{-\alpha-1}\Delta t^{k+1} + \Delta t^{k+1-\alpha} \right). \tag{2.1.25}$$

In particular, we find

$$D^{\alpha}_{k,k}u(t_n) - {}^{C}\mathcal{D}^{\alpha}u(t_n) = O(\Delta t^{k+1-\alpha}), \qquad k = 1, \cdots, 6, \tag{2.1.26}$$

where the bound is finite and uniform with respect to n.

Proof. According to (2.1.5), it holds that

$$p^k_{j,q}(t) - u(t) = u^{(k+1)}(\xi_j)\binom{s-q+k}{k+1}(\Delta t)^{k+1}, \tag{2.1.27}$$

where $t = t_{j-1} + s\Delta t$ with $0 \le s \le 1$ and $t_{j+q-k-1} \le \xi_j \le t_{j+q-1}$.

Inspired by [22], making use of the integration by part, one arrives at

$$\begin{aligned}
&D^{\alpha}_{k,i}u(t_n) - {}^{C}\mathcal{D}^{\alpha}u(t_n)\\
=&\frac{1}{\Gamma(1-\alpha)}\sum_{j=1}^{n}\int_{t_{j-1}}^{t_j}(t_n - t)^{-\alpha}\left(\frac{\mathrm{d}P_i^k(t)}{\mathrm{d}t} - \frac{\mathrm{d}u(t)}{\mathrm{d}t}\right)\mathrm{d}t\\
=&\frac{-\alpha}{\Gamma(1-\alpha)}\sum_{j=1}^{n}\int_{t_{j-1}}^{t_j}(t_n - t)^{-\alpha-1}\left(P_i^k(t) - u(t)\right)\mathrm{d}t\\
=&\frac{-\alpha(\Delta t)^{-\alpha}}{\Gamma(1-\alpha)}\sum_{j=1}^{n}\int_0^1(n-j+1-s)^{-\alpha-1}\left(P_i^k(t_{j-1}+s\Delta t) - u(t_{j-1}+s\Delta t)\right)\mathrm{d}s
\end{aligned} \tag{2.1.28}$$

as $n \ge k$, which is based on the conditions of (2.1.8) and (2.1.27). According to the general representation of $P_i^k(t)$ in (2.1.7), it is known that in the case $k - i \ge 1$, the polynomials of degree $(k-1)$ can be used on subinterval $\cup_{j=1}^{k-i} I_j$ to construct $P_i^k(t)$, and in the other case $k = i$, the polynomials of degree k are chosen on each subinterval I_j instead. Therefore, we next consider the two cases separately.

Substituting (2.1.7) and (2.1.27) into the last equivalent formula of (2.1.28) and taking $k = i$, one obtains

$$\begin{aligned}
&\left|D^{\alpha}_{k,k}u(t_n) - {}^{C}\mathcal{D}^{\alpha}u(t_n)\right|\\
\le&\frac{\alpha\,(\Delta t)^{k+1-\alpha}}{\Gamma(1-\alpha)}\max_{\xi\in I}\left|u^{(k+1)}(\xi)\right|\Bigg(\sum_{j=1}^{n-k+1}\left|\int_0^1(n-j+1-s)^{-\alpha-1}\binom{s}{k+1}\mathrm{d}s\right|\\
&+\sum_{j=n-k+2}^{n}\left|\int_0^1(n-j+1-s)^{-\alpha-1}\binom{s+k-n-1+j}{k+1}\mathrm{d}s\right|\Bigg),
\end{aligned}$$

and if $1 \leq i \leq k-1$, one has

$$\begin{aligned}
&\left|D^{\alpha}_{k,i}u(t_n) - {}^{C}\mathcal{D}^{\alpha}u(t_n)\right| \\
\leq& \frac{\alpha\,(\Delta t)^{-\alpha}}{\Gamma(1-\alpha)}\Big((\Delta t)^{k}\max_{\xi\in\cup_{j=1}^{k-i}I_j}\left|u^{(k)}(\xi)\right|\sum_{j=1}^{k-i}\left|\int_0^1(n-j+1-s)^{-\alpha-1}\binom{s+j-1}{k}\mathrm{d}s\right| \\
&+(\Delta t)^{k+1}\max_{\xi\in I}\left|u^{(k+1)}(\xi)\right|\sum_{j=k-i+1}^{n-i+1}\left|\int_0^1(n-j+1-s)^{-\alpha-1}\binom{s+k-i}{k+1}\mathrm{d}s\right| \\
&+(\Delta t)^{k+1}\max_{\xi\in I}\left|u^{(k+1)}(\xi)\right|\sum_{j=n-i+2}^{n}\left|\int_0^1(n-j+1-s)^{-\alpha-1}\binom{s+k-n-i+j}{k+1}\mathrm{d}s\right|\Big).
\end{aligned}$$

Since for any $q \leq k$ and $q, k \in \mathbb{N}^+$, the factor $(1-s)$ is included in $\binom{s-q+k}{k+1}$, the term $\frac{1}{1-s}\binom{s-q+k}{k+1}$ is bounded as $0 \leq s \leq 1$, and we obtain

$$\begin{aligned}
\left|D^{\alpha}_{k,k}u(t_n) - {}^{C}\mathcal{D}^{\alpha}u(t_n)\right| \leq& \frac{\alpha\,(\Delta t)^{k+1-\alpha}}{\Gamma(1-\alpha)}C^{(k)}\sum_{j=1}^{n}\int_0^1(n-j+1-s)^{-\alpha-1}(1-s)\mathrm{d}s \\
\leq& \frac{\alpha\,(\Delta t)^{k+1-\alpha}}{\Gamma(1-\alpha)}C^{(k)}\Big(\sum_{j=1}^{n-1}\int_0^1(n-j+1-s)^{-\alpha-1}\mathrm{d}s + \int_0^1(1-s)^{-\alpha}\mathrm{d}s\Big) \\
\leq& (\Delta t)^{k+1-\alpha}\,C^{(k)}\Big(\frac{1}{\Gamma(1-\alpha)} + \frac{1}{\Gamma(2-\alpha)}\Big),
\end{aligned}$$

where $C^{(k)}$ is bounded and depends on $u^{(k+1)}$ and k. On the other hand, if $i < k$, it holds that

$$\begin{aligned}
\left|D^{\alpha}_{k,i}u(t_n) - {}^{C}\mathcal{D}^{\alpha}u(t_n)\right| \leq& \frac{\alpha}{\Gamma(1-\alpha)}C^{(k,i)}\Big((\Delta t)^{k-\alpha}\sum_{j=1}^{k-i}\int_0^1(n-j+1-s)^{-\alpha-1}\mathrm{d}s \\
&+(\Delta t)^{k+1-\alpha}\sum_{j=1}^{n}\int_0^1(n-j+1-s)^{-\alpha-1}(1-s)\mathrm{d}s\Big) \\
\leq& C^{(k,i)}\Big(\frac{\alpha}{\Gamma(1-\alpha)}(\Delta t)^{k+1}(k-i)(t_{n-k+i})^{-\alpha-1} \\
&+(\Delta t)^{k+1-\alpha}\big(\frac{1}{\Gamma(1-\alpha)} + \frac{1}{\Gamma(2-\alpha)}\big)\Big),
\end{aligned}$$

where $C^{(k,i)}$ is a constant and depends on $u^{(k)}$, $u^{(k+1)}$ and k, i. □

Remark 2.1.3. *It is shown from formula* (2.1.25) *that the order of accuracy isn't uniform for all $n \geq k$. In the case of t_n being near the origin, the accuracy order of the local truncation error reduced to the $(k-\alpha)$ order, in view that the $(k-1)$ degree polynomials as shown in* (2.1.1) *are chosen on the subinterval $\cup_{j=1}^{k-i}I_j$. However, replacing polynomials of degree k on the corresponding subinterval can avoid this drawback, which is shown in* (2.1.26).

Remark 2.1.4. *There is need to point out that the local truncation error estimations* (2.1.25) *and* (2.1.26) *hold in the case of the solution $u(t)$ possessing proper smoothness on the closed interval $[0, T]$. In order to check the convergence rate of the global error when $f(t, u(t))$ is smooth with respect to t and u, we apply the methods* (2.1.11) *in the cases $1 \leq i \leq k \leq 3$ on the test equation*

$$ {}^{C}\mathcal{D}^{\alpha}u(t) = f(t), \qquad t \in (0, 1], \tag{2.1.29}$$

such that the exact solution is $u(t) = E_{\alpha,1}(-t^\alpha) \in C[0,1] \cap C^\infty(0,1]$*. In Tables 2.1 and 2.2, the accuracy and the convergence order of the error* $|u(t_M) - u_M|$ *are shown for different timestep and order* α*. According to the numerical experiment, the convergence order reduces to first order in the cases* $1 \le j \le k \le 3$*. Note that the solution of* (2.1.29) *is only continuous on* I*. Therefore, we next consider numerical methods on a non-uniform grid to improve the order of accuracy.*

TABLE 2.1:
Errors and convergence orders of $|u(t_M) - u_M|$ for problem (2.1.29).

α	M	$(k,i)=(1,1)$		$(k,i)=(2,1)$		$(k,i)=(2,2)$	
		$\|u(t_M) - u_M\|$	rate	$\|u(t_M) - u_M\|$	rate	$\|u(t_M) - u_M\|$	rate
0.1	20	4.70994E-03	-	9.55476E-04	-	9.67511E-04	-
	40	2.37818E-03	0.99	4.93426E-04	0.95	4.96390E-04	0.96
	80	1.21118E-03	0.97	2.53608E-04	0.96	2.54352E-04	0.96
	160	6.19034E-04	0.97	1.30008E-04	0.96	1.30197E-04	0.97
	320	3.16763E-04	0.97	6.65299E-05	0.97	6.65780E-05	0.97
0.5	20	3.59879E-02	-	1.27599E-03	-	1.24693E-03	-
	40	1.87445E-02	0.94	5.84522E-04	1.13	5.76449E-04	1.11
	80	9.67807E-03	0.95	2.79573E-04	1.06	2.77440E-04	1.06
	160	4.95832E-03	0.96	1.36716E-04	1.03	1.36166E-04	1.03
	320	2.52435E-03	0.97	6.76067E-05	1.02	6.74666E-05	1.01
0.9	20	6.28955E-02	-	2.95957E-03	-	2.96453E-03	-
	40	3.23694E-02	0.96	1.33551E-03	1.15	1.33646E-03	1.15
	80	1.64619E-02	0.98	6.25412E-04	1.09	6.25601E-04	1.10
	160	8.31769E-03	0.98	3.00737E-04	1.06	3.00775E-04	1.06
	320	4.18769E-03	0.99	1.47049E-04	1.03	1.47057E-04	1.03

TABLE 2.2:
Errors and convergence orders of $|u(t_M) - u_M|$ for problem (2.1.29).

α	M	$(k,i)=(3,1)$		$(k,i)=(3,2)$		$(k,i)=(3,3)$	
		$\|u(t_M) - u_M\|$	rate	$\|u(t_M) - u_M\|$	rate	$\|u(t_M) - u_M\|$	rate
0.1	20	9.24206E-04	-	9.17788E-04	-	9.23060E-04	-
	40	4.71821E-04	0.97	4.70329E-04	0.96	4.71636E-04	0.97
	80	2.41265E-04	0.97	2.40900E-04	0.97	2.41229E-04	0.97
	160	1.23379E-04	0.97	1.23288E-04	0.97	1.23371E-04	0.97
	320	6.30607E-05	0.97	6.30376E-05	0.97	6.30591E-05	0.97
0.5	20	2.87149E-03	-	2.85982E-03	-	2.86650E-03	-
	40	1.42015E-03	1.02	1.41730E-03	1.01	1.41912E-03	1.01
	80	7.06991E-04	1.01	7.06289E-04	1.00	7.06757E-04	1.01
	160	3.52818E-04	1.00	3.52644E-04	1.00	3.52763E-04	1.00
	320	1.76251E-04	1.00	1.76208E-04	1.00	1.76237E-04	1.00
0.9	20	1.30920E-03	-	1.30931E-03	-	1.30919E-03	-
	40	6.18111E-04	1.08	6.18099E-04	1.08	6.18098E-04	1.08
	80	3.00274E-04	1.04	3.00268E-04	1.04	3.00270E-04	1.04
	160	1.47969E-04	1.02	1.47967E-04	1.02	1.47968E-04	1.02
	320	7.34347E-05	1.01	7.34342E-05	1.01	7.34345E-05	1.01

2.2 Non-uniform grid approximation of Caputo fractional derivative

In this section, we would like to construct continuous piecewise polynomials approximation to the Caputo fractional derivative ${}^{C}\mathcal{D}^{\alpha}u(t)$ of order $0 < \alpha < 1$ on a non-uniform grid . The motivation is to obtain more precise approximate results for solutions losing regularity based on an equally computational cost. However, note that the quadrature weights generated on a non-uniform grid can't preserve the discrete convolution property, that brings severe difficulties with theoretical analyses.

Given a uniform partition of interval I by

$$0 = \tau_0 < \tau_1 < \cdots < \tau_M = T,$$

the uniform stepsize is denoted by $\Delta\tau = \frac{T}{M}$. In combination with (2.1.1), we define a strictly monotonic increasing function $\varphi : I \to I$ such that $t = \varphi(\tau)$, and for any $\tau_{i+1} > \tau_j$, it follows that $t_{i+1} > t_i$ as well. The n-th stepsize with respect to t is denoted by Δt_n, and $\Delta t_n = t_n - t_{n-1} = \varphi(\tau_n) - \varphi(\tau_{n-1})$ as $1 \le n \le M-1$.

2.2.1 Linear interpolation

We consider a class of linear interpolating polynomials $\{p_{j,1}^1(t)\}_{j=1}^M$, which are defined on I and possess compact supports $I_j = [t_{j-1}, t_j]$ for $1 \le j \le M$. In addition, the interpolating conditions

$$p_{j,1}^1(t_i) = u(t_i), \qquad i = j-1,\ j$$

are prescribed to uniquely determine the coefficients of polynomial $p_{j,1}^1(t)$. According to (2.1.3), the Lagrange form of $p_{j,1}^1(t)$ is expressed by

$$p_{j,1}^1(t) = u(t_{j-1})\frac{t-t_j}{t_{j-1}-t_j} + u(t_j)\frac{t-t_{j-1}}{t_j-t_{j-1}} = u_j + (s-1)\nabla u_j, \tag{2.2.1}$$

where $t = t_{j-1} + s\Delta t_j$ and $0 \le s \le 1$. We next define that $P_1^1(t) = \sum_{j=1}^n p_{j,1}^1(t)$ for $t \in [t_{n-1}, t_n]$. It is known that $P_1^1(t) \in C_p^1(I)$. In a similar way as (2.1.11), we propose an operator of the form

$$\begin{aligned} D_{1,1}^{\alpha}u_n =& \frac{1}{\Gamma(1-\alpha)}\sum_{j=1}^n \int_{t_{j-1}}^{t_j} (t_n - t)^{-\alpha}\frac{\mathrm{d}p_{j,1}^1}{\mathrm{d}t}\mathrm{d}t \\ =& \frac{1}{\Gamma(1-\alpha)}\sum_{j=1}^n \int_0^1 (t_n - t_{j-1} - s\Delta t_j)^{-\alpha}\frac{\mathrm{d}p_{j,1}^1(t_{j-1}+s\Delta t_j)}{\mathrm{d}s}\mathrm{d}s \\ =& \sum_{j=1}^n I_{n,j}\nabla u_j, \qquad n \ge 1, \end{aligned} \tag{2.2.2}$$

as an approximation to the Caputo derivative defined in (1.1.12), where for $1 \le j \le n$, the weights are denoted by

$$I_{n,j} = \frac{1}{\Gamma(1-\alpha)}\int_0^1 (t_n - t_{j-1} - s\Delta t_j)^{-\alpha}\mathrm{d}s = \frac{(t_n - t_{j-1})^{1-\alpha} - (t_n - t_j)^{1-\alpha}}{\Gamma(2-\alpha)\Delta t_j}. \tag{2.2.3}$$

In addition, we rewrite (2.2.2) into the equivalent form

$$D_{1,1}^{\alpha}u_n = \sum_{j=0}^n W_{n,j}^{(1,1)}u_j, \qquad n \ge 1 \tag{2.2.4}$$

in combination with

$$\begin{aligned} &W_{n,n}^{(1,1)} = I_{n,n}, \quad W_{n,j}^{(1,1)} = I_{n,j} - I_{n,j+1}, \quad 1 \le j \le n-1, \\ &W_{n,0}^{(1,1)} = -I_{n,1}, \quad n \ge 1, \qquad W_{n,j}^{(1,1)} = 0, \quad j \ge n. \end{aligned} \tag{2.2.5}$$

Remark 2.2.1. *Formula* (2.2.4) *exactly holds if* $u(t)$ *is linear polynomial, this yields*

$$\sum_{j=0}^{n} W_{n,j}^{(1,1)} = 0 \quad and \quad \sum_{j=1}^{n} W_{n,j}^{(1,1)} t_j = \frac{t_n^{1-\alpha}}{\Gamma(2-\alpha)}, \qquad n \ge 1.$$

Applying method (2.2.4) to solve the scalar problem of (2.0.1) gives

$$D_{1,1}^{\alpha} u_n = f(t_n, u_n), \qquad n \ge 1. \tag{2.2.6}$$

In addition, rewriting (2.2.6) into the matrix-vector form yields

$$\begin{bmatrix} W_{1,1}^{(1,1)} & & & \\ W_{2,1}^{(1,1)} & W_{2,2}^{(1,1)} & & \\ \vdots & \ddots & \ddots & \\ W_{M,1}^{(1,1)} & W_{M,2}^{(1,1)} & \cdots & W_{M,M}^{(1,1)} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_M \end{bmatrix} = \begin{bmatrix} f(t_1, u_1) \\ f(t_2, u_2) \\ \vdots \\ f(t_M, u_M) \end{bmatrix} - u_0 \begin{bmatrix} W_{1,0}^{(1,1)} \\ W_{2,0}^{(1,1)} \\ \vdots \\ W_{M,0}^{(1,1)} \end{bmatrix},$$

where it is obtained from (2.2.5) that

$$\begin{bmatrix} W_{1,1}^{(1,1)} & & & \\ W_{2,1}^{(1,1)} & W_{2,2}^{(1,1)} & & \\ \vdots & \ddots & \ddots & \\ W_{M,1}^{(1,1)} & W_{M,2}^{(1,1)} & \cdots & W_{M,M}^{(1,1)} \end{bmatrix} = \begin{bmatrix} I_{1,1} & & & \\ I_{2,1} & I_{2,2} & & \\ \vdots & \ddots & \ddots & \\ I_{M,1} & I_{M,2} & \cdots & I_{M,M} \end{bmatrix} \begin{bmatrix} 1 & & & \\ -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{bmatrix}.$$

2.2.2 Quadratic interpolation

In this part, we consider the approximation to the Caputo derivative based on piecewise quadratic interpolating polynomials. As mentioned in Remark 2.1.1, we consider two available approximations, $P_1^2(t), P_2^2(t) \in C_p^2(I)$ of the forms (2.1.9), to $u(t)$ on a non-uniform grid.

Case I

On the subinterval $[t_0, t_1]$, the piecewise linear interpolating polynomial $p_{1,1}^1(t)$ is chosen, where according to (2.2.1), we have $p_{1,1}^1(t) = u_1 + (s-1)\nabla u_1$. On the subinterval I_j for $2 \le j \le M$, we construct the piecewise quadratic polynomial $p_{j,1}^2(t)$, which is defined on I and has the compact support I_j. The coefficients of the quadratic polynomial are determined by

$$p_{j,1}^2(t_i) = u(t_i), \qquad i = j-2, j-1, j.$$

From (2.1.3), we obtain

$$\begin{aligned} p_{j,1}^2(t) =& u(t_{j-2}) \frac{(t_j - t)(t_{j-1} - t)}{(t_j - t_{j-2})(t_{j-1} - t_{j-2})} + u(t_{j-1}) \frac{(t - t_{j-2})(t_j - t)}{(t_{j-1} - t_{j-2})(t_j - t_{j-1})} + u(t_j) \frac{(t - t_{j-2})(t - t_{j-1})}{(t_j - t_{j-2})(t_j - t_{j-1})} \\ =& u(t_{j-2}) \frac{(s^2 - s)(\Delta t_j)^2}{\Delta t_{j-1}(\Delta t_j + \Delta t_{j-1})} + u(t_{j-1}) \frac{(s\Delta t_j + \Delta t_{j-1})(1-s)}{\Delta t_{j-1}} + u(t_j) \frac{s^2 \Delta t_j + s\Delta t_{j-1}}{\Delta t_j + \Delta t_{j-1}} \end{aligned} \tag{2.2.7}$$

in the case $t = t_{j-1} + s\Delta t_j$. In addition, it follows that

$$\begin{aligned}\frac{\mathrm{d}p_{j,1}^2}{\mathrm{d}s} &= (2s-1)u(t_{j-2})\frac{(\Delta t_j)^2}{\Delta t_{j-1}(\Delta t_j + \Delta t_{j-1})} \\ &- u(t_{j-1})\left(\frac{\Delta t_j}{\Delta t_{j-1}}(2s-1)+1\right) + u(t_j)\left(\frac{(2s-1)\Delta t_j}{\Delta t_j + \Delta t_{j-1}}+1\right).\end{aligned} \tag{2.2.8}$$

Therefore, when $t \in [t_{n-1}, t_n]$, we propose the piecewise polynomial $P_1^2(t) = p_{1,1}^1(t) + \sum_{j=2}^n p_{j,1}^2(t)$ such that $P_1^2(t) \in C_p^2(I)$ as an approximation to $u(t)$. Accordingly, as an approximation to ${}^C\mathcal{D}^\alpha u(t_n)$, the discrete operator is proposed in the form of

$$\begin{aligned}D_{2,1}^\alpha u_n =& \frac{1}{\Gamma(1-\alpha)}\Big(\int_{t_0}^{t_1}(t_n-t)^{-\alpha}\frac{\mathrm{d}p_{1,1}^1}{\mathrm{d}t}\mathrm{d}t + \sum_{j=2}^n\int_{t_{j-1}}^{t_j}(t_n-t)^{-\alpha}\frac{\mathrm{d}p_{j,1}^2}{\mathrm{d}t}\mathrm{d}t\Big) \\ =& I_{n,1}\nabla u_1 + \frac{1}{\Gamma(1-\alpha)}\sum_{j=2}^n\int_0^1(t_n - t_{j-1} - s\Delta t_j)^{-\alpha}\frac{\mathrm{d}p_{j,1}^2(t_{j-1}+s\Delta t_j)}{\mathrm{d}s}\mathrm{d}s\end{aligned} \tag{2.2.9}$$

when $n \geq 2$. Further, based on (2.2.8), it holds that

$$\begin{aligned}\frac{1}{\Gamma(1-\alpha)}\int_0^1(t_n - t_{j-1} - s\Delta t_j)^{-\alpha}\frac{\mathrm{d}p_{j,1}^2}{\mathrm{d}s}\mathrm{d}s &= u(t_{j-2})\frac{2I_{n,j}^2(\Delta t_j)^2}{\Delta t_{j-1}(\Delta t_j+\Delta t_{j-1})} \\ - u(t_{j-1})\Big(\frac{2\Delta t_j}{\Delta t_{j-1}}I_{n,j}^2 + I_{n,j}\Big) &+ u(t_j)\Big(I_{n,j}^2\frac{2\Delta t_j}{\Delta t_j + \Delta t_{j-1}} + I_{n,j}\Big),\end{aligned} \tag{2.2.10}$$

where $I_{n,j}$ are shown in (2.2.3) and the coefficients $I_{n,j}^2$ are defined by

$$\begin{aligned}I_{n,j}^2 =& \frac{1}{\Gamma(1-\alpha)}\int_0^1(t_n - t_{j-1} - s\Delta t_j)^{-\alpha}\Big(s - \frac{1}{2}\Big)\mathrm{d}s \\ =& \frac{(t_n-t_{j-1})^{2-\alpha} - (t_n-t_j)^{2-\alpha} - (1-\frac{\alpha}{2})\Delta t_j\left((t_n-t_{j-1})^{1-\alpha} + (t_n-t_j)^{1-\alpha}\right)}{\Gamma(3-\alpha)(\Delta t_j)^2}\end{aligned} \tag{2.2.11}$$

for $n \geq 1$ and $j \geq 1$. As a result, substituting (2.2.10) into (2.2.9), we deduce that

$$\begin{aligned}D_{2,1}^\alpha u_n = I_{n,1}\nabla u_1 + \sum_{j=2}^n\Big(&\frac{2I_{n,j}^2\Delta t_j^2}{\Delta t_{j-1}(\Delta t_j + \Delta t_{j-1})}u_{j-2} \\ &- (\frac{2I_{n,j}^2\Delta t_j}{\Delta t_{j-1}} + I_{n,j})u_{j-1} + (\frac{2I_{n,j}^2\Delta t_j}{\Delta t_j + \Delta t_{j-1}} + I_{n,j})u_j\Big)\end{aligned}$$

for $n \geq 2$. Equivalently, it can be rewritten as

$$D_{2,1}^\alpha u_n = \sum_{j=0}^n W_{n,j}^{(2,1)}u_j, \qquad n \geq 2, \tag{2.2.12}$$

where

$$\begin{cases} W_{n,n}^{(2,1)} = \dfrac{2I_{n,n}^2\Delta t_n}{\Delta t_n + \Delta t_{n-1}} + I_{n,n}, \quad n \geq 2, \\ W_{n,n-1}^{(2,1)} = \dfrac{2I_{n,n-1}^2\Delta t_{n-1}}{\Delta t_{n-1} + \Delta t_{n-2}} - \dfrac{2I_{n,n}^2\Delta t_n}{\Delta t_{n-1}} - I_{n,n} + I_{n,n-1}, \quad n \geq 3, \\ W_{n,j}^{(2,1)} = \dfrac{2I_{n,j+2}^2(\Delta t_{j+2})^2}{\Delta t_{j+1}(\Delta t_{j+1} + \Delta t_{j+2})} - \dfrac{2I_{n,j+1}^2\Delta t_{j+1}}{\Delta t_j} \\ \qquad + \dfrac{2I_{n,j}^2\Delta t_j}{\Delta t_j + \Delta t_{j-1}} - I_{n,j+1} + I_{n,j}, \quad 2 \leq j \leq n-2, \ n \geq 4 \end{cases}$$

and

$$\begin{cases} W_{n,0}^{(2,1)} = \dfrac{2I_{n,2}^2(\Delta t_2)^2}{\Delta t_1(\Delta t_1+\Delta t_2)} - I_{n,1}, \quad n\geq 2, \quad W_{2,1}^{(2,1)} = -\dfrac{2I_{2,2}^2\Delta t_2}{\Delta t_1} - I_{2,2}+I_{2,1}, \\ W_{n,1}^{(2,1)} = \dfrac{2I_{n,3}^2(\Delta t_3)^2}{\Delta t_2(\Delta t_2+\Delta t_3)} - \dfrac{2I_{n,2}^2\Delta t_2}{\Delta t_1} - I_{n,2}+I_{n,1}, \quad n\geq 3. \end{cases}$$

Remark 2.2.2. *If $\alpha\to 1$, from (2.2.3) and (2.2.11), we find*

$$I_{n,j} = I_{n,j}^2 = 0, \quad 1\leq j\leq n-1, \quad I_{n,n} = \frac{1}{\Delta t_n}, \quad I_{n,n}^2 = \frac{1}{2\Delta t_n} \quad n\geq 1.$$

Then for $n\geq 2$, the method (2.2.12) reduces to the BDF2 method of variable step, which is denoted by

$$Du_n = \frac{\Delta t_n}{\Delta t_{n-1}(\Delta t_{n-1}+\Delta t_n)}u_{n-2} - \left(\frac{1}{\Delta t_{n-1}}+\frac{1}{\Delta t_n}\right)u_{n-1} + \left(\frac{1}{\Delta t_{n-1}+\Delta t_n}+\frac{1}{\Delta t_n}\right)u_n.$$

Case II

We consider a class of interpolating polynomials, denoted by $p_{j,2}^2(t)$ on I. Each $p_{j,2}^2(t)$ has a compact support I_j and is expressed by a quadratic polynomial satisfying

$$p_{j,2}^2(t_i) = u(t_i), \qquad i = j-1, j, j+1. \tag{2.2.13}$$

Writing into the Lagrange form yields

$$\begin{aligned} p_{j,2}^2(t) = & u(t_{j-1})\frac{(t_j-t)(t_{j+1}-t)}{(t_j-t_{j-1})(t_{j+1}-t_{j-1})} + u(t_j)\frac{(t-t_{j-1})(t_{j+1}-t)}{(t_j-t_{j-1})(t_{j+1}-t_j)} \\ & + u(t_{j+1})\frac{(t-t_{j-1})(t-t_j)}{(t_{j+1}-t_{j-1})(t_{j+1}-t_j)} \\ = & u(t_{j-1})\frac{(1-s)\left(\Delta t_{j+1}+\Delta t_j - s\Delta t_j\right)}{(\Delta t_{j+1}+\Delta t_j)} + u(t_j)\frac{s\left(\Delta t_{j+1}+\Delta t_j-s\Delta t_j\right)}{\Delta t_{j+1}} \\ & + u(t_{j+1})\frac{s(s-1)(\Delta t_j)^2}{(\Delta t_j+\Delta t_{j+1})\,\Delta t_{j+1}}, \end{aligned}$$

where assuming $t = t_{j-1}+s\Delta t_j$ and $0\leq s\leq 1$. Moreover, we arrive at

$$\begin{aligned} \frac{\mathrm{d}p_{j,2}^2}{\mathrm{d}s} = & u(t_{j-1})\left((2s-1)\frac{\Delta t_j}{\Delta t_{j+1}+\Delta t_j} - 1\right) \\ & + u(t_j)\left(1-(2s-1)\frac{\Delta t_j}{\Delta t_{j+1}}\right) + u(t_{j+1})\frac{(2s-1)(\Delta t_j)^2}{(\Delta t_{j+1}+\Delta t_j)\Delta t_{j+1}}. \end{aligned} \tag{2.2.14}$$

Then in the case $t\in[t_{n-1},t_n]$, we construct $P_2^2(t)\in C_p^2(I)$ of the form $P_2^2(t) = \sum_{j=1}^{n-1} p_{j,2}^2(t) + p_{n,1}^2(t)$ to approximate solution $u(t)$. Consequently, we propose the discrete operator

$$\begin{aligned} D_{2,2}^{\alpha}u_n = & \frac{1}{\Gamma(1-\alpha)}\sum_{j=1}^{n}\int_{t_{j-1}}^{t_j}(t_n-t)^{-\alpha}\frac{\mathrm{d}P_2^2(t)}{\mathrm{d}t}\mathrm{d}t \\ = & \frac{1}{\Gamma(1-\alpha)}\Big(\sum_{j=1}^{n-1}\int_0^1 (t_n-t_{j-1}-s\Delta t_j)^{-\alpha}\frac{\mathrm{d}p_{j,2}^2(t_{j-1}+s\Delta t_j)}{\mathrm{d}s}\mathrm{d}s \\ & + \int_0^1 (t_n-t_{n-1}-s\Delta t_n)^{-\alpha}\frac{\mathrm{d}p_{n,1}^2(t_{n-1}+s\Delta t_n)}{\mathrm{d}s}\mathrm{d}s\Big) \end{aligned} \tag{2.2.15}$$

in the case $n \geq 2$. In addition, according to (2.2.14), one finds

$$\begin{aligned}\frac{1}{\Gamma(1-\alpha)}\int_0^1 (t_n - t_{j-1} - s\Delta t_j)^{-\alpha}\frac{\mathrm{d}p_{j,2}^2}{\mathrm{d}s}\mathrm{d}s = u(t_{j-1})\Big(\frac{2I_{n,j}^2\Delta t_j}{\Delta t_j + \Delta t_{j+1}} - I_{n,j}\Big)\\ + u(t_j)\Big(I_{n,j} - \frac{2\Delta t_j}{\Delta t_{j+1}}I_{n,j}^2\Big) + u(t_{j+1})\frac{2I_{n,j}^2(\Delta t_j)^2}{(\Delta t_j + \Delta t_{j+1})\Delta t_{j+1}}.\end{aligned} \tag{2.2.16}$$

Therefore, together with (2.2.16) and (2.2.10), formula (2.2.15) becomes

$$\begin{aligned}D_{2,2}^{\alpha}u_n = &\sum_{j=1}^{n-1}\Big(u(t_{j-1})(\frac{2I_{n,j}^2\Delta t_j}{\Delta t_j + \Delta t_{j+1}} - I_{n,j}) + u(t_j)(I_{n,j} - \frac{2\Delta t_j}{\Delta t_{j+1}}I_{n,j}^2)\\ &+ u(t_{j+1})\frac{2I_{n,j}^2(\Delta t_j)^2}{(\Delta t_j + \Delta t_{j+1})\Delta t_{j+1}}\Big) + u(t_{n-2})\frac{2I_{n,n}^2(\Delta t_n)^2}{\Delta t_{n-1}(\Delta t_n + \Delta t_{n-1})}\\ &- u(t_{n-1})(\frac{2\Delta t_n}{\Delta t_{n-1}}I_{n,n}^2 + I_{n,n}) + u(t_n)(\frac{2I_{n,n}^2\Delta t_n}{\Delta t_n + \Delta t_{n-1}} + I_{n,n}), \quad n \geq 2.\end{aligned} \tag{2.2.17}$$

Formula (2.2.17) can be rewritten as

$$D_{2,2}^{\alpha}u_n = \sum_{j=0}^{n} W_{n,j}^{(2,2)}u_j, \qquad n \geq 2, \tag{2.2.18}$$

where

$$\begin{cases} W_{n,n}^{(2,2)} = \dfrac{2I_{n,n-1}^2(\Delta t_{n-1})^2}{(\Delta t_{n-1} + \Delta t_n)\Delta t_n} + \dfrac{2I_{n,n}^2\Delta t_n}{\Delta t_n + \Delta t_{n-1}} + I_{n,n}, \quad n \geq 2,\\ W_{n,n-1}^{(2,2)} = \dfrac{2I_{n,n-2}^2(\Delta t_{n-2})^2}{(\Delta t_{n-2} + \Delta t_{n-1})\Delta t_{n-1}} - \dfrac{2I_{n,n}^2\Delta t_n}{\Delta t_{n-1}} - \dfrac{2I_{n,n-1}^2\Delta t_{n-1}}{\Delta t_n} - I_{n,n} + I_{n,n-1}, \quad n \geq 3,\\ W_{n,n-2}^{(2,2)} = \dfrac{2I_{n,n-1}^2\Delta t_{n-1}}{\Delta t_{n-1} + \Delta t_n} - \dfrac{2I_{n,n-2}^2\Delta t_{n-2}}{\Delta t_{n-1}} + \dfrac{2I_{n,n-3}^2(\Delta t_{n-3})^2}{(\Delta t_{n-3} + \Delta t_{n-2})\Delta t_{n-2}}\\ \qquad + \dfrac{2I_{n,n}^2(\Delta t_n)^2}{\Delta t_{n-1}(\Delta t_n + \Delta t_{n-1})} - I_{n,n-1} + I_{n,n-2}, \quad n \geq 4,\\ W_{n,j}^{(2,2)} = \dfrac{2I_{n,j+1}^2\Delta t_{j+1}}{\Delta t_{j+1} + \Delta t_{j+2}} - \dfrac{2I_{n,j}^2\Delta t_j}{\Delta t_{j+1}} + \dfrac{2I_{n,j-1}^2(\Delta t_{j-1})^2}{(\Delta t_{j-1} + \Delta t_j)\Delta t_j} - I_{n,j+1} + I_{n,j}, \quad 2 \leq j \leq n-3 \end{cases}$$

and

$$\begin{cases} W_{2,0}^{(2,2)} = \dfrac{2I_{2,1}^2\Delta t_1}{\Delta t_1 + \Delta t_2} + \dfrac{2I_{2,2}^2(\Delta t_2)^2}{\Delta t_1(\Delta t_2 + \Delta t_1)} - I_{2,1},\\ W_{n,0}^{(2,2)} = \dfrac{2I_{n,1}^2\Delta t_1}{\Delta t_1 + \Delta t_2} - I_{n,1}, \quad n \geq 3,\\ W_{2,1}^{(2,2)} = -\dfrac{2\Delta t_1}{\Delta t_2}I_{2,1}^2 - \dfrac{2\Delta t_2}{\Delta t_1}I_{2,2}^2 - I_{2,2} + I_{2,1},\\ W_{3,1}^{(2,2)} = \dfrac{2I_{3,2}^2\Delta t_2}{\Delta t_2 + \Delta t_3} + \dfrac{2I_{3,3}^2(\Delta t_3)^2}{\Delta t_2(\Delta t_3 + \Delta t_2)} - \dfrac{2\Delta t_1}{\Delta t_2}I_{3,1}^2 - I_{3,2} + I_{3,1},\\ W_{n,1}^{(2,2)} = \dfrac{2I_{n,2}^2\Delta t_2}{\Delta t_2 + \Delta t_3} - \dfrac{2\Delta t_1}{\Delta t_2}I_{n,1}^2 - I_{n,2} + I_{n,1}, \quad n \geq 4. \end{cases}$$

Remark 2.2.3. *The interpolating conditions (2.2.13) imply that the discrete scheme (2.2.18) exactly holds if function $u(t)$ is a quadratic polynomial. From this follows*

$$\sum_{j=0}^{n} W_{n,j}^{(2,2)} = 0, \qquad \sum_{j=1}^{n} W_{n,j}^{(2,2)}t_j = \frac{t_n^{1-\alpha}}{\Gamma(2-\alpha)}, \qquad \sum_{j=1}^{n} W_{n,j}^{(2,2)}t_j^2 = \frac{2t_n^{2-\alpha}}{\Gamma(3-\alpha)}, \qquad n \geq 2.$$

Applying methods (2.2.12) and (2.2.18) to solve a scalar version of the problem (2.0.1) gives

$$D^{\alpha}_{2,i}u_n = f(t_n, u_n), \qquad 2 \le n \le M, \;\; i = 1, 2. \tag{2.2.19}$$

In addition, rewriting (2.2.19) into a matrix-vector form yields

$$\begin{bmatrix} W^{(2,i)}_{2,2} & & & \\ W^{(2,i)}_{3,2} & W^{(2,i)}_{3,3} & & \\ \vdots & \ddots & \ddots & \\ W^{(2,i)}_{M,2} & W^{(2,i)}_{M,3} & \cdots & W^{(2,i)}_{M,M} \end{bmatrix} \begin{bmatrix} u_2 \\ u_3 \\ \vdots \\ u_M \end{bmatrix} = \begin{bmatrix} f(t_2, u_2) \\ f(t_3, u_3) \\ \vdots \\ f(t_M, u_M) \end{bmatrix} - u_0 \begin{bmatrix} W^{(2,i)}_{2,0} \\ W^{(2,i)}_{3,0} \\ \vdots \\ W^{(2,i)}_{M,0} \end{bmatrix} - u_1 \begin{bmatrix} W^{(2,i)}_{2,1} \\ W^{(2,i)}_{3,1} \\ \vdots \\ W^{(2,i)}_{M,1} \end{bmatrix},$$

In the following, we apply the proposed three methods to the problem (2.1.29) and check the order of accuracy of errors. A non-uniform grid is given by the map $t = T^{m-1}\tau^m$ for a real number $m > 1$. It is observed from Tables 2.3-2.5 that the rates of convergence of errors are improved in comparison with the results in Tables 2.1-2.2. We also find that for $(k,i) = (1,1)$, the error $|u(t_M) - u_M|$ is proportional to $\min(\Delta\tau^{2-\alpha}, \Delta\tau^m)$, and for $(k,i) = (2,1)$ and $(k,i) = (2,2)$, the error $|u(t_M)-u_M|$ is proportional to $\min(\Delta\tau^{3-\alpha}, \Delta\tau^m)$. In addition, the map from a uniform-grid to a non-uniform grid has an effect on the order of accuracy. As shown in Table 2.5, for $m = 2.5$, the convergence rate of errors reduces when α is near zero. Therefore, further investigation on the approximation for a non-uniform grid is necessary.

TABLE 2.3:
Errors and convergence orders of $|u(t_M) - u_M|$ in problem (2.1.29) for $m = 1.5$.

α	M	$(k,i) = (1,1)$		$(k,i) = (2,1)$		$(k,i) = (2,2)$	
		$\lvert u(t_M) - u_M\rvert$	rate	$\lvert u(t_M) - u_M\rvert$	rate	$\lvert u(t_M) - u_M\rvert$	rate
0.1	20	4.24074E-04	-	3.03868E-05	-	1.65985E-04	-
	40	1.55229E-04	1.45	9.83626E-06	1.63	6.13791E-05	1.44
	80	5.68023E-05	1.45	3.51169E-06	1.49	2.24842E-05	1.45
	160	2.07544E-05	1.45	1.29976E-06	1.43	8.19933E-06	1.46
	320	7.56930E-06	1.46	4.86720E-07	1.42	2.98187E-06	1.46
0.5	20	6.05261E-03	-	3.39057E-03	-	2.74362E-03	-
	40	2.42542E-03	1.32	1.19762E-03	1.50	9.62882E-04	1.51
	80	9.58293E-04	1.34	4.23772E-04	1.50	3.39847E-04	1.50
	160	3.74374E-04	1.36	1.49955E-04	1.50	1.20136E-04	1.50
	320	1.44912E-04	1.37	5.30484E-05	1.50	4.24822E-05	1.50
0.7	20	1.15902E-02	-	4.76469E-03	-	4.40747E-03	-
	40	5.05941E-03	1.20	1.64546E-03	1.53	1.51718E-03	1.54
	80	2.17440E-03	1.22	5.72575E-04	1.52	5.27385E-04	1.52
	160	9.24361E-04	1.23	2.00357E-04	1.51	1.84502E-04	1.52
	320	3.89790E-04	1.25	7.03774E-05	1.51	6.48106E-05	1.51
0.9	20	1.64344E-02	-	3.06290E-03	-	3.00979E-03	-
	40	7.92616E-03	1.05	1.03560E-03	1.56	1.01644E-03	1.57
	80	3.78257E-03	1.07	3.54105E-04	1.55	3.47422E-04	1.55
	160	1.79298E-03	1.08	1.22291E-04	1.53	1.19977E-04	1.53
	320	8.46077E-04	1.08	4.25494E-05	1.52	4.17466E-05	1.52

TABLE 2.4:
Errors and convergence orders of $|u(t_M) - u_M|$ in problem (2.1.29) for $m = 2$.

α	M	$(k,i)=(1,1)$		$(k,i)=(2,1)$		$(k,i)=(2,2)$	
		$\|u(t_M) - u_M\|$	rate	$\|u(t_M) - u_M\|$	rate	$\|u(t_M) - u_M\|$	rate
0.1	20	1.37171E-04	-	1.76398E-04	-	1.09098E-05	-
	40	3.79525E-05	1.85	4.59678E-05	1.94	2.56718E-06	2.09
	80	1.04831E-05	1.86	1.20004E-05	1.94	6.47412E-07	1.99
	160	2.88871E-06	1.86	3.12748E-06	1.94	1.62892E-07	1.99
	320	7.94108E-07	1.86	7.76604E-07	2.01	2.87452E-08	2.50
0.3	20	1.22520E-03	-	1.33591E-03	-	8.06358E-04	-
	40	3.90396E-04	1.65	3.50716E-04	1.93	2.08298E-04	1.95
	80	1.23606E-04	1.66	9.10379E-05	1.95	5.35667E-05	1.96
	160	3.89176E-05	1.67	2.33952E-05	1.96	1.36810E-05	1.97
	320	1.21972E-05	1.67	5.96263E-06	1.97	3.47175E-06	1.98
0.5	20	4.45344E-03	-	3.23064E-03	-	2.61564E-03	-
	40	1.62337E-03	1.46	8.33116E-04	1.96	6.67082E-04	1.97
	80	5.85721E-04	1.47	2.12911E-04	1.97	1.69415E-04	1.98
	160	2.09956E-04	1.48	5.40510E-05	1.98	4.28495E-05	1.98
	320	7.49359E-05	1.49	1.36579E-05	1.98	1.08026E-05	1.99
0.9	20	1.75168E-02	-	3.10129E-03	-	3.04315E-03	-
	40	8.34970E-03	1.07	8.37810E-04	1.89	8.20211E-04	1.89
	80	3.94103E-03	1.08	2.23328E-04	1.91	2.18334E-04	1.91
	160	1.85021E-03	1.09	5.90092E-05	1.92	5.76398E-05	1.92
	320	8.66098E-04	1.10	1.54876E-05	1.93	1.51196E-05	1.93

TABLE 2.5:
Errors and convergence orders of $|u(t_M) - u_M|$ in problem (2.1.29) for $m = 2.5$.

α	M	$(k,i)=(1,1)$		$(k,i)=(2,1)$		$(k,i)=(2,2)$	
		$\|u(t_M) - u_M\|$	rate	$\|u(t_M) - u_M\|$	rate	$\|u(t_M) - u_M\|$	rate
0.1	20	6.96654E-05	-	1.47414E-04	-	3.68958E-05	-
	40	1.76613E-05	1.98	2.76650E-05	2.41	6.60598E-06	2.48
	80	4.58741E-06	1.94	5.16765E-06	2.42	1.20418E-06	2.46
	160	1.21240E-06	1.92	1.12954E-06	2.19	3.73276E-07	1.69
	320	3.24257E-07	1.90	4.52415E-06	-2.00	7.98134E-06	-4.42
0.3	20	9.79566E-04	-	1.10086E-03	-	6.96699E-04	-
	40	3.00987E-04	1.70	2.11692E-04	2.38	1.29478E-04	2.43
	80	9.28719E-05	1.70	3.99920E-05	2.40	2.38040E-05	2.44
	160	2.87148E-05	1.69	7.47432E-06	2.42	4.35806E-06	2.45
	320	8.88492E-06	1.69	8.37841E-07	3.16	1.49198E-06	1.55
0.5	20	4.29413E-03	-	2.80156E-03	-	2.27568E-03	-
	40	1.53459E-03	1.48	5.53366E-04	2.34	4.39330E-04	2.37
	80	5.45785E-04	1.49	1.07885E-04	2.36	8.41140E-05	2.38
	160	1.93704E-04	1.49	2.08286E-05	2.37	1.60028E-05	2.39
	320	6.86724E-05	1.50	3.97190E-06	2.39	3.04946E-06	2.39
0.9	20	1.95780E-02	-	3.29673E-03	-	3.23631E-03	-
	40	9.31869E-03	1.07	7.83866E-04	2.07	7.66859E-04	2.08
	80	4.39196E-03	1.09	1.84283E-04	2.09	1.79839E-04	2.09
	160	2.05953E-03	1.09	4.31192E-05	2.10	4.20054E-05	2.10
	320	9.63310E-04	1.10	1.00683E-05	2.10	9.79603E-06	2.10

Chapter 3

Stability analysis

In order to study the numerical stability of the methods (2.1.24) applied to problem (2.0.1), we will examine the behaviour of the numerical method on the linear scalar equation

$$^{C}\mathcal{D}^{\alpha}u(t) = \lambda u(t), \qquad \lambda \in \mathbb{C} \tag{3.0.1}$$

with initial value $u(0) = u_0$. It is already shown that the solution of (3.0.1) satisfies that $u(t) \to 0$ as $t \to +\infty$ provided that $|\arg(\lambda)| > \frac{\alpha\pi}{2}$ $(-\pi \leq \arg(\lambda) \leq \pi)$ for arbitrary bounded initial value (see Theorems 1.2.9 and Theorem 1.2.10), accordingly, it can be studied in seeking those λ for which the corresponding numerical solutions preserve the same property as true solution. In fact, several classical numerical stability theories have been constructed on solving problem (3.0.1) in the case $\alpha = 1$ [23, 24]. Furthermore, there are some efforts on generalizing the numerical stability theory to integral equations, such as Volterra-type integral equations [41, 45, 8]. It is known that, for example, in the case $|\arg(\lambda)| > \frac{\alpha\pi}{2}$ $(0 < \alpha \leq 1)$, if the numerical solution has the same asymptotical stability property as true solution, then the numerical method is called A-stable , and in the other case $|\arg(\lambda)| \geq \theta$ $(\frac{\alpha\pi}{2} < |\theta| \leq \pi)$, the numerical method is $A(\theta)$-stable if the numerical solution is asymptotic stability for those λ. Motivated by previous work, we specialise and refine the technique pioneered in [45] to obtain some new results for the fractional case. We confirm the stability regions of the proposed numerical methods and provide a rigorous analysis on the $A(\frac{\pi}{2})$-stability of some methods. In practical implementation, it can be observed that the class of methods possesses the property of $A(\theta)$-stability uniformly for $0 < \alpha < 1$, and for some $\alpha \in (0, 1)$, A-stability can be obtained.

3.1 Stability of linear multistep methods and fractional linear multistep methods

3.1.1 Zero-stability

It is well known that the consistency of a general linear multistep method can not deduce its convergence, therefore, the so-called zero-stability analysis is taken into consideration. Generally speaking, if we consider a linear multistep method of the form

$$\sum_{i=0}^{k} \alpha_i u_{n+i} = \Delta t \sum_{i=0}^{k} \beta_i f(t_{n+i}, u_{n+i}), \qquad n \geq 0, \tag{3.1.1}$$

where the generating polynomials (ρ, σ) are defined by

$$\rho(\xi) = \sum_{i=0}^{k} \alpha_i \xi^i, \qquad \sigma(\xi) = \sum_{i=0}^{k} \beta_i \xi^i, \tag{3.1.2}$$

the zero-stability yields that for a limited stepsize $\Delta t \in (0, t_0]$, the numerical solutions $\{u_n\}_{n=0}^{\infty}$ remain bounded.

Definition 3.1.1 ([57]). *The linear multistep method of form* (3.1.1) *is zero-stable if there exist* $t_0 > 0$ *and* $C > 0$ *such that* $\forall\ \Delta t \in (0, t_0]$ *and* $\forall\ \varepsilon > 0$, *if* $|\delta_n| \leq \varepsilon$ *for* $0 \leq n \leq N$, *then*

$$|z_n - u_n| \leq C\varepsilon, \qquad 0 \leq n \leq N_h, \tag{3.1.3}$$

and the sequences $\{z_n\}$ *and* $\{u_n\}$ *are, respectively, the solution of problems*

$$\begin{cases} \sum_{i=0}^{k} \alpha_i u_{n+i} = \Delta t \sum_{i=0}^{k} \beta_i f(t_{n+i}, u_{n+i}) \\ u_k = w_k, \quad k = 0, \cdots, p-1 \end{cases} \tag{3.1.4}$$

and

$$\begin{cases} \sum_{i=0}^{k} \alpha_i z_{n+i} = \Delta t \sum_{i=0}^{k} \beta_i f(t_{n+i}, z_{n+i}) + \Delta t \delta_n, \\ z_k = w_k + \delta_k, \quad k = 0, \cdots, p-1, \end{cases} \tag{3.1.5}$$

where $p \leq n \leq N$.

We next revisit the definitions of the root condition and the strong root condition in terms of a generating polynomial and the related equivalence theorem.

Definition 3.1.2. *The generating polynomial* $\rho(\xi)$ *defined in* (3.1.2) *satisfies the root condition, if*

i). *The zeros of* $\rho(\xi)$ *lie on or within the unit circle;*

ii). *The zeros on the unit circle are simple.*

Definition 3.1.3. *The generating polynomial* $\rho(\xi)$ *satisfies the strong root condition, if*

i). *The zeros on the unit circle is only* $\xi = 1$ *and simple,*

ii). *The rest zeros of* $\rho(\xi)$ *lie inside the unit circle;*

Theorem 3.1.1 ([57]). *The root condition is equivalent to zero-stability for the consistent linear multistep methods.*

Theorem 3.1.2 ([24]). *The* k*-step BDF formulae are zero-stable for* $1 \leq k \leq 6$, *and unstable for* $k \geq 7$.

3.1.2 A-stability and $A(\theta)$-stability

In numerical analysis, to explain the asymptotic behavior of the numerical solution $\{u_n\}$ to the discretized scheme

$$\sum_{i=0}^{k} \alpha_i u_{n+i} = \lambda \Delta t \sum_{i=0}^{k} \beta_i u_{n+i}, \qquad n \geq 0, \tag{3.1.6}$$

the concept absolute-stability is needed. It yields that for arbitrary fixed $\Delta t > 0$, solutions $\{u_n\}$ remain bounded. More precisely, for some time stepsize Δt and $\lambda \in \mathbb{C}$, the region of absolute stability is defined by

$$\mathcal{S} = \{\mu = \lambda \Delta t \in \mathbb{C} : \ |u_n| \to 0 \ \text{ as } \ t_n \to +\infty\}.$$

Moreover, in terms of the linear multistep method (ρ, σ), the stability region can be expressed equivalently by the set

$$\mathcal{S} = \{\mu \in \mathbb{C} : \ \rho(\xi) - \mu\sigma(\xi) = 0 \text{ with all zeros } |\xi(\mu)| < 1\}. \tag{3.1.7}$$

According to (3.1.6), we define a generating polynomial by

$$\omega(\xi, \mu) = \xi^k \left(\rho(\xi^{-1}) - \mu\sigma(\xi^{-1})\right), \tag{3.1.8}$$

and consider some analytical properties with respect to its reciprocal.

Lemma 3.1.1. *Let $r(\xi, \mu)$ be the reciprocal of the generating polynomial $\omega(\xi)$ defined by (3.1.8), then in the case $\mu \in \mathcal{S}$, we find that the series $r(\xi, \mu)$ is absolutely convergent.*

Proof. Since $\mu \in \mathcal{S}$, according to the definition of $\omega(\xi, \mu)$, the polynomial can be decomposed in the form of

$$\omega(\xi, \mu) = (\alpha_0 - \mu\beta_0) \prod_{n=1}^{k} (\xi - \xi_n(\mu)) = (\alpha_k - \mu\beta_k) \prod_{n=1}^{k} (1 - \xi_n(\mu)^{-1}\xi), \tag{3.1.9}$$

and it implies that $|\xi_n(\mu)| > 1$ for $1 \leq n \leq k$. If we define

$$r^{(m)}(\xi, \mu) = \sum_{i=0}^{\infty} r_i^{(m)}(\mu)\xi^i = \prod_{n=1}^{m} \frac{1}{1 - \xi_n(\mu)^{-1}\xi}, \qquad 1 \leq m \leq k, \tag{3.1.10}$$

in the case $m = 1$, it yields that $r_i^{(1)}(\mu) = (\xi_1(\mu))^{-i}$ for any $i \geq 0$, and consequently,

$$\sum_{i=0}^{\infty} |r_i^{(1)}(\mu)| \leq \sum_{i=0}^{\infty} |\xi_1(\mu)|^{-i} = \frac{1}{1 - |\xi_1(\mu)|^{-1}}.$$

If we assume that $\sum_{i=0}^{\infty} |r_i^{(m-1)}(\mu)| \leq \prod_{n=1}^{m-1} \frac{1}{1-|\xi_n(\mu)|^{-1}}$ in the case $m \geq 2$, then according to formula (3.1.10), it follows that

$$\begin{aligned}
\sum_{i=0}^{\infty} |r_i^{(m)}(\mu)| &= \sum_{i=0}^{\infty} \Big| \sum_{j=0}^{i} r_{i-j}^{(m-1)}(\mu) \left(\xi_m(\mu)\right)^{-j} \Big| \\
&\leq \sum_{j=0}^{\infty} |\xi_m(\mu)|^{-j} \sum_{i=0}^{\infty} |r_i^{(m-1)}(\mu)| \\
&\leq \prod_{n=1}^{m} \frac{1}{1 - |\xi_n(\mu)|^{-1}}.
\end{aligned}$$

Therefore, an induction process yields

$$\sum_{i=0}^{\infty} |r_i(\mu)| \leq \frac{1}{|\alpha_k - \mu\beta_k|} \prod_{n=1}^{k} \frac{1}{1 - |\xi_n(\mu)|^{-1}},$$

which proves the result. □

Remark 3.1.1. *In the situation of the stability region being defined by the set of $\mu \in \mathbb{C}$ satisfying $\rho(\xi) - \mu\sigma(\xi) = 0$ with all zeros $|\xi(\mu)| \leq 1$ and the zeros $|\xi(\mu)| = 1$ is simple, we can obtain the boundedness of the coefficients $\{r_n(\mu)\}_{n=0}^{\infty}$ by partial fractional decomposition (see Appendix A.2).*

Motivated by the fractional linear multistep method whose convolution quadrature weights are generated by power function of order $\alpha \in \mathbb{R}$ of the polynomial $\omega(\xi, \mu)$ in (3.1.8), we next consider the absolutely convergent property of its reciprocal, from which we can deduce that the property of the linear multistep method shown in Lemma 3.1.1 is preserved.

Lemma 3.1.2. *Let the series $r_\alpha(\xi, \mu)$ be defined by the reciprocal of the generating power series $(\omega(\xi, \mu))^\alpha$, where the polynomial $\omega(\xi, \mu)$ is defined by (3.1.8) and $\alpha \in \mathrm{R}^+$. Suppose that $\mu \in \mathrm{S}$, then it holds that the coefficients of the series $r_\alpha(\xi, \mu)$ belong to l^1 space.*

Proof. According to the definition of $\omega(\xi, \mu)$, there exists a factorization of the form

$$r_\alpha(\xi, \mu) = \frac{1}{(\alpha_k - \mu\beta_k)^\alpha} \prod_{n=1}^{k} \frac{1}{(1 - \xi_n(\mu)^{-1}\xi)^\alpha},$$

and in the case $\mu \in \mathcal{S}$, equivalently, it holds that $|\xi_n(\mu)| > 1$ for $1 \leq n \leq k$. Therefore, define that

$$r^{(m)}(\xi, \mu, \alpha) = \sum_{i=0}^{\infty} r_i^{(m)}(\mu, \alpha)\xi^i = \prod_{n=1}^{m} \frac{1}{(1 - \xi_n(\mu)^{-1}\xi)^\alpha}, \qquad 1 \leq m \leq k,$$

and we deduce $r_i^{(1)}(\mu, \alpha) = \binom{-\alpha}{i} (\xi_1(\mu))^{-i}$ as $i \geq 0$. In addition, we obtain

$$\sum_{i=0}^{\infty} |r_i^{(1)}(\mu, \alpha)| \leq \sum_{i=0}^{\infty} \binom{-\alpha}{i} |\xi_1(\mu)|^{-i} = \frac{1}{(1 - |\xi_1(\mu)|^{-1})^\alpha},$$

where $\binom{-\alpha}{i} \geq 0$ in the case $\alpha \in \mathbb{R}^+$ and $i \geq 0$. If we assume that $\sum_{j=0}^{\infty} |r_j^{(m-1)}(\mu, \alpha)| \leq \prod_{i=1}^{m-1} \frac{1}{(1-|\xi_i(\mu)|^{-1})^\alpha}$ for $m \geq 2$, then by induction, it yields

$$\begin{aligned}
\sum_{i=0}^{\infty} |r_i^{(m)}(\mu, \alpha)| &\leq \sum_{i=0}^{\infty}\sum_{j=0}^{i} \binom{-\alpha}{j} |r_{i-j}^{(m-1)}(\mu, \alpha)||\xi_m(\mu)|^{-j} \\
&\leq \sum_{i=0}^{\infty} |r_i^{(m-1)}(\mu, \alpha)| \sum_{j=0}^{\infty} \binom{-\alpha}{j} |\xi_m(\mu)|^{-j} \\
&\leq \prod_{i=1}^{m} \frac{1}{(1 - |\xi_i(\mu)|^{-1})^\alpha},
\end{aligned}$$

correspondingly, from which the desired result follows. □

In the following, As remarked in [59, 68], the analytical property of the generating polynomial $\omega(\xi, \mu)$ can be generalized to an absolutely convergent power series.

Theorem 3.1.3. *Suppose that*

$$\omega(\xi) = \sum_{n=0}^{\infty} \omega_n \xi^n, \quad \sum_{n=0}^{\infty} |\omega_n| < \infty,$$

and $\omega(\xi) \neq 0$ for every $|\xi| \leq 1$. Then

$$\frac{1}{\omega(\xi)} = \sum_{n=0}^{\infty} r_n \xi^n \ \textit{with} \ \sum_{n=0}^{\infty} |r_n| < \infty.$$

Remark 3.1.2. *Since the coefficients of the series $\omega(\xi)$ belong to the space l^1, we can find polynomials $\omega_N(\xi)$ arbitrarily near $\omega(\xi)$, where $\omega_N(\xi)=\sum_{n=0}^{N}\omega_n\xi^n$ is regarded as a partial sum of $\omega(\xi)$ with respect to N. Rigorously speaking, for any $\epsilon>0$, there exists $N=N(\epsilon)\in\mathbb{N}^+$, such that for all $n>N$ and all $|\xi|\le 1$, $|\omega(\xi)-\omega_N(\xi)|<\epsilon$ holds. This yields $\omega_N(\xi)\in B(\omega(\xi),\epsilon)$. For fixed $N>0$, the polynomial $\omega_N(\xi)$ can be factored as*

$$\omega_N(\xi)=\omega_N\prod_{n=0}^{N}(\xi-\xi_n)=\omega_0\prod_{n=0}^{N}(1-\xi_n^{-1}\xi).$$

According to the assumption that $\omega(\xi)\neq 0$ for all $|\xi|\le 1$, we can choose N such that $|\xi_n|>1$ for $1\le n\le N$. Therefore, an induction process deduces

$$\sum_{i=0}^{\infty}|\hat{r}_i|\le\frac{1}{|\omega_0|}\prod_{n=0}^{N}\frac{1}{1-|\xi_n|^{-1}},$$

where $\frac{1}{\omega_N(\xi)}=\sum_{n=0}^{\infty}\hat{r}_n\xi^n$.

Definition 3.1.4 ([23]). *A convergent linear multistep method is $A(\theta)$-stable, $0<\theta<\frac{\pi}{2}$, if the sector*

$$\mathcal{S}_\theta=\{\mu:|\arg(-\mu)|\le\theta,\ \ \mu\neq 0\}\tag{3.1.11}$$

is included in the stability region $\mathcal{S}$.

It is well known that there exists an angle $0<\theta_k\le\frac{\pi}{2}$ such that the k-step BDF method defined in (1.3.16) satisfies $A(\theta_k)$-stability for $1\le k\le 6$. In particular, the backward Euler method and the two-step BDF method are A-stable.

3.2 Stability of proposed methods

As a generalization of the stability analysis in the usual sense, we next consider the numerical stability of schemes (2.1.24) with initial value $u(0)=u_0$. The analysis on the linear difference equation

$$D_{k,i}^{\alpha}u_n=\lambda u_n,\qquad n\ge k\tag{3.2.1}$$

is given in the following steps. We equivalently rewrite (3.2.1) into a formal power series form

$$\sum_{n=0}^{\infty}D_{k,i}^{\alpha}u_{n+k}\xi^n=\lambda\sum_{n=0}^{\infty}u_{n+k}\xi^n.$$

Substituting (2.1.11), one has

$$\omega^{(k,i)}(\xi)u(\xi)=zu(\xi)+g^{(k,i)}(\xi),\tag{3.2.2}$$

where $z:=\lambda(\Delta t)^\alpha$. The formal power series are denoted by

$$\begin{aligned}u(\xi)&=\sum_{n=0}^{\infty}u_{n+k}\xi^n,\quad \omega^{(k,i)}(\xi)=\sum_{n=0}^{\infty}\omega_n^{(k,i)}\xi^n,\\ g^{(k,i)}(\xi)&=-\sum_{j=0}^{k-1}u_j\sum_{n=0}^{\infty}(w_{n+k,j}^{(k,i)}+\omega_{n+k-j}^{(k,i)})\xi^n.\end{aligned}\tag{3.2.3}$$

Inspired by [41, 45], we list the following preliminary conclusions.

Lemma 3.2.1 ([45]). *Assume that the coefficient sequence of $a(\xi)$ is in l^1. Let $|\xi_0| \leq 1$. Then the coefficient sequence of*

$$b(\xi) = \frac{a(\xi) - a(\xi_0)}{\xi - \xi_0}$$

converges to zero.

Theorem 3.2.1 ([2, 64]). *The moment problem*

$$s_k = \int_0^1 u^k \mathrm{d}\sigma(u), \qquad k = 0, 1, \cdots$$

is solvable within the class of non-decreasing functions iff the inequalities

$$(-1)^m \nabla^m s_k \geq 0$$

hold for $k \geq m$.

3.2.1 Stability regions

Lemma 3.2.2. *The coefficient sequences of series $g^{(k,i)}(\xi)$ converge to zero.*

Proof. The expression of $\nabla^k I^r_{n,q}$ in Lemma 2.1.1 yields

$$\lim_{n\to\infty} \nabla^k I^r_{n,q} = \frac{(-\alpha)_k}{\Gamma(1-\alpha)} \int_{[0,1]^{k+1}} \lim_{n\to\infty} \left(\sum_{i=1}^k \xi_i + n - k + 1 - s\right)^{-\alpha-k} \mathrm{d}^k\xi \mathrm{d}\binom{s-q+r-1}{r} = 0$$

or

$$\lim_{n\to\infty} \nabla^k I^r_{n,q} = \frac{(-\alpha)_{k+1}}{\Gamma(1-\alpha)} \int_{[0,1]^{k+1}} \lim_{n\to\infty} \left(\sum_{i=1}^k \xi_i + n - k + 1 - s\right)^{-\alpha-k-1} \binom{s-q+r-1}{r} \mathrm{d}^k\xi \mathrm{d}s = 0$$

for $k, q, r \in \mathbb{N}^+$ that are independent of n and $\alpha > 0$. Note that $g_n^{(k,i)} = -\sum_{j=0}^{k-1} u_j(\omega^{(k,i)}_{n+k,j} + \omega^{(k,i)}_{n+k-j})$ is the finite linear combination of $\nabla^k I^r_{j,q}$ for finite k. This gives $g_n^{(k,i)} \to 0$ as $n \to \infty$ if $\{u_j\}_{j=0}^{k-1}$ are bounded. □

Lemma 3.2.3. *For $1 \leq i \leq k \leq 6$, the coefficient sequence of $\omega^{(k,i)}(\xi)$ belongs to l^1 space.*

Proof. As indicated in Lemma 2.1.1 and Lemma 3.2.2, the following relationship

$$\sum_{n=p}^{\infty} |\nabla^k I^r_{n,q}| = |\sum_{n=p}^{\infty} (\nabla^{k-1} I^r_{n,q} - \nabla^{k-1} I^r_{n-1,q})| = |\nabla^{k-1} I^r_{p-1,q}| \tag{3.2.4}$$

holds for $p \geq k \geq 1$. Therefore, according to the definition of the sequence $\{\omega_n^{(k,i)}\}_{n=0}^{\infty}$, there exists finite positive integer $M = M(k,i)$, such that

$$\begin{aligned}\sum_{n=0}^{\infty} |\omega_n^{(k,i)}| &\leq \sum_{n=0}^{M} |\omega_n^{(k,i)}| + \sum_{m=1}^{k} \sum_{n=m}^{\infty} |\nabla^m I^m_{n,i}| \\ &\leq \sum_{n=0}^{M} |\omega_n^{(k,i)}| + \sum_{m=1}^{k} |\nabla^{m-1} I^m_{m-1,i}|,\end{aligned}$$

which implies the result. □

Lemma 3.2.4. *In the cases $1 \le i \le k \le 6$ and $|\xi_0| \le 1$, the coefficient sequence of $(1-\xi)\frac{\omega^{(k,i)}(\xi)-\omega^{(k,i)}(\xi_0)}{\xi-\xi_0}$ belongs to the space l^1.*

Proof. Using the expression for $\omega^{(k,i)}(\xi)$, the following series can be rewritten as

$$\begin{aligned}(1-\xi)\frac{\omega^{(k,i)}(\xi)-\omega^{(k,i)}(\xi_0)}{\xi-\xi_0} &= (1-\xi)\sum_{n=0}^{\infty}\omega_n^{(k,i)}\frac{\xi^n-\xi_0^n}{\xi-\xi_0}\\ &= (1-\xi)\sum_{n=1}^{\infty}\omega_n^{(k,i)}\sum_{m=0}^{n-1}\xi_0^{n-1-m}\xi^m\\ &= (1-\xi)\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\omega_{n+m+1}^{(k,i)}\xi_0^n\xi^m\\ &= \sum_{n=0}^{\infty}\omega_{n+1}^{(k,i)}\xi_0^n + \sum_{m=1}^{\infty}\Big(\sum_{n=0}^{\infty}\nabla\omega_{n+m+1}^{(k,i)}\xi_0^n\Big)\xi^m.\end{aligned}$$

On the one hand, from Lemma 3.2.3, we have

$$\Big|\sum_{n=0}^{\infty}\omega_{n+1}^{(k,i)}\xi_0^n\Big| \le \sum_{n=0}^{\infty}|\omega_{n+1}^{(k,i)}||\xi_0|^n \le \sum_{n=0}^{\infty}|\omega_{n+1}^{(k,i)}| < +\infty.$$

On the other hand, by the definition of $\{\nabla^{k+1}I_{n,q}^r\}_{n=k+1}^{\infty}$ in Lemma 2.1.1, it can be verified that

$$\begin{aligned}\sum_{m=p}^{\infty}\sum_{n=0}^{\infty}|\nabla^{k+1}I_{m+n+1,q}^r| &= \Big|\sum_{m=p}^{\infty}\sum_{n=0}^{\infty}(\nabla^k I_{m+n+1,q}^r - \nabla^k I_{m+n,q}^r)\Big|\\ &= \Big|\sum_{m=p}^{\infty}(\nabla^{k-1}I_{m,q}^r - \nabla^{k-1}I_{m-1,q}^r)\Big|\\ &= \nabla^{k-1}I_{p-1,q}^r|\end{aligned}$$

for $p \ge k \ge 1$. Therefore, there exists $M_1 = M_1(k,i) \ge 1$ and $M_2 = M_2(k,i) \ge 0$ such that

$$\begin{aligned}\sum_{m=1}^{\infty}\sum_{n=0}^{\infty}|\nabla\omega_{n+m+1}^{(k,i)}| &\le \sum_{m=1}^{M_1}\sum_{n=0}^{M_2}|\nabla\omega_{n+m+1}^{(k,i)}| + \sum_{p=1}^{k}\sum_{m=p}^{\infty}\sum_{n=0}^{\infty}|\nabla^{p+1}I_{m+n+1,i}^p|\\ &\le \sum_{m=1}^{M_1}\sum_{n=0}^{M_2}|\nabla\omega_{n+m+1}^{(k,i)}| + \sum_{p=1}^{k}|\nabla^{p-1}I_{p-1,i}^p|.\end{aligned}$$

Combining this with

$$\Big|\sum_{n=0}^{\infty}\omega_{n+1}^{(k,i)}\xi_0^n\Big| + \sum_{m=1}^{\infty}\Big|\sum_{n=0}^{\infty}\nabla\omega_{n+m+1}^{(k,i)}\xi_0^n\Big| \le \sum_{n=0}^{\infty}|\omega_{n+1}^{(k,i)}| + \sum_{m=1}^{\infty}\sum_{n=0}^{\infty}|\nabla\omega_{n+m+1}^{(k,i)}|,$$

we arrive at the conclusion. □

Corollary 3.2.2. *Assume that $|\xi_0| \le 1$ and $1 \le i \le k \le 6$, then the sequence*

$$(1-\xi)(1-\xi_0)\frac{\varphi^{(k,i)}(\xi)-\varphi^{(k,i)}(\xi_0)}{\xi-\xi_0}$$

belongs to the space l^1, where the series $\varphi^{(k,i)}(\xi)$ satisfies the relation $\omega^{(k,i)}(\xi) = (1-\xi)\varphi^{(k,i)}(\xi)$.

Proof. Based on the definition of $\varphi^{(k,i)}(\xi)$, we obtain

$$(1-\xi)\frac{\omega^{(k,i)}(\xi)-\omega^{(k,i)}(\xi_0)}{\xi-\xi_0} = (1-\xi)\frac{(1-\xi)\varphi^{(k,i)}(\xi)-(1-\xi_0)\varphi^{(k,i)}(\xi_0)}{\xi-\xi_0}$$
$$= (1-\xi)(1-\xi_0)\frac{\varphi^{(k,i)}(\xi)-\varphi^{(k,i)}(\xi_0)}{\xi-\xi_0} - \omega^{(k,i)}(\xi),$$

From the absolute convergence of sequences $(1-\xi)\frac{\omega^{(k,i)}(\xi)-\omega^{(k,i)}(\xi_0)}{\xi-\xi_0}$ and $\omega^{(k,i)}(\xi)$ shown in Lemma 3.2.3 and Lemma 3.2.4, respectively, we arrive at the result. □

Lemma 3.2.5. *Assume that sequence* $\{l_n\}$ *belongs to the space* l^1, *with limit* L, *and sequence* $c_n \to c$ *as* $n \to \infty$, *then* $\sum_{j=0}^{n} l_j c_{n-j} \to cL$ *if* $n \to \infty$.

Proof. According to the assumptions, for any $\varepsilon > 0$, there exists $N_1 > 0$, such that for all $N_p > N_q > N_1$, $\sum_{n=N_q}^{N_p} |l_n| < \varepsilon$ holds. And for any $\varepsilon > 0$, there exists $N_2 > 0$, such that for all $n > N_2$, $|c_n - c| < \varepsilon$. Therefore, for any $\varepsilon > 0$, there exists $N = N_1 + N_2$, such that for all $n > N$,

$$|\sum_{j=0}^{n} l_j c_{n-j} - c\sum_{j=0}^{n} l_j - c\sum_{j=n+1}^{\infty} l_j| \leq |\sum_{j=0}^{n} l_j\,(c_{n-j}-c)| + |c\sum_{j=n+1}^{\infty} l_j|$$
$$\leq \sum_{j=0}^{N_1} |l_j||c_{n-j}-c| + \sum_{j=N_1+1}^{n} |l_j||c_{n-j}| + |c|\sum_{j=n+1}^{\infty} |l_j|$$
$$\leq L\varepsilon + \|c_n\|_\infty \varepsilon + |c|\varepsilon \leq C\varepsilon,$$

which yields the result. □

Theorem 3.2.3. *The stability region of method* $D^\alpha_{k,i}u_n = \lambda u_n$ *is* $\mathrm{S}^{(k,i)} = \mathbb{C}\backslash\{\omega^{(k,i)}(\xi) : |\xi| \leq 1\}$ *in the cases* $1 \leq i \leq k \leq 6$.

Remark 3.2.1. *The definition of stability region* $\mathrm{S}^{(k,i)}$ *of method* $D^\alpha_{k,i}u_n = \lambda u_n$ *is the set of* $z = \lambda(\Delta t)^\alpha \in \mathbb{C}$ *with* $\Delta t > 0$ *for which there is* $u_n \to 0$ *as* $n \to \infty$ *whenever the starting values* $u_0, \cdots, u_{k-1}$ *are bounded.*

Proof. The proof that $S^{(k,i)} = \mathbb{C}\backslash\{\omega^{(k,i)}(\xi) : |\xi| \leq 1\}$ is equivalent with proving both $S^{(k,i)} \supseteq \mathbb{C}\backslash\{\omega^{(k,i)}(\xi) : |\xi| \leq 1\}$ and $S^{(k,i)} \subseteq \mathbb{C}\backslash\{\omega^{(k,i)}(\xi) : |\xi| \leq 1\}$, i.e., to prove that for any $z \in \mathbb{C}\backslash\{\omega^{(k,i)}(\xi) : |\xi| \leq 1\}$, there is $z \in S^{(k,i)}$ and for any $z \notin \mathbb{C}\backslash\{\omega^{(k,i)}(\xi) : |\xi| \leq 1\}$, there is $z \notin S^{(k,i)}$.

On one hand, if $z \in \mathbb{C}\backslash\{\omega^{(k,i)}(\xi) : |\xi| \leq 1\}$ and $|z| \leq 1$, then $z - \omega^{(k,i)}(\xi) \neq 0$ for $|\xi| \leq 1$. Thus according to Lemma 3.2.2, Lemma 3.2.3 and Theorem 3.1.3, the sequence of coefficients of reciprocal of $z - \omega^{(k,i)}(\xi)$ is in l^1 and coefficients of series $g^{(k,i)}(\xi)$ tend to zero.

If $|z| > 1$, formula (3.2.2) can be rewritten to

$$u(\xi) = \frac{\frac{g^{(k,i)}(\xi)}{z}}{\frac{\omega^{(k,i)}(\xi)}{z} - 1},$$

in which case the coefficient sequence of the reciprocal of $\frac{\omega^{(k,i)}(\xi)}{z} - 1$ is in l^1, and the coefficient sequence of series $\frac{g^{(k,i)}(\xi)}{z}$ converges to zero. In addition, assume that $\lim_{n\to\infty}\sum_{j=0}^{n} |l_i| = L < +\infty$

and $\lim_{j\to\infty} c_j = 0$, then from Lemma 3.2.5 it follows that $\lim_{n\to\infty} \sum_{j=0}^{n} l_{n-j}c_j = 0$. This implies that $u_n \to 0$ as $n \to \infty$.

On the other hand, assume that for any $z = \omega^{(k,i)}(\xi_0)$ with $|\xi_0| \le 1$, according to (3.2.2) the solution satisfies

$$\left(\omega^{(k,i)}(\xi) - \omega^{(k,i)}(\xi_0)\right) u(\xi) = g^{(k,i)}(\xi). \tag{3.2.5}$$

Note that method (2.1.11) is exact for a constant function, which leads to

$$\sum_{j=0}^{k-1} w_{n,j}^{(k,i)} + \sum_{j=0}^{n} \omega_{n-j}^{(k,i)} = 0, \qquad n \ge k,$$

and the corresponding formal power series satisfies

$$\begin{aligned}
&\sum_{n=k}^{\infty} \left(\sum_{j=0}^{k-1} w_{n,j}^{(k,i)} + \sum_{j=0}^{n} \omega_{n-j}^{(k,i)} \right) \xi^{n-k} \\
&= \sum_{n=0}^{\infty} \left(\sum_{j=0}^{k-1} w_{n+k,j}^{(k,i)} + \sum_{j=0}^{n+k} \omega_{n+k-j}^{(k,i)} \right) \xi^{n} \\
&= \sum_{n=0}^{\infty} \sum_{j=0}^{k-1} \left(w_{n+k,j}^{(k,i)} + \omega_{n+k-j}^{(k,i)} \right) \xi^{n} + \frac{\omega^{(k,i)}(\xi)}{1-\xi} = 0.
\end{aligned}$$

Assume that $u_0 = \cdots = u_{k-1} \ne 0$, then according to the expression of $g^{(k,i)}(\xi)$, we find $g^{(k,i)}(\xi) = u_0 \frac{\omega^{(k,i)}(\xi)}{1-\xi}$. In the case $\omega^{(k,i)}(\xi_0) = 0$, this gives $u(\xi) = \frac{u_0}{1-\xi}$, which means that $u_n = u_0$ for any $n \in \mathbb{N}$. And for the other cases, we have

$$u(\xi)(1-\xi)\frac{\omega^{(k,i)}(\xi) - \omega^{(k,i)}(\xi_0)}{\xi - \xi_0} = u_0 \frac{\omega^{(k,i)}(\xi) - \omega^{(k,i)}(\xi_0)}{\xi - \xi_0} + u_0 \frac{\omega^{(k,i)}(\xi_0)}{\xi - \xi_0}.$$

If we assume that $u_n \to 0$ as $n \to \infty$, then applying Lemma 3.2.4, it follows that the coefficient sequence of $(1-\xi)\frac{\omega^{(k,i)}(\xi)-\omega^{(k,i)}(\xi_0)}{\xi-\xi_0}$ is in l_1. This indicates that the coefficients of series $u(\xi)(1-\xi)\frac{\omega^{(1,1)}(\xi)-\omega^{(1,1)}(\xi_0)}{\xi-\xi_0}$ tend to zero. In addition, according to Lemma 3.2.1, the sequence of coefficients of $\frac{\omega^{(k,i)}(\xi)-\omega^{(k,i)}(\xi_0)}{\xi-\xi_0}$ converges to zero. However, the divergence of the coefficients of $\frac{1}{\xi-\xi_0}$ for $|\xi_0| \le 1$ leads to a contradiction. Thus, there exist some nonzero bounded initial values $\{u_i\}_{i=0}^{k-1}$ such that $u_n \not\to 0$ as $n \to \infty$, which indicates that $z \notin \mathrm{S}^{(k,i)}$. □

3.2.2 $A(\theta)$-stability analysis

According to the definition of $A(\theta)$-stability [23] in the ordinary case, we define the $A(\theta)$-stability in the following sense for $0 < \alpha < 1$:

Definition 3.2.1. *A method is said to be $A(\theta)$-stable for $\theta \in [0, \pi - \frac{\alpha\pi}{2})$, if the sector*

$$S_\theta = \{z : |\arg(-z)| \le \theta, \ z \ne 0\}$$

is contained in the stability region.

Theorem 3.2.4. *The methods (3.2.1) are $A(\frac{\pi}{2})$-stable for $1 \le i \le k \le 2$.*

Proof. In view of the definition of $A(\theta)$-stability, in particular, when $\theta = \frac{\pi}{2}$, it suffices to prove that $S_{\frac{\pi}{2}} \subseteq S^{(k,i)}$ for $1 \le i \le k \le 2$, i.e., to prove $\omega^{(k,i)}(\xi) = 0$ for some $|\xi| \le 1$ and $\mathrm{Re}(\omega^{(k,i)}(\xi)) > 0$ otherwise.

First of all, $\omega^{(k,i)}(1) = 0$ can be easily checked, which implies $0 \notin S_{\frac{\pi}{2}}$. In the case $(k,i) = (1,1)$, from the expression of $\omega^{(1,1)}(\xi)$, we have

$$\omega^{(1,1)}(\xi) = I_0 + \sum_{j=1}^{\infty} \nabla I_j \xi^j = (1-\xi)I(\xi), \tag{3.2.6}$$

where $I(\xi) = \sum\limits_{n=0}^{\infty} I_n \xi^n$. According to Lemma 2.1.1, it follows that I_n is a completely monotonic sequence. Then from Theorem 3.2.1, one has

$$I_n = \int_0^1 r^n \mathrm{d}\sigma(r), \quad n \in \mathbb{N}, \tag{3.2.7}$$

where $\sigma(r)$ is a non-decreasing function. Suppose that $|\xi| < 1$, substituting (3.2.7) into (3.2.6) yields

$$\Re\left(\omega^{(1,1)}(\xi)\right) = \Re\left((1-\xi)\sum_{n=0}^{\infty}\int_0^1 r^n \mathrm{d}\sigma(r)\xi^n\right) = \int_0^1 \Re\left(\frac{1-\xi}{1-r\xi}\right)\mathrm{d}\sigma(r).$$

Let $\xi = |\xi|(\cos\theta + i\sin\theta)$, then

$$\begin{aligned}
\frac{1-\xi}{1-r\xi} &= \frac{(1-\xi)(\overline{1-r\xi})}{(1-r\xi)(\overline{1-r\xi})} \\
&= \frac{(1-|\xi|\cos\theta - i|\xi|\sin\theta)(1-r|\xi|\cos\theta + ir|\xi|\sin\theta)}{(1-r|\xi|\cos\theta - ir|\xi|\sin\theta)(1-r|\xi|\cos\theta + ir|\xi|\sin\theta)} \\
&= \frac{\left(1-(r+1)|\xi|\cos\theta + r|\xi|^2\right) + i\left((r-1)|\xi|\sin\theta\right)}{(1-r|\xi|\cos\theta)^2 + (r|\xi|\sin\theta)^2}.
\end{aligned}$$

In the cases $0 \le r \le 1$ and $|\xi| < 1$, we find

$$\begin{aligned}
&1-(r+1)|\xi|\cos\theta + r|\xi|^2 \ge \min\left((1-|\xi|\cos\theta)^2, 1-|\xi|\cos\theta\right), \\
&1-2r|\xi|\cos\theta + r^2|\xi|^2 \le (1+r|\xi|)^2 \le 4,
\end{aligned}$$

which gives us

$$\int_0^1 \Re\left(\frac{1-\xi}{1-r\xi}\right)\mathrm{d}\sigma(r) \ge \frac{\min\left((1-|\xi|\cos\theta)^2, 1-|\xi|\cos\theta\right)}{4} I_0.$$

In the case $(k,i) = (2,1)$, using the definition of $\omega^{(2,1)}(\xi)$, we observe

$$\begin{aligned}
\omega^{(2,1)}(\xi) &= \sum_{n=0}^{\infty}\left(\nabla I_n + \nabla^2 I_{n,1}^2\right)\xi^n \\
&= (1-\xi)I(\xi) + (1-\xi)^2 I_1^2(\xi) \\
&= (1-\xi)\left(I(\xi) - 2I_1^2(\xi) + (3-\xi)I_1^2(\xi)\right),
\end{aligned} \tag{3.2.8}$$

where

$$I(\xi) = \sum_{n=0}^{\infty} I_n \xi^n, \qquad I_1^2(\xi) = \sum_{n=0}^{\infty} I_{n,1}^2 \xi^n.$$

Since it is known that

$$I_n - 2I_{n,1}^2 = \frac{2}{\Gamma(1-\alpha)} \int_0^1 (n+1-s)^{-\alpha}(1-s)\mathrm{d}s,$$

based on Lemma 2.1.1, Corollary 2.1.1 and Theorem 3.2.1, there exist non-decreasing functions v and γ, respectively, such that

$$I_n - 2I_{n,1}^2 = \int_0^1 r^n \mathrm{d}v(r), \quad n = 0, 1, \cdots, \tag{3.2.9}$$

and

$$I_{n,1}^2 = \int_0^1 r^n \mathrm{d}\gamma(r), \qquad n = 0, 1, \cdots. \tag{3.2.10}$$

Then for $|\xi| < 1$,

$$\Re\left(\omega^{(2,1)}(\xi)\right) = \int_0^1 \Re\left(\frac{1-\xi}{1-r\xi}\right)\mathrm{d}v(r) + \int_0^1 \Re\left(\frac{(1-\xi)(3-\xi)}{1-r\xi}\right)\mathrm{d}\gamma(r).$$

Moreover, this indicates

$$\begin{aligned}
\frac{(1-\xi)(3-\xi)}{1-r\xi} =& \frac{(1-\xi)(3-\xi)\overline{(1-r\xi)}}{(1-r\xi)\overline{(1-r\xi)}} \\
=& \frac{(1-|\xi|\cos\theta - i|\xi|\sin\theta)\,(3-|\xi|\cos\theta - i|\xi|\sin\theta)\,(1-r|\xi|\cos\theta + ir|\xi|\sin\theta)}{(1-r|\xi|\cos\theta - ir|\xi|\sin\theta)\,(1-r|\xi|\cos\theta + ir|\xi|\sin\theta)} \\
=& \frac{(3-4|\xi|\cos\theta + |\xi|^2\cos 2\theta)(1-r|\xi|\cos\theta) + (4-2|\xi|\cos\theta)r|\xi|^2\sin^2\theta}{(1-r|\xi|\cos\theta)^2 + (r|\xi|\sin\theta)^2} \\
&+ i\frac{(3r-|\xi|^2 r - 4 + 2|\xi|\cos\theta)|\xi|\sin\theta}{(1-r|\xi|\cos\theta)^2 + (r|\xi|\sin\theta)^2}.
\end{aligned}$$

Since

$$3 - 4|\xi|\cos\theta + |\xi|^2\cos 2\theta = 3 - 4|\xi|\cos\theta + 2|\xi|^2\cos^2\theta - |\xi|^2 \geq 2(1-|\xi|\cos\theta)^2,$$

we get

$$\int_0^1 \Re\left(\frac{(1-\xi)(3-\xi)}{1-r\xi}\right)\mathrm{d}\gamma(r) \geq \frac{\min\left((1-|\xi|\cos\theta)^3, (1-|\xi|\cos\theta)^2\right)}{2} I_{0,1}^2.$$

In the case $(k,i) = (2,2)$, we first propose the equivalent form of $\omega^{(2,2)}(\xi)$, which satisfies

$$\begin{aligned}
\omega^{(2,2)}(\xi) =& I_0(1-\xi) + I_{0,1}^2(1-\xi)^2 + (1-\xi)\sum_{n=0}^{\infty} I_{n+1}\xi^n + (1-\xi)^2\sum_{n=0}^{\infty} I_{n+1,2}^2\xi^n \\
=& I_{0,1}^2(1-\xi)(3-\xi) + (1-\xi^2)\sum_{n=0}^{\infty} I_{n+1,1}^2\xi^n + (1-\xi)\left(I(\xi) - 2I_1^2(\xi)\right).
\end{aligned} \tag{3.2.11}$$

Since for any $n \geq 0$, using the relation $I_n + I_{n,2}^2 = I_{n,1}^2$, this yields

$$\begin{aligned}
&(1-\xi)\sum_{n=0}^{\infty} I_{n+1}\xi^n + (1-\xi)^2\sum_{n=0}^{\infty} I_{n+1,2}^2\xi^n \\
=&(1-\xi)\Big(\sum_{n=0}^{\infty} I_{n+1,1}^2\xi^n - \xi\sum_{n=0}^{\infty} I_{n+1,2}^2\xi^n\Big) \\
=&(1-\xi^2)\sum_{n=0}^{\infty} I_{n+1,1}^2\xi^n + (1-\xi)\sum_{n=0}^{\infty}\left(I_{n+1} - 2I_{n+1,1}^2\right)\xi^{n+1} \\
=&(1-\xi^2)\sum_{n=0}^{\infty} I_{n+1,1}^2\xi^n + (1-\xi)\left(I(\xi) - 2I_1^2(\xi) - (I_0 - 2I_{0,1}^2)\right).
\end{aligned}$$

Next, suppose that $|\xi| < 1$, substituting (3.2.9) and (3.2.10) into the expression of $\omega^{(2,2)}(\xi)$, one obtains

$$\begin{aligned}
\Re\left(\omega^{(2,2)}(\xi)\right) =& \int_0^1 \Re\left((1-\xi)(3-\xi)\right)\mathrm{d}\gamma(r) \\
&+ \int_0^1 r\Re\left(\frac{1-\xi^2}{1-r\xi}\right)\mathrm{d}\gamma(r) + \int_0^1 \Re\left(\frac{1-\xi}{1-r\xi}\right)\mathrm{d}v(r).
\end{aligned}$$

Furthermore, it follows that

$$\begin{aligned}
\frac{1-\xi^2}{1-r\xi} =& \frac{(1-\xi^2)\overline{(1-r\xi)}}{(1-r\xi)\overline{(1-r\xi)}} \\
=& \frac{\left(1-|\xi|^2\cos 2\theta - i|\xi|^2\sin 2\theta\right)\left(1-r|\xi|\cos\theta + ir|\xi|\sin\theta\right)}{\left(1-r|\xi|\cos\theta - ir|\xi|\sin\theta\right)\left(1-r|\xi|\cos\theta + ir|\xi|\sin\theta\right)} \\
=& \frac{(1-|\xi|^2\cos 2\theta)(1-r|\xi|\cos\theta) + r|\xi|^3\sin\theta\sin 2\theta}{(1-r|\xi|\cos\theta)^2 + (r|\xi|\sin\theta)^2} \\
&+ i\frac{(1-|\xi|^2\cos 2\theta)r|\xi|\sin\theta - (1-r|\xi|\cos\theta)\rho^2\sin 2\theta}{(1-r|\xi|\cos\theta)^2 + (r|\xi|\sin\theta)^2}.
\end{aligned}$$

Since for $0 \leq r \leq 1$, we have

$$\begin{aligned}
&(1-|\xi|^2\cos 2\theta)(1-r|\xi|\cos\theta) + r|\xi|^3\sin\theta\sin 2\theta \\
=&1 - |\xi|^2\cos 2\theta - r|\xi|\cos\theta + r|\xi|^3\cos\theta \\
\geq&1 - |\xi|^2 - r|\xi|\cos\theta(1-|\xi|^2) \\
=&(1-|\xi|^2)(1-|\xi||\cos\theta|),
\end{aligned}$$

we may see that

$$\begin{aligned}
\int_0^1 r\Re\left(\frac{1-\xi^2}{1-r\xi}\right)\mathrm{d}\gamma(r) \geq& \frac{(1-|\xi|^2)(1-|\xi||\cos\theta|)}{4}\int_0^1 r\mathrm{d}\gamma(r) \\
=& \frac{(1-|\xi|^2)(1-|\xi||\cos\theta|)}{4}I_{1,1}^2.
\end{aligned} \tag{3.2.12}$$

As a result, for $1 \leq i \leq k \leq 2$, this demonstrates that

$$\Re\left(\omega^{(k,i)}(\xi)\right) \geq \frac{\min\left((1-|\xi|\cos\theta)^2, 1-|\xi|\cos\theta\right)}{4}I_0 > 0, \qquad |\xi| < 1.$$

In addition, according to Lemma 3.2.4, there exists a constant $M^{(k,i)} > 0$ such that

$$\left|\omega^{(k,i)}(\xi) - \omega^{(k,i)}(\xi_0)\right| \leq \frac{M^{(k,i)}}{|1-\xi|}|\xi - \xi_0|, \qquad \xi \neq 1,$$

which shows the pointwise continuity of $\omega^{(k,i)}(\xi)$ for $|\xi| \leq 1$ with the exception of $\xi = 1$. Therefore, for any fixed ξ lying on the unit circle, and the angle satisfying $\arg(\xi) = \theta_\xi \neq 0$, there exists a sequence $\xi_n = (1 - \frac{1}{n})\xi$ with $|\xi_n| < 1$ for any $n = 1, 2, \cdots$, such that

$$\Re\left(\omega^{(k,i)}(\xi)\right) = \lim_{n\to\infty} \Re\left(\omega^{(k,i)}(\xi_n)\right) \geq \frac{I_0}{4}\min\left((1-\cos\theta_\xi)^2, 1-\cos\theta_\xi\right) > 0.$$

□

In [30], A_0-stability of a method is introduced. In the following part, we generalize the stability property to the proposed methods.

Definition 3.2.2 ([30]). *A method is A_0-stable iff $\mathbb{R}^- \subset \mathrm{S}$, where* S *is denoted by the stability region.*

Remark 3.2.2. *The following statements are equivalent:*

i). *The method $D^\alpha_{k,i}u_n = \lambda u_n$ is A_0-stable;*

ii). *For any $z \in \mathbb{R}^-$, $z - \omega^{(k,i)}(\xi) \neq 0$ with $|\xi| \leq 1$;*

iii). *For arbitrary $|\xi| \leq 1$, $\omega^{(k,i)}(\xi) \notin \mathbb{R}^-$ holds;*

iv). *For those $|\xi| \leq 1$ such that $\Im(\omega^{(k,i)}(\xi)) = 0$, one obtains $\Re(\omega^{(k,i)}(\xi)) \geq 0$.*

Theorem 3.2.5. *In the cases $1 \leq i \leq k \leq 3$, the methods $D^\alpha_{k,i}u_n = \lambda u_n$ are A_0-stable.*

Proof. In accordance with the expression of $\omega^{(k,i)}(\xi)$ in (3.2.14) with $\xi = 1$, it is known that $\omega^{(k,i)}(1) = 0$. In this case $\Im(\omega^{(k,i)}(1)) = \Re(\omega^{(k,i)}(1)) = 0$ holds. Besides, for those $|\xi| \leq 1$ with $\xi \neq 1$, one has

$$\Re(1-\xi)\Im(\varphi^{(k,i)}(\xi)) + \Re(\varphi^{(k,i)}(\xi))\Im(1-\xi) = 0. \tag{3.2.13}$$

Therefore, substituting (3.2.13) into the real part of $\omega^{(k,i)}(\xi)$, and using the fact that $|\varphi^{(k,i)}(\xi)| \geq \Re(\varphi^{(k,i)}(\xi)) > 0$ for all $|\xi| \leq 1$ in Theorem 3.2.6, we obtain

$$\Re(\omega^{(k,i)}(\xi)) = \frac{\Re(1-\xi)}{\Re(\varphi^{(k,i)}(\xi))}|\varphi^{(k,i)}(\xi)|^2 > 0.$$

□

3.2.3 Generalized strong root condition

It is shown in Theorem 3.2.4 that all the remaining zeros of series $\omega^{(k,i)}(\xi)$ $(1 \leq i \leq k \leq 2)$ are outside the unit disc except the zero $\xi = 1$. We next consider the location of zeros of series $\omega^{(k,i)}(\xi)$ in the case $1 \leq i \leq k \leq 3$ and confirm that $\xi = 1$ is a simple zero. The following result can be considered as an extension of the strong root condition presented in Definition 3.1.3.

Theorem 3.2.6. *In the cases $1 \leq i \leq k \leq 3$, the series $\omega^{(k,i)}(\xi)$ satisfies the following conditions:*

i). *$\omega^{(k,i)}(\xi) \neq 0$ within the unit circle $|\xi| \leq 1$ and $\xi \neq 1$;*

ii). $\xi = 1$ *is a simple zero.*

Proof. It can be easily checked that $\omega^{(k,i)}(1) = 0$, yielding that $\xi = 1$ is a zero, if we rewrite the series $\omega^{(k,i)}(\xi)$ in the form

$$\omega^{(k,i)}(\xi) = (1-\xi)\varphi^{(k,i)}(\xi), \tag{3.2.14}$$

it remains to prove that $\varphi^{(k,i)}(\xi) \neq 0$ for $|\xi| \leq 1$, which suffices to prove that $\mathrm{Re}(\varphi^{(k,i)}(\xi)) > 0$ for all $|\xi| \leq 1$. We first consider the integral of form $\int_0^1 \frac{\psi(\xi)}{1-r\xi}\mathrm{d}g(r)$. In the case where $g(r)$ is non-decreasing with respect to r, $\Re\left(\frac{\psi(\xi)}{1-r\xi}\right) \geq 0$ yields $\Re\left(\int_0^1 \frac{\psi(\xi)}{1-r\xi}\mathrm{d}g(r)\right) \geq 0$. Assume that $\xi = |\xi|e^{i\theta} = |\xi|(\cos\theta + i\sin\theta)$ as $|\xi| < 1$, then

$$\begin{aligned}\frac{\psi(\xi)}{1-r\xi} &= \frac{(\Re\psi + i\Im\psi)(1 - r|\xi|\cos\theta + ir|\xi|\sin\theta)}{(1 - r|\xi|\cos\theta - ir|\xi|\sin\theta)(1 - r|\xi|\cos\theta + ir|\xi|\sin\theta)} \\ &= \frac{(1-r|\xi|\cos\theta)\Re\psi - r|\xi|\sin\theta\Im\psi}{1 - 2r|\xi|\cos\theta + r^2|\xi|^2} + i\frac{\Im\psi(1-r|\xi|\cos\theta) + r|\xi|\sin\theta\Re\psi}{1 - 2r|\xi|\cos\theta + r^2|\xi|^2}.\end{aligned} \tag{3.2.15}$$

In the case $(k,i) = (1,1)$, it is deduced from (3.2.6) and (3.2.7) that

$$\varphi^{(1,1)}(\xi) = I(\xi) = \int_0^1 \frac{1}{1-r\xi}\mathrm{d}\sigma(\mathrm{r}),$$

and furthermore,

$$\Re\left(\varphi^{(1,1)}(\xi)\right) = \int_0^1 \Re\left(\frac{1}{1-r\xi}\right)\mathrm{d}\sigma(\mathrm{r}) = \int_0^1 f(r,|\xi|,\theta)\mathrm{d}\sigma(\mathrm{r}),$$

where by choosing $\psi(\xi) = 1$ in (3.2.15), we see that $f(r,|\xi|,\theta) = \frac{1-r|\xi|\cos\theta}{1-2r|\xi|\cos\theta + r^2|\xi|^2}$. In view of

$$\frac{\partial f}{\partial \theta}(r,|\xi|,\theta) = \frac{-r|\xi|\sin\theta(1-r^2|\xi|^2)}{(1-2r|\xi|\cos\theta + r^2|\xi|^2)^2},$$

for $0 \leq r \leq 1$ and $0 \leq |\xi| < 1$, it follows that $0 < f(r,|\xi|,\pi) \leq f(r,|\xi|,\theta) \leq f(r,|\xi|,0)$. Thus

$$\Re\left(\varphi^{(1,1)}(\xi)\right) \geq \int_0^1 \frac{1}{1+r|\xi|}\mathrm{d}\sigma(\mathrm{r}) \geq \frac{I_0}{2}.$$

In the case $(k,i) = (2,1)$, according to formulae (3.2.8), (3.2.9) and (3.2.10), one obtains

$$\begin{aligned}\varphi^{(2,1)}(\xi) =& I(\xi) - 2I_1^2(\xi) + (3-\xi)I_1^2(\xi) \\ =& \int_0^1 \frac{1}{1-r\xi}\mathrm{d}\upsilon(r) + \int_0^1 \frac{3-\xi}{1-r\xi}\mathrm{d}\gamma(r),\end{aligned}$$

therefore

$$\begin{aligned}\Re\left(\varphi^{(2,1)}(\xi)\right) &= \int_0^1 \Re\left(\frac{1}{1-r\xi}\right)\mathrm{d}\upsilon(r) + \int_0^1 \Re\left(\frac{3-\xi}{1-r\xi}\right)\mathrm{d}\gamma(r) \\ &\geq \int_0^1 \frac{1}{1+r|\xi|}\mathrm{d}\upsilon(r) + 2\int_0^1 \frac{1}{1+r|\xi|}\mathrm{d}\gamma(r) + \int_0^1 \Re\left(\frac{1-\xi}{1-r\xi}\right)\mathrm{d}\gamma(r) > \frac{I_0}{2}.\end{aligned}$$

In the case $(k,i) = (2,2)$, it is obtained from (3.2.11) that

$$\varphi^{(2,2)}(\xi) = I_{0,1}^2(3-\xi) + (1+\xi)\sum_{n=0}^{\infty} I_{n+1,1}^2\xi^n + I(\xi) - 2I_1^2(\xi).$$

Based on (3.2.9) and (3.2.10), the real part of the series can be expressed by

$$\Re\left(\varphi^{(2,2)}(\xi)\right) = I_{0,1}^2 \Re(3-\xi) + \int_0^1 r\Re\left(\frac{1+\xi}{1-r\xi}\right) \mathrm{d}\gamma(r) + \int_0^1 \Re\left(\frac{1}{1-r\xi}\right) \mathrm{d}\upsilon(r).$$

Substituting $\psi(\xi)$ in (3.2.15) by $1+\xi$, we have $\Re\psi = 1 + |\xi|\cos\theta$ and $\Im\psi = |\xi|\sin\theta$. Then

$$\Re\left(\frac{1+\xi}{1-r\xi}\right) = \frac{1 - r|\xi|\cos\theta + |\xi|\cos\theta - r|\xi|^2}{1 - 2r|\xi|\cos\theta + r^2|\xi|^2} = f(r, |\xi|, \theta).$$

The relation

$$\frac{\partial f}{\partial \theta}(r, |\xi|, \theta) = \frac{-|\xi|\sin\theta(r+1)(1-r^2|\xi|^2)}{(1-2r|\xi|\cos\theta + r^2|\xi|^2)^2}$$

implies that $f(r,|\xi|,\theta) \geq f(r,|\xi|,\pi) > 0$ for $0 \leq r \leq 1$ and $0 \leq |\xi| < 1$, which means $\int_0^1 r\Re\left(\frac{1+\xi}{1-r\xi}\right)\mathrm{d}\gamma(r) \geq 0$ accordingly. In addition, one finds $I_{0,1}^2\Re(3-\xi) \geq 2I_{0,1}^2$ as $\Re(3-\xi) \geq 2$ for $|\xi| \leq 1$. Therefore, we obtain $\Re\left(\varphi^{(2,2)}(\xi)\right) \geq \frac{I_0}{2} + I_{0,1}^2 > 0$.

In the case $(k,i) = (3,1)$, based on (2.1.13), a rewritten form of series $\omega^{(3,1)}(\xi)$ is

$$\omega^{(3,1)}(\xi) = (1-\xi)I(\xi) + (1-\xi)^2 I_1^2(\xi) + (1-\xi)^3 I_1^3(\xi),$$

and consequently $\varphi^{(3,1)}(\xi)$ is given by

$$\begin{aligned}\varphi^{(3,1)}(\xi) &= I(\xi) + (1-\xi)I_1^2(\xi) + (1-\xi)^2 I_1^3(\xi) \\ &= I(\xi) - 3I_1^3(\xi) + (1-\xi)I_1^2(\xi) + (4 - 2\xi + \xi^2)I_1^3(\xi).\end{aligned} \tag{3.2.16}$$

According to Lemma 2.1.2, we obtain that

$$\begin{aligned}I_n - 3I_{n,1}^3 &= \frac{1}{\Gamma(1-\alpha)}\int_0^1 (n+1-s)^{-\alpha}\left(1 - \frac{3s^2-1}{2}\right)\mathrm{d}s \\ &= \frac{3}{2}\frac{1}{\Gamma(1-\alpha)}\int_0^1 (n+1-s)^{-\alpha}(1-s^2)\mathrm{d}s, \qquad n \geq 0\end{aligned}$$

is a completely monotonic sequence. From Theorem 3.2.1 there exists a non-decreasing function, named η, such that

$$I_n - 3I_{n,1}^3 = \int_0^1 r^n \mathrm{d}\eta(r), \qquad n = 0, 1, \cdots.$$

In addition, we have from Lemma 2.1.1 that the sequence $\{I_{n,1}^3\}_{n=0}^{\infty}$ is a complete monotonic sequence, therefore it can be represented by

$$I_{n,1}^3 = \int_0^1 r^n \mathrm{d}\beta(r), \qquad n = 0, 1, \cdots, \tag{3.2.17}$$

where the function $\beta(r)$ is non-decreasing on $[0,1]$. We thus represent the series into the integral form and take the real part,

$$\Re\left(\varphi^{(3,1)}(\xi)\right) = \int_0^1 \Re\left(\frac{1}{1-r\xi}\right)\mathrm{d}\eta(r) + \int_0^1 \Re\left(\frac{1-\xi}{1-r\xi}\right)\mathrm{d}\gamma(r) + \int_0^1 \Re\left(\frac{4-2\xi+\xi^2}{1-r\xi}\right)\mathrm{d}\beta(r).$$

Assume that $\psi(\xi) = \frac{3}{2} - 2\xi + \xi^2$, where $\Re\psi = \frac{3}{2} - 2|\xi|\cos\theta + |\xi|^2\cos 2\theta$ and $\Im\psi = |\xi|^2\sin 2\theta - 2|\xi|\sin\theta$. From (3.2.15) we see that

$$\Re\left(\frac{\frac{3}{2} - 2\xi + \xi^2}{1 - r\xi}\right) = \frac{(1 - r|\xi|\cos\theta)(\frac{3}{2} - 2|\xi|\cos\theta + |\xi|^2\cos 2\theta) + 2r|\xi|^2\sin^2\theta(1 - |\xi|\cos\theta)}{1 - 2r|\xi|\cos\theta + r^2|\xi|^2}.$$

Since

$$\frac{3}{2} - 2|\xi|\cos\theta + |\xi|^2\cos 2\theta = \frac{1}{2}(1-2|\xi|\cos\theta)^2 + (1-|\xi|^2) \geq 0$$

as $|\xi| \leq 1$ and $\theta \in \mathbb{R}$, it follows that

$$\Re\left(\varphi^{(3,1)}(\xi)\right) \geq \int_0^1 \frac{1}{1+r|\xi|}\mathrm{d}\eta(r) + \frac{5}{2}\int_0^1 \frac{1}{1+r|\xi|}\mathrm{d}\beta(r) \geq \frac{1}{2}I_0 - \frac{1}{4}I_{0,1}^3.$$

In the case $(k,i) = (3,2)$, according to the representation of $\{\omega_n^{(2,2)}\}_{n=0}^{\infty}$ in (2.1.14), we derive the following expression for $\varphi^{(3,2)}(\xi)$:

$$\begin{aligned}\varphi^{(3,2)}(\xi) =& I_0 + \sum_{j=0}^{\infty} I_{j+1}\xi^j + I_{0,1}^2(1-\xi) + (1-\xi)\sum_{j=0}^{\infty} I_{j+1,2}^2\xi^j \\ &+(1-\xi)^2 I_{0,1}^3 + (1-\xi)^2\sum_{j=0}^{\infty} I_{j+1,2}^3\xi^j.\end{aligned} \tag{3.2.18}$$

Substituting the relations $I_{n,2}^2 = I_{n,1}^2 - I_n$ and $I_{n,2}^3 = I_{n,1}^3 - I_{n,1}^2$ into (3.2.18), one finds

$$\begin{aligned}\varphi^{(3,2)}(\xi) =& I(\xi) + (1-\xi)I_1^2(\xi) + (1-\xi^2)\sum_{j=0}^{\infty} I_{j+1,1}^3\xi^j \\ &-2(1-\xi)I_1^3(\xi) + (3-\xi)(1-\xi)I_{0,1}^3 \\ =& \left(\frac{5}{6}+\frac{1}{6}\xi\right)I(\xi) + (1-\xi)\left(I_1^2(\xi) - 2I_1^3(\xi) + \frac{1}{6}I(\xi)\right) \\ &+ (1-\xi^2)\sum_{j=0}^{\infty} I_{j+1,1}^3\xi^j + (3-\xi)(1-\xi)I_{0,1}^3.\end{aligned}$$

Based on Lemma 2.1.2, one hence obtains that

$$I_{n,1}^2 - 2I_{n,1}^3 + \frac{1}{6}I_n = \frac{1}{\Gamma(1-\alpha)}\int_0^1 (n+1-s)^{-\alpha}s(1-s)\mathrm{d}s, \quad n \geq 0$$

is a completely monotonic sequence. Therefore the sequence is expressed by

$$I_{n,1}^2 - 2I_{n,1}^3 + \frac{1}{6}I_n = \int_0^1 r^n \mathrm{d}\mu(r), \quad n = 0, 1, \cdots. \tag{3.2.19}$$

Note that the function $\mu(r)$ is non-decreasing on interval $[0,1]$. From formulae (3.2.7), (3.2.19) and (3.2.17), it follows that

$$\begin{aligned}\Re\left(\varphi^{(3,2)}(\xi)\right) =& \int_0^1 \Re\left(\frac{\frac{5}{6}+\frac{1}{6}\xi}{1-r\xi}\right)\mathrm{d}\sigma(r) + \int_0^1 \Re\left(\frac{1-\xi}{1-r\xi}\right)\mathrm{d}\mu(r) \\ &+ \int_0^1 r\Re\left(\frac{1-\xi^2}{1-r\xi}\right)\mathrm{d}\beta(r) + \Re\left((3-\xi)(1-\xi)\right)I_{0,1}^3 \\ \geq& \frac{2}{3}\int_0^1 \frac{1}{1+r|\xi|}\mathrm{d}\sigma(r) \geq \frac{I_0}{3}.\end{aligned}$$

In the case $(k,i) = (3,3)$, the definition of the series $\omega^{(3,3)}(\xi)$ coincides with

$$\begin{aligned}\omega^{(3,3)}(\xi) =& (1-\xi)(I_0+I_1) + (1-\xi)\sum_{j=0}^{\infty} I_{j+2}\xi^j + (1-\xi)^2(I_{0,1}^2 + I_{1,2}^2) \\ &+ (1-\xi)^2\sum_{j=0}^{\infty} I_{j+2,3}^2\xi^j + (1-\xi)^3(I_{0,1}^3 + I_{1,2}^3) + (1-\xi)^3\sum_{j=0}^{\infty} I_{j+2,3}^3\xi^j.\end{aligned} \tag{3.2.20}$$

Therefore it follows that

$$\begin{aligned}\varphi^{(3,3)}(\xi) =& I_0 + I_1 + \sum_{j=0}^{\infty} I_{j+2}\xi^j + (1-\xi)\left(I_{0,1}^2 + I_{1,2}^2\right) + (1-\xi)\sum_{j=0}^{\infty} I_{j+2,3}^2\xi^j \\ &+ (1-\xi)^2\left(I_{0,1}^3 + I_{1,2}^3\right) + (1-\xi)^2\sum_{j=0}^{\infty} I_{j+2,3}^3\xi^j.\end{aligned} \tag{3.2.21}$$

In addition, substituting the relations

$$\begin{aligned}I_{n,3}^2 &= I_{n,2}^2 - I_n = I_{n,1}^2 - 2I_n, \\ I_{n,3}^3 &= I_{n,2}^3 - I_{n,2}^2 = I_{n,1}^3 - 2I_{n,1}^2 + I_n, \qquad n \geq 0\end{aligned}$$

into (3.2.21) shows that

$$\begin{aligned}\varphi^{(3,3)}(\xi) =& I_0 + I_1 + \sum_{j=0}^{\infty} I_{j+2}\xi^j + (1-\xi)\left(I_{0,1}^2 + I_{1,1}^2 - I_1\right) + (1-\xi)\sum_{j=0}^{\infty}\left(I_{j+2,1}^2 - 2I_{j+2}\right)\xi^j \\ &+ (1-\xi)^2\left(I_{0,1}^3 + I_{1,1}^3 - I_{1,1}^2\right) + (1-\xi)^2\sum_{j=0}^{\infty}\left(I_{j+2,1}^3 - 2I_{j+2,1}^2 + I_{j+2}\right)\xi^j \\ =& I(\xi) + (1-\xi)I_1^2(\xi) - 2(1-\xi)I_1^3(\xi) + (1-\xi^2)\sum_{j=0}^{\infty} I_{j+2,2}^3\xi^j - (3 - 4\xi + \xi^2)\sum_{j=0}^{\infty} I_{j+1,2}^3\xi^j \\ &+ (3-\xi)(1-\xi)\left(I_{0,1}^3 + I_{1,2}^3\right) + (1-\xi^2)\sum_{j=0}^{\infty} I_{j+1,1}^3\xi^j.\end{aligned}$$

In view of Lemma 2.1.1, the sequence $\{-I_{n,2}^3\}_{n=0}^{\infty}$ is completely monotonic. Thus there exists a non-decreasing function $\vartheta(r)$ defined on $[0,1]$ such that

$$-I_{n,2}^3 = \int_0^1 r^n \mathrm{d}\vartheta(r), \qquad n = 0, 1, \cdots.$$

This yields that

$$(1-\xi^2)\sum_{j=0}^{\infty} I_{j+2,2}^3\xi^j - (3 - 4\xi + \xi^2)\sum_{j=0}^{\infty} I_{j+1,2}^3\xi^j = \int_0^1 \frac{(3r - r^2) - 4r\xi + (r^2 + r)\xi^2}{1 - r\xi}\mathrm{d}\vartheta(r)$$

in the case $|\xi| < 1$. Substituting $\psi(\xi)$ by $\frac{(3r-r^2)-4r\xi+(r^2+r)\xi^2}{1-r\xi}$ in (3.2.15), one thus obtains

$$\begin{aligned}&\Re\left(\frac{(3r - r^2) - 4r\xi + (r^2 + r)\xi^2}{1 - r\xi}\right) \\ =&\frac{(1 - r|\xi|\cos\theta)\left(3r - r^2 - 4r|\xi|\cos\theta + (r^2 + r)|\xi|^2\cos 2\theta\right) - r|\xi|\sin\theta\left(-4r|\xi|\sin\theta + (r^2 + r)|\xi|^2\sin 2\theta\right)}{1 - 2r|\xi|\cos\theta + r^2|\xi|^2} \\ =&\frac{(3r - r^2)(1 - r|\xi|\cos\theta) + 4r^2|\xi|^2 - 4r|\xi|\cos\theta + (r^2 + r)|\xi|^2\cos 2\theta - (r^3 + r^2)|\xi|^3\cos\theta}{1 - 2r|\xi|\cos\theta + r^2|\xi|^2} \\ =& f(r, |\xi|, \theta).\end{aligned}$$

Taking the derivative with respect to θ, one obtains

$$\frac{\partial f}{\partial \theta}(r,|\xi|,\theta) = \frac{4r|\xi|\sin\theta - 2(r+r^2)|\xi|^2\sin 2\theta + (3r-r^2)r|\xi|\sin\theta + (r+r^2)r|\xi|^3\sin\theta}{1-2r|\xi|\cos\theta + r^2|\xi|^2}$$

$$-2r|\xi|\sin\theta\frac{(3r-r^2)(1-r|\xi|\cos\theta) + 4r^2|\xi|^2 - 4r|\xi|\cos\theta + (r^2+r)|\xi|^2\cos 2\theta - (r^3+r^2)|\xi|^3\cos\theta}{(1-2r|\xi|\cos\theta + r^2|\xi|^2)^2}$$

$$= \frac{r|\xi|\sin\theta}{(1-2r|\xi|\cos\theta + r^2|\xi|^2)^2} g(r,|\xi|,\theta), \tag{3.2.22}$$

where

$$g(r,|\xi|,\theta) = \left(4+3r-r^2-4(r+1)|\xi|\cos\theta + (r^2+r)|\xi|^2\right)\left(1-2r|\xi|\cos\theta + r^2|\xi|^2\right)$$
$$-2\left((3r-r^2)(1-r|\xi|\cos\theta) + 4r^2|\xi|^2 - 4r|\xi|\cos\theta + (r^2+r)|\xi|^2\cos 2\theta - (r^3+r^2)|\xi|^3\cos\theta\right),$$

and

$$\frac{\partial g}{\partial \theta}(r,|\xi|,\theta) = 4|\xi|\sin\theta(r+1)(1-2r|\xi|\cos\theta + r^2|\xi|^2).$$

We thus know that $g(r,|\xi|,0) \le g(r,|\xi|,\theta) \le g(r,|\xi|,\pi)$. In addition, we have

$$g(r,|\xi|,0) = (4-3r+r^2) - 4(1+r)|\xi| + (7r+3r^2+3r^3-r^4)|\xi|^2 - 4(r^3+r^2)|\xi|^3 + (r^3+r^4)|\xi|^4,$$

and

$$\frac{\partial g}{\partial |\xi|}(r,|\xi|,0) = -4(1+r) + 2(7r+3r^2+3r^3-r^4)|\xi| - 12(r^3+r^2)|\xi|^2 + 4(r^3+r^4)|\xi|^3. \tag{3.2.23}$$

In view of

$$\frac{\partial^2 g}{\partial |\xi|^2}(r,|\xi|,0) = r\left(12(r+1)(r|\xi|-1)^2 + 2(1-r)^3\right) \ge 0$$

for all $0 \le r \le 1$ and $0 \le |\xi| < 1$, we obtain that $\frac{\partial g}{\partial|\xi|}(r,|\xi|,0) < \frac{\partial g}{\partial|\xi|}(r,1,0)$. In addition, formula (3.2.23) shows that

$$\frac{\partial g}{\partial |\xi|}(r,1,0) = 2(r^3-3r+2)(r-1) \le 0$$

for all $0 \le r \le 1$. From this one derives that $\frac{\partial g}{\partial|\xi|}(r,|\xi|,0) < \frac{\partial g}{\partial|\xi|}(r,1,0) \le 0$ for all $0 \le r \le 1$ and $0 \le |\xi| < 1$. We finally get

$$g(r,|\xi|,0) > g(r,1,0) = 0, \qquad 0 \le r \le 1, \ \ 0 \le |\xi| < 1.$$

Hence, it holds that $g(r,|\xi|,\theta) \ge g(r,|\xi|,0) > 0$ in the cases $0 \le r \le 1$ and $0 \le |\xi| < 1$. According to formula (3.2.22), we have that $f(r,|\xi|,0) \le f(r,|\xi|,\theta) \le f(r,|\xi|,\pi)$ for all $0 \le r \le 1$ and $0 \le |\xi| < 1$. The definition of $f(r,|\xi|,\theta)$ states

$$f(r,|\xi|,0) = \frac{3r-r^2-4r|\xi| + r^2|\xi|^2 + r|\xi|^2}{1-r|\xi|}.$$

Taking the derivative with respect to $|\xi|$, one obtains

$$\frac{\partial f}{\partial |\xi|}(r,|\xi|,0) = \frac{r}{(1-r|\xi|)^2}\left(-4+3r-r^2+2(r+1)|\xi| - (r^2+r)|\xi|^2\right) = \frac{r}{(1-r|\xi|)^2}h(r,|\xi|).$$

It can be easily checked that $\frac{\partial h}{\partial|\xi|}(r,|\xi|) \geq 2(1-r^2) \geq 0$ for $0 \leq r \leq 1$. In combination with $h(r,1) = -2(1-r)^2 \leq 0$, we have that $h(r,|\xi|) \leq h(r,1) \leq 0$ for $0 \leq r \leq 1$. Consequently, the result $\frac{\partial f}{\partial|\xi|}(r,|\xi|,0) \leq 0$ suggests that $f(r,|\xi|,0) \geq f(r,1,0)$ for $0 \leq r \leq 1$ and $0 \leq |\xi| < 1$. In combination with $f(r,1,0) = 0$, we can obtain

$$f(r,|\xi|,\theta) \geq f(r,|\xi|,0) \geq 0, \quad \forall\, 0 \leq r \leq 1,\ |\xi| < 1,\ \theta \in \mathbb{R}.$$

Therefore, it follows that

$$\int_0^1 \Re\left(\frac{(3r-r^2) - 4r\xi + (r^2+r)\xi^2}{1-r\xi}\right) \mathrm{d}\vartheta(r) \geq 0, \qquad |\xi| < 1,$$

and consequently,

$$\begin{aligned}\Re(\varphi^{(3,3)}(\xi)) = &\int_0^1 \Re(\frac{\frac{5}{6}+\frac{1}{6}\xi}{1-r\xi})\mathrm{d}\sigma(r) + \int_0^1 \Re(\frac{1-\xi}{1-r\xi})\mathrm{d}\mu(r) + \int_0^1 r\Re(\frac{1-\xi^2}{1-r\xi})\mathrm{d}\beta(r)\\ &+ \int_0^1 \Re\left(\frac{(3r-r^2) - 4r\xi + (r^2+r)\xi^2}{1-r\xi}\right) \mathrm{d}\vartheta(r) + \Re\left((3-\xi)(1-\xi)\right)(I_{0,1}^3 + I_{1,2}^3)\\ \geq &\frac{2}{3}\int_0^1 \frac{1}{1+r|\xi|}\mathrm{d}\sigma(r) \geq \frac{I_0}{3},\end{aligned}$$

since $I_{0,1}^3 + I_{1,2}^3 = \frac{2^{1-\alpha}(\alpha^2+\alpha)}{3\Gamma(4-\alpha)} \geq 0$ for all $0 \leq \alpha \leq 1$.

In addition, for $\xi = 1$, assume that $\varphi^{(k,i)}(1) = 0$, we know from the definition of $\varphi^{(k,i)}(\xi)$ that

$$\varphi^{(k,i)}(\xi) = I(\xi) + l^{(k,i)}(\xi), \tag{3.2.24}$$

where the series $l^{(k,i)}(\xi)$ is absolutely convergent. The definition of coefficients of $I(\xi)$ yields that $\sum_{i=0}^n I_i$ is arbitrary large as increasing n. However, the boundedness of $l^{(k,i)}(1)$ contradicts identity (3.2.24) for $\xi = 1$, which shows that $\varphi^{(k,i)}(1) \neq 0$.

In the case $|\xi| = 1$ and $\xi \neq 1$, we get from Corollary 3.2.2 that the series $\varphi^{(k,i)}(\xi)$ is pointwise continuous on $|\xi| \leq 1$ except at $\xi = 1$. Then for the sequence $\xi_n = (1-\frac{1}{n})\xi$ satisfying $|\xi_n| < 1$ for all $n \in \mathbb{N}^+$, $\varphi^{(k,i)}(\xi)$ is the limit point of the sequence $\varphi^{(k,i)}(\xi_n)$, and thus

$$\Re(\varphi^{(k,i)}(\xi)) = \lim_{n\to+\infty} \Re(\varphi^{(k,i)}(\xi_n)) \geq c^{(k,i)} > 0,$$

where the constants $c^{(k,i)}$ are independent of n. □

Remark 3.2.3. *Motivated by [50, 31], the integral representation of the series generated by the convolution weights of the so-called L1 method are provided explicitly. As a generalization, we present the equivalent integral representations of the series $\omega^{(k,i)}(\xi)$ for $1 \leq i \leq k \leq 3$. Based on the definition of the Gamma function (see Appendix A.1.1), it holds that*

$$\int_0^\infty e^{-\xi t}\xi^p \mathrm{d}\xi = \frac{\Gamma(p+1)}{t^{p+1}}, \tag{3.2.25}$$

where $\Re(t) \geq 0$ and $-1 < \Re(p) < 0$. Substituting (3.2.25) into the expression of a sequence $\{s_n\}_{n=0}^\infty$ gives

$$\begin{aligned}s_n &= \frac{1}{\Gamma(1-\alpha)}\int_0^1 (n+1-s)^{-\alpha}\varphi(s)\mathrm{d}s\\ &= \frac{1}{\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^1 \varphi(s)\int_0^\infty e^{-\tau(n+1-s)}\tau^{\alpha-1}\mathrm{d}\tau\mathrm{d}s\\ &= \frac{1}{\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^\infty \tau^{\alpha-1}e^{-\tau(n+1)}\int_0^1 e^{\tau s}\varphi(s)\mathrm{d}s\mathrm{d}\tau.\end{aligned} \tag{3.2.26}$$

Hence, replacing $e^{-\tau}$ *by* x*, one obtains from the definition of the sequence* $\{I^r_{n,q}\}_{n=0}^{\infty}$ *that*

$$I^r_{n,q} = \int_0^1 x^n \mu^r_q(x)\mathrm{d}x, \qquad n \geq 0, \tag{3.2.27}$$

where

$$\mu^r_q(x) = \frac{1}{\Gamma(1-\alpha)\Gamma(\alpha)}(-\ln x)^{\alpha-1}\int_0^1 x^{-s}\mathrm{d}\binom{s-q+r-1}{r}. \tag{3.2.28}$$

Assuming that $|\xi| < 1$ *and using* (3.2.27)*, one gets*

$$\begin{aligned}\omega^{(1,1)}(\xi) &= \frac{1}{\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^1 \frac{1-\xi}{1-x\xi}\frac{(-\ln x)^{\alpha-2}(1-x)}{x}\mathrm{d}x \\ &= \frac{1-\xi}{\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^\infty \frac{\tau^{\alpha-2}(1-e^{-\tau})}{1-e^{-\tau}\xi}\mathrm{d}\tau.\end{aligned} \tag{3.2.29}$$

In the case $(k,i) = (2,1)$*, the series expression of* $\omega^{(2,1)}(\xi)$ *yields*

$$\begin{aligned}\omega^{(2,1)}(\xi) &= \int_0^1 \frac{1-\xi}{1-x\xi}\left(\mu(x) - 2\mu_1^2(x)\right)\mathrm{d}x + \int_0^1 \frac{(1-\xi)(3-\xi)}{1-x\xi}\mu_1^2(x)\mathrm{d}x \\ &= \frac{1}{2\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^1 \frac{1-\xi}{1-x\xi}\frac{(-\ln x)^{\alpha-3}(2x-2-\ln x - x\ln x)}{x}\mathrm{d}x \\ &+ \frac{2}{\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^1 \frac{(1-\xi)(3-\xi)}{1-x\xi}\frac{(-\ln x)^{\alpha-3}(1-x+x\ln x)}{x}\mathrm{d}x \\ &= \frac{1-\xi}{2\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^\infty \frac{\tau^{\alpha-3}(2e^{-\tau}-2+\tau+\tau e^{-\tau})}{1-e^{-\tau}\xi}\mathrm{d}\tau \\ &+ \frac{2(1-\xi)(3-\xi)}{\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^\infty \frac{\tau^{\alpha-3}(1-e^{-\tau}-\tau e^{-\tau})}{1-e^{-\tau}\xi}\mathrm{d}\tau.\end{aligned} \tag{3.2.30}$$

In the case $(k,i) = (2,2)$*, based on* (3.2.11)*, one has*

$$\begin{aligned}\omega^{(2,2)}(\xi) &= (1-\xi)(3-\xi)\int_0^1 \mu_1^2(x)\mathrm{d}x + \int_0^1 x\frac{1-\xi^2}{1-x\xi}\mu_1^2(x)\mathrm{d}x + \int_0^1 \frac{1-\xi}{1-x\xi}\left(\mu(x)-2\mu_1^2(x)\right)\mathrm{d}x \\ &= \frac{(1-\xi)(3-\xi)}{2\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^1 \frac{(-\ln x)^{\alpha-3}(2x-2-\ln x - x\ln x)}{x}\mathrm{d}x \\ &+ \frac{1-\xi^2}{2\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^1 \frac{(-\ln x)^{\alpha-3}(2x-2-\ln x-x\ln x)}{1-x\xi}\mathrm{d}x \\ &+ \frac{2}{\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^1 \frac{1-\xi}{1-x\xi}\frac{(-\ln x)^{\alpha-3}(1-x+x\ln x)}{x}\mathrm{d}x,\end{aligned}$$

or equivalently,

$$\begin{aligned}\omega^{(2,2)}(\xi) &= \frac{(1-\xi)(3-\xi)}{2\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^\infty \tau^{\alpha-3}\left(2e^{-\tau}-2+\tau+e^{-\tau}\tau\right)\mathrm{d}\tau \\ &+ \frac{1-\xi^2}{2\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^\infty \frac{\tau^{\alpha-3}e^{-\tau}\left(2e^{-\tau}-2+\tau+e^{-\tau}\tau\right)}{1-e^{-\tau}\xi}\mathrm{d}\tau \\ &+ \frac{2(1-\xi)}{\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^\infty \frac{\tau^{\alpha-3}(1-e^{-\tau}-\tau e^{-\tau})}{1-e^{-\tau}\xi}\mathrm{d}\tau.\end{aligned}$$

Here it is noted that the functions $\omega^{(k,i)}(\xi)$ *are considered as analytic continuition of the power series* $\sum_{n=0}^{\infty}\omega_n^{(k,i)}\xi^n$ *onto the domain* $\mathbb{C}/(1,+\infty)$*. In addition, in view of the formula* (3.2.14)*, we* *consider the integral expressions of* $\varphi^{(k,i)}(\xi)$ *instead in the case* $k=3$. *According to the definition of* $\varphi^{(3,1)}(\xi)$ *shown in* (3.2.16), *one obtains*

$$\begin{aligned}
\varphi^{(3,1)}(\xi) &= \int_0^1 \frac{1}{1-x\xi}\left(\mu(x)-3\mu_1^3(x)\right)\mathrm{d}x + \int_0^1 \frac{1-\xi}{1-x\xi}\mu_1^2(x)\mathrm{d}x + \int_0^1 \frac{4-2\xi+\xi^2}{1-x\xi}\mu_1^3(x)\mathrm{d}x \\
&= \frac{3}{2\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^1 \frac{(-\ln x)^{\alpha-4}(2x-2-2\ln x-x(\ln x)^2)}{(1-x\xi)x}\mathrm{d}x \\
&+ \frac{1}{2\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^1 \frac{1-\xi}{1-x\xi}\frac{(-\ln x)^{\alpha-3}\left(2x-2-\ln x-x\ln x\right)}{x}\mathrm{d}x \\
&+ \frac{1}{\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^1 \frac{4-2\xi+\xi^2}{1-x\xi}\frac{(-\ln x)^{\alpha-4}\left(x-1-\ln x-\frac{2+x}{6}(\ln x)^2\right)}{x}\mathrm{d}x.
\end{aligned}$$

In the case $(k,i)=(3,2)$, *we find*

$$\begin{aligned}
\varphi^{(3,2)}(\xi) &= \int_0^1 \frac{\frac{5}{6}+\frac{1}{6}\xi}{1-x\xi}\mu(x)\mathrm{d}x + \int_0^1 \frac{1-\xi}{1-x\xi}\left(\mu_1^2(x)-2\mu_1^3(x)+\frac{1}{6}\mu(x)\right)\mathrm{d}x \\
&+ \int_0^1 x\frac{1-\xi^2}{1-x\xi}\mu_1^3(x)\mathrm{d}x + (3-\xi)(1-\xi)\int_0^1 \mu_1^3(x)\mathrm{d}x \\
&= \frac{1}{\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^1 \frac{\frac{5}{6}+\frac{1}{6}\xi}{1-x\xi}\frac{(-\ln x)^{\alpha-2}(1-x)}{x}\mathrm{d}x \\
&+ \frac{1}{\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^1 \frac{1-\xi}{1-x\xi}\frac{(-\ln x)^{\alpha-4}\left(2x-2-\ln x-x\ln x\right)}{x}\mathrm{d}x \\
&+ \frac{1}{\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^1 \frac{1-\xi^2}{1-x\xi}(-\ln x)^{\alpha-4}\left(x-1-\ln x-\frac{2+x}{6}(\ln x)^2\right)\mathrm{d}x \\
&+ \frac{1}{\Gamma(1-\alpha)\Gamma(\alpha)}(3-\xi)(1-\xi)\int_0^1 \frac{(-\ln x)^{\alpha-4}\left(x-1-\ln x-\frac{2+x}{6}(\ln x)^2\right)}{x}\mathrm{d}x.
\end{aligned}$$

In the case $(k,i)=(3,3)$, *according to* (3.2.20), *we get*

$$\begin{aligned}
\varphi^{(3,3)}(\xi) &= \int_0^1 \frac{\frac{5}{6}+\frac{1}{6}\xi}{1-x\xi}\mu(x)\mathrm{d}x + \int_0^1 \frac{1-\xi}{1-x\xi}\left(\mu_1^2(x)-2\mu_1^3(x)+\frac{1}{6}\mu(x)\right)\mathrm{d}x \\
&+ \int_0^1 x\frac{1-\xi^2}{1-x\xi}\mu_1^3(x)\mathrm{d}x + (3-\xi)(1-\xi)\int_0^1 \left(\mu_1^3(x)+x\mu_2^3(x)\right)\mathrm{d}x \\
&- \int_0^1 \frac{(3x-x^2)-4x\xi+(x^2+x)\xi^2}{1-x\xi}\mu_2^3(x)\mathrm{d}x,
\end{aligned}$$

where

$$\begin{aligned}
\mu_2^3(x) &= \frac{1}{6\Gamma(1-\alpha)\Gamma(\alpha)}(-\ln x)^{\alpha-1}\int_0^1 x^{-s}\left(3s^2-6s+2\right)\mathrm{d}s \\
&= \frac{(-\ln x)^{\alpha-4}\left(1-x+x\ln x-\frac{1+2x}{6}(\ln x)^2\right)}{\Gamma(1-\alpha)\Gamma(\alpha)x}.
\end{aligned}$$

In this chapter, we mainly generalize the stability properties of the k-step BDF methods such as the stability region, $A(\theta)$-stability and strong root condition to the methods on a uniform-grid proposed in chapter 2. In the next chapter, we will study the convergence of these numerical schemes for time-fractional differential equations.

Chapter 4

Convergence analysis

4.1 Convergence for time-fractional ordinary differential equation

In this section, we consider the global error estimation for the nonlinear time-fractional ordinary differential equation of the form

$$\begin{cases} {}^C\mathcal{D}^\alpha u(t) = f(t, u(t)), & t \in (0, T], \\ u(0) = u_0, \end{cases} \tag{4.1.1}$$

where $\alpha \in (0,1)$ and the fractional derivative ${}^C\mathcal{D}^\alpha$ in the Caputo's sense is defined by (1.1.12). The function f is given and assumed to satisfy the Lipschitz continuous condition with respect to the second variable. The existence and uniqueness properties of the continuous solution of (4.1.1) are guaranteed by Theorem 1.2.5. As discussed in section 2.1, the numerical approximations for (4.1.1) are constructed in the form of

$$D^\alpha_{k,i} u_n^{(k,i)} = f(t_n, u_n^{(k,i)}), \tag{4.1.2}$$

and the exact solution $u(t)$ satisfies

$$D^\alpha_{k,i} u(t_n) = f(t_n, u(t_n)) + \tau_n^{(k,i)} \tag{4.1.3}$$

for $k \le n \le N$, where $\tau_n^{(k,i)}$ denotes the local truncation error at $t = t_n$. Define the global error by

$$e_n^{(k,i)} = u(t_n) - u_n^{(k,i)} \qquad \text{for } 0 \le n \le N, \tag{4.1.4}$$

then subtracting (4.1.2) by (4.1.3) implies

$$D^\alpha_{k,i} e_n^{(k,i)} = \delta f_n^{(k,i)} + \tau_n^{(k,i)}, \qquad k \le n \le N, \tag{4.1.5}$$

where $\delta f_n^{(k,i)} = f(t_n, u(t_n)) - f(t_n, u_n^{(k,i)})$. In addition, substituting (2.1.11) into (4.1.5) yields

$$\sum_{j=0}^{k-1} w_{n,j}^{(k,i)} e_j^{(k,i)} + \sum_{j=0}^{n} \omega_{n-j}^{(k,i)} e_j^{(k,i)} = (\Delta t)^\alpha \delta f_n^{(k,i)} + (\Delta t)^\alpha \tau_n^{(k,i)}, \qquad k \le n \le N. \tag{4.1.6}$$

Multiplying ξ^{n-k} on both sides of (4.1.6) and summing up for all $n \ge k$, one obtains

$$\begin{aligned} &\sum_{n=0}^{\infty} \sum_{j=0}^{k-1} \left(w_{n+k,j}^{(k,i)} + \omega_{n+k-j}^{(k,i)} \right) e_j^{(k,i)} \xi^n + \sum_{n=0}^{\infty} \sum_{j=k}^{n+k} \omega_{n+k-j}^{(k,i)} e_j^{(k,i)} \xi^n \\ =& (\Delta t)^\alpha \sum_{n=0}^{\infty} \delta f_{n+k}^{(k,i)} \xi^n + (\Delta t)^\alpha \sum_{n=0}^{\infty} \tau_{n+k}^{(k,i)} \xi^n. \end{aligned}$$

Since

$$\sum_{n=0}^{\infty}\sum_{j=k}^{n+k}\omega_{n+k-j}^{(k,i)}e_j^{(k,i)}\xi^n=\sum_{n=0}^{\infty}\sum_{j=0}^{n}\omega_{n-j}^{(k,i)}e_{j+k}^{(k,i)}\xi^n=\sum_{j=0}^{\infty}e_{j+k}^{(k,i)}\xi^j\sum_{n=0}^{\infty}\omega_n^{(k,i)}\xi^n,$$

it follows that

$$\omega^{(k,i)}(\xi)e^{(k,i)}(\xi)=\sum_{m=0}^{k-1}e_m^{(k,i)}s_m^{(k,i)}(\xi)+(\Delta t)^\alpha\delta f^{(k,i)}(\xi)+(\Delta t)^\alpha\tau^{(k,i)}(\xi), \tag{4.1.7}$$

where

$$\begin{aligned} &s_m^{(k,i)}(\xi):=\sum_{n=0}^{\infty}s_{n,m}^{(k,i)}\xi^n=-\sum_{n=0}^{\infty}\left(w_{n+k,m}^{(k,i)}+\omega_{n+k-m}^{(k,i)}\right)\xi^n, \quad e^{(k,i)}(\xi)=\sum_{n=0}^{\infty}e_{n+k}^{(k,i)}\xi^n,\\ &\omega^{(k,i)}(\xi)=\sum_{n=0}^{\infty}\omega_n^{(k,i)}\xi^n, \quad \delta f^{(k,i)}(\xi)=\sum_{n=0}^{\infty}\delta f_{n+k}^{(k,i)}\xi^n, \quad \tau^{(k,i)}(\xi)=\sum_{n=0}^{\infty}\tau_{n+k}^{(k,i)}\xi^n. \end{aligned} \tag{4.1.8}$$

Based on the definitions of series $s_m^{(k,i)}(\xi)$ in (4.1.8) for $1\le i\le k\le 3$, we derive explicit expressions of the coefficients $\{s_{n,m}^{(k,i)}\}_{n=0}^{\infty}$ by means of $I_{n,q}^r$ defined in (2.1.12), i.e.,

$$\begin{cases} (k,i)=(1,1): & s_{n,0}=I_n, \quad n\ge 0,\\ (k,i)=(2,1): & s_{n,0}=I_{n+1}-I_{n,1}^2, \quad n\ge 0,\\ & s_{0,1}=-\nabla I_1+2I_{0,1}^2,\\ & s_{n,1}=-\nabla I_{n+1}+2I_{n,1}^2-I_{n-1,1}^2, \quad n\ge 1,\\ (k,i)=(2,2): & s_{0,0}=I_1-I_{1,1}^2-I_{0,1}^2,\\ & s_{n,0}=I_{n+1}-I_{n+1,1}^2, \quad n\ge 1,\\ & s_{0,1}=-\nabla I_1+2I_{1,1}^2+2I_{0,1}^2,\\ & s_{1,1}=-\nabla I_2+2I_{2,1}^2-I_{1,1}^2-I_{0,1}^2,\\ & s_{n,1}=-\nabla I_{n+1}+2I_{n+1,1}^2-I_{n,1}^2, \quad n\ge 2 \end{cases} \tag{4.1.9}$$

and

i) $(k,i)=(3,1)$:

$$\begin{cases} s_{n,0}=I_{n+2}-I_{n+2,1}^2-I_{n+1,1}^2+I_{n,1}^3, \quad n\ge 0,\\ s_{0,1}=-\nabla I_2+2I_{2,1}^2+2I_{1,1}^2-I_{0,1}^2-3I_{0,1}^3,\\ s_{n,1}=-\nabla I_{n+2}+2I_{n+2,1}^2+2I_{n+1,1}^2-I_{n,1}^2-3I_{n,1}^3+I_{n-1,1}^3, \quad n\ge 1,\\ s_{0,2}=-\nabla I_1-I_{2,1}^2-I_{1,1}^2+2I_{0,1}^2+3I_{0,1}^3,\\ s_{1,2}=-\nabla I_2-I_{3,1}^2-\nabla^2 I_{2,1}^2+3I_{1,1}^3-3I_{0,1}^3,\\ s_{n,2}=-\nabla I_{n+1}-\nabla^2 I_{n+1,1}^2-\nabla^3 I_{n+1,1}^3-I_{n+2,1}^2+I_{n+1,1}^3, \quad n\ge 2, \end{cases} \tag{4.1.10}$$

ii) $(k,i) = (3,2)$:

$$\begin{cases} s_{0,0} = I_2 - I_{2,1}^2 - I_{1,1}^2 + I_{1,1}^3 + I_{0,1}^3, \\ s_{n,0} = I_{n+2} - I_{n+2,1}^2 - I_{n+1,1}^2 + I_{n+1,1}^3, \quad n \geq 1, \\ s_{0,1} = -\nabla I_2 + 2I_{2,1}^2 + 2I_{1,1}^2 - I_{0,1}^2 - 3I_{0,1}^3 - 3I_{1,1}^3, \\ s_{1,1} = -\nabla I_3 + 2I_{3,1}^2 + 2I_{2,1}^2 - I_{1,1}^2 - 3I_{2,1}^3 + I_{1,1}^3 + I_{0,1}^3, \\ s_{n,1} = -\nabla I_{n+2} + 2I_{n+2,1}^2 + 2I_{n+1,1}^2 - I_{n,1}^2 - 3I_{n+1,1}^3 + I_{n,1}^3, \quad n \geq 2, \\ s_{0,2} = -\nabla I_1 - I_{2,1}^2 - I_{1,1}^2 + 2I_{0,1}^2 + 3I_{0,1}^3 + 3I_{1,1}^3, \\ s_{1,2} = -\nabla I_2 - I_{3,1}^2 - \nabla^2 I_{2,1}^2 + 3I_{2,1}^3 - 3I_{1,1}^3 - 3I_{0,1}^3, \\ s_{2,2} = -\nabla I_3 - I_{4,1}^2 - \nabla^2 I_{3,1}^2 - \nabla^3 I_{4,1}^3 + I_{4,1}^3 + I_{0,1}^3, \\ s_{n,2} = -\nabla I_{n+1} - \nabla^2 I_{n+1,1}^2 - I_{n+2,1}^2 - \nabla^3 I_{n+2,1}^3 + I_{n+2,1}^3, \quad n \geq 3, \end{cases} \tag{4.1.11}$$

iii) $(k,i) = (3,3)$:

$$\begin{cases} s_{0,0} = I_2 - 2I_{2,1}^2 - I_{1,1}^2 + I_{2,1}^3 + I_{1,1}^3 + I_{0,1}^3, \\ s_{n,0} = I_{n+2} - 2I_{n+2,1}^2 + I_{n+2,1}^3, \quad n \geq 1, \\ s_{0,1} = -I_{2,3}^2 - I_{1,2}^2 - I_{0,1}^2 - 3I_{2,3}^3 - 3I_{0,1}^3 - 3I_{1,2}^3, \\ s_{1,1} = -I_{3,3}^2 - 3I_{3,3}^3 + I_{2,3}^3 + I_{1,2}^3 + I_{0,1}^3, \\ s_{n,1} = -\nabla I_{n+2} + 2I_{n+2,1}^2 + 2I_{n+1,1}^2 - I_{n,1}^3 - 3I_{n,1}^3 + I_{n-1,1}^3, \quad n \geq 2, \\ s_{0,2} = I_0 + I_1 + I_2 + 2I_{0,1}^2 + 2I_{1,2}^2 + 2I_{2,3}^2 + 3I_{0,1}^3 + 3I_{1,2}^3 + 3I_{2,3}^3, \\ s_{1,2} = I_3 + 2I_{3,3}^2 - I_{2,3}^2 - I_{0,1}^2 - I_{1,2}^2 - 3I_{1,2}^3 - 3I_{0,1}^3 - 3I_{2,3}^3 + 3I_{3,3}^3, \\ s_{2,2} = I_4 + 2I_{4,3}^2 - 2I_{3,3}^2 + 3I_{4,3}^3 - 3I_{3,3}^3 + I_{2,3}^3 + I_{1,2}^3 + I_{0,1}^3, \\ s_{n,2} = -\nabla I_{n+1} - \nabla^2 I_{n+1,1}^2 - \nabla^3 I_{n+1,1}^3 - I_{n-1,1}^2 + I_{n-2,1}^3, \quad n \geq 3. \end{cases} \tag{4.1.12}$$

Lemma 4.1.1. *For $1 \leq i \leq k \leq 3$ and $0 \leq m \leq k-1$, the coefficients $\{s_{n,m}^{(k,i)}\}_{n=0}^{\infty}$ are defined by (4.1.9)-(4.1.12). Then for $n \geq 0$, $s_{n,m}^{(k,i)}$ is bounded, and moreover, there exist bounded constants $c_m^{(k,i)} > 0$ independent of n and α, such that*

$$|s_{n,0}^{(k,i)}| \leq c_0^{(k,i)} \frac{n^{-\alpha}}{\Gamma(1-\alpha)} \qquad \text{and} \qquad |s_{n,m}^{(k,i)}| \leq c_m^{(k,i)} \frac{n^{-\alpha-1}}{|\Gamma(-\alpha)|}$$

for $n \geq 1$ and $m \geq 1$.

Proof. It is known from (2.1.12) that for any finite $q, r \in \mathbb{N}^+$, $I_{n,q}^r$ is bounded for all $n \in \mathbb{Z}$. Since the coefficients $s_{n,m}^{(k,i)}$ are written as linear combinations of $I_{n,q}^r$, we can immediately obtain the boundedness of $s_{n,m}^{(k,i)}$ for all integer $n \geq 0$.

Moreover, in the cases $1 \leq i \leq k \leq 3$, each $s_{n,0}^{(k,i)}$ can be expressed as a linear combination of I_l and $I_{l,1}^r$ with $l \geq n$ and $2 \leq r \leq 3$. Using formulae (2.1.19) and (2.1.21), we obtain $I_n = O\left(\frac{n^{-\alpha}}{\Gamma(1-\alpha)}\right)$ and $I_{n,1}^r = O\left(\frac{n^{-\alpha-1}}{\Gamma(-\alpha)}\right) = o\left(\frac{n^{-\alpha}}{\Gamma(1-\alpha)}\right)$ for $r \geq 2$ and $n \geq 1$, This implies that there is a uniform bound independent of n, denoted by $c_0^{(k,i)} > 0$, such that $|s_{n,0}^{(k,i)}| \leq \frac{c_0^{(k,i)} n^{-\alpha}}{\Gamma(1-\alpha)}$ as $n \geq 1$.

In terms of $m \geq 1$, observe that $s_{n,m}^{(k,i)}$ are linear combinations of ∇I_l, $I_{l,1}^r$ and $\nabla^p I_{l,1}^r$ in the cases $l \geq n+1$, $r \geq 2$ and $1 \leq p \leq 3$. From formulae (2.1.20) and (2.1.22), we know that

$\nabla I_n = O\left(\frac{(n-1)^{-\alpha-1}}{\Gamma(-\alpha)}\right) = O\left(\frac{n^{-\alpha-1}}{\Gamma(-\alpha)}\right)$ and $\nabla^p I_{n,1}^r = O\left(\frac{(n-p)^{-\alpha-p-1}}{\Gamma(-\alpha-p+1)}\right) = o\left(\frac{n^{-\alpha-1}}{\Gamma(-\alpha)}\right)$ for $r \geq 2$. Therefore one gets $s_{n,m}^{(k,i)} = O\left(\frac{n^{-\alpha-1}}{\Gamma(-\alpha)}\right)$, and hence there exist constants $c_m^{(k,i)} > 0$ such that (4.1.1) is satisfied. □

Recall the definition of the series $\omega^{(k,i)}(\xi)$. It is important to notice its decomposed form

$$\omega^{(k,i)}(\xi) = (1-\xi)\varphi^{(k,i)}(\xi) = (1-\xi)^{\alpha}\psi^{(k,i)}(\xi), \tag{4.1.13}$$

where the series $\varphi^{(k,i)}(\xi)$ is defined by (3.2.14) and

$$\psi^{(k,i)}(\xi) = (1-\xi)^{1-\alpha}\varphi^{(k,i)}(\xi). \tag{4.1.14}$$

Formula (4.1.13) indicates a relationship between the proposed methods and the fractional Euler method mentioned in [44]. In what follows, we discuss the relevant properties of the series $\psi^{(k,i)}(\xi)$ as preliminaries.

Lemma 4.1.2. *Assume that $\{g_n^{(\beta)}\}_{n=0}^{\infty}$ are generated by the power series $(1-\xi)^{\beta}$ for $\beta \in \mathbb{R}$, i.e.,*

$$(1-\xi)^{\beta} = \sum_{n=0}^{\infty}(-1)^n\binom{\beta}{n}\xi^n = \sum_{n=0}^{\infty} g_n^{(\beta)}\xi^n.$$

Then the following relations hold

$$\begin{cases} \beta \in (-1,0): & g_0^{(\beta)} = 1, \quad g_0^{(\beta)} > g_1^{(\beta)} > \cdots > 0, \\ & \sum_{i=0}^{n} g_i^{(\beta)} = g_n^{(\beta-1)}, \quad n \geq 0; \\ \beta \in (0,1): & g_0^{(\beta)} = 1, \quad g_n^{(\beta)} < 0, \quad n \geq 1, \\ & 1 > |g_1^{(\beta)}| > |g_2^{(\beta)}| > \cdots > 0, \\ & \sum_{i=0}^{\infty} g_i^{(\beta)} = 0, \quad \sum_{i=0}^{n} g_i^{(\beta)} = g_n^{(\beta-1)}, \quad n \geq 0. \end{cases} \tag{4.1.15}$$

Lemma 4.1.3. *In the case $1 \leq i \leq k \leq 6$, the coefficients of the power series $\psi^{(k,i)}(\xi)$ belong to the space l^1.*

Proof. Using the expression of $\varphi^{(k,i)}(\xi)$ presented in Theorem 3.2.6, one obtains

$$\varphi^{(k,i)}(\xi) = I(\xi) + l^{(k,i)}(\xi), \qquad \text{with } \sum_{n=0}^{\infty}|l_n^{(k,i)}| < \infty. \tag{4.1.16}$$

In addition, together with (4.1.14), it follows that

$$\psi^{(k,i)}(\xi) = (1-\xi)^{(1-\alpha)}I(\xi) + (1-\xi)^{(1-\alpha)}l^{(k,i)}(\xi).$$

Therefore, it suffices to prove that the coefficients of series $(1-\xi)^{1-\alpha}I(\xi)$ belong to l^1.

From the definition of Gamma function (see Appendix A.1.1)

$$\Gamma(\beta) = \lim_{n\to\infty}\frac{n^{\beta}}{(-1)^n\binom{-\beta}{n}(n+\beta)}, \qquad \beta \neq 0, -1, -2, \cdots,$$

one obtains the asymptotic relation

$$\frac{n^{\beta-1}}{\Gamma(\beta)} \cong (-1)^n \binom{-\beta}{n}, \qquad \text{as } n \to \infty, \tag{4.1.17}$$

where the notation $\cong$ means that the ratio $\left(n^{\beta-1}/\Gamma(\beta)\right)/(-1)^n\binom{-\beta}{n} \to 1$ as $n \to \infty$. Furthermore, it is known from [20, 45] that

$$(-1)^n \binom{-\beta}{n} = \frac{n^{\beta-1}}{\Gamma(\beta)}\left(1 + O\left(\frac{\beta-1}{n}\right)\right). \tag{4.1.18}$$

Also, based on the definition of I_n, one finds $I_n \cong \frac{n^{-\alpha}}{\Gamma(1-\alpha)}$ as $n \to \infty$, and, therefore,

$$\begin{aligned}
\sum_{n=1}^{\infty}\left|I_n - \frac{n^{-\alpha}}{\Gamma(1-\alpha)}\right| &= \frac{1}{\Gamma(1-\alpha)}\sum_{n=1}^{\infty}\int_0^1 \left(n^{-\alpha} - (n+1-s)^{-\alpha}\right) \mathrm{d}s \\
&= \frac{\alpha}{\Gamma(1-\alpha)}\int_0^1\int_0^{1-s}\sum_{n=1}^{\infty}(n+t)^{-\alpha-1}\mathrm{d}t\mathrm{d}s \\
&\le \frac{\alpha}{\Gamma(1-\alpha)}\sum_{n=1}^{\infty} n^{-\alpha-1} \\
&\le \frac{\alpha}{\Gamma(1-\alpha)}\left(1 + \int_1^{\infty} x^{-\alpha-1}\mathrm{d}x\right) \\
&= \frac{\alpha+1}{\Gamma(1-\alpha)} < +\infty.
\end{aligned} \tag{4.1.19}$$

Combining this with (4.1.18), we obtain

$$I_n = g_n^{(\alpha-1)} + v_n, \quad \text{with } \sum_{n=0}^{\infty}|v_n| < \infty. \tag{4.1.20}$$

Hence,

$$(1-\xi)^{1-\alpha} I(\xi) = \sum_{n=0}^{\infty}\left(\sum_{k=0}^{n} g_{n-k}^{(1-\alpha)} I_k\right)\xi^n$$

in combination with the relation

$$\begin{aligned}
\sum_{n=0}^{\infty}\left|\sum_{k=0}^{n} g_{n-k}^{(1-\alpha)} I_k\right| &= \sum_{n=0}^{\infty}\left|\sum_{k=0}^{n} g_{n-k}^{(1-\alpha)}\left(g_k^{(\alpha-1)} + v_k\right)\right| \\
&\le \sum_{n=0}^{\infty}\left|\sum_{k=0}^{n} g_{n-k}^{(1-\alpha)} g_k^{(\alpha-1)}\right| + \sum_{n=0}^{\infty}\left|\sum_{k=0}^{n} g_{n-k}^{(1-\alpha)} v_k\right| \\
&\le 1 + \sum_{n=0}^{\infty}|g_n^{(1-\alpha)}|\sum_{k=0}^{\infty}|v_k| < \infty,
\end{aligned}$$

yields the result. □

Lemma 4.1.4. *In the cases $1 \le i \le k \le 3$, it holds that $\psi^{(k,i)}(\xi) \neq 0$ for any $|\xi| \le 1$.*

Proof. In the proof of Theorem 3.2.6, it is noticed $\varphi^{(k,i)}(\xi) \neq 0$ for all $|\xi| \le 1$ and $1 \le i \le k \le 3$. For any prescribed $|\xi| \le 1$, $(1-\xi)^{1-\alpha}$ is located within the sector $S_\alpha = \{z : \ |\arg(z)| \le \frac{(1-\alpha)\pi}{2}\}$.

In addition, note that $(1-\xi)^{1-\alpha}=0$ if and only if $\xi=1$. Thus, it remains to find the value of the series $(1-\xi)^{1-\alpha}\varphi^{(k,i)}(\xi)$ at $\xi=1$. In fact, from the formulae (4.1.16) and (4.1.20), it follows that

$$\begin{aligned}\sum_{n=0}^{\infty}\sum_{l=0}^{n} g_{n-l}^{(1-\alpha)}\varphi_l^{(k,i)} &= \sum_{n=0}^{\infty}\sum_{l=0}^{n} g_{n-l}^{(1-\alpha)}\left(g_l^{(\alpha-1)}+v_l+l_l^{(k,i)}\right)\\ &= \sum_{n=0}^{\infty}\sum_{l=0}^{n} g_{n-l}^{(1-\alpha)}g_l^{(\alpha-1)}+\sum_{n=0}^{\infty}\sum_{l=0}^{n} g_{n-l}^{(1-\alpha)}\left(v_l+l_l^{(k,i)}\right)\\ &= 1+\sum_{n=0}^{\infty} g_n^{(1-\alpha)}\sum_{l=0}^{\infty}\left(v_l+l_l^{(k,i)}\right)=1,\end{aligned}$$

where the last equality holds based on Lemma 4.1.2. □

As a result, in combination with the conclusions of Theorem 3.1.3, Lemma 4.1.3 and Lemma 4.1.4, we can obtain the following result.

Proposition 4.1.1. *In the case $1\le i\le k\le 3$ and $0<\alpha<1$, let*

$$\frac{1}{\psi^{(k,i)}(\xi)}=r^{(k,i)}(\xi)=\sum_{n=0}^{\infty} r_n^{(k,i)}\xi^n, \tag{4.1.21}$$

then there exist bounded positive constants $M_\alpha^{(k,i)}$, such that $\sum_{n=0}^{\infty}|r_n^{(k,i)}|=M_\alpha^{(k,i)}$.

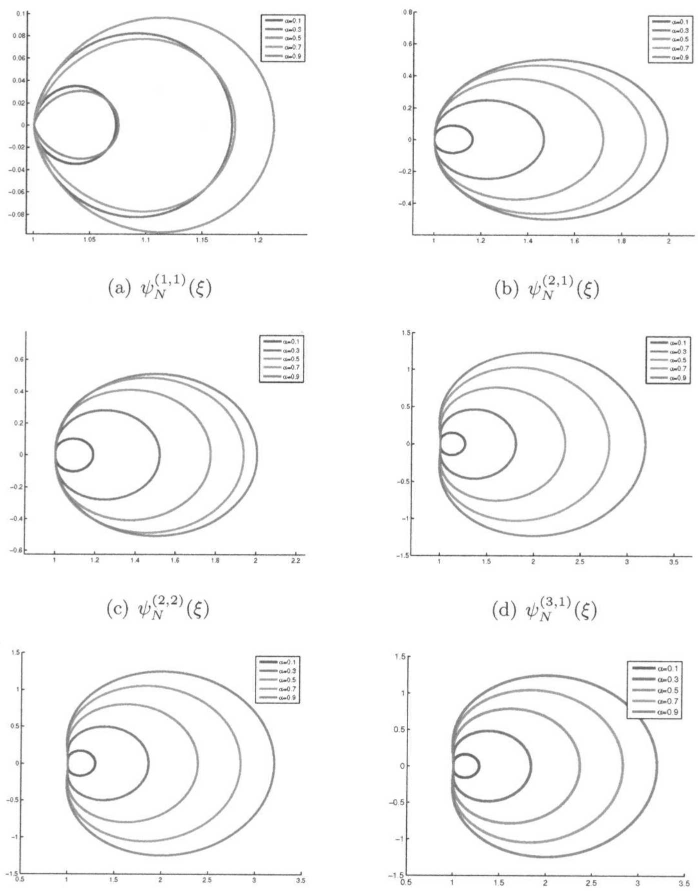
Remark 4.1.1. *It can be seen from Proposition 4.1.1 that a qualitative analysis is provided on the absolute convergence of the coefficients of the reciprocal of the series $\psi^{(k,i)}(\xi)$. On the other hand, we would like to get the bounds $M_\alpha^{(k,i)}$ in a numerical approach to confirm the theoretical analysis. Note that the equality (4.1.13) can be represented in a matrix form with arbitrary $N\in\mathbb{N}^+$, i.e.,*

$$\begin{aligned}\begin{bmatrix}\omega_0^{(k,i)} & & & \\ \omega_1^{(k,i)} & \omega_0^{(k,i)} & & \\ \vdots & \ddots & \ddots & \\ \omega_N^{(k,i)} & \omega_{N-1}^{(k,i)} & \cdots & \omega_0^{(k,i)}\end{bmatrix} &= \begin{bmatrix}1 & & & \\ -1 & 1 & & \\ \vdots & \ddots & \ddots & \\ 0 & \cdots & -1 & 1\end{bmatrix}\begin{bmatrix}\varphi_0^{(k,i)} & & & \\ \varphi_1^{(k,i)} & \varphi_0^{(k,i)} & & \\ \vdots & \ddots & \ddots & \\ \varphi_N^{(k,i)} & \varphi_{N-1}^{(k,i)} & \cdots & \varphi_0^{(k,i)}\end{bmatrix}\\ &= \begin{bmatrix}g_0^{(\alpha)} & & & \\ g_1^{(\alpha)} & g_0^{(\alpha)} & & \\ \vdots & \ddots & \ddots & \\ g_N^{(\alpha)} & g_{N-1}^{(\alpha)} & \cdots & g_0^{(\alpha)}\end{bmatrix}\begin{bmatrix}\psi_0^{(k,i)} & & & \\ \psi_1^{(k,i)} & \psi_0^{(k,i)} & & \\ \vdots & \ddots & \ddots & \\ \psi_N^{(k,i)} & \psi_{N-1}^{(k,i)} & \cdots & \psi_0^{(k,i)}\end{bmatrix}.\end{aligned}$$

Equivalently, we may write $\Omega_N^{(k,i)}=G_N^{(\alpha)}\Psi_N^{(k,i)}$ for any $N>0$. From this follows

$$\sum_{n=0}^{N}|r_n^{(k,i)}|=\|(\Psi_N^{(k,i)})^{-1}\|_1=\|(\Omega_N^{(k,i)})^{-1}G_N^{(\alpha)}\|_1.$$

In Table 4.1, we display the L^1 (or L^∞) norm of the inverse of the matrix $\Psi_N^{(k,i)}$ for increasing values of N, where $0<\alpha<1$ and $1\le i\le k\le 3$. It shows that the value goes to a limit for refined N, which also implies the absolute convergence of the series $r^{(k,i)}(\xi)$.



(a) $\psi_N^{(1,1)}(\xi)$ (b) $\psi_N^{(2,1)}(\xi)$

(c) $\psi_N^{(2,2)}(\xi)$ (d) $\psi_N^{(3,1)}(\xi)$

(e) $\psi_N^{(3,2)}(\xi)$ (f) $\psi_N^{(3,3)}(\xi)$

FIGURE 4.1:
The locations of the truncated curves $\psi_N^{(k,i)}(e^{i\theta})$ with $N = 5000$.

Theorem 4.1.2. *In the cases* $1 \leq i \leq k \leq 2$, *for* $|\xi| \leq 1$, $\psi^{(k,i)}(\xi)$ *is in the sector* $\Sigma_{\frac{\pi}{2}} = \{x \in \mathbb{C} : |\arg x| \leq \frac{\pi}{2}\}$.

Proof. We first express that $(1-\xi) = \rho(\xi)e^{i\theta(\xi)}$ and $\varphi^{(k,i)}(\xi) = \rho_\varphi(\xi)e^{i\theta_\varphi(\xi)}$ for $|\xi| \leq 1$. According to Theorem 3.2.4 and Theorem 3.2.5, it follows that $\Re\omega^{(k,i)}(\xi) \geq 0$ and $\Re\varphi^{(k,i)}(\xi) > 0$, which implies $|\theta(\xi) + \theta_\varphi(\xi)| \leq \frac{\pi}{2}$ and $|\theta_\varphi(\xi)| \leq \frac{\pi}{2}$, respectively. Thus

$$|(1-\alpha)\theta(\xi) + \theta_\varphi(\xi)| \leq (1-\alpha)|\theta(\xi) + \theta_\varphi(\xi)| + \alpha|\theta_\varphi(\xi)| \leq \frac{\pi}{2},$$

which is equivalent to $\Re\psi^{(k,i)}(\xi) \geq 0$ for all $|\xi| \leq 1$. □

Theorem 4.1.3. *Let* $u(t)$ *and* $\{u_n\}_{n=k}^N$ *be the solutions of equations* (4.1.1) *and* (4.1.6), *respectively. The function* $f(t, u(t))$ *in* (4.1.1) *is assumed to satisfy the Lipschitz continuous condition with respect to the second variable* $u(t)$. *If* $u(t) \in C^{k+1}[0,T]$, *then*

TABLE 4.1:
The L^1 or L^∞ norm of the inverse matrix of $\Psi_N^{(k,i)}$.

α	N	$\|(\Psi^{(k,i)})^{-1}\|_p,\ p=1,\infty$					
		$(k,i)=(1,1)$	$(k,i)=(2,1)$	$(k,i)=(2,2)$	$(k,i)=(3,1)$	$(k,i)=(3,2)$	$(k,i)=(3,3)$
0.0001	10	1.000000	1.000031	1.000048	1.000099	1.000122	1.000110
	100	1.000000	1.000031	1.000048	1.000099	1.000122	1.000110
	1000	1.000000	1.000031	1.000048	1.000114	1.000138	1.000128
	10000	1.000000	1.000069	1.000085	1.189345	1.189482	1.201595
0.10	10	0.999884	1.018469	1.029129	1.064680	1.076031	1.070190
	100	0.999998	1.018482	1.029132	1.064683	1.076031	1.070192
	1000	1.000000	1.018482	1.029132	1.064690	1.076038	1.070200
	10000	1.000000	1.018493	1.029143	1.116970	1.127403	1.135033
0.30	10	0.999277	1.017407	1.023508	1.089001	1.106180	1.098806
	100	0.999985	1.017480	1.023541	1.089017	1.106188	1.098817
	1000	1.000000	1.017480	1.023541	1.089018	1.106189	1.098818
	10000	1.000000	1.017482	1.023542	1.095718	1.112733	1.105976
0.50	10	0.997958	1.011762	1.018412	1.083218	1.089780	1.086681
	100	0.999934	1.011961	1.018565	1.083274	1.089839	1.086736
	1000	0.999998	1.011962	1.018566	1.083274	1.089839	1.086737
	10000	1.000000	1.011962	1.018566	1.083921	1.090478	1.087412
0.70	10	0.996339	1.006427	1.008625	1.084779	1.088936	1.087241
	100	0.999810	1.006774	1.008952	1.084842	1.089003	1.087305
	1000	0.999990	1.006775	1.008953	1.084842	1.089003	1.087305
	10000	1.000000	1.006776	1.008953	1.084940	1.089100	1.087410
0.90	10	0.996942	1.001263	1.001437	1.059819	1.060335	1.060095
	100	0.999742	1.001543	1.001724	1.059858	1.060374	1.060134
	1000	0.999979	1.001544	1.001726	1.059859	1.060374	1.060134
	10000	0.999998	1.001544	1.001726	1.059876	1.060391	1.060153

i) *in the cases* $1 \le k \le 3$*:*

$$|e_n^{(k,k)}| \le C^{(k,k)} \left(\sum_{m=0}^{k-1} |e_m^{(k,k)}| + (\Delta t)^{k+1-\alpha}\, t_{n-1}^{\alpha} \right), \qquad k \le n \le N$$

ii) *in the cases* $1 \le i < k \le 3$*:*

$$|e_n^{(k,i)}| \le C^{(k,i)} \left(\sum_{m=0}^{k-1} |e_m^{(k,i)}| + (\Delta t)^{k} + (\Delta t)^{k+1-\alpha}\, t_{n-1}^{\alpha} \right), \qquad k \le n \le N$$

for sufficiently small $\Delta t > 0$*, where* $N\Delta t = T$ *is fixed and the constant* $C^{(k,i)} > 0$ *is independent of* N*.*

Proof. Substituting formula (4.1.13) into (4.1.7) and using (4.1.21), one has

$$e^{(k,i)}(\xi) = \frac{r^{(k,i)}(\xi)}{(1-\xi)^{\alpha}} \left(\sum_{m=0}^{k-1} e_m^{(k,i)} s_m^{(k,i)}(\xi) + (\Delta t)^{\alpha} \delta f^{(k,i)}(\xi) + (\Delta t)^{\alpha} \tau^{(k,i)}(\xi) \right), \tag{4.1.22}$$

which can also be written into a matrix-vector form

$$\begin{bmatrix} e_k^{(k,i)} \\ e_{k+1}^{(k,i)} \\ \vdots \\ e_N^{(k,i)} \end{bmatrix} = \begin{bmatrix} r_0^{(k,i)} & & & \\ r_1^{(k,i)} & r_0^{(k,i)} & & \\ \vdots & \ddots & \ddots & \\ r_{N-k}^{(k,i)} & \cdots & r_1^{(k,i)} & r_0^{(k,i)} \end{bmatrix} \begin{bmatrix} g_0^{(-\alpha)} & & & \\ g_1^{(-\alpha)} & g_0^{(-\alpha)} & & \\ \vdots & \ddots & \ddots & \\ g_{N-k}^{(-\alpha)} & \cdots & g_1^{(-\alpha)} & g_0^{(-\alpha)} \end{bmatrix}$$

$$\left(e_0^{(k,i)} \begin{bmatrix} s_{0,0}^{(k,i)} \\ s_{1,0}^{(k,i)} \\ \vdots \\ s_{N-k,0}^{(k,i)} \end{bmatrix} + \cdots + e_{k-1}^{(k,i)} \begin{bmatrix} s_{0,k-1}^{(k,i)} \\ s_{1,k-1}^{(k,i)} \\ \vdots \\ s_{N-k,k-1}^{(k,i)} \end{bmatrix} + (\Delta t)^\alpha \begin{bmatrix} \delta f_k^{(k,i)} \\ \delta f_{k+1}^{(k,i)} \\ \vdots \\ \delta f_N^{(k,i)} \end{bmatrix} + (\Delta t)^\alpha \begin{bmatrix} \tau_k^{(k,i)} \\ \tau_{k+1}^{(k,i)} \\ \vdots \\ \tau_N^{(k,i)} \end{bmatrix} \right) \tag{4.1.23}$$

with arbitrary $N \in \mathbb{N}$. Therefore for any $k \le n \le N$, we obtain

$$\begin{aligned} e_n^{(k,i)} = & \sum_{m=0}^{k-1} e_m^{(k,i)} \sum_{j=0}^{n-k} r_{n-k-j}^{(k,i)} \sum_{i=0}^{j} g_{j-i}^{(-\alpha)} s_{i,m}^{(k,i)} + (\Delta t)^\alpha \sum_{j=0}^{n-k} r_{n-k-j}^{(k,i)} \sum_{i=0}^{j} g_{j-i}^{(-\alpha)} \delta f_{i+k}^{(k,i)} \\ & + (\Delta t)^\alpha \sum_{j=0}^{n-k} r_{n-k-j}^{(k,i)} \sum_{i=0}^{j} g_{j-i}^{(-\alpha)} \tau_{i+k}^{(k,i)}, \end{aligned} \tag{4.1.24}$$

where $\{g_n^{(-\alpha)}\}$ are given in Lemma 4.1.2. Since it is assumed that the function $f(t, u(t))$ satisfies a Lipschitz continuous condition, there exists a constant $L^{(k,i)} > 0$ such that $|\delta f_n^{(k,i)}| \le L^{(k,i)} |e_n^{(k,i)}|$ for $k \le n \le N$. It follows that

$$\begin{aligned} |e_n^{(k,i)}| \le & \sum_{m=0}^{k-1} |e_m^{(k,i)}| \sum_{j=0}^{n-k} |r_{n-k-j}^{(k,i)}| \sum_{i=0}^{j} g_{j-i}^{(-\alpha)} |s_{i,m}^{(k,i)}| \\ & + (\Delta t)^\alpha \sum_{j=0}^{n-k} g_{n-k-j}^{(-\alpha)} \sum_{i=0}^{j} |r_{j-i}^{(k,i)}| \left(L^{(k,i)} |e_{i+k}^{(k,i)}| + |\tau_{i+k}^{(k,i)}| \right). \end{aligned} \tag{4.1.25}$$

On the one hand, based on the relations (4.1.1) and (4.1.20), there exists a constant $\tilde{c}_{k,i} > 0$, such that $|s_{n,0}^{(k,i)}| \le c_{k,i} \frac{n^{-\alpha}}{\Gamma(1-\alpha)} \le \tilde{c}_{k,i} g_n^{(\alpha-1)}$. One hence obtains

$$\begin{aligned} \sum_{j=0}^{n-k} |r_{n-k-j}^{(k,i)}| \sum_{i=0}^{j} g_{j-i}^{(-\alpha)} |s_{i,0}^{(k,i)}| & \le \tilde{c}_{k,i} \sum_{j=0}^{n-k} |r_{n-k-j}^{(k,i)}| \sum_{i=0}^{j} g_{j-i}^{(-\alpha)} g_i^{(\alpha-1)} \\ & \le \tilde{c}_{k,i} \sum_{j=0}^{\infty} |r_j^{(k,i)}| = \tilde{c}_{k,i} M_\alpha^{(k,i)}, \end{aligned} \tag{4.1.26}$$

where $\sum_{i=0}^{j} g_{j-i}^{(-\alpha)} g_i^{(\alpha-1)} = 1$ for any $j \ge 0$ in view of the equality $(1-\xi)^{-\alpha}(1-\xi)^{\alpha-1} = (1-\xi)^{-1}$. On the other hand, there exist constants $\tilde{c}_m^{(k,i)} > 0$ for $m \ge 1$, such that $|s_{n,m}^{(k,i)}| \le c_m^{(k,i)} \frac{n^{-\alpha-1}}{|\Gamma(-\alpha)|} \le \tilde{c}_m^{(k,i)} |g_n^{(\alpha)}|$, respectively. This gives

$$\begin{aligned} \sum_{j=0}^{n-k} |r_{n-k-j}^{(k,i)}| \sum_{l=0}^{j} g_{j-l}^{(-\alpha)} |s_{l,m}^{(k,i)}| & \le \tilde{c}_m^{(k,i)} \sum_{j=0}^{n-k} |r_{n-k-j}^{(k,i)}| \sum_{l=0}^{j} g_{j-l}^{(-\alpha)} |g_l^{(\alpha)}| \\ & \le 2\tilde{c}_m^{(k,i)} \sum_{j=0}^{n-k} |r_{n-k-j}^{(k,i)}| g_j^{(-\alpha)}, \end{aligned} \tag{4.1.27}$$

where the last inequality holds since it satisfies that $\sum_{l=0}^{j} g_{j-l}^{(-\alpha)} g_l^{(\alpha)} = 0$ for any $j \geq 1$, and $\sum_{l=0}^{j} g_{j-l}^{(-\alpha)} |g_l^{(\alpha)}| = g_j^{(-\alpha)} g_0^{(\alpha)} - \sum_{l=1}^{j} g_{j-l}^{(-\alpha)} g_l^{(\alpha)} = 2g_j^{(-\alpha)}$ holds by Lemma 4.1.2. In addition, the sequences $\{r_n^{(k,i)}\}$ belong to l^1, and $g_n^{(-\alpha)} \to 0$ as $n \to \infty$. Therefore, based on Lemma 3.2.5, we know that $\sum_{j=0}^{n-k} |r_{n-k-j}^{(k,i)}| g_j^{(-\alpha)} \to 0$ as $n \to \infty$. Then, the sequences $\sum_{j=0}^{n-k} |r_{n-k-j}^{(k,i)}| \sum_{l=0}^{j} g_{j-l}^{(-\alpha)} |s_{l,m}^{(k,i)}|$ can be bounded by $2\tilde{c}_m^{(k,i)} M_\alpha^{(k,i)}$.

In the cases $1 \leq k \leq 3$, recalling $|\tau_n^{(k,k)}| \leq C_\alpha^{(k)} (\Delta t)^{k+1-\alpha}$ uniformly for $n \geq k$ in Theorem 2.1.2, together with (4.1.17), we have

$$
\begin{aligned}
(\Delta t)^\alpha \sum_{j=0}^{n-k} |r_{n-k-j}^{(k,k)}| \sum_{i=0}^{j} g_{j-i}^{(-\alpha)} |\tau_{i+k}^{(k,k)}| &= (\Delta t)^\alpha \sum_{j=0}^{n-k} g_{n-k-j}^{(-\alpha)} \sum_{i=0}^{j} |r_{j-i}^{(k,k)}| |\tau_{i+k}^{(k,k)}| \\
&\leq (\Delta t)^{k+1} C_\alpha^{(k)} M_\alpha^{(k,k)} \sum_{j=0}^{n-k} g_j^{(-\alpha)} \\
&\leq (\Delta t)^{k+1} C_\alpha^{(k)} M_\alpha^{(k,k)} \Big(1 + C \sum_{j=1}^{n-k} \frac{j^{\alpha-1}}{\Gamma(\alpha)}\Big) \\
&\leq (\Delta t)^{k+1} C_\alpha^{(k)} M_\alpha^{(k,k)} \Big(1 + \frac{C}{\Gamma(\alpha)} \int_0^{n-k} t^{\alpha-1} \mathrm{d}t\Big) \\
&\leq \tilde{C}_\alpha^{(k,k)} \left((\Delta t)^{k+1} + (\Delta t)^{k+1-\alpha} t_{n-k}^\alpha \right).
\end{aligned} \tag{4.1.28}
$$

In the other cases $1 \leq i < k \leq 3$, according to Theorem 2.1.2, there exists a constant $C_\alpha^{(k,i)} > 0$, such that

$$
|\tau_n^{(k,i)}| \leq C_\alpha^{(k,i)} \left((\Delta t)^{k-\alpha} \frac{(n-k)^{-\alpha-1}}{|\Gamma(-\alpha)|} + \frac{(\Delta t)^{k+1-\alpha}}{\Gamma(1-\alpha)} \right),
$$

if $n \geq k$. Together with (4.1.17), it follows that

$$
\begin{aligned}
(\Delta t)^\alpha \sum_{j=0}^{n-k} |r_{n-k-j}^{(k,i)}| \sum_{l=0}^{j} g_{j-l}^{(-\alpha)} |\tau_{l+k}^{(k,i)}| &\leq C_\alpha^{(k,i)} \Big((\Delta t)^k \tilde{c}_\alpha \sum_{j=0}^{n-k} |r_{n-k-j}^{(k,i)}| \sum_{l=0}^{j} g_{j-l}^{(-\alpha)} |g_l^{(\alpha)}| \\
&\quad + (\Delta t)^{k+1} \sum_{j=0}^{n-k} |r_{n-k-j}^{(k,i)}| \sum_{l=0}^{n-k} g_l^{(-\alpha)} \Big) \\
&\leq C_\alpha^{(k,i)} \Big(2(\Delta t)^k \tilde{c}_\alpha \sum_{j=0}^{n-k} |r_{n-k-j}^{(k,i)}| g_j^{(-\alpha)} \\
&\quad + (\Delta t)^{k+1} \sum_{j=0}^{n-k} |r_{n-k-j}^{(k,i)}| g_{n-k}^{(-\alpha-1)} \Big) \\
&\leq \tilde{C}_\alpha^{(k,i)} \left((\Delta t)^k + (\Delta t)^{k+1-\alpha} t_{n-k}^\alpha \right).
\end{aligned} \tag{4.1.29}
$$

Therefore, formula (4.1.30) becomes

$$
\begin{aligned}
|e_n^{(k,i)}| \leq (\Delta t)^\alpha L^{(k,i)} \Big(&\sum_{j=0}^{n-k-1} g_{n-k-j}^{(-\alpha)} \sum_{l=0}^{j} |r_{j-l}^{(k,i)}| |e_{l+k}^{(k,i)}| + g_0^{(-\alpha)} \sum_{l=0}^{n-k-1} |r_{n-k-l}^{(k,i)}| |e_{l+k}^{(k,i)}| \\
&+ g_0^{(-\alpha)} |r_0^{(k,i)}| |e_n^{(k,i)}| \Big) + \delta_n^{(k,i)}, \qquad n \geq k.
\end{aligned}
$$

If the time step $\Delta t > 0$ is chosen sufficiently small, there exist bounded constants $c^*_{k,i}$ such that $0 < \frac{1}{1-(\Delta t)^\alpha L^{(k,i)} g_0^{(-\alpha)} |r_0^{(k,i)}|} \le c^*_{k,i}$, and it follows that

$$\begin{cases} |e_k^{(k,i)}| \le \tilde{\delta}_k^{(k,i)}, \\ |e_n^{(k,i)}| \le \tilde{\delta}_n^{(k,i)} + (\Delta t)^\alpha c^*_{k,i} L^{(k,i)} \Big(\sum_{j=0}^{n-k-1} g_{n-k-j}^{(-\alpha)} \sum_{l=0}^{j} |r_{j-l}^{(k,i)}||e_{l+k}^{(k,i)}| \\ \qquad + g_0^{(-\alpha)} \sum_{l=0}^{n-k-1} |r_{n-k-l}^{(k,i)}||e_{l+k}^{(k,i)}| \Big), \qquad n \ge k+1, \end{cases} \tag{4.1.30}$$

where we denote $\tilde{\delta}_n^{(k,i)} = c^*_{k,i} \delta_n^{(k,i)}$. In the cases $1 \le k \le 3$, one obtains from (4.1.26), (4.1.27) and (4.1.28) that

$$\delta_n^{(k,k)} = C_\alpha^{(k,k)} \left(\sum_{m=0}^{k-1} |e_m^{(k,k)}| + (\Delta t)^{k+1-\alpha} t_{n-1}^\alpha \right), \qquad n \ge k.$$

In the cases $1 \le i < k \le 3$, from formulae (4.1.26), (4.1.27) and (4.1.29), it yields

$$\delta_n^{(k,i)} = C_\alpha^{(k,i)} \left(\sum_{m=0}^{k-1} |e_m^{(k,i)}| + (\Delta t)^k + (\Delta t)^{k+1-\alpha} t_{n-1}^\alpha \right), \qquad n \ge k.$$

The constants satisfy $C_\alpha^{(k,i)} = \max\{\tilde{c}_{k,i} M_\alpha^{(k,i)}, 2\tilde{c}_m^{(k,i)} M_\alpha^{(k,i)}, \tilde{C}_\alpha^{(k,i)}\}$. Next, assume that the non-negative sequence $\{p_n^{(k,i)}\}_{n\ge 0}$ satisfies

$$\begin{cases} p_0^{(k,i)} = \tilde{\delta}_k^{(k,i)}, \\ p_n^{(k,i)} = \tilde{\delta}_{n+k}^{(k,i)} + \dfrac{(\Delta t)^\alpha \tilde{L}^{(k,i)}}{\Gamma(\alpha)} \sum_{j=0}^{n-1} (n-j)^{\alpha-1} p_j^{(k,i)}, \qquad n \ge 1, \end{cases} \tag{4.1.31}$$

where the coefficient $\tilde{L}^{(k,i)}$ is chosen such that

$$\tilde{L}^{(k,i)} = \max\{c^*_{k,i} L^{(k,i)} M_\alpha^{(k,i)} \left(1 + \Gamma(\alpha) g_1^{(-\alpha)}\right), c^*_{k,i} L^{(k,i)} M_\alpha^{(k,i)} g_n^{(-\alpha)} n^{1-\alpha} \Gamma(\alpha)\}.$$

Therefore, according to Theorem A.4.3, the monotonic increasing property of sequence $\{\tilde{\delta}_n^{(k,i)}\}_{n\ge 0}$ yields that the sequence $\{p_n^{(k,i)}\}_{n\ge 1}$ is monotonic increasing with respect to n for each $1 \le i \le k \le 3$, and correspondingly, it follows that

$$p_n^{(k,i)} \le \tilde{\delta}_{n+k}^{(k,i)} E_\alpha \left(\tilde{L}^{(k,i)} (n\Delta t)^\alpha \right), \qquad n \ge 1,$$

where $E_\alpha(\cdot)$ is denoted by the Mittag-Leffler function (see Appendix A.1.2). In addition, according to (4.1.30) and (4.1.31), it is readily known that $|e_k^{(k,i)}| \le p_0^{(k,i)}$. If assume that $|e_n^{(k,i)}| \le p_{n-k}^{(k,i)}$ for $n \ge k$, then, by induction, together with (4.1.17), it follows that

$$\begin{aligned} |e_{n+1}^{(k,i)}| &\le \tilde{\delta}_{n+1}^{(k,i)} + (\Delta t)^\alpha c^*_{k,i} L^{(k,i)} \Big(\sum_{j=0}^{n-k} g_{n+1-k-j}^{(-\alpha)} \sum_{l=0}^{j} |r_{j-l}^{(k,i)}| p_l^{(k,i)} + g_0^{(-\alpha)} \sum_{l=0}^{n-k} |r_{n+1-k}^{(k,i)}| p_l^{(k,i)} \Big) \\ &\le \tilde{\delta}_{n+1}^{(k,i)} + (\Delta t)^\alpha c^*_{k,i} L^{(k,i)} M_\alpha^{(k,i)} \Big(\sum_{j=0}^{n-k} g_{n+1-k-j}^{(-\alpha)} p_j^{(k,i)} + g_0^{(-\alpha)} p_{n-k}^{(k,i)} \Big) \\ &\le \tilde{\delta}_{n+1}^{(k,i)} + \frac{(\Delta t)^\alpha \tilde{L}^{(k,i)}}{\Gamma(\alpha)} \sum_{j=0}^{n-k} (n+1-k-j)^{\alpha-1} p_j^{(k,i)}. \end{aligned}$$

Thus, one obtains that

$$|e_n^{(k,i)}| \le \tilde{\delta}_n^{(k,i)} E_\alpha\left(\tilde{L}^{(k,i)}(n-k)^\alpha \Delta t^\alpha\right) \le \tilde{\delta}_n^{(k,i)} E_\alpha\left(\tilde{L}^{(k,i)} T^\alpha\right), \qquad k \le n \le N.$$

□

Remark 4.1.2. *Note that the error is convergent of $(k+1-\alpha)$-order uniformly for all $n \ge k$, especially for the step t_n near the origin. On the other hand, for those t_n away from origin, the convergence result can be better. For example, it can be observed that if the computed starting values satisfy $u_i = u(t_i) + O((\Delta t)^k)$ for $1 \le i \le k-1$, then $|u(t_M) - u_M| = O((\Delta t)^{k+1-\alpha})$ in the cases $1 \le i \le k \le 3$.*

4.2 Convergence for linear time-fractional partial differential equations

In this section, we mainly consider the linear fractional partial differential equations of order $\alpha \in (0,1)$, whose semi-discretized form is expressed by

$$^C\mathcal{D}^\alpha \mathbf{u}(t) = A\mathbf{u}(t) + \mathbf{f}(t), \qquad 0 \le t \le T, \tag{4.2.1}$$

together with a given initial vector $\mathbf{u}(0)$, where the fractional derivative $^C\mathcal{D}^\alpha u$ is defined in (1.1.12), and the vectors are denoted by

$$\mathbf{u}(t) = \begin{bmatrix} u_1(t) & u_2(t) & \cdots & u_M(t) \end{bmatrix}^T, \qquad \mathbf{f}(t) = \begin{bmatrix} f_1(t) & f_2(t) & \cdots & f_M(t) \end{bmatrix}^T.$$

Here A is defined by a $M \times M$ square matrix with real constant elements. We restrict A to be a symmetric semi-positive definite matrix.

We make use of formula (2.1.11) on a uniform mesh $\{t_n\}_{n=0}^N$ in time. Then the discrete form of equation (4.2.1) is given by

$$D_{k,i}^\alpha \mathbf{u}^n = A\mathbf{u}^n + \mathbf{f}^n, \qquad k \le n \le N, \tag{4.2.2}$$

where $\mathbf{u}^n = [u_1^n \ \ u_2^n \ \ \cdots \ \ u_M^n]^T \in \mathbb{C}^M$, or equivalently,

$$(\Delta t)^{-\alpha} \sum_{l=0}^{k-1} w_{n,l}^{(k,i)} \mathbf{u}^l + (\Delta t)^{-\alpha} \sum_{l=0}^{n} \omega_{n-l}^{(k,i)} \mathbf{u}^l = A\mathbf{u}^n + \mathbf{f}^n, \quad k \le n \le N. \tag{4.2.3}$$

The assumption on matrix A implies that there exists an orthogonal matrix $Q \in \mathbb{R}^{M\times M}$ and a diagonal matrix Λ with non-negative entries $\{\lambda_m\}_{m=1}^M$ such that $A = Q^{-1}\Lambda Q$. Multiplying Q on both sides of (4.2.3) and substituting $\tilde{\mathbf{u}}^n = Q\mathbf{u}^n$ and $\tilde{\mathbf{f}}^n = Q\mathbf{f}^n$, one then obtains

$$(\Delta t)^{-\alpha} \sum_{l=0}^{k-1} w_{n,l}^{(k,i)} \tilde{\mathbf{u}}^l + (\Delta t)^{-\alpha} \sum_{l=0}^{n} \omega_{n-l}^{(k,i)} \tilde{\mathbf{u}}^l = \Lambda\tilde{\mathbf{u}}^n + \tilde{\mathbf{f}}^n, \qquad k \le n \le N, \tag{4.2.4}$$

which can be rewritten into the decoupled form:

$$(\Delta t)^{-\alpha} \sum_{l=0}^{k-1} w_{n,l}^{(k,i)} \tilde{u}_j^l + (\Delta t)^{-\alpha} \sum_{l=0}^{n} \omega_{n-l}^{(k,i)} \tilde{u}_j^l = \lambda_j \tilde{u}_j^n + \tilde{f}_j^n, \quad 1 \le j \le M, \ k \le n \le N. \tag{4.2.5}$$

In addition, define the discrete L^2-norm of a vector function $\mathbf{u} \in \mathbb{C}^M$ on a uniform mesh in space by

$$\|\mathbf{u}\| = \sqrt{\Delta x \sum_{j=1}^{M} (u_j)^2}. \tag{4.2.6}$$

Note that, the relation $\|Q\mathbf{u}\| = \|\mathbf{u}\|$ holds for any $1 \le n \le N$.

Remark 4.2.1. *As an example, we consider the one-dimensional time-fractional diffusion equation of the form*

$$\begin{cases} {}^C\mathcal{D}^\alpha u(x,t) = \kappa\frac{\partial^2 u}{\partial x^2}(x,t) + f(x,t), & (x,t) \in [a,b]\times(0,T], \\ u(a,t) = g_a(t), \quad u(b,t) = g_b(t), & (x,t) \in [a,b]\times[0,T], \\ u(0,x) = u^0(x), & x \in [a,b], \end{cases} \tag{4.2.7}$$

where $\kappa > 0$ is given as the diffusion constant. Denoting $x_j = a + j\Delta x$ with $\Delta x = \frac{b-a}{M+1}$ for $0 \le j \le M+1$, we discretize the second-order operator $\frac{\partial^2 u}{\partial x^2}$ by a central difference scheme, and utilize (2.1.11) *to get the discrete form*

$$(\Delta t)^{-\alpha}\sum_{l=0}^{k-1} w_{n,l}^{(k,i)} u_j^l + (\Delta t)^{-\alpha}\sum_{l=0}^{n} \omega_{n-l}^{(k,i)} u_j^l = \frac{\kappa}{(\Delta x)^2}\left(u_{j+1}^n - 2u_j^n + u_{j-1}^n\right) + f_j^n \tag{4.2.8}$$

for $1 \le j \le M$ and $k \le n \le N$, together with

$$u_0^n = g_a(t_n), \quad u_{M+1}^n = g_b(t_n), \qquad u_j^0 = u^0(x_j), \quad 0 \le n \le N, \ \ 0 \le j \le M+1. \tag{4.2.9}$$

Here, define $A = \mathrm{tridiag}(1,-2,1)$. Then A has a decomposition $A = Q\Lambda Q^{-1}$, where $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \cdots, \lambda_M)$ with the eigenvalues expressed by

$$\lambda_k = -4\sin^2\frac{k\pi}{M+1}, \qquad k = 1, 2, \cdots, M$$

and

$$Q = [\mathbf{v}^{(1)} \ \ \mathbf{v}^{(2)} \ \ \cdots \ \ \mathbf{v}^{(M)}]$$

with orthonormal eigenvectors $\mathbf{v}^{(k)} = [v_1^{(k)} \ \ v_2^{(k)} \ \ \cdots \ \ v_M^{(k)}]^T$ denoted by

$$v_j^{(k)} = \sqrt{\frac{2}{M+1}}\sin\frac{jk\pi}{M+1}, \qquad j = 1, 2, \cdots, M.$$

This implies that Q is a symmetric matrix. Substituting $\tilde{\mathbf{u}}^n = Q\mathbf{u}^n$, $\tilde{\mathbf{f}}^n = Q\mathbf{f}^n$ and $\tilde{\mathbf{b}}^n = Q\mathbf{b}^n$, then for each j, $\{\tilde{u}_j^n\}_{n=k}^N$ can be solved independently in accordance with

$$(\Delta t)^{-\alpha}\sum_{l=0}^{k-1} w_{n,l}^{(k,i)} \tilde{u}_j^l + (\Delta t)^{-\alpha}\sum_{l=0}^{n} \omega_{n-l}^{(k,i)} \tilde{u}_j^l = \lambda_j\kappa(\Delta x)^{-2}\tilde{u}_j^n + \tilde{f}_j^n + \tilde{b}_j^n,$$

where $\mathbf{b}^n = [\frac{\kappa}{(\Delta x)^2}u_0^n \ \ 0 \ \ \cdots \ \ 0 \ \ \frac{\kappa}{(\Delta x)^2}u_{M+1}^n]^T \in \mathbb{C}^M$ for each $k \le n \le N$.

As a complementary result, we provide the orthogonal property of the matrix Q.

Lemma 4.2.1. *The following orthogonality relation holds:*

$$\sum_{l=1}^{M}\sin\frac{lj\pi}{M+1}\sin\frac{lk\pi}{M+1} = \frac{M+1}{2}\delta_{jk} \quad j,k = 1, \cdots M. \tag{4.2.10}$$

Proof. Substituting the identity $\sin x = \frac{e^{ix}-e^{-ix}}{2i}$ in the left hand side (LHS) of (4.2.10), one arrives at

$$
\begin{aligned}
&\sum_{l=1}^{M} \frac{e^{\frac{ílj\pi}{M+1}}-e^{-\frac{ilj\pi}{M+1}}}{2i}\cdot\frac{e^{\frac{ilk\pi}{M+1}}-e^{-\frac{ilk\pi}{M+1}}}{2i}\\
&=-\frac{1}{4}\sum_{l=1}^{M}\left(e^{\frac{il(j+k)\pi}{M+1}}-e^{\frac{il(k-j)\pi}{M+1}}-e^{\frac{il(j-k)\pi}{M+1}}+e^{-\frac{il(j+k)\pi}{M+1}}\right)\\
&=-\frac{1}{4}\Bigg(\frac{(-1)^{j+k}-e^{\frac{i(j+k)\pi}{M+1}}}{e^{\frac{i(j+k)\pi}{M+1}}-1}+\frac{(-1)^{j+k}e^{\frac{i(j+k)\pi}{M+1}}-1}{1-e^{\frac{i(j+k)\pi}{M+1}}}\\
&\quad-\frac{(-1)^{j-k}-e^{\frac{i(j-k)\pi}{M+1}}}{e^{\frac{i(j-k)\pi}{M+1}}-1}-\frac{(-1)^{k-j}-e^{\frac{i(k-j)\pi}{M+1}}}{e^{\frac{i(k-j)\pi}{M+1}}-1}\Bigg)=0
\end{aligned}
$$

in the case $j \neq k$. Note that $j+k$ and $j-k$ can be both odd or even, respectively. Otherwise, if $j=k$, then

$$
\text{LHS} = -\frac{1}{4}\sum_{l=1}^{M}\left(e^{\frac{2ilj\pi}{M+1}}-2+e^{-\frac{2ilj\pi}{M+1}}\right)=\frac{M}{2}-\frac{1}{4}\left(\frac{1-e^{\frac{2ij\pi}{M+1}}}{e^{\frac{2ij\pi}{M+1}}-1}+\frac{e^{\frac{2ij\pi}{M+1}}-1}{1-e^{\frac{2ij\pi}{M+1}}}\right)=\frac{M+1}{2}.
$$

This gives the result. □

Motivated by (4.2.5), we next focus on the linear scalar cases

$$
(\Delta t)^{-\alpha}\sum_{l=0}^{k-1} w_{n,l}^{(k,i)}u^l + (\Delta t)^{-\alpha}\sum_{l=0}^{n}\omega_{n-l}^{(k,i)}u^l = \lambda u^n + f^n, \qquad k \le n \le N \tag{4.2.11}
$$

for some k, i, which are considered as a class of approximations of the fractional linear ordinary differential equation

$$
\begin{cases} {}^{C}\mathcal{D}^{\alpha}u(t) = \lambda u(t) + f(t), & t \in (0,T],\\ u(0) = u^0. \end{cases} \tag{4.2.12}
$$

Multiplying (4.2.11) by $(\Delta t)^{\alpha}$ and rewriting it into a formal power series form yields

$$
\left(\omega^{(k,i)}(\xi) - z\right)u(\xi) = \sum_{l=0}^{k-1} u^l s_l^{(k,i)}(\xi) + (\Delta t)^{\alpha} f(\xi), \qquad z = \lambda(\Delta t)^{\alpha}, \tag{4.2.13}
$$

where $\{s_l^{(k,i)}(\xi)\}_{l=0}^{k-1}$ are defined by (4.1.8), $u(\xi) = \sum_{n=0}^{\infty} u^{n+k}\xi^n$ and $f(\xi) = \sum_{n=0}^{\infty} f^{n+k}\xi^n$. If we define the reciprocal of the series $\left(\omega^{(k,i)}(\xi) - z\right)$ by $\tilde{\omega}_z^{(k,i)}(\xi) = \sum_{n=0}^{\infty}\tilde{\omega}_n^{(k,i)}(z)\xi^n$ such that

$$
\tilde{\omega}_z^{(k,i)}(\xi)\left(\omega^{(k,i)}(\xi) - z\right) = \left(\omega^{(k,i)}(\xi) - z\right)\tilde{\omega}_z^{(k,i)}(\xi) = 1,
$$

then using Cauchy integral formula , we find

$$
\begin{aligned}
\tilde{\omega}_n^{(k,i)}(z) &= \frac{1}{2\pi i}\int_{|\xi|=\rho}\frac{1}{\left(\omega^{(k,i)}(\xi)-z\right)\xi^{n+1}}d\xi\\
&= \frac{\Delta t}{2\pi i}\int_{-\frac{\ln\rho}{\Delta t}-i\frac{\pi}{\Delta t}}^{-\frac{\ln\rho}{\Delta t}+i\frac{\pi}{\Delta t}} e^{st_n}\frac{1}{\omega^{(k,i)}(e^{-s\Delta t})-z}ds
\end{aligned} \tag{4.2.14}
$$

where we choose $0<\rho<1$ and appropriate $z\in\mathbb{C}$ such that the function $\omega^{(k,i)}(\xi)-z$ is analytic and has no zero on $|\xi|\leq\rho$. In addition, the last equality is derived from the change of variable $\xi=e^{-s\Delta t}$. If $\lambda\in\mathbb{R}^-$, deforming the integral interval into an equivalent contour, we can obtain an alternative expression of the form

$$\tilde{\omega}_n^{(k,i)}(z)=\frac{\Delta t}{2\pi i}\int_\Gamma e^{st_n}\frac{1}{\omega^{(k,i)}(e^{-s\Delta t})-z}\mathrm{d}s,$$

where $\Gamma=\Gamma^+\cup\Gamma^-\cup\Gamma_u\cup\Gamma_b\cup S_\epsilon$. The curves are defined by $\Gamma^+=\{xe^{i\vartheta}:\ \epsilon\leq x\leq\frac{\pi}{\Delta t\sin(\pi-\vartheta)}\}$, $\Gamma^-=\{xe^{-i\vartheta}:\ \frac{\pi}{\Delta t\sin(\pi-\vartheta)}\leq x\leq\epsilon\}$, $\Gamma_u=\{x+i\frac{\pi}{\Delta t}:\ -\frac{\pi}{\Delta t}\cot(\pi-\vartheta)\leq x\leq-\frac{\ln\rho}{\Delta t}\}$, $\Gamma_b=\{x-i\frac{\pi}{\Delta t}:\ -\frac{\ln\rho}{\Delta t}\leq x\leq-\frac{\pi}{\Delta t}\cot(\pi-\vartheta)\}$ and $S_\epsilon=\{\epsilon e^{ix}:\ |x|\leq\vartheta\}$. Here the angle $\vartheta\in(\frac{\pi}{2},\pi)$ and $\epsilon>0$ are chosen such that $\left(\omega^{(k,i)}(e^{-s\Delta t})-z\right)^{-1}$ is analytic on $s\in\Gamma$ and $\lambda\in\mathbb{R}^-$.

Making use of the fact that

$$\int_{\Gamma_u}e^{st_n}\frac{1}{\omega^{(k,i)}(e^{-s\Delta t})-z}\mathrm{d}s=-\int_{\Gamma_b}e^{st_n}\frac{1}{\omega^{(k,i)}(e^{-s\Delta t})-z}\mathrm{d}s,$$

we then obtain

$$\tilde{\omega}_n^{(k,i)}(z)=\frac{\Delta t}{2\pi i}\int_{\Gamma^+\cup\Gamma^-\cup S_\epsilon}e^{st_n}\frac{1}{\omega^{(k,i)}(e^{-s\Delta t})-z}\mathrm{d}s. \tag{4.2.15}$$

Next, we would like to find the range of values of $\omega^{(k,i)}(e^{-s\Delta t})$ for $s\in\Gamma^+\cup\Gamma^-\cup S_\epsilon$. According to the decomposition of power series $\omega^{(k,i)}(\xi)$ defined by (4.1.13), we will consider the corresponding range of values of series $(1-\xi)^\alpha$ and $\psi^{(k,i)}(\xi)$ respectively.

Lemma 4.2.2. *Assume that $\rho\in\Delta t(\Gamma^+\cup\Gamma^-\cup S_\epsilon)$ and $0<\alpha<1$, then there exists $c>0$, independently of ρ, such that*

$$\left|\left(\frac{1-e^{-\rho}}{\rho}\right)^\alpha\right|\geq c. \tag{4.2.16}$$

Proof. The proof is a direct generalization of the result in [31]. If $\rho\in\Delta t\Gamma^+$, we denote $\rho=xe^{i\vartheta}$ for $\epsilon\Delta t\leq x\leq\frac{\pi}{\sin\vartheta}$. This yields

$$\begin{aligned}\left|\left(\frac{1-e^{-\rho}}{\rho}\right)^\alpha\right|&=\left(\frac{|1-e^{-xe^{i\vartheta}}|}{x}\right)^\alpha=\left(\frac{|1-e^{-x\cos\vartheta}e^{iy}|}{x}\right)^\alpha\\&=\left(\frac{\sqrt{(1-e^{-x\cos\vartheta}\cos y)^2+e^{-2x\cos\vartheta}\sin^2 y}}{x}\right)^\alpha\\&=\left(\frac{\sqrt{1-2e^{-x\cos\vartheta}\cos y+e^{-2x\cos\vartheta}}}{x}\right)^\alpha\\&\geq\left(\frac{e^{-x\cos\vartheta}-1}{x}\right)^\alpha\geq(-\cos\vartheta)^\alpha>0,\end{aligned}$$

where $y=-x\sin\vartheta\in(0,-\pi]$. If $\rho\in\Delta t\Gamma^-$, choosing $\rho=xe^{-i\vartheta}$ for $\epsilon\Delta t\leq x\leq\frac{\pi}{\sin\vartheta}$, we can readily obtain the result in an analogous way. Moreover, in the remaining case $\rho\in\Delta tS_\epsilon$, if we denote $\rho=\tilde{\epsilon}e^{ix}$ as $|x|\leq\vartheta$, where $\tilde{\epsilon}=\Delta t\epsilon$, then

$$\begin{aligned}\left|\left(\frac{1-e^{-\rho}}{\rho}\right)^\alpha\right|&=\left(\frac{|1-e^{-\tilde{\epsilon}\cos x}e^{-i\tilde{\epsilon}\sin x}|}{\tilde{\epsilon}}\right)^\alpha\\&=\left(\frac{\sqrt{1-2e^{-\tilde{\epsilon}\cos x}\cos(\tilde{\epsilon}\sin x)+e^{-2\tilde{\epsilon}\cos x}}}{\tilde{\epsilon}}\right)^\alpha:=g(x,\tilde{\epsilon}).\end{aligned}$$

If we assume that $\tilde{\epsilon} \in (0, \pi]$, then in the case that $x \in [0, \frac{\pi}{2}]$, it is clear that the functions $\sin x$ and $\cos x$ are non-negative and monotonically increasing and decreasing, respectively, and correspondingly, the function $\cos(\tilde{\epsilon} \sin x)$ is monotonically decreasing as well. This implies $g(x, \tilde{\epsilon}) \geq g(0, \tilde{\epsilon})$. In the case $x \in [-\frac{\pi}{2}, 0]$, because of the symmetry of the function g with respect to x, we can obtain an analogous result. In summary, for $x \in [-\frac{\pi}{2}, \frac{\pi}{2}]$, we obtain

$$\left| \left(\frac{1 - e^{-\rho}}{\rho} \right)^{\alpha} \right| \geq \left(\frac{1 - e^{-\tilde{\epsilon}}}{\tilde{\epsilon}} \right)^{\alpha}.$$

Further, we see that $(\frac{1-e^{-\tilde{\epsilon}}}{\tilde{\epsilon}})^{\alpha} \to 1$ as $\tilde{\epsilon} \to 0$. On the other hand, if $x \in [\frac{\pi}{2}, \vartheta]$ for arbitrary $\vartheta \in (\frac{\pi}{2}, \pi)$, we define

$$f(x, \tilde{\epsilon}) = 1 - 2e^{-\tilde{\epsilon} \cos x} \cos(\tilde{\epsilon} \sin x) + e^{-2\tilde{\epsilon} \cos x}.$$

Then it can be derived that

$$\begin{aligned} \frac{\partial f}{\partial x}(x, \tilde{\epsilon}) &= 2\tilde{\epsilon} e^{-\tilde{\epsilon} \cos x} \left(\sin x e^{-\tilde{\epsilon} \cos x} + \sin\left(\tilde{\epsilon} \sin x - x\right) \right) \\ &\geq 2\tilde{\epsilon} e^{-\tilde{\epsilon} \cos x} \left(\sin x (1 - \cos(\tilde{\epsilon} \sin x)) - \cos x (\tilde{\epsilon} \sin x - \sin(\tilde{\epsilon} \sin x)) \right) \geq 0 \end{aligned}$$

for all $\tilde{\epsilon} \geq 0$. Thus $f(x, \tilde{\epsilon}) \geq f(\frac{\pi}{2}, \tilde{\epsilon})$, and consequently

$$\left| \left(\frac{1 - e^{-\rho}}{\rho} \right)^{\alpha} \right| \geq \left(\frac{\sin \frac{\tilde{\epsilon}}{2}}{\frac{\tilde{\epsilon}}{2}} \right)^{\alpha}.$$

It follows that $\frac{\sin \tilde{\epsilon}/2}{\tilde{\epsilon}/2} \to 1$ as $\tilde{\epsilon} \to 0$. In view of the symmetric property of g in terms of the variable x, we can obtain the same result in the case $x \in [-\vartheta, -\frac{\pi}{2}]$ as well. □

Theorem 4.2.1. *Assume that for $1 \leq i \leq k \leq 3$, there exist $\theta_{\omega}(k, i) \in (\frac{\pi}{2}, \pi)$ and $\theta_{\psi}(k, i) \in (\frac{\pi}{2}, \pi)$ such that $\omega^{(k,i)}(e^{-\rho}) \in \Sigma_{\theta_{\omega}(k,i)}$ and $\psi^{(k,i)}(e^{-\rho}) - 1 \in \Sigma_{\theta_{\psi}(k,i)}$ for $\rho \in \Delta t\,(\Gamma^{+} \cup \Gamma^{-} \cup S_{\epsilon})$, respectively, then there exists constants $C^{(k,i)} = C^{(k,i)}(\vartheta) > 0$ such that*

$$|\tilde{\omega}_n^{(k,i)}(z)| \leq \frac{C^{(k,i)}}{\Gamma(\alpha)} n^{\alpha-1}, \qquad n \geq 1$$

uniformly for $\Re\lambda \leq 0$ and $z = \lambda(\Delta t)^{\alpha}$.

Proof. From (4.2.15), we obtain

$$\begin{aligned} \tilde{\omega}_n^{(k,i)}(z) = \frac{\Delta t}{2\pi i} \Bigg(&\int_{\epsilon}^{\frac{\pi}{\Delta t \sin(\pi - \vartheta)}} \frac{e^{x e^{i\vartheta} t_n} e^{i\vartheta}}{\omega^{(k,i)}(e^{-x e^{i\vartheta} \Delta t}) - \lambda(\Delta t)^{\alpha}} \mathrm{d}x \\ &+ \int_{\frac{\pi}{\Delta t \sin(\pi - \vartheta)}}^{\epsilon} \frac{e^{x e^{-i\vartheta} t_n} e^{-i\vartheta}}{\omega^{(k,i)}(e^{-x e^{-i\vartheta} \Delta t}) - \lambda(\Delta t)^{\alpha}} \mathrm{d}x + \int_{-\vartheta}^{\vartheta} \frac{e^{\epsilon e^{ix} t_n} \epsilon i e^{ix}}{\omega^{(k,i)}(e^{-\epsilon e^{ix} \Delta t}) - \lambda(\Delta t)^{\alpha}} \mathrm{d}x \Bigg) \\ := l_n^{(k,i)} + ll_n^{(k,i)} + lll_n^{(k,i)}. \end{aligned}$$

From the assumption follows that there exists $\theta^{(k,i)} \in (\frac{\pi}{2}, \pi)$, such that $\omega^{(k,i)}(e^{-\rho}) \in \Sigma_{\theta^{(k,i)}}$ for $\rho \in \Delta t\,(\Gamma^{+} \cup \Gamma^{-} \cup S_{\epsilon})$. Hence, for $\Re\lambda \leq 0$, one has the following estimate

$$\begin{aligned} |l_n^{(k,i)}| &\leq \frac{\Delta t}{2\pi} \int_{\epsilon}^{\frac{\pi}{\Delta t \sin(\pi - \vartheta)}} e^{x \cos \vartheta t_n} \frac{1}{|\omega^{(k,i)}(e^{-x e^{i\vartheta} \Delta t})|} \mathrm{d}x \\ &\leq \frac{(\Delta t)^{1-\alpha}}{2\pi c^{(k,i)} \Gamma(1-\alpha)\Gamma(\alpha)} \int_0^{\infty} e^{x \cos \vartheta t_n} x^{-\alpha} \mathrm{d}x \leq \frac{\tilde{c}_l^{(k,i)}}{\Gamma(\alpha)} n^{\alpha-1}, \end{aligned}$$

and in view of the symmetry of the interval of integration, the same result holds for $ll_n^{(k,i)}$. In addition, we find

$$|lll_n^{(k,i)}| \leq \frac{\Delta t}{\pi} \int_0^{\vartheta} \epsilon e^{\epsilon \cos x t_n} \frac{1}{|\omega^{(k,i)}(e^{-\epsilon e^{ix}\Delta t})|} \mathrm{d}x$$
$$\leq \frac{(\Delta t)^{1-\alpha}}{\pi c^{(k,i)}\Gamma(1-\alpha)\Gamma(\alpha)} \int_0^{\vartheta} \epsilon^{1-\alpha} e^{\epsilon \cos x t_n} \mathrm{d}x \leq \frac{\tilde{c}_{lll}^{(k,i)}}{\Gamma(\alpha)} n^{\alpha-1}.$$

Here $\epsilon = \min(b, 1/t_n)$, and b is a positive constant. Therefore, the result is satisfied by choosing $C^{(k,i)} = \max(\tilde{c}_l^{(k,i)}, \tilde{c}_{ll}^{(k,i)}, \tilde{c}_{lll}^{(k,i)})$. □

Remark 4.2.2. *The proposed result of the coefficients of the series $\tilde{\omega}^{(k,i)}(e^{-\rho})$ is crucial for the error estimate. From this we can obtain a similar conclusion in Theorem 4.1.3 for the problem 4.2.1 without a restriction to the time stepsize.*

In this chapter, we mainly study the convergence of the numerical methods on a uniform grid proposed in chapter 2 for a time-fractional ordinary differential equation and a system of time-fractional ordinary differential equations. Next, we will carry out lots of numerical experiments to verify our theoretical results.

Chapter 5

Numerical experiments

In this section, we utilize the methods proposed in Chapter 2 to numerical approximate several time-fractional differential equations, and confirm the error accuracy and convergence order corresponding to variable stepsizes. Without loss of generalization, we prescribe the starting values exactly. In practical computations, the starting values can be obtained numerically in advance and have no influence on the numerical stability of the methods.

5.1 Time-fractional ordinary differential equations

Example 5.1.1. *We consider the linear fractional ordinary differential equation*

$$\begin{cases} {}^{C}\mathcal{D}^{\alpha}u(t) = \lambda u(t) + f(t), \quad t \in (0,1], \\ u(0) = u_0 \end{cases} \tag{5.1.1}$$

in the case $0 < \alpha < 1$. *The exact solution is given by*

i). $u(t) = e^{-t} \in C^{\infty}[0,1]$, *if* $f(t) = -t^{1-\alpha}E_{1,2-\alpha}(-t) - \lambda e^{-t} \in C[0,1] \cap C^{\infty}(0,1]$,

ii). $u(x,t) = E_{\alpha,1}(\lambda t^{\alpha}) \in C[0,1] \cap C^{\infty}(0,1]$, *if* $f(t) = 0 \in C^{\infty}[0,1]$,

where the Mittag-Leffler functions are defined in Definition A.1.2.

In Figures 5.1(a)-5.1(d), we plot the truncated boundary locus curves $\sum_{n=0}^{6000} \omega_n^{(k,i)} e^{in\theta}$ $(0 \leq \theta \leq 2\pi)$ in the cases $1 \leq i \leq k \leq 3$ for different $\alpha \in (0,1)$. It is known from Theorem 3.2.3 that the stability regions of methods (3.2.1) lie outside the corresponding curves. Here, we introduce the points $z_n = \lambda(\Delta t_n)^{\alpha}$ for $1 \leq n \leq 5$, where $\Delta t_n = 1/2^{n+6}$ denote different time steps. Table 5.1 and Table 5.2 list the accuracy and convergence rate of $|e_M^{(k,i)}| = |u(t_M) - u_M^{(k,i)}|$ in Example 5.1.1, where $t_M = 1$ is fixed and $M = 2^j$ for $7 \leq j \leq 11$, $u(t_M)$ and u_M are the exact solution and the computed solution, respectively.

By comparing Figures 5.1(a)-5.1(d) and Tables 5.1-5.2, we can see the influence of the stability of the numerical methods on the error accuracy. In Figure 5.1(a), the points z_n for $1 \leq n \leq 5$ all lie in the stability regions in the case $\alpha = 0.5$ and $\lambda = -50$, in which situation the reliable accuracy is obtained. It is observed that $|e_M^{(k,i)}| = O(\Delta t^{k+1-\alpha})$ in Table 5.1-5.2 as mentioned in Remark 4.1.2. In Figure 5.1(b)-5.1(c), z_n are chosen on the half line with angle $\frac{\pi\alpha}{2}$ and different λ. It is observed that when all $\{z_n\}_{n=1}^{5}$ fall out of the instability region (cf. Figure 5.1(b)), correspondingly, as shown in Table 5.1-5.2, then the global error e_M agrees with the expected accuracy. On the other hand, due to the fact that points z_4 and z_5 outside the stability regions of $k = 3$ (cf. Figure 5.1(c)), the perturbation errors are magnified and accumulated significantly, which are shown in Table 5.1-5.2 as well. In Figure 5.1(d), $\{z_n\}$ are chosen on the imaginary axis with imaginary number λ, according to Theorem 3.2.4, all the $\{z_n\}$ belong to the stability region of the methods (3.2.1) in the case $k = 1, 2$, and the error accuracy and the convergence order are obtained (cf. Table 5.1).

As a counter example, when z_3 doesn't belong to the stability region for $\alpha = 0.98$ in Figure 5.1(d), the corresponding error e_M, shown in Table 5.2, can't ensure the desirable accuracy. In fact, it can be observed that for $k = 3$, methods (3.2.1) don't possess $A(\frac{\pi}{2})$-stability when α tends to 1, which appears to be predictable, since it is well known that BDF3 method for ODEs is not $A(\frac{\pi}{2})$-stable.

Table 5.3 and Table 5.4 display the error accuracy and convergence rate at the fixed time step t_4, to further explain the theoretical result in Theorem 4.1.3. As we know, the theoretical order of error accuracy $e_n^{(k,i)}$ is not uniform for all $n \geq k$. In contrast to the case n being large enough, for those n near the origin, the error satisfies $|e_n^{(k,k)}| = O\left((\Delta t)^{k+1}\right)$ and $|e_n^{(k,i)}| = O\left((\Delta t^k)\right)$ for $1 \leq i < k \leq 3$, which can be observed from Table 5.3 and Table 5.4 accordingly.

In Table 5.5 and Table 5.6, we show the error accuracy and convergence order of e_M for different values of α in the case $\lambda = -50$ and $\lambda = i$, respectively. It implies that in case ii). of Example 5.1.1, the arbitrary order derivatives of the exact solution tend to infinity near the origin. Therefore in practical implementation, making use of the approximating schemes on a uniform grid constructed in Chapter 2 Section 2.1 we can't find the desired convergence rate as that in the case i). of Example 5.1.1. We thus apply the schemes on a nonuniform grid introduced in Chapter 2 Section 2.2, where the map from the uniform grid to the nonuniform grid is chosen by $t = T\tau^2$. It is known that the convolution structure of the differential matrix to ${}^C\mathcal{D}^\alpha u$ isn't preserved, and the stability region shown in Figures 5.1 can't apply to this case. We therefore check two specific values of λ, which are either included in $\mathbb{R}^-$ or on imaginary axis. It is observed that the convergence order of the error is $\min(M^{-(k+1-\alpha)}, M^{-2})$ without considering the stability.

Example 5.1.2. *Consider the nonlinear equation*

$$\begin{cases} {}^C\mathcal{D}^\alpha u(t) = -Ku^p + f(t), \quad t \in (0, T] \\ u(0) = u_0. \end{cases} \tag{5.1.2}$$

with $p > 0, K > 0$ and the source function is prescribed by $f(t) = \mu t^{1-\alpha} E_{1,2-\alpha}(\mu t) + K e^{p\mu t}$ such that the exact solution reads $u(t) = e^{\mu t}$.

Tables 5.7-5.10 plot the global error $|e_M^{(k,i)}| = |u(t_M) - u_M^{(k,i)}|$ in Example 5.1.2 for different μ and α, where $t_M = 1$ is fixed and $\Delta t = 1/M$ with $M = 2^j$, $2 \leq j \leq 11$. It is observed that $|e_M^{(k,i)}| = O(\Delta t^{k+1-\alpha})$ in the cases $1 \leq i \leq k \leq 3$, when using discretisation formula (2.1.24) in combination with Newton-Raphson method for the nonlinear equation behind the implicit method. The detailed process is as follows. Define a linear function $\mathbf{F}^{(k,i)} : \mathbb{R}^M \to \mathbb{R}^M$ such that

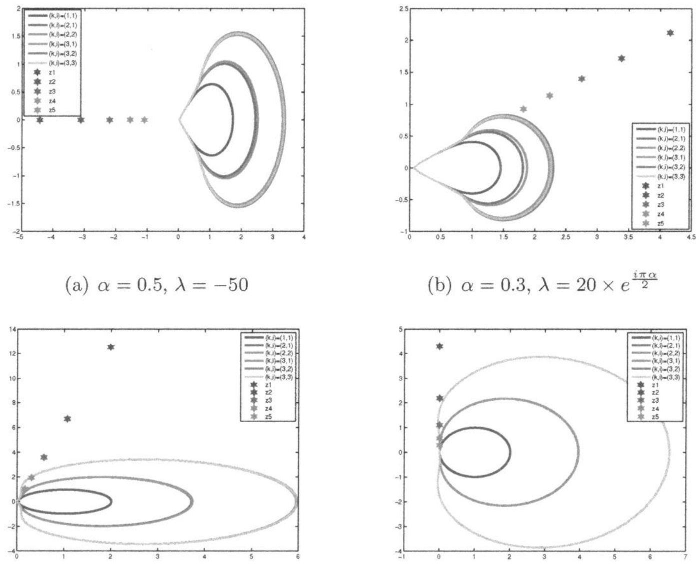
$$F_n^{(k,i)} = (\Delta t)^{-\alpha} \sum_{j=0}^{k-1} w_{n,j}^{(k,i)} u_j + (\Delta t)^{-\alpha} \sum_{j=0}^{n} \omega_{n-j}^{(k,i)} u_j + K(u_n)^p - f_n = 0, \quad n = k, \cdots, M,$$

we prescribe the exact starting values by $u_j^{(m)} = u_j$ for $0 \leq j \leq k-1$ of every iteration step m. The Newton's method therefore yields that

$$\mathbf{u}^{(m+1)} = \mathbf{u}^{(m)} + \delta \mathbf{u}^{(m)}, \qquad m \geq 0 \tag{5.1.3}$$

together with initial value $\mathbf{u}^{(0)} = \mathbf{u}_0$, where $\delta \mathbf{u}^{(m)}$ is obtained by

$$J_{F^{(k,i)}}(\mathbf{u}^{(m)}) \delta \mathbf{u}^{(m)} = -\mathbf{F}^{(k,i)}(\mathbf{u}^{(m)})$$



(a) $\alpha = 0.5$, $\lambda = -50$

(b) $\alpha = 0.3$, $\lambda = 20 \times e^{\frac{i\pi\alpha}{2}}$

(c) $\alpha = 0.9$, $\lambda = 1000 \times e^{\frac{i\pi\alpha}{2}}$

(d) $\alpha = 0.98$, $\lambda = 500i$

FIGURE 5.1:
The boundary of the numerical stability region of formula (2.1.11) for different α and λ.

TABLE 5.1:
Errors and convergence rates of $|u(t_M) - u_M|$ in Example 5.1.1. i) for different α, λ.

α	λ	M	$(k,i)=(1,1)$		$(k,i)=(2,1)$		$(k,i)=(2,2)$	
			$\|u(t_M)-u_M\|$	rate	$\|u(t_M)-u_M\|$	rate	$\|u(t_M)-u_M\|$	rate
0.5	-1	128	1.59038E-04	-	1.60073E-07	-	1.34983E-07	-
		256	5.53407E-05	1.52	2.86635E-08	2.48	2.37399E-08	2.51
		512	1.93502E-05	1.52	5.11315E-09	2.49	4.18230E-09	2.50
		1024	6.78837E-06	1.51	9.09687E-10	2.49	7.37621E-10	2.50
		2048	2.38698E-06	1.51	1.61541E-10	2.49	1.30187E-10	2.50
0.3	$20 \times e^{\frac{i\pi\alpha}{2}}$	128	1.34901E-06	-	2.69029E-09	-	1.08970E-09	-
		256	3.73401E-07	1.85	4.44355E-10	2.60	1.62447E-10	2.75
		512	1.04588E-07	1.84	7.14993E-11	2.64	2.44242E-11	2.73
		1024	2.96205E-08	1.82	1.13426E-11	2.66	3.69238E-12	2.73
		2048	8.47625E-09	1.81	1.78666E-12	2.67	5.57796E-13	2.73
0.9	$1000 \times e^{\frac{i\pi\alpha}{2}}$	128	7.84215E-07	-	3.94997E-09	-	3.83098E-09	-
		256	3.63985E-07	1.11	9.18845E-10	2.10	8.91101E-10	2.10
		512	1.69345E-07	1.10	2.14033E-10	2.10	2.07571E-10	2.10
		1024	7.88889E-08	1.10	4.98901E-11	2.10	4.83852E-11	2.10
		2048	3.67748E-08	1.10	1.16334E-11	2.10	1.12827E-11	2.10
0.98	$500i$	128	2.55224E-06	-	1.32455E-08	-	1.31778E-08	-
		256	1.25624E-06	1.02	3.25627E-09	2.02	3.23963E-09	2.02
		512	6.18899E-07	1.02	8.01689E-10	2.02	7.97599E-10	2.02
		1024	3.05047E-07	1.02	1.97518E-10	2.02	1.96512E-10	2.02
		2048	1.50388E-07	1.02	4.86819E-11	2.02	4.84347E-11	2.02

TABLE 5.2:
Errors and convergence rates of $|u(t_M) - u_M|$ in Example 5.1.1. i) for different α, λ.

α	λ	M	$(k,i)=(3,1)$ $\lvert u(t_M)-u_M\rvert$	rate	$(k,i)=(3,2)$ $\lvert u(t_M)-u_M\rvert$	rate	$(k,i)=(3,3)$ $\lvert u(t_M)-u_M\rvert$	rate
0.5	-1	128	1.04028E-09	-	9.41107E-10	-	9.99698E-10	-
		256	9.23186E-11	3.49	8.25515E-11	3.51	8.86817E-11	3.49
		512	8.18229E-12	3.50	7.25575E-12	3.51	7.85577E-12	3.50
		1024	7.25420E-13	3.50	6.37490E-13	3.51	6.92002E-13	3.50
		2048	6.82232E-14	3.41	5.34572E-14	3.58	5.85643E-14	3.56
0.3	$20\times e^{\frac{i\pi\alpha}{2}}$	128	1.73101E-11	-	1.03070E-11	-	1.53161E-11	-
		256	1.33740E-12	3.69	7.55245E-13	3.77	1.18503E-12	3.69
		512	1.03673E-13	3.69	5.58325E-14	3.76	9.13054E-14	3.70
		1024	6.13266E-15	4.08	4.40825E-15	3.66	7.52355E-15	3.60
		2048	1.20505E-15	2.35	6.86635E-16	2.68	1.12983E-15	2.74
0.9	$1000\times e^{\frac{i\pi\alpha}{2}}$	128	2.28884E-11	-	2.24089E-11	-	2.26564E-11	-
		256	2.65645E-12	3.11	2.60061E-12	3.11	2.62969E-12	3.11
		512	3.09069E-13	3.10	3.02593E-13	3.10	3.05970E-13	3.10
		1024	9.71032E-07	-21.58	4.20376E-06	-23.73	4.42542E-07	-20.46
		2048	6.28199E+34	-135.57	1.41894E+35	-134.63	1.09390E+34	-134.18
0.98	$500i$	128	7.76488E-11	-	7.73754E-11	-	7.75095E-11	-
		256	9.52734E-12	3.03	9.49401E-12	3.03	9.51047E-12	3.03
		512	9.64788E-07	-16.63	1.77544E-06	-17.51	1.37083E-06	-17.14
		1024	3.88686E-14	24.57	1.83022E-13	23.21	1.31363E-13	23.31
		2048	1.75624E-14	1.15	1.70830E-14	3.42	1.66951E-14	2.98

TABLE 5.3:
Errors and convergence rates of $|u(t_n) - u_n|$ in Example 5.1.1. i) for $n = 4$ and $\lambda = -1$.

α	M	$(k,i)=(1,1)$ $\lvert u(t_n)-u_n\rvert$	rate	$(k,i)=(2,1)$ $\lvert u(t_n)-u_n\rvert$	rate	$(k,i)=(2,2)$ $\lvert u(t_n)-u_n\rvert$	rate
0.20	32	5.58923E-05	-	2.05711E-06	-	5.84786E-07	-
	64	1.54138E-05	1.86	6.68846E-07	1.62	8.09660E-08	2.85
	128	4.13739E-06	1.90	1.93717E-07	1.79	1.08862E-08	2.89
	256	1.09335E-06	1.92	5.32015E-08	1.86	1.43946E-09	2.92
	512	2.86124E-07	1.93	1.42182E-08	1.90	1.88391E-10	2.93
0.40	32	1.87911E-04	-	3.93148E-06	-	2.45377E-06	-
	64	5.27143E-05	1.83	1.48758E-06	1.40	3.42086E-07	2.84
	128	1.42703E-05	1.89	4.55312E-07	1.71	4.60557E-08	2.89
	256	3.77655E-06	1.92	1.27610E-07	1.84	6.06659E-09	2.92
	512	9.84358E-07	1.94	3.42230E-08	1.90	7.87671E-10	2.95
0.60	32	4.50936E-04	-	2.50300E-06	-	6.42064E-06	-
	64	1.25419E-04	1.85	1.61936E-06	0.63	8.80026E-07	2.87
	128	3.34912E-05	1.90	5.52956E-07	1.55	1.16318E-07	2.92
	256	8.72552E-06	1.94	1.59495E-07	1.79	1.50476E-08	2.95
	512	2.23905E-06	1.96	4.28808E-08	1.90	1.92163E-09	2.97
0.80	32	9.15296E-04	-	5.94225E-06	-	1.30634E-05	-
	64	2.50043E-04	1.87	1.86219E-07	5.00	1.75401E-06	2.90
	128	6.56454E-05	1.93	2.80309E-07	-0.59	2.27927E-07	2.94
	256	1.68606E-05	1.96	1.01234E-07	1.47	2.90987E-08	2.97
	512	4.27858E-06	1.98	2.93601E-08	1.79	3.67946E-09	2.98

and for $k \le l, j \le M$, we find

$$\left(J_{F^{(k,i)}}(\mathbf{u}^{(m)})\right)_{l,j} = \frac{\partial F_l^{(k,i)}}{\partial u_j}(\mathbf{u}^{(m)}) = \begin{cases} (\Delta t)^{-\alpha}\omega_{l-j}^{(k,i)}, & l > j, \\ (\Delta t)^{-\alpha}\omega_0^{(k,i)} + Kp(u_l^{(m)})^{p-1}, & l = j, \\ 0, \quad l < j. \end{cases}$$

TABLE 5.4:
Errors and convergence rates of $|u(t_n) - u_n|$ in Example 5.1.1. i) for $n = 4$ and $\lambda = -1$.

α	M	$(k,i) = (3,1)$		$(k,i) = (3,2)$		$(k,i) = (3,3)$	
		$\|u(t_n) - u_n\|$	rate	$\|u(t_n) - u_n\|$	rate	$\|u(t_n) - u_n\|$	rate
0.20	32	9.14994E-09	-	5.51519E-08	-	1.64392E-08	-
	64	2.42728E-09	1.91	6.42201E-09	3.10	1.12084E-09	3.87
	128	4.03404E-10	2.59	7.83026E-10	3.04	7.46285E-11	3.91
	256	5.84484E-11	2.79	9.82220E-11	2.99	4.90119E-12	3.93
	512	7.98961E-12	2.87	1.25016E-11	2.97	3.19411E-13	3.94
0.40	32	1.26782E-08	-	1.24811E-07	-	5.36460E-08	-
	64	5.51808E-09	1.20	1.34429E-08	3.21	3.67132E-09	3.87
	128	9.87881E-10	2.48	1.54587E-09	3.12	2.43886E-10	3.91
	256	1.45819E-10	2.76	1.86139E-10	3.05	1.59049E-11	3.94
	512	1.99211E-11	2.87	2.30072E-11	3.02	1.02496E-12	3.96
0.60	32	2.68046E-08	-	1.87580E-07	-	1.15160E-07	-
	64	4.22127E-09	2.67	1.75211E-08	3.42	7.75606E-09	3.89
	128	1.06505E-09	1.99	1.78408E-09	3.30	5.06726E-10	3.94
	256	1.69853E-10	2.65	1.96676E-10	3.18	3.25280E-11	3.96
	512	2.36985E-11	2.84	2.29382E-11	3.10	2.06590E-12	3.98
0.80	32	1.35202E-07	-	2.43799E-07	-	2.00876E-07	-
	64	4.58705E-09	4.88	1.89979E-08	3.68	1.33122E-08	3.92
	128	2.68518E-10	4.09	1.59166E-09	3.58	8.58451E-10	3.95
	256	8.88215E-11	1.60	1.47762E-10	3.43	5.45584E-11	3.98
	512	1.46531E-11	2.60	1.51970E-11	3.28	3.44014E-12	3.99

TABLE 5.5:
Errors and convergence rates of $|u(t_M) - u_M|$ in Example 5.1.1. ii) for different α in the case $\lambda = -50$.

α	M	$(k,i) = (1,1)$		$(k,i) = (2,1)$		$(k,i) = (2,2)$	
		$\|u(t_M) - u_M\|$	rate	$\|u(t_M) - u_M\|$	rate	$\|u(t_M) - u_M\|$	rate
0.1	32	9.08004E-07	-	1.13807E-06	-	7.73661E-07	-
	64	2.28357E-07	1.99	2.84570E-07	2.00	1.92219E-07	2.01
	128	5.74856E-08	1.99	7.14167E-08	1.99	4.77832E-08	2.01
	256	1.44839E-08	1.99	1.66445E-08	2.10	1.16600E-08	2.03
	512	3.65247E-09	1.99	6.85139E-09	1.28	1.11785E-08	0.06
0.3	32	2.71639E-06	-	3.61952E-06	-	1.09348E-06	-
	64	7.33468E-07	1.89	9.85194E-07	1.88	1.78487E-07	2.62
	128	2.02231E-07	1.86	2.72721E-07	1.85	1.37364E-08	3.70
	256	5.69643E-08	1.83	7.67263E-08	1.83	5.91421E-09	1.22
	512	1.63723E-08	1.80	1.36611E-08	2.49	1.06870E-08	-0.85
0.5	32	5.44629E-06	-	8.20975E-06	-	2.83191E-06	-
	64	1.78078E-06	1.61	2.44542E-06	1.75	1.23700E-06	1.19
	128	6.01284E-07	1.57	6.88610E-07	1.83	4.24454E-07	1.54
	256	2.06771E-07	1.54	1.85405E-07	1.89	1.27529E-07	1.73
	512	7.18401E-08	1.53	4.83963E-08	1.94	3.56950E-08	1.84
0.7	32	9.49358E-06	-	1.07784E-05	-	7.65164E-06	-
	64	3.69505E-06	1.36	2.78723E-06	1.95	2.22306E-06	1.78
	128	1.46419E-06	1.34	7.10775E-07	1.97	6.03356E-07	1.88
	256	5.86245E-07	1.32	1.81393E-07	1.97	1.59076E-07	1.92
	512	2.36144E-07	1.31	4.64107E-08	1.97	4.13219E-08	1.94

TABLE 5.6:
Errors and convergence rates of $|u(t_M) - u_M|$ in Example 5.1.1. ii) for different α in the case $\lambda = i$.

α	M	$(k,i)=(1,1)$ $\lvert u(t_M)-u_M\rvert$	rate	$(k,i)=(2,1)$ $\lvert u(t_M)-u_M\rvert$	rate	$(k,i)=(2,2)$ $\lvert u(t_M)-u_M\rvert$	rate
0.1	32	4.56340E-05	-	5.03581E-05	-	1.07742E-05	-
	64	1.24719E-05	1.87	1.26788E-05	1.99	2.40596E-06	2.16
	128	3.40835E-06	1.87	3.19738E-06	1.99	5.38353E-07	2.16
	256	9.30702E-07	1.87	8.00102E-07	2.00	1.19274E-07	2.17
	512	2.53869E-07	1.87	1.69302E-07	2.24	9.39923E-08	0.34
0.3	32	5.22797E-04	-	3.31179E-04	-	1.92248E-04	-
	64	1.64525E-04	1.67	8.18577E-05	2.02	4.71408E-05	2.03
	128	5.16103E-05	1.67	2.03453E-05	2.01	1.16945E-05	2.01
	256	1.61361E-05	1.68	5.07034E-06	2.00	2.91455E-06	2.00
	512	5.03031E-06	1.68	1.26480E-06	2.00	7.28087E-07	2.00
0.5	32	2.79060E-03	-	9.26472E-04	-	7.41150E-04	-
	64	1.00762E-03	1.47	2.30809E-04	2.01	1.83155E-04	2.02
	128	3.61406E-04	1.48	5.76192E-05	2.00	4.55372E-05	2.01
	256	1.29060E-04	1.49	1.43937E-05	2.00	1.13527E-05	2.00
	512	4.59503E-05	1.49	3.59668E-06	2.00	2.83396E-06	2.00
0.7	32	8.24001E-03	-	1.35931E-03	-	1.24727E-03	-
	64	3.42317E-03	1.27	3.58621E-04	1.92	3.27610E-04	1.93
	128	1.40796E-03	1.28	9.37144E-05	1.94	8.53503E-05	1.94
	256	5.75965E-04	1.29	2.42821E-05	1.95	2.20674E-05	1.95
	512	2.34903E-04	1.29	6.24810E-06	1.96	5.66932E-06	1.96

TABLE 5.7:
Errors and convergence orders of $|e_M|$ for $\mu = -1$ in Example 5.1.2 in the cases $K = 1$ and $p = 2$.

α	M	$(k,i)=(1,1)$ $\lvert u(t_M)-u_M\rvert$	rate	$(k,i)=(2,1)$ $\lvert u(t_M)-u_M\rvert$	rate	$(k,i)=(2,2)$ $\lvert u(t_M)-u_M\rvert$	rate
0.1	32	1.77420E-05	-	1.34563E-07	-	1.44620E-08	-
	64	5.02145E-06	1.82	2.09471E-08	2.68	5.84367E-10	4.63
	128	1.41283E-06	1.83	3.17430E-09	2.72	3.71249E-10	0.65
	256	3.95463E-07	1.84	4.71557E-10	2.75	8.48118E-11	2.13
	512	1.10196E-07	1.84	6.89781E-11	2.77	1.56365E-11	2.44
0.3	32	1.02368E-04	-	1.16950E-06	-	7.44373E-07	-
	64	3.21104E-05	1.67	1.92603E-07	2.60	1.07277E-07	2.79
	128	1.00362E-05	1.68	3.12510E-08	2.62	1.57091E-08	2.77
	256	3.12764E-06	1.68	5.01368E-09	2.64	2.32621E-09	2.76
	512	9.72370E-07	1.69	7.97379E-10	2.65	3.47263E-10	2.74
0.5	32	3.61074E-04	-	5.29046E-06	-	4.57737E-06	-
	64	1.28284E-04	1.49	9.63089E-07	2.46	7.97338E-07	2.52
	128	4.55113E-05	1.50	1.73854E-07	2.47	1.39694E-07	2.51
	256	1.61301E-05	1.50	3.11964E-08	2.48	2.45589E-08	2.51
	512	5.71284E-06	1.50	5.57391E-09	2.48	4.32640E-09	2.51
0.7	32	1.13040E-03	-	1.95934E-05	-	1.88894E-05	-
	64	4.59858E-04	1.30	4.02983E-06	2.28	3.82681E-06	2.30
	128	1.86904E-04	1.30	8.24864E-07	2.29	7.76005E-07	2.30
	256	7.59344E-05	1.30	1.68344E-07	2.29	1.57456E-07	2.30
	512	3.08447E-05	1.30	3.42933E-08	2.30	3.19602E-08	2.30

TABLE 5.8:
Errors accuracy and convergence orders of $|e_M|$ for $\mu = -1$ in Example 5.1.2 in the cases $K = 1$ and $p = 2$.

α	M	$(k,i)=(3,1)$ $\lvert u(t_M)-u_M \rvert$	rate	$(k,i)=(3,2)$ $\lvert u(t_M)-u_M \rvert$	rate	$(k,i)=(3,3)$ $\lvert u(t_M)-u_M \rvert$	rate
0.1	32	5.97442E-09	-	4.12374E-09	-	5.22481E-09	-
	64	4.22608E-10	3.82	2.53599E-10	4.02	3.70957E-10	3.82
	128	2.96461E-11	3.83	1.56801E-11	4.02	2.61735E-11	3.83
	256	2.06629E-12	3.84	9.72611E-13	4.01	1.83664E-12	3.83
	512	1.51434E-13	3.77	5.90084E-14	4.04	1.25844E-13	3.87
0.3	32	3.63586E-08	-	2.98609E-08	-	3.32377E-08	-
	64	2.85491E-09	3.67	2.18534E-09	3.77	2.60248E-09	3.67
	128	2.22890E-10	3.68	1.61522E-10	3.76	2.03176E-10	3.68
	256	1.73471E-11	3.68	1.20285E-11	3.75	1.58175E-11	3.68
	512	1.35003E-12	3.68	9.01168E-13	3.74	1.22508E-12	3.69
0.5	32	1.38110E-07	-	1.27455E-07	-	1.32024E-07	-
	64	1.23087E-08	3.49	1.10139E-08	3.53	1.17199E-08	3.49
	128	1.09270E-09	3.49	9.57697E-10	3.52	1.03891E-09	3.50
	256	9.68335E-11	3.50	8.36696E-11	3.52	9.20156E-11	3.50
	512	8.57364E-12	3.50	7.33291E-12	3.51	8.14260E-12	3.50
0.7	32	4.71501E-07	-	4.61657E-07	-	4.64497E-07	-
	64	4.82158E-08	3.29	4.66544E-08	3.31	4.73668E-08	3.29
	128	4.91018E-09	3.30	4.71769E-09	3.31	4.81794E-09	3.30
	256	4.99217E-10	3.30	4.77606E-10	3.30	4.89591E-10	3.30
	512	5.07119E-11	3.30	4.84126E-11	3.30	4.97420E-11	3.30

TABLE 5.9:
Errors and convergence orders of $|e_M|$ for $\mu = i$ in Example 5.1.2 in the cases $K = 1$ and $p = 2$.

α	M	$(k,i)=(1,1)$ $\lvert u(t_M)-u_M \rvert$	rate	$(k,i)=(2,1)$ $\lvert u(t_M)-u_M \rvert$	rate	$(k,i)=(2,2)$ $\lvert u(t_M)-u_M \rvert$	rate
0.1	32	2.54121E-05	-	3.52358E-07	-	8.56779E-08	-
	64	7.32713E-06	1.79	5.14268E-08	2.78	8.08705E-09	3.41
	128	2.09321E-06	1.81	7.42653E-09	2.79	7.38063E-10	3.45
	256	5.93428E-07	1.82	1.06282E-09	2.80	8.51842E-11	3.12
	512	1.67161E-07	1.83	1.50938E-10	2.82	1.47554E-11	2.53
0.3	32	1.44121E-04	-	2.21534E-06	-	1.22445E-06	-
	64	4.58574E-05	1.65	3.56433E-07	2.64	1.77215E-07	2.79
	128	1.44905E-05	1.66	5.68067E-08	2.65	2.58224E-08	2.78
	256	4.55432E-06	1.67	8.98792E-09	2.66	3.78933E-09	2.77
	512	1.42539E-06	1.68	1.41404E-09	2.67	5.59864E-10	2.76
0.5	32	4.89012E-04	-	8.26670E-06	-	6.43523E-06	-
	64	1.75193E-04	1.48	1.49308E-06	2.47	1.12324E-06	2.52
	128	6.25162E-05	1.49	2.67884E-07	2.48	1.96610E-07	2.51
	256	2.22470E-05	1.49	4.78471E-08	2.49	3.44997E-08	2.51
	512	7.90153E-06	1.49	8.51955E-09	2.49	6.06569E-09	2.51
0.7	32	1.47058E-03	-	2.70727E-05	-	2.47625E-05	-
	64	6.00118E-04	1.29	5.55402E-06	2.29	5.02488E-06	2.30
	128	2.44431E-04	1.30	1.13475E-06	2.29	1.01945E-06	2.30
	256	9.94448E-05	1.30	2.31281E-07	2.29	2.06856E-07	2.30
	512	4.04305E-05	1.30	4.70707E-08	2.30	4.19810E-08	2.30

TABLE 5.10:
Errors and convergence orders of $|e_M|$ for $\mu = i$ in Example 5.1.2 in the cases $K = 1$ and $p = 2$.

α	M	$(k,i)=(3,1)$ $\lvert u(t_M)-u_M\rvert$	rate	$(k,i)=(3,2)$ $\lvert u(t_M)-u_M\rvert$	rate	$(k,i)=(3,3)$ $\lvert u(t_M)-u_M\rvert$	rate
0.1	32	8.71434E-09	-	4.79960E-09	-	7.47072E-09	-
	64	6.27059E-10	3.80	2.95994E-10	4.02	5.39926E-10	3.79
	128	4.46205E-11	3.81	1.81797E-11	4.03	3.86592E-11	3.80
	256	3.15064E-12	3.82	1.11308E-12	4.03	2.74569E-12	3.82
	512	2.15830E-13	3.87	6.89707E-14	4.01	1.94223E-13	3.82
0.3	32	5.23976E-08	-	3.73908E-08	-	4.68436E-08	-
	64	4.16942E-09	3.65	2.78549E-09	3.75	3.72285E-09	3.65
	128	3.28853E-10	3.66	2.08205E-10	3.74	2.93824E-10	3.66
	256	2.57840E-11	3.67	1.56249E-11	3.74	2.30683E-11	3.67
	512	2.01141E-12	3.68	1.17766E-12	3.73	1.80270E-12	3.68
0.5	32	1.90898E-07	-	1.62656E-07	-	1.78745E-07	-
	64	1.71443E-08	3.48	1.42466E-08	3.51	1.60163E-08	3.48
	128	1.53023E-09	3.49	1.24931E-09	3.51	1.42842E-09	3.49
	256	1.36106E-10	3.49	1.09734E-10	3.51	1.27023E-10	3.49
	512	1.20810E-11	3.49	9.65029E-12	3.51	1.12707E-11	3.49
0.7	32	6.21914E-07	-	5.86156E-07	-	6.04267E-07	-
	64	6.37330E-08	3.29	5.95612E-08	3.30	6.18239E-08	3.29
	128	6.50169E-09	3.29	6.04415E-09	3.30	6.30254E-09	3.29
	256	6.61800E-10	3.30	6.13212E-10	3.30	6.41338E-10	3.30
	512	6.72836E-11	3.30	6.22274E-11	3.30	6.52096E-11	3.30

5.2 Time-fractional partial differential equations

In this part, we apply the proposed numerical methods with respect to time discretization on the linear time-fractional advection-diffusion equation, and confirm the error accuracy and convergence order corresponding to proper norms. Without loss of generalization, we prescribe the starting values exactly.

Example 5.2.1. *Consider the time-fractional advection-diffusion equation*

$$ {}^{C}\mathcal{D}^{\alpha}u(x,t) = \kappa_d \frac{\partial^2 u}{\partial x^2}(x,t) + \kappa_a \frac{\partial u}{\partial x}(x,t) + f(x,t), \qquad (x,t) \in \Omega \times (0,T]. \tag{5.2.1} $$

We examine two cases with exact solution and prescribed source term:

i). $u(x,t) = e^{-t}\sin x \in C^{\infty}([0,T]\times\Omega)$ *and* $f(x,t) = -t^{1-\alpha}E_{1,2-\alpha}(-t)\sin x + \kappa_d e^{-t}\sin x - \kappa_a e^{-t}\cos x \in C^{0,\infty}([0,T]\times\Omega)$;

ii). $u(x,t) = E_{\alpha,1}(-t^{\alpha})\cos x \in C^{0,\infty}([0,T]\times\Omega)$ *and* $f(x,t) = -E_{\alpha,1}(-t^{\alpha})\cos x + \kappa_d E_{\alpha,1}(-t^{\alpha})\cos x + \kappa_a E_{\alpha,1}(-t^{\alpha})\sin x \in C^{0,\infty}([0,T]\times\Omega)$.

In addition, the initial value and boundary value are prescribed consistently.

Case 1. If applying the uniform grid approximation (2.1.11) to ${}^{C}\mathcal{D}^{\alpha}u(x,t)$ in the time-direction, and the central difference method for the spatial discretization, one obtains

$$ (\Delta t)^{-\alpha}\sum_{l=0}^{k-1}\left(w_{n,l}^{(k,i)} + \omega_{n-l}^{(k,i)}\right)\mathbf{u}^{l} + (\Delta t)^{-\alpha}\sum_{l=k}^{n}\omega_{n-l}^{(k,i)}\mathbf{u}^{l} = A\mathbf{u}^{n} + \mathbf{f}^{n} + \mathbf{r}^{n} \tag{5.2.2} $$

for $k \le n \le N$, where

$$\mathbf{u}^n = \left[\begin{array}{cccc} u_1^n & u_2^n & \cdots & u_M^n \end{array}\right]^T, \qquad \mathbf{f}^n = \left[\begin{array}{cccc} f_1^n & f_2^n & \cdots & f_M^n \end{array}\right]^T,$$
$$\mathbf{r}^n = \left[\begin{array}{ccccc} \left(\frac{\kappa_d}{(\Delta x)^2} - \frac{\kappa_a}{2\Delta x}\right) u_0^n & 0 & \cdots & 0 & \left(\frac{\kappa_d}{(\Delta x)^2} + \frac{\kappa_a}{2\Delta x}\right) u_{M+1}^n \end{array}\right]^T,$$

and matrix $A \in \mathbb{C}^{M\times M}$ is denoted by

$$A = \frac{\kappa_d}{(\Delta x)^2}\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix} + \frac{\kappa_a}{2\Delta x}\begin{bmatrix} 0 & 1 & & & \\ -1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 0 & 1 \\ & & & -1 & 0 \end{bmatrix}. \tag{5.2.3}$$

In terms of numerical implementation, for given starting vectors $\mathbf{u}^l, 0 \le l \le k-1$, we compute $\mathbf{u}^k, \mathbf{u}^{k+1}, \cdots, \mathbf{u}^N$ iteratively by

$$\left(\omega_0^{(k,i)} - (\Delta t)^\alpha A\right)\mathbf{u}^k = -\sum_{l=0}^{k-1}\left(w_{k,l}^{(k,i)} + \omega_{k-l}^{(k,i)}\right)\mathbf{u}^l + (\Delta t)^\alpha \mathbf{f}^k + (\Delta t)^\alpha \mathbf{r}^k,$$
$$\left(\omega_0^{(k,i)} - (\Delta t)^\alpha A\right)\mathbf{u}^n = -\sum_{l=0}^{k-1}\left(w_{n,l}^{(k,i)} + \omega_{n-l}^{(k,i)}\right)\mathbf{u}^l - \sum_{l=k}^{n-1}\omega_{n-l}^{(k,i)}\mathbf{u}^l + (\Delta t)^\alpha \mathbf{f}^n + (\Delta t)^\alpha \mathbf{r}^n.$$

Case 2. If utilizing the linear interpolation (2.2.4), quadratic interpolations (2.2.12) and (2.2.18) on a nonuniform grid, a general discretized form to (5.2.1) is

$$\sum_{l=0}^{n} W_{n,l}^{(k,i)}\mathbf{u}^l = A\mathbf{u}^n + \mathbf{f}^n + \mathbf{r}^n, \qquad k \le n \le N, \tag{5.2.4}$$

and $\mathbf{u}^l$, $l \ge k$ can be computed based on

$$\left(W_{k,k}^{(k,i)} - A\right)\mathbf{u}^k = -\sum_{l=0}^{k-1} W_{k,l}^{(k,i)}\mathbf{u}^l + \mathbf{f}^k + \mathbf{r}^k,$$
$$\left(W_{n,n}^{(k,i)} - A\right)\mathbf{u}^n = -\sum_{l=0}^{n-1} W_{n,l}^{(k,i)}\mathbf{u}^l + \mathbf{f}^n + \mathbf{r}^n, \qquad n = k+1, \cdots, N.$$

From Table 5.11 to Table 5.18, we take the case $\kappa_d = 1$ and $\kappa_a = 0$ as an example of Example 5.2.1 i), and confirm the error accuracy and convergence rate with respect to time and space. We first define two norms,

$$\|\mathbf{u}\|_\infty = \max_{1\le i\le M}|u_i|, \qquad \|\mathbf{u}\|_2 = \sqrt{\Delta x \sum_{i=1}^{M} u_i^2}.$$

According to the spatial discretization, the matrix A defined in (5.2.3) has negative and real eigenvalues for arbitrary $M > 1$. Thus based on the stability analysis in Chapter 3, we make use of all the schemes on a uniform grid for $1 \le i \le k \le 3$, and check the error accuracy $\|\mathbf{e}^N\|$ with respect to L^∞- and L^2- norms, respectively, for different values of α and stepsize N. This can be seen in Table 5.11-Table 5.14. Here we choose the spatial stepsize sufficiently small such that the convergence rate with respect to the temporal direction dominates. Therefore, in the case $\Omega = [0, 0.1]$ and $M = 2^9$, it is observed that the convergence rate $\|\mathbf{e}^N\| = O\left((\Delta t)^{k+1-\alpha}\right)$ is obtained. In Table 5.15-Table 5.18, we define the spatial interval $\Omega = [0, 1]$ and choose $\Delta t = \Delta x$, to check the error accuracy and convergence order for different α and space partition M. It is observed in the case $(k, i) = (1, 1)$, the $(2 - \alpha)$ order in time dominates, while in the remaining cases, the second order in space dominates instead.

In Table 5.19-Table 5.24, we utilize the discretized schemes on a nonuniform grid to solve the problem of Example 5.2.1 ii), where the map in time is defined by $t = T\tau^2$. In the case $\kappa_d = 0$ and $\kappa_a = 1$, the spatial discretization matrix A has eigenvalues on the imaginary axis. For fixed spatial stepsize $M = 2^9$ and $\Omega = [0, 0.1]$, the error accuracy and convergence order in terms of L^∞ and L^2 norms are displayed in Table 5.19 and Table 5.20, it is observed that $\|\mathbf{e}^N\| = O\left(\min(N^{-k-1+\alpha}, N^{-2})\right)$. In addition, we choose $M = N$ and $\Omega = [0, 1]$ to check the error accuracy and convergence rate for different α and M, it implies that $\|\mathbf{e}^N\| = O\left(N^{-k-1+\alpha} + M^{-2}\right)$. In the other case $\kappa_d = 1$ and $\kappa_a = 1$, the corresponding matrix A possesses the eigenvalues laying on left half complex plane. For $M = 2^9$ and $\Omega = [0, 0.1]$, it is shown in Table 5.23 and Table 5.24 that the error accuracy and convergence rate are improved.

TABLE 5.11:
Errors and convergence orders of $\|\mathbf{e}^N\|_\infty$ in Example 5.2.1. i) of different α and N on interval $\Omega = [0, 0.1]$ and $T = 1$ in the case $M = 512$, $\kappa_d = 1$ and $\kappa_a = 0$.

α	N	$(k,i)=(1,1)$ $\|\mathbf{u}(t_N) - \mathbf{u}^N\|_\infty$	rate	$(k,i)=(2,1)$ $\|\mathbf{u}(t_N) - \mathbf{u}^N\|_\infty$	rate	$(k,i)=(2,2)$ $\|\mathbf{u}(t_N) - \mathbf{u}^N\|_\infty$	rate
0.1	8	2.33408E-08	-	5.97555E-10	-	3.65079E-10	-
	16	6.66550E-09	1.81	1.01649E-10	2.56	2.49825E-11	3.87
	32	1.89239E-09	1.82	1.61548E-11	2.65	9.69863E-13	4.69
	64	5.34088E-10	1.83	2.32578E-12	2.80	9.47263E-14	3.36
	128	1.50041E-10	1.83	3.13853E-13	2.89	1.36974E-13	-0.53
0.3	8	1.00979E-07	-	4.76892E-09	-	3.56281E-09	-
	16	3.15109E-08	1.68	8.07207E-10	2.56	4.69890E-10	2.92
	32	9.82683E-09	1.68	1.33813E-10	2.59	6.52361E-11	2.85
	64	3.05967E-09	1.68	2.18499E-11	2.61	9.34745E-12	2.80
	128	9.50995E-10	1.69	3.53620E-12	2.63	1.31598E-12	2.83
0.5	8	2.52051E-07	-	1.60620E-08	-	1.35656E-08	-
	16	8.80211E-08	1.52	2.89681E-09	2.47	2.22330E-09	2.61
	32	3.09055E-08	1.51	5.21558E-10	2.47	3.78468E-10	2.55
	64	1.08827E-08	1.51	9.36800E-11	2.48	6.55335E-11	2.53
	128	3.83821E-09	1.50	1.68070E-11	2.48	1.13321E-11	2.53
0.7	8	5.44685E-07	-	4.11926E-08	-	3.79843E-08	-
	16	2.16424E-07	1.33	8.18199E-09	2.33	7.30158E-09	2.38
	32	8.68171E-08	1.32	1.64533E-09	2.31	1.44465E-09	2.34
	64	3.50105E-08	1.31	3.32643E-10	2.31	2.89738E-10	2.32
	128	1.41607E-08	1.31	6.73349E-11	2.30	5.84505E-11	2.31

In the last chapter, a large amount of numerical experiments are performed to examine the order of accuracy of the proposed numerical methods for various time-fractional differential equations. From the experimental results, we see that the proposed numerical schemes on a uniform grid exhibit higher-order temporal accuracy for a smooth solution, and the numerical schemes on a non-uniform grid show higher-order accuracy in time for a non-smooth solution.

TABLE 5.12:
Errors and convergence orders of $\|\mathbf{e}^N\|_2$ in Example 5.2.1. i) of different α and N on interval $\Omega = [0, 0.1]$ and $T = 1$ in the case $M = 512$, $\kappa_d = 1$ and $\kappa_a = 0$.

α	N	$(k,i)=(1,1)$ $\|\mathbf{u}(t_N)-\mathbf{u}^N\|_2$	rate	$(k,i)=(2,1)$ $\|\mathbf{u}(t_N)-\mathbf{u}^N\|_2$	rate	$(k,i)=(2,2)$ $\|\mathbf{u}(t_N)-\mathbf{u}^N\|_2$	rate
0.1	8	5.29320E-09	-	1.35513E-10	-	8.27924E-11	-
	16	1.51160E-09	1.81	2.30517E-11	2.56	5.66548E-12	3.87
	32	4.29155E-10	1.82	3.66354E-12	2.65	2.19805E-13	4.69
	64	1.21120E-10	1.83	5.27432E-13	2.80	2.14899E-14	3.35
	128	3.40263E-11	1.83	7.11349E-14	2.89	3.10758E-14	-0.53
0.3	8	2.28999E-08	-	1.08149E-09	-	8.07972E-10	-
	16	7.14602E-09	1.68	1.83058E-10	2.56	1.06561E-10	2.92
	32	2.22852E-09	1.68	3.03460E-11	2.59	1.47942E-11	2.85
	64	6.93870E-10	1.68	4.95506E-12	2.61	2.11982E-12	2.80
	128	2.15666E-10	1.69	8.01940E-13	2.63	2.98384E-13	2.83
0.5	8	5.71601E-08	-	3.64252E-09	-	3.07641E-09	-
	16	1.99614E-08	1.52	6.56937E-10	2.47	5.04199E-10	2.61
	32	7.00874E-09	1.51	1.18279E-10	2.47	8.58288E-11	2.55
	64	2.46797E-09	1.51	2.12447E-11	2.48	1.48617E-11	2.53
	128	8.70427E-10	1.50	3.81149E-12	2.48	2.56981E-12	2.53
0.7	8	1.23523E-07	-	9.34163E-09	-	8.61407E-09	-
	16	4.90805E-08	1.33	1.85551E-09	2.33	1.65585E-09	2.38
	32	1.96883E-08	1.32	3.73127E-10	2.31	3.27618E-10	2.34
	64	7.93965E-09	1.31	7.54367E-11	2.31	6.57066E-11	2.32
	128	3.21135E-09	1.31	1.52701E-11	2.30	1.32554E-11	2.31

TABLE 5.13:
Errors and convergence orders of $\|\mathbf{e}^N\|_\infty$ in Example 5.2.1. i) of different α and N on interval $\Omega = [0, 0.1]$ and $T = 1$ in the case $M = 512$, $\kappa_d = 1$ and $\kappa_a = 0$.

α	N	$(k,i)=(3,1)$ $\|\mathbf{u}(t_N)-\mathbf{u}^N\|_\infty$	rate	$(k,i)=(3,2)$ $\|\mathbf{u}(t_N)-\mathbf{u}^N\|_\infty$	rate	$(k,i)=(3,3)$ $\|\mathbf{u}(t_N)-\mathbf{u}^N\|_\infty$	rate
0.1	4	1.48573E-09	-	2.18396E-09	-	1.11940E-10	-
	8	1.24735E-10	3.57	1.19075E-10	4.20	7.95367E-12	3.81
	16	9.16431E-12	3.77	6.92256E-12	4.10	6.30038E-13	3.66
	32	6.84709E-13	3.74	4.50109E-13	3.94	1.08951E-13	2.53
	64	7.98771E-14	3.10	6.19123E-14	2.86	7.14359E-14	0.61
0.3	4	7.29572E-09	-	9.05989E-09	-	5.54403E-10	-
	8	6.07875E-10	3.59	5.56270E-10	4.03	4.18198E-11	3.73
	16	4.73018E-11	3.68	3.70520E-11	3.91	3.17303E-12	3.72
	32	3.77134E-12	3.65	2.72899E-12	3.76	3.24015E-13	3.29
	64	4.29067E-13	3.14	2.19116E-13	3.64	9.43932E-14	1.78
0.5	4	1.98078E-08	-	2.19812E-08	-	1.59639E-09	-
	8	1.70126E-09	3.54	1.57482E-09	3.80	1.33615E-10	3.58
	16	1.44559E-10	3.56	1.23626E-10	3.67	1.16692E-11	3.52
	32	1.24175E-11	3.54	1.03228E-11	3.58	1.05644E-12	3.47
	64	1.17056E-12	3.41	8.68399E-13	3.57	1.27776E-13	3.05
0.7	4	4.46029E-08	-	4.63958E-08	-	3.95428E-09	-
	8	4.08959E-09	3.45	3.91254E-09	3.57	3.74145E-10	3.40
	16	3.89450E-10	3.39	3.61457E-10	3.44	3.68020E-11	3.35
	32	3.81358E-11	3.35	3.50060E-11	3.37	3.67449E-12	3.32
	64	3.91312E-12	3.28	3.52515E-12	3.31	5.13495E-13	2.84

Table 5.14:

Errors and convergence orders of $\|\mathbf{e}^N\|_2$ in Example 5.2.1. i) of different α and N on interval $\Omega = [0, 0.1]$ and $T = 1$ in the case $M = 512$, $\kappa_d = 1$ and $\kappa_a = 0$.

α	N	$(k,i) = (3,1)$		$(k,i) = (3,2)$		$(k,i) = (3,3)$	
		$\|\mathbf{u}(t_N) - \mathbf{u}^N\|_2$	rate	$\|\mathbf{u}(t_N) - \mathbf{u}^N\|_2$	rate	$\|\mathbf{u}(t_N) - \mathbf{u}^N\|_2$	rate
0.1	4	3.36933E-10	-	4.95278E-10	-	2.53857E-11	-
	8	2.82874E-11	3.57	2.70038E-11	4.20	1.80380E-12	3.81
	16	2.07816E-12	3.77	1.56987E-12	4.10	1.42821E-13	3.66
	32	1.55179E-13	3.74	1.01988E-13	3.94	2.46248E-14	2.54
	64	1.81306E-14	3.10	1.40725E-14	2.86	1.62132E-14	0.60
0.3	4	1.65452E-09	-	2.05460E-09	-	1.25727E-10	-
	8	1.37853E-10	3.59	1.26151E-10	4.03	9.48390E-12	3.73
	16	1.07272E-11	3.68	8.40263E-12	3.91	7.19637E-13	3.72
	32	8.55279E-13	3.65	6.18813E-13	3.76	7.35183E-14	3.29
	64	9.73339E-14	3.14	4.97042E-14	3.64	2.13049E-14	1.79
0.5	4	4.49200E-09	-	4.98488E-09	-	3.62029E-10	-
	8	3.85811E-10	3.54	3.57137E-10	3.80	3.03012E-11	3.58
	16	3.27828E-11	3.56	2.80359E-11	3.67	2.64635E-12	3.52
	32	2.81609E-12	3.54	2.34100E-12	3.58	2.39507E-13	3.47
	64	2.65354E-13	3.41	1.96922E-13	3.57	2.89318E-14	3.05
0.7	4	1.01150E-08	-	1.05216E-08	-	8.96749E-10	-
	8	9.27435E-10	3.45	8.87283E-10	3.57	8.48484E-11	3.40
	16	8.83193E-11	3.39	8.19711E-11	3.44	8.34595E-12	3.35
	32	8.64841E-12	3.35	7.93859E-12	3.37	8.33306E-13	3.32
	64	8.87467E-13	3.28	7.99375E-13	3.31	1.16435E-13	2.84

Table 5.15:

Errors and convergence orders of $\|\mathbf{e}^N\|_\infty$ in Example 5.2.1. i) for $T = 1$ and $\Omega = [0, 1]$ in the case $M = N$, $\kappa_d = 1$ and $\kappa_a = 0$.

α	M	$(k,i) = (1,1)$		$(k,i) = (2,1)$		$(k,i) = (2,2)$	
		$\|\mathbf{u}(t_N) - \mathbf{u}^N\|_\infty$	rate	$\|\mathbf{u}(t_N) - \mathbf{u}^N\|_\infty$	rate	$\|\mathbf{u}(t_N) - \mathbf{u}^N\|_\infty$	rate
0.1	8	2.67337E-05	-	2.62665E-05	-	2.62687E-05	-
	16	6.77083E-06	1.98	6.63998E-06	1.98	6.64034E-06	1.98
	32	1.69665E-06	2.00	1.66032E-06	2.00	1.66037E-06	2.00
	64	4.25505E-07	2.00	4.15414E-07	2.00	4.15422E-07	2.00
	128	1.06652E-07	2.00	1.03858E-07	2.00	1.03859E-07	2.00
0.5	8	3.84565E-05	-	2.82999E-05	-	2.83231E-05	-
	16	1.07875E-05	1.83	7.17872E-06	1.98	7.18316E-06	1.98
	32	3.06746E-06	1.81	1.79634E-06	2.00	1.79717E-06	2.00
	64	8.98049E-07	1.77	4.49398E-07	2.00	4.49548E-07	2.00
	128	2.70946E-07	1.73	1.12423E-07	2.00	1.12450E-07	2.00
0.9	8	1.38897E-04	-	2.97690E-05	-	2.97999E-05	-
	16	5.88011E-05	1.24	7.57686E-06	1.97	7.58427E-06	1.97
	32	2.56854E-05	1.19	1.89846E-06	2.00	1.90019E-06	2.00
	64	1.15481E-05	1.15	4.75648E-07	2.00	4.76054E-07	2.00
	128	5.27897E-06	1.13	1.19152E-07	2.00	1.19247E-07	2.00

TABLE 5.16:
Errors and convergence orders of $\|\mathbf{e}^N\|_2$ in Example 5.2.1. i) for $T = 1$ and $\Omega = [0, 1]$ in the case $M = N$, $\kappa_d = 1$ and $\kappa_a = 0$.

α	M	$(k,i) = (1,1)$ $\|\mathbf{u}(t_N) - \mathbf{u}^N\|_2$	rate	$(k,i) = (2,1)$ $\|\mathbf{u}(t_N) - \mathbf{u}^N\|_2$	rate	$(k,i) = (2,2)$ $\|\mathbf{u}(t_N) - \mathbf{u}^N\|_2$	rate
0.1	8	1.93893E-05	-	1.90504E-05	-	1.90520E-05	-
	16	4.85934E-06	2.00	4.76544E-06	2.00	4.76570E-06	2.00
	32	1.21768E-06	2.00	1.19160E-06	2.00	1.19164E-06	2.00
	64	3.05164E-07	2.00	2.97927E-07	2.00	2.97933E-07	2.00
	128	7.64886E-08	2.00	7.44849E-08	2.00	7.44857E-08	2.00
0.5	8	2.79500E-05	-	2.05681E-05	-	2.05849E-05	-
	16	7.73747E-06	1.85	5.14903E-06	2.00	5.15222E-06	2.00
	32	2.20019E-06	1.81	1.28846E-06	2.00	1.28905E-06	2.00
	64	6.44096E-07	1.77	3.22316E-07	2.00	3.22424E-07	2.00
	128	1.94280E-07	1.73	8.06125E-08	2.00	8.06319E-08	2.00
0.9	8	1.01196E-04	-	2.16883E-05	-	2.17107E-05	-
	16	4.21562E-05	1.26	5.43207E-06	2.00	5.43738E-06	2.00
	32	1.84147E-05	1.19	1.36107E-06	2.00	1.36231E-06	2.00
	64	8.27920E-06	1.15	3.41008E-07	2.00	3.41299E-07	2.00
	128	3.78467E-06	1.13	8.54242E-08	2.00	8.54921E-08	2.00

TABLE 5.17:
Errors and convergence orders of $\|\mathbf{e}^N\|_\infty$ in Example 5.2.1. i) for $T = 1$ and $\Omega = [0, 1]$ in the case $M = N$, $\kappa_d = 1$ and $\kappa_a = 0$.

α	M	$(k,i) = (3,1)$ $\|\mathbf{u}(t_N) - \mathbf{u}^N\|_\infty$	rate	$(k,i) = (3,2)$ $\|\mathbf{u}(t_N) - \mathbf{u}^N\|_\infty$	rate	$(k,i) = (3,3)$ $\|\mathbf{u}(t_N) - \mathbf{u}^N\|_\infty$	rate
0.1	8	2.61950E-05	-	2.61918E-05	-	2.61848E-05	-
	16	6.62548E-06	1.98	6.62366E-06	1.98	6.62445E-06	1.98
	32	1.65812E-06	2.00	1.65792E-06	2.00	1.65804E-06	2.00
	64	4.15113E-07	2.00	4.15096E-07	2.00	4.15108E-07	2.00
	128	1.03818E-07	2.00	1.03817E-07	2.00	1.03818E-07	2.00
0.5	8	2.92217E-05	-	2.91561E-05	-	2.91516E-05	-
	16	7.24300E-06	2.01	7.22680E-06	2.01	7.23394E-06	2.01
	32	1.80045E-06	2.01	1.79859E-06	2.01	1.79963E-06	2.01
	64	4.49651E-07	2.00	4.49465E-07	2.00	4.49579E-07	2.00
	128	1.12443E-07	2.00	1.12426E-07	2.00	1.12437E-07	2.00
0.9	8	3.89800E-05	-	3.88887E-05	-	3.89058E-05	-
	16	8.78889E-06	2.15	8.77320E-06	2.15	8.77931E-06	2.15
	32	2.06595E-06	2.09	2.06387E-06	2.09	2.06483E-06	2.09
	64	5.01916E-07	2.04	5.01663E-07	2.04	5.01789E-07	2.04
	128	1.23827E-07	2.02	1.23798E-07	2.02	1.23813E-07	2.02

TABLE 5.18:
Errors and convergence orders of $\|\mathbf{e}^N\|_2$ in Example 5.2.1. i) for $T = 1$ and $\Omega = [0, 1]$ in the case $M = N$, $\kappa_d = 1$ and $\kappa_a = 0$.

α	M	$(k,i) = (3,1)$		$(k,i) = (3,2)$		$(k,i) = (3,3)$	
		$\|\mathbf{u}(t_N) - \mathbf{u}^N\|_2$	rate	$\|\mathbf{u}(t_N) - \mathbf{u}^N\|_2$	rate	$\|\mathbf{u}(t_N) - \mathbf{u}^N\|_2$	rate
0.1	8	1.89949E-05	-	1.89925E-05	-	1.89875E-05	-
	16	4.75516E-06	2.00	4.75386E-06	2.00	4.75442E-06	2.00
	32	1.19004E-06	2.00	1.18990E-06	2.00	1.18998E-06	2.00
	64	2.97711E-07	2.00	2.97698E-07	2.00	2.97707E-07	2.00
	128	7.44565E-08	2.00	7.44555E-08	2.00	7.44562E-08	2.00
0.5	8	2.12231E-05	-	2.11764E-05	-	2.11727E-05	-
	16	5.19554E-06	2.03	5.18391E-06	2.03	5.18904E-06	2.03
	32	1.29145E-06	2.01	1.29012E-06	2.01	1.29086E-06	2.01
	64	3.22496E-07	2.00	3.22363E-07	2.00	3.22444E-07	2.00
	128	8.06272E-08	2.00	8.06145E-08	2.00	8.06228E-08	2.00
0.9	8	2.83674E-05	-	2.83007E-05	-	2.83131E-05	-
	16	6.30117E-06	2.17	6.28992E-06	2.17	6.29430E-06	2.17
	32	1.48117E-06	2.09	1.47967E-06	2.09	1.48037E-06	2.09
	64	3.59842E-07	2.04	3.59661E-07	2.04	3.59751E-07	2.04
	128	8.87764E-08	2.02	8.87549E-08	2.02	8.87658E-08	2.02

TABLE 5.19:
Errors and convergence orders of $\|\mathbf{e}^N\|_\infty$ in Example 5.2.1. ii) of different α and N on interval $\Omega = [0, 0.1]$ and $T = 1$ in the case $M = 512$, $\kappa_d = 0$ and $\kappa_a = 1$.

α	N	$(k,i) = (1,1)$		$(k,i) = (2,1)$		$(k,i) = (2,2)$	
		$\|\mathbf{u}(t_N) - \mathbf{u}^N\|_\infty$	rate	$\|\mathbf{u}(t_N) - \mathbf{u}^N\|_\infty$	rate	$\|\mathbf{u}(t_N) - \mathbf{u}^N\|_\infty$	rate
0.1	8	7.70477E-04	-	1.09695E-03	-	1.14790E-04	-
	16	2.12000E-04	1.86	2.77099E-04	1.99	2.09056E-05	2.46
	32	5.85537E-05	1.86	7.18404E-05	1.95	4.73173E-06	2.14
	64	1.61586E-05	1.86	1.87176E-05	1.94	1.16309E-06	2.02
	128	4.45018E-06	1.86	4.87179E-06	1.94	2.92979E-07	1.99
0.3	8	5.57693E-03	-	7.79424E-03	-	4.89729E-03	-
	16	1.78807E-03	1.64	2.05689E-03	1.92	1.24774E-03	1.97
	32	5.70355E-04	1.65	5.40866E-04	1.93	3.22086E-04	1.95
	64	1.80814E-04	1.66	1.40758E-04	1.94	8.29640E-05	1.96
	128	5.69954E-05	1.67	3.62557E-05	1.96	2.12289E-05	1.97
0.5	8	1.66432E-02	-	1.92505E-02	-	1.59758E-02	-
	16	6.21495E-03	1.42	4.99478E-03	1.95	4.05849E-03	1.98
	32	2.27394E-03	1.45	1.29065E-03	1.95	1.03535E-03	1.97
	64	8.22329E-04	1.47	3.30476E-04	1.97	2.63233E-04	1.98
	128	2.95207E-04	1.48	8.40185E-05	1.98	6.66478E-05	1.98
0.7	8	3.29820E-02	-	2.63109E-02	-	2.46025E-02	-
	16	1.42771E-02	1.21	6.90892E-03	1.93	6.36622E-03	1.95
	32	6.00275E-03	1.25	1.80223E-03	1.94	1.64790E-03	1.95
	64	2.48537E-03	1.27	4.66157E-04	1.95	4.24367E-04	1.96
	128	1.02052E-03	1.28	1.19752E-04	1.96	1.08731E-04	1.96
0.9	8	4.68170E-02	-	1.69684E-02	-	1.67457E-02	-
	16	2.28666E-02	1.03	4.77972E-03	1.83	4.69446E-03	1.83
	32	1.09383E-02	1.06	1.29520E-03	1.88	1.26857E-03	1.89
	64	5.17289E-03	1.08	3.45807E-04	1.91	3.38182E-04	1.91
	128	2.43113E-03	1.09	9.14029E-05	1.92	8.92950E-05	1.92

TABLE 5.20:
Errors and convergence orders of $\|\mathbf{e}^N\|_2$ in Example 5.2.1. ii) of different α and N on interval $\Omega = [0, 0.1]$ and $T = 1$ in the case $M = 512$, $\kappa_d = 0$ and $\kappa_a = 1$.

α	N	$(k,i)=(1,1)$ $\|\mathbf{u}(t_N)-\mathbf{u}^N\|_2$	rate	$(k,i)=(2,1)$ $\|\mathbf{u}(t_N)-\mathbf{u}^N\|_2$	rate	$(k,i)=(2,2)$ $\|\mathbf{u}(t_N)-\mathbf{u}^N\|_2$	rate
0.1	8	1.67968E-04	-	2.40097E-04	-	2.29536E-05	-
	16	4.63137E-05	1.86	6.08434E-05	1.98	4.02570E-06	2.51
	32	1.28153E-05	1.85	1.58130E-05	1.94	9.07047E-07	2.15
	64	3.54216E-06	1.86	4.12847E-06	1.94	2.25332E-07	2.01
	128	9.76862E-07	1.86	1.07644E-06	1.94	5.75647E-08	1.97
0.3	8	1.22939E-03	-	1.72973E-03	-	1.09376E-03	-
	16	3.94725E-04	1.64	4.57756E-04	1.92	2.78501E-04	1.97
	32	1.26034E-04	1.65	1.20567E-04	1.92	7.19065E-05	1.95
	64	3.99841E-05	1.66	3.14099E-05	1.94	1.85288E-05	1.96
	128	1.26104E-05	1.66	8.09595E-06	1.96	4.74276E-06	1.97
0.5	8	3.66752E-03	-	4.28043E-03	-	3.56100E-03	-
	16	1.37146E-03	1.42	1.11324E-03	1.94	9.06045E-04	1.97
	32	5.02198E-04	1.45	2.88020E-04	1.95	2.31286E-04	1.97
	64	1.81701E-04	1.47	7.38020E-05	1.96	5.88224E-05	1.98
	128	6.52499E-05	1.48	1.87713E-05	1.98	1.48961E-05	1.98
0.7	8	7.22560E-03	-	5.83367E-03	-	5.45941E-03	-
	16	3.13381E-03	1.21	1.53613E-03	1.93	1.41625E-03	1.95
	32	1.31888E-03	1.25	4.01344E-04	1.94	3.67110E-04	1.95
	64	5.46350E-04	1.27	1.03915E-04	1.95	9.46220E-05	1.96
	128	2.24403E-04	1.28	2.67139E-05	1.96	2.42591E-05	1.96
0.9	8	1.01092E-02	-	3.71466E-03	-	3.66683E-03	-
	16	4.94834E-03	1.03	1.05035E-03	1.82	1.03173E-03	1.83
	32	2.36971E-03	1.06	2.85557E-04	1.88	2.79731E-04	1.88
	64	1.12134E-03	1.08	7.63917E-05	1.90	7.47115E-05	1.90
	128	5.27166E-04	1.09	2.02358E-05	1.92	1.97709E-05	1.92

TABLE 5.21:
Errors and convergence orders of $\|\mathbf{e}^N\|_\infty$ in Example 5.2.1. ii) for $T = 1$ and $\Omega = [0, 1]$ in the case $M = N$, $\kappa_d = 0$ and $\kappa_a = 1$.

α	M	$(k,i)=(1,1)$ $\|\mathbf{u}(t_N)-\mathbf{u}^N\|_\infty$	rate	$(k,i)=(2,1)$ $\|\mathbf{u}(t_N)-\mathbf{u}^N\|_\infty$	rate	$(k,i)=(2,2)$ $\|\mathbf{u}(t_N)-\mathbf{u}^N\|_\infty$	rate
0.1	16	2.11578E-04	-	2.76320E-04	-	2.03843E-05	-
	32	5.85234E-05	1.85	7.17315E-05	1.95	4.65152E-06	2.13
	64	1.61605E-05	1.86	1.87000E-05	1.94	1.14903E-06	2.02
	128	4.45175E-06	1.86	4.86859E-06	1.94	2.90248E-07	1.99
	256	1.22339E-06	1.86	1.25384E-06	1.96	7.55759E-08	1.94
0.5	16	6.20525E-03	-	4.99265E-03	-	4.05753E-03	-
	32	2.27234E-03	1.45	1.29045E-03	1.95	1.03524E-03	1.97
	64	8.22073E-04	1.47	3.30453E-04	1.97	2.63216E-04	1.98
	128	2.95170E-04	1.48	8.40148E-05	1.98	6.66446E-05	1.98
	256	1.05464E-04	1.48	2.12518E-05	1.98	1.68154E-05	1.99
0.9	16	2.27768E-02	-	4.76945E-03	-	4.68444E-03	-
	32	1.09182E-02	1.06	1.29407E-03	1.88	1.26747E-03	1.89
	64	5.16854E-03	1.08	3.45673E-04	1.90	3.38052E-04	1.91
	128	2.43027E-03	1.09	9.13881E-05	1.92	8.92806E-05	1.92
	256	1.13856E-03	1.09	2.40368E-05	1.93	2.34682E-05	1.93

TABLE 5.22:
Errors and convergence orders of $\|\mathbf{e}^N\|_2$ in Example 5.2.1. ii) for $T = 1$ and $\Omega = [0, 1]$ in the case $M = N$, $\kappa_d = 0$ and $\kappa_a = 1$.

α	M	$(k,i)=(1,1)$ $\|\mathbf{u}(t_N)-\mathbf{u}^N\|_2$	rate	$(k,i)=(2,1)$ $\|\mathbf{u}(t_N)-\mathbf{u}^N\|_2$	rate	$(k,i)=(2,2)$ $\|\mathbf{u}(t_N)-\mathbf{u}^N\|_2$	rate
0.1	16	4.63513E-05	-	6.08064E-05	-	3.98837E-06	-
	32	1.28246E-05	1.85	1.58037E-05	1.94	8.97789E-07	2.15
	64	3.54446E-06	1.86	4.12616E-06	1.94	2.23046E-07	2.01
	128	9.77410E-07	1.86	1.07589E-06	1.94	5.70198E-08	1.97
	256	2.68877E-07	1.86	2.77648E-07	1.95	1.51183E-08	1.92
0.5	16	1.37151E-03	-	1.11321E-03	-	9.06009E-04	-
	32	5.02209E-04	1.45	2.88010E-04	1.95	2.31276E-04	1.97
	64	1.81704E-04	1.47	7.37994E-05	1.96	5.88198E-05	1.98
	128	6.52505E-05	1.48	1.87707E-05	1.98	1.48955E-05	1.98
	256	2.33168E-05	1.48	4.74939E-06	1.98	3.75881E-06	1.99
0.9	16	4.94840E-03	-	1.05031E-03	-	1.03169E-03	-
	32	2.36972E-03	1.06	2.85546E-04	1.88	2.79720E-04	1.88
	64	1.12134E-03	1.08	7.63889E-05	1.90	7.47087E-05	1.90
	128	5.27167E-04	1.09	2.02351E-05	1.92	1.97702E-05	1.92
	256	2.46956E-04	1.09	5.32155E-06	1.93	5.19592E-06	1.93

TABLE 5.23:
Errors and convergence orders of $\|\mathbf{e}^N\|_\infty$ in Example 5.2.1. ii) of different α and N on interval $\Omega = [0, 0.1]$ and $T = 1$ in the case $M = 512$, $\kappa_d = 1$ and $\kappa_a = 1$.

α	N	$(k,i)=(1,1)$ $\|\mathbf{u}(t_N)-\mathbf{u}^N\|_\infty$	rate	$(k,i)=(2,1)$ $\|\mathbf{u}(t_N)-\mathbf{u}^N\|_\infty$	rate	$(k,i)=(2,2)$ $\|\mathbf{u}(t_N)-\mathbf{u}^N\|_\infty$	rate
0.2	8	1.07280E-06	-	1.05387E-06	-	3.57518E-07	-
	16	2.86396E-07	1.91	1.99930E-07	2.40	8.82804E-08	2.02
	32	7.76907E-08	1.88	3.94148E-08	2.34	1.93221E-08	2.19
	64	2.13064E-08	1.87	7.81271E-09	2.33	4.03102E-09	2.26
	128	5.89228E-09	1.85	1.54118E-09	2.34	8.20356E-10	2.30
0.4	8	3.51360E-06	-	1.96415E-06	-	3.62379E-07	-
	16	1.09888E-06	1.68	2.98414E-07	2.72	2.12135E-08	4.09
	32	3.50087E-07	1.65	4.71959E-08	2.66	7.73444E-10	4.78
	64	1.12739E-07	1.63	7.55363E-09	2.64	2.55411E-11	4.92
	128	3.65562E-08	1.62	1.21410E-09	2.64	2.22444E-12	3.52
0.6	8	1.02514E-05	-	3.90646E-06	-	2.71867E-06	-
	16	3.72958E-06	1.46	6.26066E-07	2.64	4.19713E-07	2.70
	32	1.38079E-06	1.43	1.07964E-07	2.54	7.29190E-08	2.53
	64	5.16122E-07	1.42	1.93608E-08	2.48	1.34128E-08	2.44
	128	1.93975E-07	1.41	3.55119E-09	2.45	2.52870E-09	2.41
0.8	8	2.67054E-05	-	7.65886E-06	-	7.13280E-06	-
	16	1.13155E-05	1.24	1.50011E-06	2.35	1.38596E-06	2.36
	32	4.85536E-06	1.22	3.09545E-07	2.28	2.85435E-07	2.28
	64	2.09749E-06	1.21	6.55740E-08	2.24	6.04866E-08	2.24
	128	9.09342E-07	1.21	1.40782E-08	2.22	1.29961E-08	2.22

TABLE 5.24:
Errors and convergence orders of $\|\mathbf{e}^N\|_2$ in Example 5.2.1. ii) of different α and N on interval $\Omega = [0, 0.1]$ and $T = 1$ in the case $M = 512$, $\kappa_d = 1$ and $\kappa_a = 1$.

α	N	$(k,i)=(1,1)$		$(k,i)=(2,1)$		$(k,i)=(2,2)$	
		$\|\mathbf{u}(t_N)-\mathbf{u}^N\|_2$	rate	$\|\mathbf{u}(t_N)-\mathbf{u}^N\|_2$	rate	$\|\mathbf{u}(t_N)-\mathbf{u}^N\|_2$	rate
0.2	8	2.47734E-07	-	2.43354E-07	-	8.25761E-08	-
	16	6.61350E-08	1.91	4.61651E-08	2.40	2.03900E-08	2.02
	32	1.79403E-08	1.88	9.10072E-09	2.34	4.46289E-09	2.19
	64	4.92003E-09	1.87	1.80382E-09	2.33	9.31090E-10	2.26
	128	1.36062E-09	1.85	3.55806E-10	2.34	1.89495E-10	2.30
0.4	8	8.11353E-07	-	4.53517E-07	-	8.36305E-08	-
	16	2.53750E-07	1.68	6.88956E-08	2.72	4.88572E-09	4.10
	32	8.08407E-08	1.65	1.08944E-08	2.66	1.75340E-10	4.80
	64	2.60331E-08	1.63	1.74319E-09	2.64	6.79921E-12	4.69
	128	8.44136E-09	1.62	2.80071E-10	2.64	5.05368E-13	3.75
0.6	8	2.36725E-06	-	9.02022E-07	-	6.27735E-07	-
	16	8.61232E-07	1.46	1.44553E-07	2.64	9.69034E-08	2.70
	32	3.18850E-07	1.43	2.49261E-08	2.54	1.68341E-08	2.53
	64	1.19182E-07	1.42	4.46948E-09	2.48	3.09613E-09	2.44
	128	4.47924E-08	1.41	8.19698E-10	2.45	5.83632E-10	2.41
0.8	8	6.16686E-06	-	1.76858E-06	-	1.64710E-06	-
	16	2.61301E-06	1.24	3.46402E-07	2.35	3.20040E-07	2.36
	32	1.12121E-06	1.22	7.14785E-08	2.28	6.59111E-08	2.28
	64	4.84357E-07	1.21	1.51418E-08	2.24	1.39671E-08	2.24
	128	2.09987E-07	1.21	3.25080E-09	2.22	3.00092E-09	2.22

Appendix A

A.1 Special functions

In the section, we review several equivalent definitions and the related properties of some special functions.

A.1.1 The Gamma function

Definition A.1.1 ([20]). *The Gamma function , denoted by $\Gamma(z)$ as $z \in \mathbb{C}$, is defined in the equivalent forms of*

i) $\Gamma(z) = \lim_{n\to\infty} \frac{n^z n!}{z(z+1)\cdots(z+n)}$,

ii) $\Gamma(z) = \int_0^\infty e^{-t}t^{z-1}\mathrm{d}t, \qquad \Re z > 0,$

iii) $\Gamma(z) = s^z \int_0^\infty e^{-st}t^{z-1}\mathrm{d}t, \qquad \Re z > 0, \quad \Re s > 0.$

Property A.1.1. *The following properties relevant to $\Gamma(z)$ hold:*

i). *$\Gamma(z)$ is an analytic function with isolated singular points $z = 0, -1, -2, \cdots$.*

ii). *$1/\Gamma(z)$ is an entire function since $\Gamma(z)$ is nonzero and analytic on $\mathbb{C}$.*

iii). *For $\Re z > 0$, it holds that $\Gamma(z+1) = z\Gamma(z)$, hence if $n \in \mathbb{N}^+$, there follows*

$$\Gamma(z+n) = (z+n-1)\cdots(z+1)z\Gamma(z).$$

iv). *For fixed $\alpha, \beta \in \mathbb{C}$, the asymptotic expansion holds*

$$\frac{\Gamma(z+\alpha)}{\Gamma(z+\beta)} = z^{\alpha-\beta}\left(1 + \frac{(\alpha-\beta)(\alpha+\beta-1)}{2z} + O(z^{-2})\right).$$

iiv). *For $0 < \Re z < 1$, there is $\Gamma(1-z)\Gamma(z) = \frac{\pi}{\sin \pi z}$.*

A.1.2 The Mittag-Leffler function

Definition A.1.2. *The Mittag-Leffler function is defined by*

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\beta+\alpha k)} \qquad \alpha > 0, \ \beta > 0. \tag{A.1.1}$$

In particular, we denote the one-parameter Mittag-Leffler function by

$$E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(1+\alpha k)}. \tag{A.1.2}$$

Remark A.1.1. *Note that the exponential function is a special case of the Mittag-Leffler function, since $E_1(z) = e^z$ holds.*

A.1.3 The Fox function

Definition A.1.3. *The H-function (Fox-function) is defined by*

$$\begin{aligned} H_{p,q}^{m,n}(z) =& H_{p,q}^{m,n}\left(z\middle|\begin{matrix}(a_j,\alpha_j), & j=1,\cdots,p\\ (b_j,\beta_j), & j=1,\cdots,q\end{matrix}\right)\\ =&\frac{1}{2\pi i}\int_L \frac{A(s)B(s)}{C(s)D(s)}z^s \mathrm{d}s, \end{aligned} \tag{A.1.3}$$

where

$$\frac{A(s)B(s)}{C(s)D(s)} = \frac{\prod_{j=1}^m \Gamma(b_j-\beta_j s)\prod_{j=1}^n \Gamma(1-a_j+\alpha_j s)}{\prod_{j=m+1}^q \Gamma(1-b_j+\beta_j s)\prod_{j=n+1}^p \Gamma(a_j-\alpha_j s)}. \tag{A.1.4}$$

A.2 Partial fractional decomposition

Theorem A.2.1 (fundamental theorem of algebra [21]). *Every complex polynomial of degree n has n complex roots (some of which can be repeated).*

Theorem A.2.2 (binomial theorem). *Assume that x and y are real with $|x| > |y|$ ($|x| \geq |y|$ if $\sum\limits_{k=0}^{\infty}\binom{\alpha}{k} < +\infty$), and α is a complex number, then*

$$(x+y)^\alpha = \sum_{k=0}^{\infty}\binom{\alpha}{k}x^{\alpha-k}y^k = x^\alpha \sum_{k=0}^{\infty}\binom{\alpha}{k}\left(\frac{x}{y}\right)^k.$$

Remark A.2.1. *Here $|x| > |y|$ in Theorem A.2.2 is to guarantee convergence. however, the series may also converge sometimes when $|x| = |y|$.*

Theorem A.2.3 ([1]). *If Q is a polynomial of degree $n > 0$ with distinct roots $\alpha_1, \cdots, \alpha_n$, and if P is a polynomial of degree $< n$, then*

$$\frac{P(z)}{Q(z)} = \sum_{k=1}^{n}\frac{P(\alpha_k)}{Q'(\alpha_k)(z-\alpha_k)},$$

where coefficients $\frac{P(\alpha_k)}{Q'(\alpha_k)}$ are the residues of $\frac{P(z)}{Q(z)}$ at $\xi = \alpha_k$.

Proof. Without loss of generality, we assume that $Q(z)$ is a monic polynomial of form

$$Q(z) = (z-\alpha_1)(z-\alpha_2)\cdots(z-\alpha_n),$$

and also define

$$P(z) = b_0 + b_1 z + \cdots + b_m z^m, \qquad m < n.$$

Then for $z - \alpha_i = \frac{1}{\xi}$, it yields

$$\begin{aligned} \xi^n P(\alpha_i + \frac{1}{\xi}) =& \xi^n \sum_{k=0}^{m} b_k(\alpha_i + \frac{1}{\xi})^k\\ =& \xi^n \sum_{k=0}^{m} b_k \sum_{p=0}^{k}\binom{k}{p}(\alpha_i)^p\left(\frac{1}{\xi}\right)^{k-p}\\ =& \xi^n \sum_{k=0}^{m} b_k\,(\alpha_i)^k + P_{n-1}(\xi)\\ =& \xi^n P(\alpha_i) + P_{n-1}(\xi), \end{aligned}$$

where

$$P_{n-1}(\xi) = \sum_{k=1}^{m} b_k \sum_{p=0}^{k-1} \binom{k}{p} (\alpha_i)^p \xi^{n-k+p} = \sum_{p=0}^{m-1} (\alpha_i)^p \sum_{k=p+1}^{m} b_k \binom{k}{p} \xi^{n-k+p}$$

is a polynomial of degree not exceeding $(n-1)$. Thus according to the polynomial reminder theorem, we get

$$\begin{aligned}\frac{P(z)}{Q(z)} &= \frac{P(\alpha_i + \frac{1}{\xi})}{\frac{1}{\xi}\prod\limits_{\substack{k=1\\k\neq i}}^{n}(\alpha_i + \frac{1}{\xi} - \alpha_k)} = \frac{\xi^n P(\alpha_i + \frac{1}{\xi})}{\prod\limits_{\substack{k=1\\k\neq i}}^{n}\Big((\alpha_i - \alpha_k)\xi + 1\Big)} \\ &= \frac{P(\alpha_i)}{Q'(\alpha_i)(z-\alpha_i)} + H_i\left(\frac{1}{z-\alpha_i}\right),\end{aligned}$$

where $Q'(\alpha_i) = \prod\limits_{\substack{k=1\\k\neq i}}^{n} (\alpha_i - \alpha_k) \neq 0$ and $H_i(\infty)$ is finite. It demonstrates that the rational function

$$r(z) := \frac{P(z)}{Q(z)} - \sum_{i=1}^{n} \frac{P(\alpha_i)}{Q'(\alpha_i)(z-\alpha_i)}$$

has no poles, thus reduces to constant zero in view of $r(\infty) = 0$. In the case when all the roots are real, an alternative viewpoint is to interpolate polynomial $P(z)$ at points $\{\alpha_i\}_{i=1}^n$, which are the distinct roots of $Q(z)$. As the degree of $P(z)$ is less than n, the Lagrange interpolation polynomial interpolating on arbitrary points $\{\alpha_i\}_{i=1}^n$ approximates $P(z)$ exactly, which yields

$$P(z) = \sum_{k=1}^{n} \frac{P(\alpha_k) Q(z)}{Q'(\alpha_k)(z-\alpha_k)}, \quad Q(z) = \prod_{i=1}^{n} (z - \alpha_i).$$

□

Corollary A.2.4. *Let $P(z)/Q(z)$ be a rational function. If* $\deg P < \deg Q$, *then the coefficients $c_{k,j}$ in the partial fraction expansion*

$$\frac{P(z)}{Q(z)} = \frac{P(z)}{\prod\limits_{k=1}^{n}(z-\alpha_k)^{m_k}} = \sum_{k=1}^{n}\sum_{j=0}^{m_k-1} \frac{c_{k,j}}{(z-\alpha_k)^{m_k-j}},$$

are given by the formula

$$c_{k,j} = \frac{1}{j!} \frac{\mathrm{d}^j}{\mathrm{d}z^j}\left[\frac{P(z)}{Q_k(z)}\right]\Big|_{z=\alpha_k}, \quad Q_k(z) = \frac{Q(z)}{(z-\alpha_k)^{m_k}},$$

where $\alpha_1, \alpha_2, \cdots, \alpha_n$ are the distinct repeated roots of $Q(z)$ with multiplicities m_k $(k = 1, \cdots, n)$, respectively.

Proof. We begin with the following expression

$$P(z) = b_0 + b_1 z + b_2 z^2 + \cdots + b_m z^m \quad \text{with} \quad b_k = \frac{P^{(k)}(0)}{k!}, \ 1 \le k \le m$$

and consequently,

$$P(\alpha_i + \xi) = \tilde{b}_0 + \tilde{b}_1 \xi + \cdots + \tilde{b}_m \xi^m \quad \text{with} \quad \tilde{b}_k = \frac{P^{(k)}(\alpha_i)}{k!}, \ 1 \le k \le m.$$

Taking $z = \alpha_i + \frac{1}{\xi}$ $(1 \le i \le n)$, we get

$$\frac{\prod_{k=1}^{n} \xi^{m_k} P(\alpha_i + \frac{1}{\xi})}{\prod_{\substack{k=1\\k\neq i}}^{n} \Big((\alpha_i - \alpha_k)\xi + 1\Big)^{m_k}} = \sum_{j=0}^{m_i} c_{i,j}\xi^{m_i - j} + \frac{P^{(i)}(\xi)}{Q^{(i)}(\xi)},$$

with $\deg P^{(i)}(\xi) < \deg Q^{(i)}(\xi)$. On the other hand, based on the definition of $Q_i(z)$ we obtain

$$\frac{P(z)}{Q_i(z)} = \frac{P(\alpha_i + \frac{1}{\xi})}{\prod_{\substack{k=1\\k\neq i}}^{n} \Big(\alpha_i - \alpha_k + \frac{1}{\xi}\Big)^{m_k}} = \sum_{j=0}^{m_i} c_{i,j}\xi^{-j} + \frac{1}{\xi^{m_i}}\frac{P^{(i)}(\xi)}{Q^{(i)}(\xi)}$$

with $c_{i,j} = \frac{1}{j!}\frac{\mathrm{d}^j}{\mathrm{d}z^j}\left[\frac{P(z)}{Q_i(z)}\right]\Big|_{z=\alpha_i}$. □

Lemma A.2.1 ([33]). *Given $a_0, a_1, a, b \in \mathbb{C}$, define a_n by*

$$a_n = a a_{n-1} + b a_{n-2}, \qquad n \ge 2. \tag{A.2.1}$$

If we have a factorisation

$$T^2 - aT - b = (T - \alpha_1)(T - \alpha_2), \quad \textit{and} \quad \alpha_1 \neq \alpha_2,$$

it can be shown that the numbers a_n are given by

$$a_n = A\alpha_1^n + B\alpha_2^n,$$

with suitable A and B in terms of a_0, a_1, α_1 and α_2.

Proof. Observe that the formal power series generated by the coefficients $\{a_n\}_{n=0}^{\infty}$ satisfies

$$\sum_{n=0}^{\infty} a_n \xi^n = \frac{-a_0 + (aa_0 - a_1)\,\xi}{b\xi^2 + a\xi - 1},$$

under the assumption of (A.2.1). Thus according to Theorem A.2.3, there exist two constants

$$A = \frac{-a_0 + (aa_0 - a_1)\beta_1}{2\beta_1 b + a}, \qquad B = \frac{-a_0 + (aa_0 - a_1)\beta_2}{2\beta_2 b + a}$$

such that

$$\frac{-a_0 + (aa_0 - a_1)\,\xi}{b\xi^2 + a\xi - 1} = \frac{A}{\xi - \beta_1} + \frac{B}{\xi - \beta_2},$$

where β_1 and β_2 are the roots of polynomial $b\xi^2 + a\xi - 1$, i. e.,

$$b\xi^2 + a\xi - 1 = b(\xi - \beta_1)(\xi - \beta_2).$$

Therefore,

$$a_n = -A\big(\alpha_1\big)^{n+1} - B\big(\alpha_2\big)^{n+1},$$

where $\alpha_1 = \frac{1}{\beta_1}$ and $\alpha_2 = \frac{1}{\beta_2}$ are the roots of polynomial $\xi^2 - a\xi - b$. □

Lemma A.2.2. *Let $\alpha_0, \cdots, \alpha_r$ be given complex numbers, and let $c_0, \cdots, c_{r-1}$ be complex numbers such that the polynomial*

$$P(T) = T^r - c_{r-1}T^{r-1} - \cdots - c_1 T - c_0,$$

has distinct roots $\alpha_1, \cdots, \alpha_r$. Define

$$a_n = \sum_{j=0}^{r-1} c_j a_{n-1-j}, \quad n \geq r.$$

Then there exist $A_1, \cdots, A_r$ such that

$$a_n = \sum_{j=1}^{r} A_j \alpha_j^n, \quad \forall\, n \geq 0.$$

Example A.2.1. *Given $a_1, c \in \mathrm{C}$, define z_n by*

$$z_0 = c, \qquad z_n = a_1 z_{n-1} + c, \quad n \geq 1, \tag{A.2.2}$$

then there exist bounded constants $C_1 > 0$ and $C_2 > 0$, such that

$$z_n = C_1 + C_2(a_1)^n, \qquad \text{all } n \geq 0.$$

Proof. Multiplying ξ^n on both sides of (A.2.2) and summing them up give

$$\sum_{n=0}^{\infty} z_n \xi^n = a_1 \xi \sum_{n=0}^{\infty} z_n \xi^n + c \sum_{n=0}^{\infty} \xi^n \Rightarrow$$
$$z(\xi) = \frac{c}{(1-a_1\xi)(1-\xi)} = \frac{c}{1-a_1}\frac{1}{1-\xi} + \frac{ca_1}{a_1-1}\frac{1}{1-a_1\xi} \Rightarrow z_n = c\frac{a_1^{n+1}-1}{a_1-1},$$

where $C_1 = \frac{c}{1-a_1}$ and $C_2 = \frac{ca_1}{a_1-1}$. □

A.3 Complex integration

In this part, we will recall some basic results on complex analysis for a single-valued complex function [1]. The statement begins with the definition of an analytic function that is defined on the complex plane $\mathbb{C}$ and then a series of relevant results on complex integration, for instance, Cauchy theorem, Cauchy integral formula and the residue theorem. Moreover, the Laplace transform and the Fourier transform with respect to the fractional derivatives are mentioned as an application in Chapter 1.

Definition A.3.1 (analytic at a point). *A function $f: \mathbb{C} \to \mathbb{C}$ is analytic at z_0 if and only if f is defined and has a derivative in an open neighborhood of z_0.*

Definition A.3.2 (analytic on a open set). *A function $f: \Omega \subset \mathbb{C} \to \mathbb{C}$, defined on an open set Ω, is analytic in Ω, if f has a complex-valued derivative at each point of Ω.*

Definition A.3.3 (analytic on an arbitrary set). *A function f is analytic on an arbitrary set A, where A is a closed set, if f is the restriction to A of a function which is analytic in some open set containing A.*

Remark A.3.1. *Let f be a function defined in some neighbourhood of a point z_0. If there exists some $r > 0$ such that for all $|z - z_0| < r$, $f(z)$ has a power series expansion at z_0, i.e.,*

$$f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n,$$

then $f(z)$ is analytic at z_0. Furthermore, $f(z)$ is analytic on disc $|z - z_0| < r$.

Theorem A.3.1 (Cauchy theorem). *If a complex-valued function $f(x)$ is analytic in a region R, then for an arbitrary closed curve γ in the region,*

$$\int_\gamma f(x)dx = 0.$$

Example A.3.1. *The following identity holds:*

$$\frac{1}{2\pi i}\int_{|\xi - c| = \rho} (\xi - c)^m \mathrm{d}\xi = \frac{1}{2\pi}\int_0^{2\pi} \rho^{m+1} e^{i(m+1)\theta} \mathrm{d}\theta = \delta_{m,-1},$$

where the radius $\rho \in \mathbb{R}^+$ and origin $c \in \mathbb{C}$ can be arbitrary.

Theorem A.3.2 (Cauchy integral formula). *Assume that a complex-valued function $f(x)$ is analytic at a point $\alpha \in \mathbb{C}$, then $f(x)$ has the power expansion at α,*

$$f(x) = \sum_{n=0}^{\infty} c_n (x - \alpha)^n,$$

where the expansion is unique. Consequently, the corresponding coefficients are unique. According to the residue theorem, the coefficients $c_n = \frac{f^{(n)}(\alpha)}{n!}$ can be expressed by

$$c_n = \frac{1}{2\pi i}\int_C \frac{f(x)}{(x - \alpha)^{n+1}} dx,$$

where the contour curve $C = |x - \alpha| = \rho$ is a circle with origin at α and radius ρ.

Assume that a complex-valued function $f(z)$ is analytic in a region R except at a point z_0. In addition assume that z_0 is an isolated singularity of $f(z)$. Then there exists a function $p(z)$ which is analytic on the region R such that $f(z)$ has the Laurent series at z_0:

$$\begin{aligned} f(z) =& \frac{p(z)}{z - z_0} = \sum_{n=0}^{\infty} a_{n-1} (z - z_0)^{n-1} \\ =& \frac{a_{-1}}{z - z_0} + a_0 + a_1 (z - z_0) + \cdots . \end{aligned} \tag{A.3.1}$$

since $p(z)$ is analytic on R, it is of course analytic at point z_0, hence $p(z)$ has the power series expansion at z_0, i.e., $p(z) = \sum\limits_{n=0}^{\infty} a_{n-1}(z - z_0)^n$.

We then define the residue of function $f(z)$ at an isolated singular point z_0 by a_{-1}, that is

$$\mathrm{Res}_{z_0} f := a_{-1},$$

where a_{-1} is a coefficient of the Laurent series of $f(z)$ shown in (A.3.1).

Theorem A.3.3 (the residue theorem). *Assume that $f(x)$ is analytic on Ω except at isolated singularities $\alpha_1, \alpha_2, \cdots, \alpha_k$. Then for any closed curve γ included in Ω and not passing through the points $\alpha_1, \alpha_2, \cdots, \alpha_k$,*

$$\frac{1}{2\pi i}\int_\gamma f(x)\mathrm{d}\gamma = \sum_{i=1}^{k} \mathrm{Res}_{x=\alpha_i} f(x).$$

A.4 Discrete Gronwall inequalities and their generalization

In this part, we will provide a series of equivalent discrete Gronwall inequalities and their generalizations, which are often used to estimate the upper bounds of sequences.

Lemma A.4.1 ([65]). *Let a non-negative sequence $\{z_n\}_{n=0}^{\infty}$ satisfy*

$$z_{n+1} \le \rho z_n + \delta, \qquad n \ge 0$$

for some constants ρ and δ with $\rho > 0$ and $\delta > 0$. Then

$$z_n \le \frac{\delta}{1-\rho}(1-\rho^n) + z_0\rho^n, \qquad n \ge 0, \qquad 0 < \rho < 1,$$

and

$$z_n \le n\delta + z_0 \quad \forall\, n = 0, \cdots, N, \qquad \rho = 1.$$

Lemma A.4.2 ([58]). *Assume that a non-negative sequence $\{z_n\}_{n=0}^{\infty}$ satisfies*

$$\begin{cases} z_0 \le \delta, \\ z_n \le \displaystyle\sum_{j=0}^{n-1} a_n z_j + \delta, \qquad n \ge 1, \end{cases}$$

if $\delta \ge 0$ and $a_n \ge 0$ for $n \ge 0$, it follows that

$$z_n \le \exp\left(\sum_{s=0}^{n-1} a_s\right)\delta, \qquad n \ge 1.$$

Corollary A.4.1 ([18]). *Let a non-negative sequence $\{z_n\}_{i=0}^{N}$ satisfy*

$$\begin{cases} z_0 \le \delta, \\ z_n \le Mh\displaystyle\sum_{j=0}^{n-1} z_j + \delta, \qquad n = 1, \cdots, N, \end{cases}$$

where $\delta > 0$, $M > 0$ is bounded independently of h and Mh is bounded. Then

$$z_n \le \exp(Mnh)\,\delta, \qquad 0 \le n \le N.$$

Corollary A.4.2 ([36]). *If the positive sequence $\{z_n\}_{n=0}^{\infty}$ satisfies*

$$z_n \le \sum_{j=0}^{n-1} a_{n,j} z_j + \delta, \qquad n = k, k+1, \cdots,$$

with $a_{n,j} > 0, \delta > 0$, $z_i \le \epsilon$ for $i = 0, 1, \cdots, k-1$ and

$$\sum_{j=0}^{n-1} a_{n,j} \le M < 1, \qquad n = 1, 2, \cdots, \tag{A.4.1}$$

then

$$|z_n| \le \frac{\delta + M\epsilon}{1-M}, \qquad n = k, k+1, \cdots.$$

As a generalization, extended discrete Gronwall inequalities are introduced in [18, 17] to solve the integral equations with weakly singular kernel $t_+^{-\alpha}(0 < \alpha < 1)$. It should be noted that the structure of the iteration rules is different from the discrete Gronwall inequalities. We first provide a comparison result, and then revisit the generalized discrete Gronwall inequality by means of a generating power series approach.

Lemma A.4.3. *Assume that the non-negative sequence $\{z_n\}_{n=0}^{\infty}$ satisfies*

$$z_0 \leq \delta_0, \qquad z_n \leq \sum_{j=0}^{n-1} a_{n,j} z_j + \delta_n, \qquad n \geq 1 \tag{A.4.2}$$

in combination with $a_{n,j} \geq 0$ and $\delta_n \geq 0$. Then one has the inequality $z_n \leq p_n$ for all $n \geq 1$, where the non-negative sequence $\{p_n\}_{n=0}^{\infty}$ satisfies

$$p_0 = \delta_0, \qquad p_n = \sum_{j=0}^{n-1} a_{n,j} p_j + \delta_n, \qquad n \geq 1. \tag{A.4.3}$$

Proof. The proof is given by an induction process. It is obvious that, for $n = 0$, $z_0 \leq \delta = p_0$. Suppose that $z_k \leq p_k$ for all $0 \leq k \leq n$, then

$$z_{n+1} \leq \sum_{j=0}^{n} a_{n+1,j} z_j + \delta \leq \sum_{j=0}^{n} a_{n+1,j} p_j + \delta = p_{n+1},$$

which implies the result. □

Theorem A.4.3 (generalized discrete Gronwall). *Let $\{z_n\}_{n=0}^{N}$ be a sequence of non-negative real numbers satisfying*

$$\begin{cases} z_0 \leq \delta_0, \\ z_n \leq \delta_n + Mh^{\alpha} \displaystyle\sum_{j=0}^{n-1} \frac{z_j}{(n-j)^{1-\alpha}}, \qquad 1 \leq n \leq N, \end{cases}$$

where $0 < \alpha < 1$ and $M > 0$, is bounded independent of h, and δ_n, $0 \leq n \leq N$ is a monotonically increasing sequence of non-negative real numbers. Then

$$z_n \leq \delta_n E_{\alpha}\left(M\Gamma(\alpha)(nh)^{\alpha}\right), \qquad 0 \leq n \leq N.$$

Remark A.4.1. *It can be deduced that the coefficients $k_{i,j} = Mh^{\alpha-1}(i-j)^{\alpha-1}$ with $0 \leq j \leq i-1 \leq N-1$, satisfy the following conditions:*

i). $k_{i,j} \geq 0$ for all $0 \leq j \leq i-1$,

ii). $h \sum_{j=0}^{i-1} k_{i,j}$ is bounded and independent of h for each $1 \leq i \leq N$,

iii). there exists $\mu \in \mathbb{N}^+$ such that the μ-th iterated discrete kernel $k_{i,j}^{(\mu)}$, recursively defined by

$$k_{i,j}^{(1)} = k_{i,j}, \qquad k_{i,j}^{(n)} = h \sum_{l=j+1}^{i-1} k_{i,l} k_{l,j}^{(n-1)}, \quad n \geq 2$$

is bounded for each i and j, independently of h.

There is a unique sequence $\{y_n\}_{n=0}^{\infty}$ *satisfying*

$$\begin{cases} y_0 = \delta_0, \\ y_n = \delta_n + Mh^\alpha \sum_{j=0}^{n-1} \frac{y_j}{(n-j)^{1-\alpha}}, \qquad 1 \le n \le N, \end{cases} \tag{A.4.4}$$

and the result of Lemma A.4.3 yields that

$$z_n \le y_n, \qquad 0 \le n \le N.$$

Therefore, it remains to solve formula (A.4.4) *exactly. Formula* (A.4.4) *can be equivalently rewritten into*

$$(1 - hK(\xi))\, y(\xi) = \delta(\xi), \tag{A.4.5}$$

where

$$y(\xi) = \sum_{n=0}^{\infty} y_n \xi^n, \qquad \delta(\xi) = \sum_{n=0}^{\infty} \delta_n \xi^n, \qquad K(\xi) = Mh^{\alpha-1} \sum_{n=1}^{\infty} n^{\alpha-1} \xi^n.$$

An iteration process yields

$$y(\xi) = \delta(\xi) \sum_{n=0}^{\infty} (hK(\xi))^n = \delta(\xi)\kappa(\xi),$$

and equivalently, we obtain $y_n = \sum_{j=0}^{n} \kappa_{n-j}\delta_j$. *In addition, it follows that*

$$\nabla y_n = \kappa_0 \delta_n + \sum_{j=0}^{n-1} \nabla \kappa_{n-j} \delta_j = \kappa_n \delta_0 + \sum_{j=0}^{n-1} \nabla \delta_{n-j} \kappa_j.$$

This yields that the sequence $\{y_n\}$ *is monotonic iff* $\{\delta_n\}$ *or* $\{\kappa_n\}$ *possesses the same monotonic property.*

A.5 Formal power series

In this section, we will revisit a useful mathematical tool called formal power series (fps). We refer to [26] for some related definitions and algebraic properties.

Definition A.5.1. *A formal power series over a field* $\mathcal{F}$ *is an infinite sequence*

$$(a_0, a_1, a_2, \cdots) \to \mathcal{F},$$

which is often written in the form

$$P = a_0 + a_1 x + a_2 x^2 + \cdots.$$

The element a_n *is called the* n*-th coefficient of fps* P.

Next, some algebraic operations defined on fps are enumerated to generate the set of fps. Given two fps P and Q,

$$P = a_0 + a_1 x + a_2 x^2 + \cdots,$$
$$Q = b_0 + b_1 x + b_2 x^2 + \cdots.$$

The addition of two fps is prescribed by

$$P + Q = (a_0 + b_0) + (a_1 + b_1)x + (a_2 + b_2)x^2 + \cdots .$$

And the product of two fps P and Q is defined by

$$\begin{aligned} P \cdot Q :=& c_0 + c_1 x + c_2 x^2 + \cdots \\ =& a_0 b_0 + (a_0 b_1 + a_1 b_0)\, x + (a_0 b_2 + a_1 b_1 + a_2 b_0)\, x^2 + \cdots , \end{aligned}$$

where

$$c_n := \sum_{i=0}^{n} a_{n-i} b_i = \sum_{i=0}^{n} a_i b_{n-i}, \qquad n = 0, 1, 2, \cdots .$$

This is called the Cauchy product.

Denote $\mathcal{S}$ a set of fps, we have the following properties:

i). for all fps P and Q, the Cauchy product $P \cdot Q$ is also a fps;

ii). for all P, Q and R in $\mathcal{S}$, it holds that $(P \cdot Q) \cdot R = P \cdot (Q \cdot R)$;

iii). there exists an identity element $e = 1$ here, such that $e \cdot P = P \cdot e = P$ holds for all $P \in \mathcal{S}$.

Additionally, not every fps P possesses an inverse element P^{-1} such that $P \cdot P^{-1} = P^{-1} \cdot P = e = 1$, for example, if P is a fps whose first coefficient $a_0 \neq 0$, then P^{-1} doesn't exist. Therefore, the set $\mathcal{S}$ together with Cauchy product can't form a group in general. However the following theorem tells us $(\mathcal{S}, \cdot)$ can be a group.

Theorem A.5.1. $(\mathcal{S}, \cdot)$ *forms a group if and only if the first coefficient of the fps is nonzero.*

Another equivalent representation of formal power series is the infinite lower (or upper) triangular toeplitz matrix, which can be represented by the following $n \times n$ matrix

$$P_n = \begin{bmatrix} a_0 & & & & \\ a_1 & a_0 & & & \\ \vdots & \ddots & \ddots & & \\ \vdots & & \ddots & a_0 & \\ a_n & \cdots & \cdots & a_1 & a_0 \end{bmatrix}$$

with arbitrary $n \in \mathbb{N}^+$. And for any n-dimensional square matrix, it yields that

$$\begin{aligned} &\text{addition:} \quad P_n + Q_n = (P + Q)_n, \\ &\text{product:} \quad P_n Q_n = (PQ)_n, \\ &\text{inverse:} \quad (P_n)^{-1} = (P^{-1})_n, \qquad \text{if } a_0 \neq 0. \end{aligned}$$

It is also known from Theorem A.5.1 that the set of the infinite lower (or upper) triangular Toeplitz matrices $\mathcal{M}$ in combination with the operation of matrix multiplication form an Abelian group .

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Summary

Fractional calculus, as a generalization of ordinary calculus, has been an interesting topic since the end of the 17th century. In comparison with ordinary derivatives and integrals, the fractional derivatives and fractional integrals are introduced in various kinds of ways, and possess some interesting mathematical properties. Recently, there arose some attractive applications in the fields of physics, chemistry and engineering by applying fractional integrals and derivatives to construct mathematical models that describe anomalous diffusion processes, for instance, subdiffusion, which is slower than the Brownian diffusion or *Lévy* flight. As a consequence, a variety of differential-integral equations have been derived such as the fractional diffusion equation, the fractional diffusion-advection equation, the fractional Fokker-Planck equation and the fractional Klein-Kramers equation. These fractional models provide a straightforward way of implementing some phenomena in real world.

In this thesis, the main objective is to investigate the numerical approximation for the fractional equations with respect to time, which is used to describe the sub-diffusive phenomenon. As a preliminary, we first step into the world of fractional calculus. There are some different definitions on the fractional integral and fractional derivatives, such as in the sense of Riemann-Louville or the sense of Caputo. Rigorous definitions are shown in Chapter 1. It is necessary to study its relevant properties. Some properties are considered as the generalization of the ordinary calculus, while some properties reveal very different and new aspects, and show the advantages of the fractional calculus when encountering specific problem. Another issue is on the application of fractional calculus. In this part, we mainly consider two aspects, the mathematical models of fractional approach and the numerical implementation of the models, which are briefly introduced in Chapter 1. Dating back to the physical background of the problem, the fractional differential equation is derived from the continuous time random walk process, whose detailed derivation is provided. We also apply the integral transform, particularly, the Laplace transform and the Fourier transform on the fractional operators to analytically obtain special solutions of the fractional equations, just as the approach for the ordinary differential equations. As a consequence, some generalized results with respect to the integral transform are proposed in a rigorously proved way. However, it is known that in most practical situations, we can not get an explicit representation of the solutions of a differential-integral equation, and the numerical implementation thus plays a dominant role. In order to design the numerical approximation for the problem, we study the analytical properties of the exact solution of the problem in advance. The essential concern is about the regularity of the exact solution. On the one hand, if the known term and initial and boundary conditions of the equations are sufficiently regular, the exact solution is less regular near the origin, on the other hand, we can obtain the exact solution with sufficient regular property even if the known conditions are less regular. In these cases, two numerical approaches, called the product integration methods and the fractional linear multistep methods, are introduced to construct the discrete schemes. They both have their own advantages and disadvantages in different situations. In theoretical analyses, there are also close connections between the two approaches. We introduce the two methods and spend the majority of the remaining part of the thesis to improve the product integration approach and design a class of numerical approximations to the fractional models.

The main work in the thesis consists of the derivation of the numerical approximation to the fractional derivative in the Caputo's sense, and its application to the numerical discretization to the time-fractional differential equations. Besides the consistency of the numerical schemes, their corresponding numerical stability analyses and the convergence analyses are respectively shown in a rigorous way. In Chapter 2, we construct a class of numerical approximations to the Caputo fractional derivative by means of a series of continuous piecewise polynomials on a uniform grid. The class of numerical methods can be considered as a generalization of the well-known BDF methods to ordinary differential equations. We discuss the local truncation error in terms of a sufficiently regular solution. In the case where the solution is less regular, to obtain high order of accuracy, we construct the numerical approximation by making use of continuous piecewise polynomials approximations on non-uniform grids. The numerical implementation shows the efficiency and high-order accuracy of the schemes. Furthermore, we apply the numerical approximations to the fractional derivative on the time fractional differential equations and obtain the semi-discretized schemes in combination with the proper discretization for the spatial direction. It is known that the numerical stability has a crucial effect on the final approximation. In Chapter 3, we focus on the stability analysis of the proposed numerical methods. In a rigorous way, we generalize the classical stability results of the linear multistep methods to the new cases. We confirm and prove the numerical stability region of the proposed methods, and provide the $A(\theta)$-stability analysis of them. In addition, we generalize the strong root condition of the BDF methods and prove the property of the proposed schemes defined in Chapter 2. In addition, in Chapter 4, we establish global error estimates for nonlinear time-fractional ordinary differential equations and time-fractional diffusion equations, respectively. It is proved that high-order convergence with respect to the time can be obtained when the exact solutions of the equations are sufficiently regular. Furthermore, for the case of the fractional diffusion equations, we can also obtain satisfactory orders of accuracy without restrictions on the temporal stepsize. In Chapter 5, we implement the proposed numerical schemes on a uniform grid and non-uniform grid in the examples of time fractional ordinary differential equations and time fractional partial differential equations. We confirm the effect of the stability on the global errors and check the error accuracy and corresponding convergence rate with respect to both temporal and spatial stepsize. The desired error accuracy order shows the efficiency of the proposed numerical methods. As a complementary, some useful results are also given in the Appendix such as the introduction of some special functions, the definition and the algebraic properties of formal power series and its application to the partial fractional decomposition. Furthermore, we revisit a series of important conclusions in terms of the complex integration. Some results from the discrete Gronwall inequality to the generalized discrete Gronwall inequality are used in the convergence analysis.

Samenvatting

Dit proefschrift behandelt een nieuwe klasse van hogere-orde eindige differentie methoden voor tijds-fractionele differentiaalvergelijkingen.

In hoofdstuk 1 worden fractionele integralen en afgeleiden geïntroduceeerd. Wiskundige modellen met tijds-fractionele differentiaalvergelijkingen en enkele relevante eigenschappen komen daar aan bod. Tevens worden twee bestaande numerieke discretisatiemethoden beschreven, n.l. de produkt-integratie methode en de fractionele lineaire multistapsmethode.

In hoofdstuk 2 stellen we een nieuwe klasse van impliciete eindige differentie methoden voor, die gerelateerd zijn aan de backward-differentiation-formules voor gewone (niet-fractionele) differentiaalvergelijkingen. Deze nieuwe methoden zijn gebaseerd op een continue stuksgewijze polynomiale benadering van de onderliggende oplossing. Eerst wordt een uniforme rooster benadering van de Caputo fractionele afgeleide uitgewerkt. De lokale afbreekfout hiervan wordt uitgebreid geanalyseerd. Daarnaast komt ook een niet-uniforme roosterbenadering ter sprake. Deze wordt bestudeerd voor het lineaire en kwadratische geval.

In hoofdstuk 3 richten we ons op de numerieke stabiliteit van de voorgestelde methoden. Begrippen als nul-stabiliteit, A-stabiliteit en A(θ)-stabiliteit spelen hierbij een belangrijke rol. De stabiliteitsgebieden en een gegeneraliseerde root-conditie komen aan de orde.

In hoofdstuk 4 wordt de convergentie van de numerieke methoden bewezen. Er wordt onderscheid gemaakt tussen een scalaire niet-lineaire tijds-fractionele differentiaalvergelijking en lineaire tijds-fractionele partiele differentiaalvergelijkingen.

Hoofdstuk 5 illustreert de numerieke eigenschappen van de hogere-orde methoden, zoals de nauwkeurigheid, de (in)stabiliteit en de convergentie. Dit wordt gedaan aan de hand van een uitgebreide reeks van numerieke experimenten.

Een Appendix sluit het proefschrift af met enkele belangrijke wiskundige hulpmiddelen, zoals de Gamma functie, de Mittag-Leffler functie en de partiële fractionele decompositie. Tot slot worden discrete Gronwall ongelijkheden en een aantal nuttige resultaten uit de complexe integratie behandeld, die bij de bewijzen van de lemma's en stellingen in hoofdstukken 2 t/m 4 zijn gebruikt.

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Curriculum Vitae

Han Zhou was born in Lanzhou city, Gansu province, China on 13 October, 1987. From the year of 2006 to 2010, she received a Bachelor degree in applied mathematics in the department of mathematics and statistics, Lanzhou university. Later on from the year of 2010 to 2013, she obtained a master degree in computational mathematics in the department of mathematics and statistics, Lanzhou university. The title of her master thesis is "The high order methods for solving parabolic equation and space fractional diffusion equation". From the year of 2013, she pursued for a PhD diploma on the topic of scientific computing in the mathematical institute of Utrecht University.

In the meantime, she took part in some conferences in Netherlands and international conferences relevant to numerical analysis and applications of the fractional differential equations. In 2014, she attended the International Conference on Fractional Differentiation and its Applications (ICFDA) in Italy. From the year of 2014 to 2016, she also took part in the thirty-ninth, the fortieth and the forty-first Woudschoten conference of the Dutch and Flemish numerical analysis communities in Zeist, the Netherlands. Han took part in the 106th Europe study group mathematics with industry (SWI) hosted by Utrecht University in 2015. In the years 2015 and 2016, she also participated in the NDNS workshop at Twente University. In 2015, she attended and reported on the International Conference on Scientific Computation And Differential Equations (SciCADE) in the University of Potsdam in Germany. Recently, she gave a contributed talk at the 14th International Conference of Numerical Analysis and Applied Mathematics (ICNAAM), in Greece.